



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 01:58 AM UTC

PDB ID : 7BKB / pdb_00007bkb
EMDB ID : EMD-12206
Title : Formate dehydrogenase - heterodisulfide reductase - formylmethanofuran dehydrogenase complex from Methanospirillum hungatei (hexameric, composite structure)
Authors : Pfeil-Gardiner, O.; Watanabe, T.; Shima, S.; Murphy, B.J.
Deposited on : 2021-01-15
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

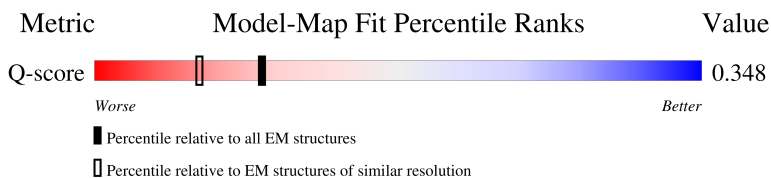
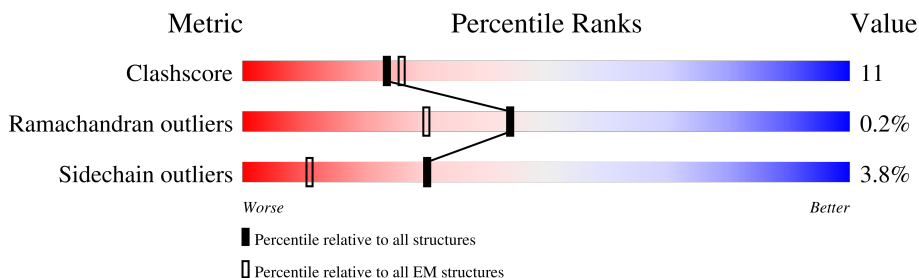
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



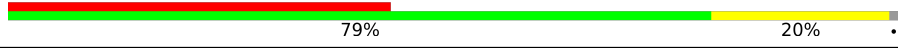
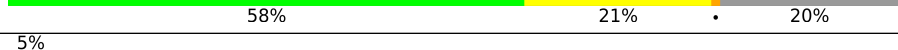
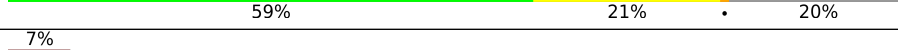
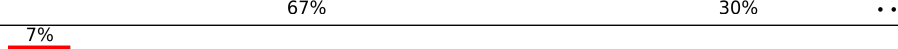
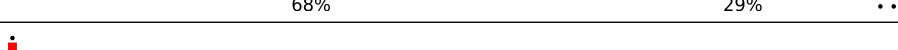
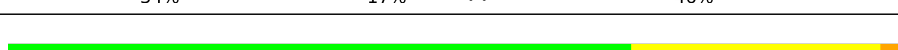
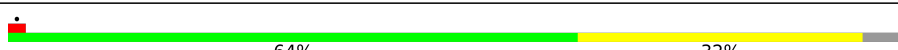
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	A	671	
1	a	671	
2	F	140	
2	f	140	

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Mol	Chain	Length	Quality of chain
3	E	414	
3	e	414	
4	C	191	
4	c	191	
5	B	296	
5	b	296	
6	D	686	
6	d	686	
7	I	266	
7	i	266	
8	L	146	
8	l	146	
9	G	571	
9	g	571	
10	J	137	
10	j	137	
11	K	388	
11	k	388	
12	H	443	
12	h	443	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	SF4	A	703	-	-	X	-
13	SF4	a	703	-	-	X	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 64126 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 CoB–CoM heterodisulfide reductase iron-sulfur subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	662	Total	C	N	O	S	0	0
			5011	3168	851	935	57		
1	a	662	Total	C	N	O	S	0	0
			5011	3168	851	935	57		

- Molecule 2 is a protein called F420-non-reducing hydrogenase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	137	Total	C	N	O	S	0	0
			1073	687	188	186	12		
2	f	137	Total	C	N	O	S	0	0
			1073	687	188	186	12		

- Molecule 3 is a protein called Formate dehydrogenase, beta subunit (F420).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	411	Total	C	N	O	S	0	0
			3151	1985	542	589	35		
3	e	411	Total	C	N	O	S	0	0
			3151	1985	542	589	35		

- Molecule 4 is a protein called CoB–CoM heterodisulfide reductase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	189	Total	C	N	O	S	0	0
			1498	936	271	278	13		
4	c	189	Total	C	N	O	S	0	0
			1498	936	271	278	13		

- Molecule 5 is a protein called CoB–CoM heterodisulfide reductase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	296	Total	C	N	O	S	0	0
			2304	1470	387	426	21		
5	b	296	Total	C	N	O	S	0	0
			2304	1470	387	426	21		

- Molecule 6 is a protein called Formate dehydrogenase.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	549	Total	C	N	O	S	0	0
			4251	2691	737	795	28		
6	d	549	Total	C	N	O	S	0	0
			4251	2691	737	795	28		

- Molecule 7 is a protein called Formylmethanofuran dehydrogenase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	264	Total	C	N	O	S	0	0
			1996	1270	336	380	10		
7	i	264	Total	C	N	O	S	0	0
			1996	1270	336	380	10		

- Molecule 8 is a protein called Formylmethanofuran dehydrogenase, subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	79	Total	C	N	O	S	0	0
			576	357	98	112	9		
8	l	79	Total	C	N	O	S	0	0
			576	357	98	112	9		

- Molecule 9 is a protein called Formylmethanofuran dehydrogenase, subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	568	Total	C	N	O	S	0	0
			4455	2840	751	841	23		
9	g	568	Total	C	N	O	S	0	0
			4455	2840	751	841	23		

- Molecule 10 is a protein called Formylmethanofuran dehydrogenase, subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	131	Total	C	N	O	S	0	0
			1007	629	179	190	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	131	Total	C	N	O	S	0	0
			1007	629	179	190	9		

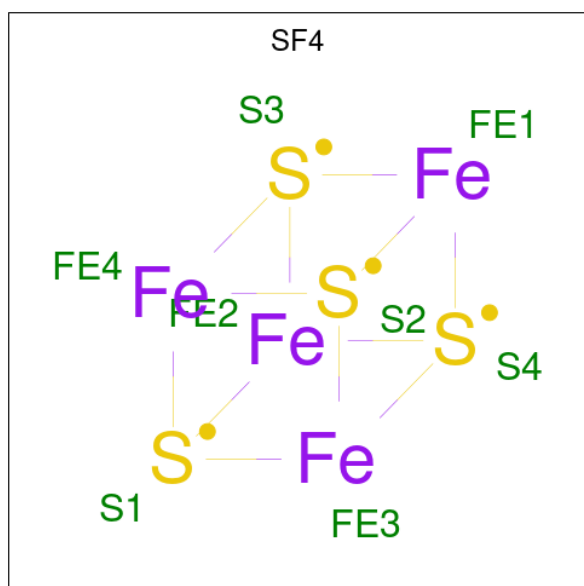
- Molecule 11 is a protein called Formylmethanofuran dehydrogenase, subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	386	Total	C	N	O	S	0	0
			2910	1815	488	571	36		
11	k	386	Total	C	N	O	S	0	0
			2910	1815	488	571	36		

- Molecule 12 is a protein called Formylmethanofuran dehydrogenase, subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	438	Total	C	N	O	S	0	0
			3416	2155	600	629	32		
12	h	438	Total	C	N	O	S	0	0
			3416	2155	600	629	32		

- Molecule 13 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total	Fe	S	0
			8	4	4	
13	A	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total 8	Fe 4	S 4	0
13	A	1	Total 8	Fe 4	S 4	0
13	A	1	Total 8	Fe 4	S 4	0
13	A	1	Total 8	Fe 4	S 4	0
13	E	1	Total 8	Fe 4	S 4	0
13	E	1	Total 8	Fe 4	S 4	0
13	E	1	Total 8	Fe 4	S 4	0
13	E	1	Total 8	Fe 4	S 4	0
13	C	1	Total 8	Fe 4	S 4	0
13	C	1	Total 8	Fe 4	S 4	0
13	D	1	Total 8	Fe 4	S 4	0
13	L	1	Total 8	Fe 4	S 4	0
13	L	1	Total 8	Fe 4	S 4	0
13	K	1	Total 8	Fe 4	S 4	0
13	K	1	Total 8	Fe 4	S 4	0
13	K	1	Total 8	Fe 4	S 4	0
13	K	1	Total 8	Fe 4	S 4	0
13	K	1	Total 8	Fe 4	S 4	0
13	K	1	Total 8	Fe 4	S 4	0
13	K	1	Total 8	Fe 4	S 4	0
13	K	1	Total 8	Fe 4	S 4	0

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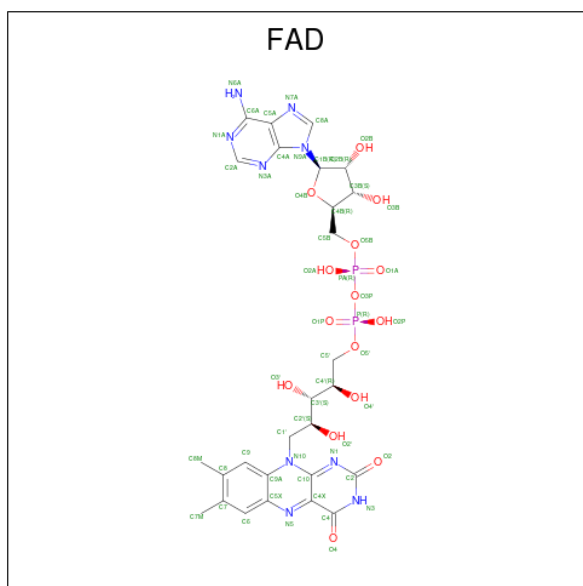
Mol	Chain	Residues	Atoms			AltConf
13	H	1	Total 8	Fe 4	S 4	0
13	a	1	Total 8	Fe 4	S 4	0
13	a	1	Total 8	Fe 4	S 4	0
13	a	1	Total 8	Fe 4	S 4	0
13	a	1	Total 8	Fe 4	S 4	0
13	a	1	Total 8	Fe 4	S 4	0
13	a	1	Total 8	Fe 4	S 4	0
13	e	1	Total 8	Fe 4	S 4	0
13	e	1	Total 8	Fe 4	S 4	0
13	e	1	Total 8	Fe 4	S 4	0
13	e	1	Total 8	Fe 4	S 4	0
13	c	1	Total 8	Fe 4	S 4	0
13	c	1	Total 8	Fe 4	S 4	0
13	d	1	Total 8	Fe 4	S 4	0
13	l	1	Total 8	Fe 4	S 4	0
13	l	1	Total 8	Fe 4	S 4	0
13	k	1	Total 8	Fe 4	S 4	0
13	k	1	Total 8	Fe 4	S 4	0
13	k	1	Total 8	Fe 4	S 4	0
13	k	1	Total 8	Fe 4	S 4	0
13	k	1	Total 8	Fe 4	S 4	0

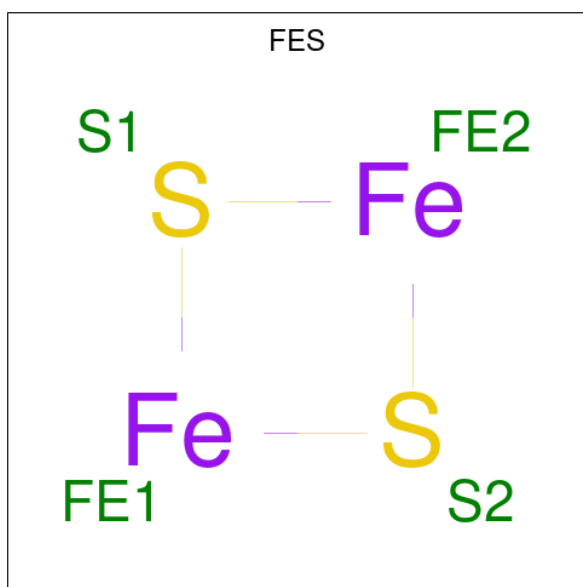
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Mol	Chain	Residues	Atoms			AltConf
13	k	1	Total	Fe	S	0
			8	4	4	
13	k	1	Total	Fe	S	0
			8	4	4	
13	k	1	Total	Fe	S	0
			8	4	4	
13	h	1	Total	Fe	S	0
			8	4	4	

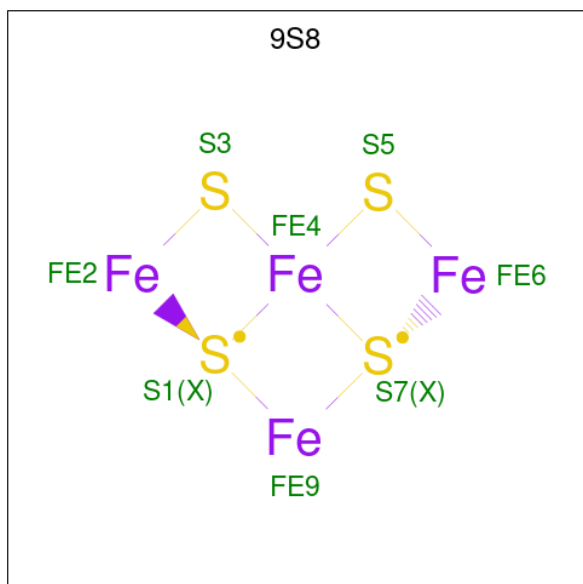
- Molecule 14 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms			AltConf
15	F	1	Total	Fe	S	0
			4	2	2	
15	f	1	Total	Fe	S	0
			4	2	2	

- Molecule 16 is Non-cubane [4Fe-4S]-cluster (CCD ID: 9S8) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
16	B	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
16	B	1	Total	Fe	S	0
			8	4	4	
16	b	1	Total	Fe	S	0
			8	4	4	
16	b	1	Total	Fe	S	0
			8	4	4	

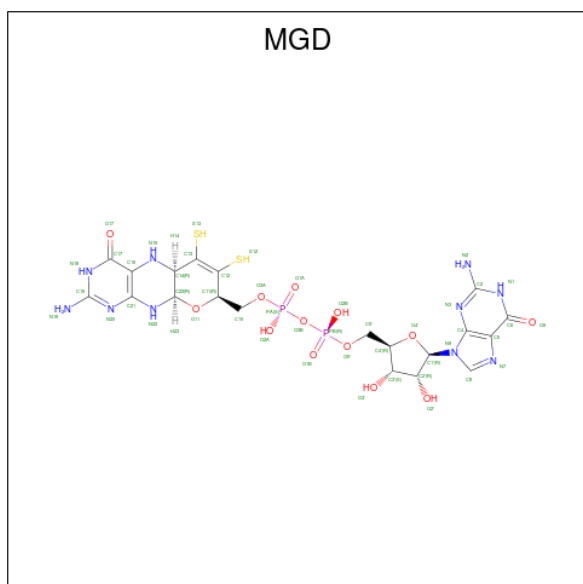
- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	G	2	Total	Zn	0
			2	2	
17	g	2	Total	Zn	0
			2	2	

- Molecule 18 is MOLYBDENUM ATOM (CCD ID: MO) (formula: Mo).

Mol	Chain	Residues	Atoms		AltConf
18	H	1	Total	Mo	0
			1	1	
18	h	1	Total	Mo	0
			1	1	

- Molecule 19 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂) (labeled as "Ligand of Interest" by depositor).

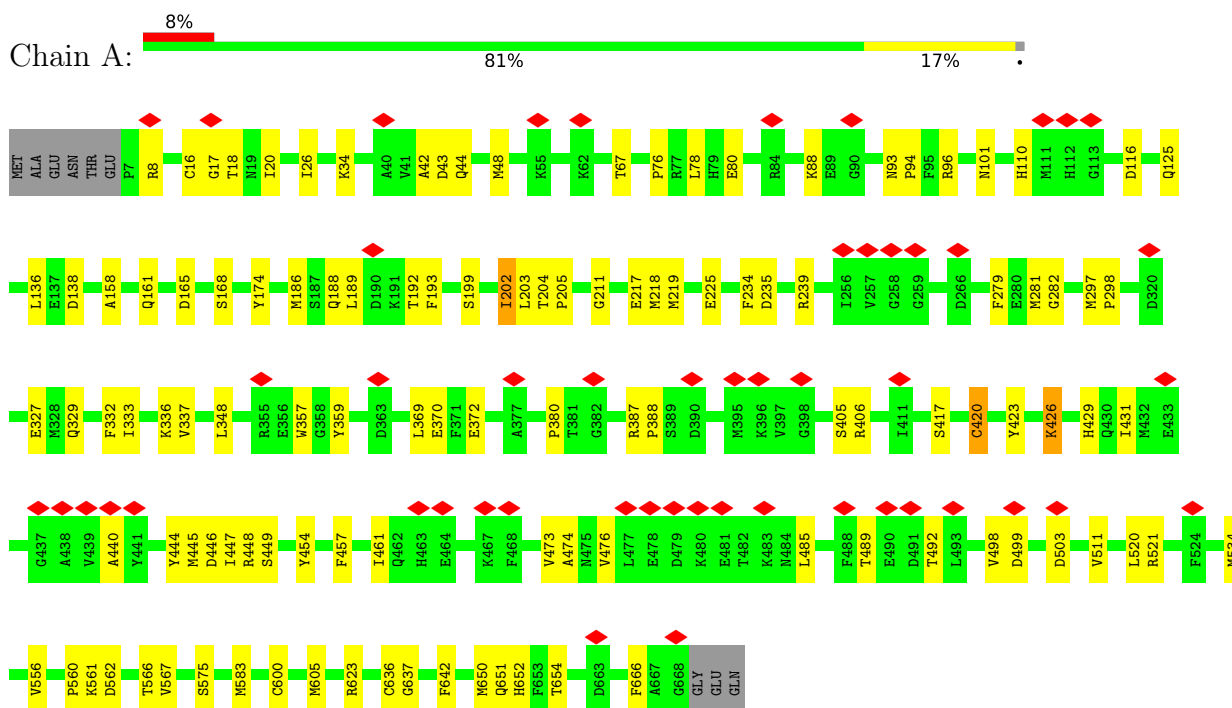


Mol	Chain	Residues	Atoms						AltConf
19	H	1	Total 47	C 20	N 10	O 13	P 2	S 2	0
19	H	1	Total 47	C 20	N 10	O 13	P 2	S 2	0
19	h	1	Total 47	C 20	N 10	O 13	P 2	S 2	0
19	h	1	Total 47	C 20	N 10	O 13	P 2	S 2	0

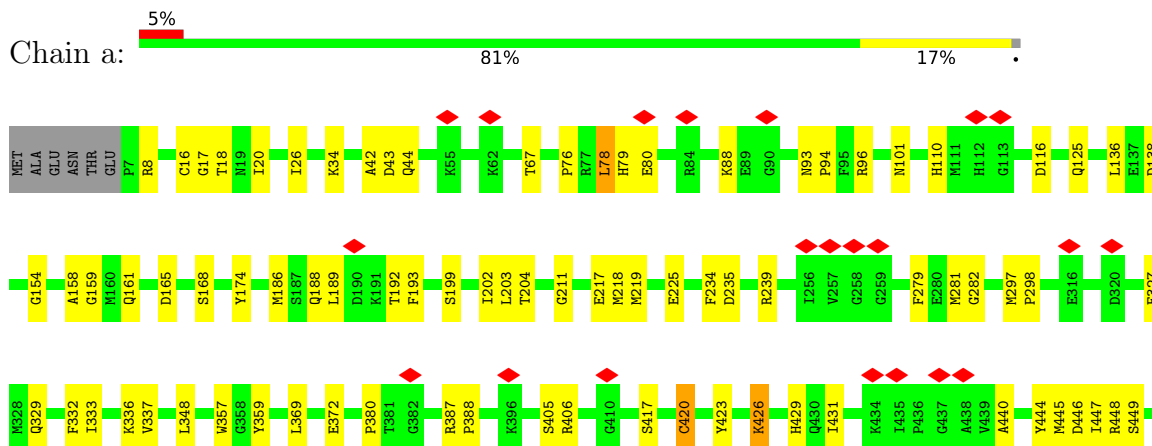
3 Residue-property plots

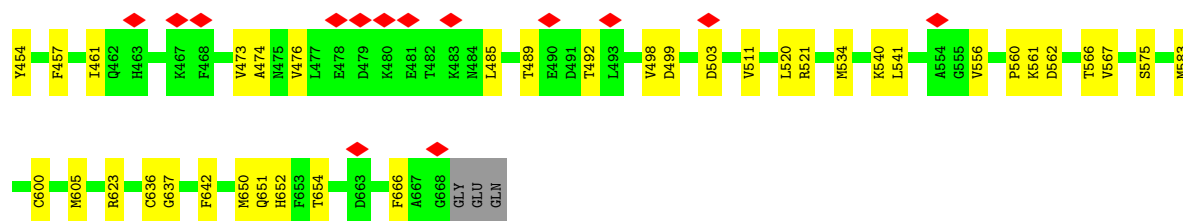
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: CoB–CoM heterodisulfide reductase iron-sulfur subunit A

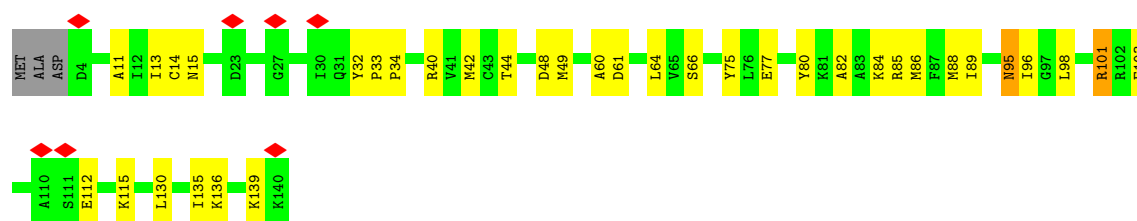
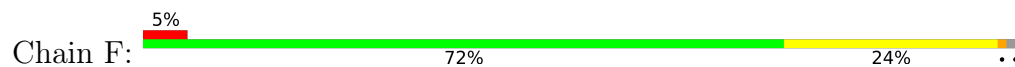


- Molecule 1: CoB–CoM heterodisulfide reductase iron-sulfur subunit A

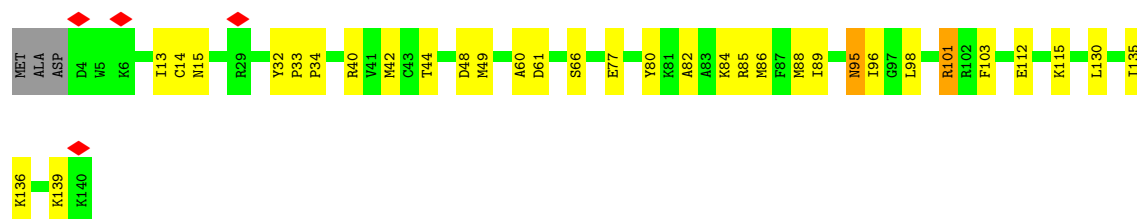
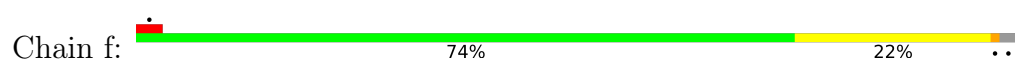




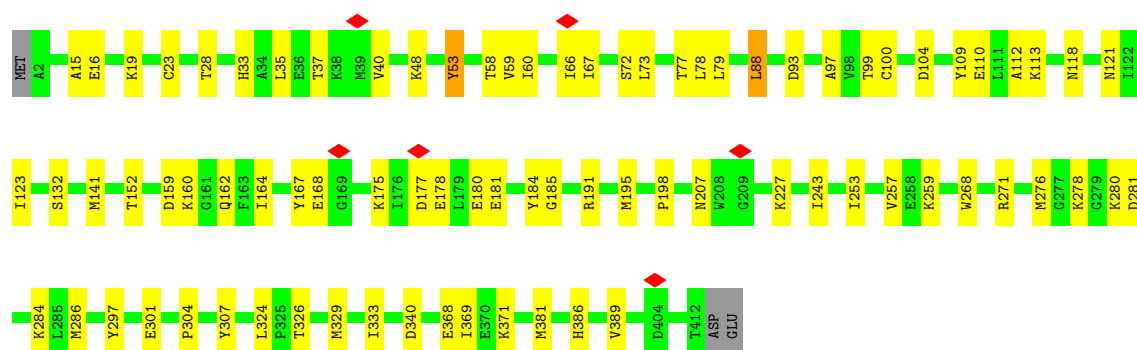
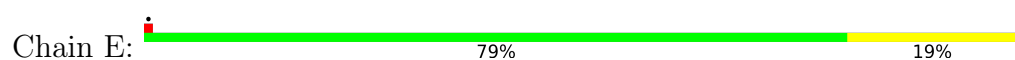
- Molecule 2: F420-non-reducing hydrogenase subunit D



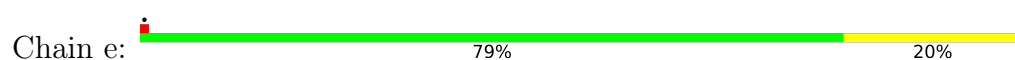
- Molecule 2: F420-non-reducing hydrogenase subunit D

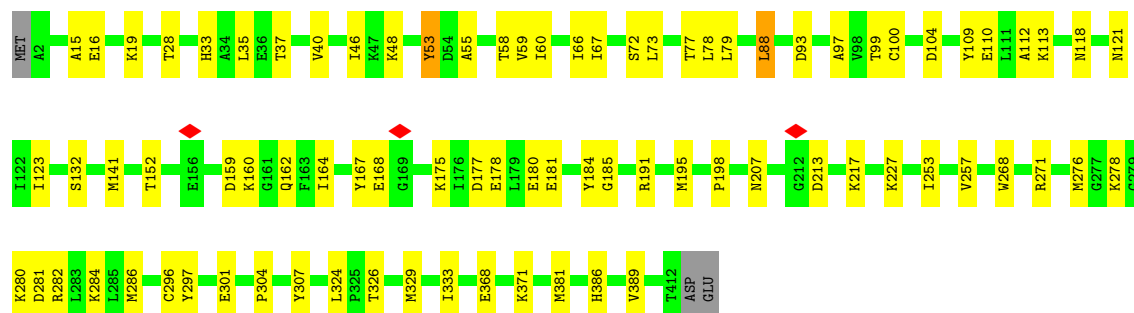


- Molecule 3: Formate dehydrogenase, beta subunit (F420)

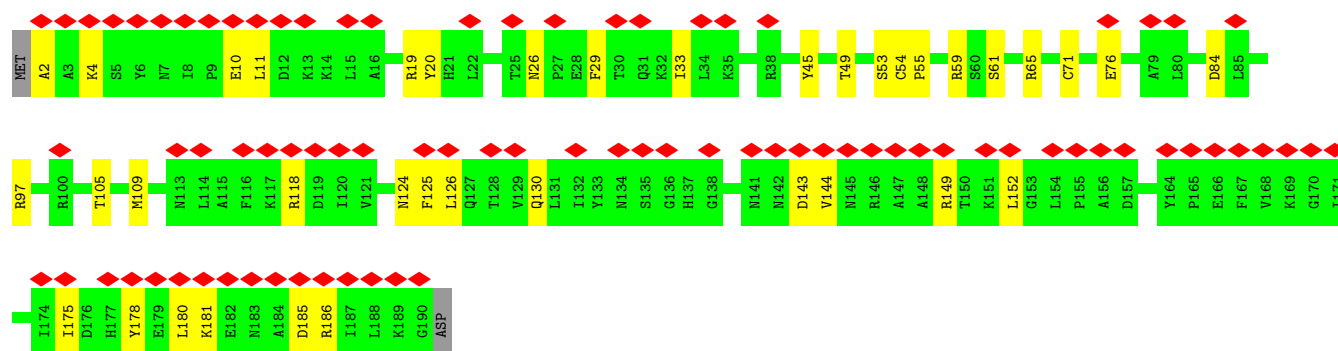
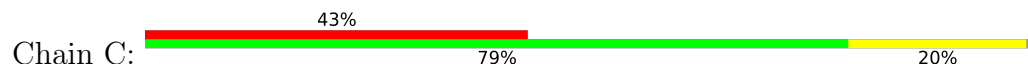


- Molecule 3: Formate dehydrogenase, beta subunit (F420)

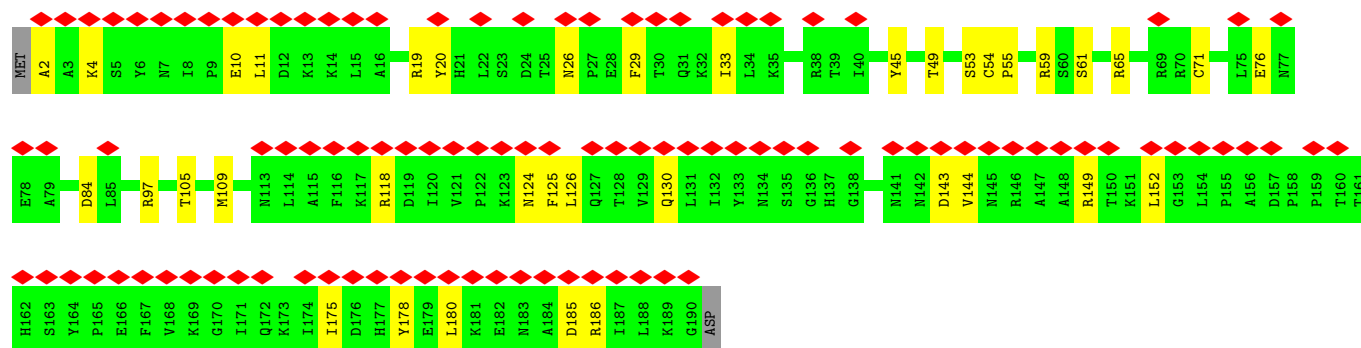
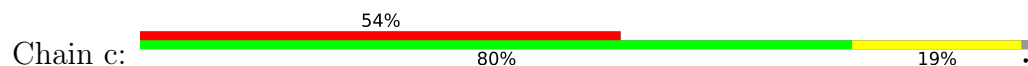




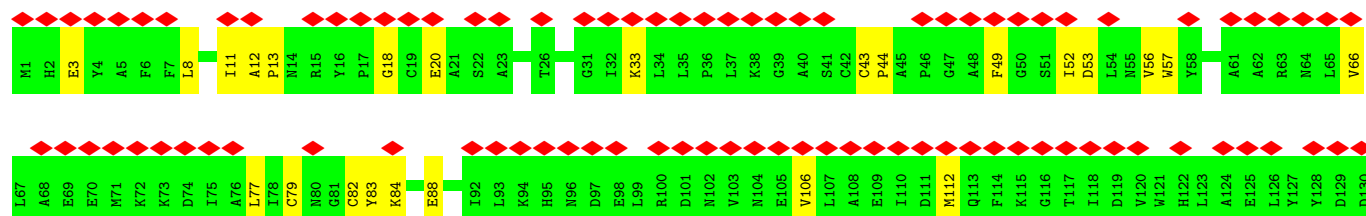
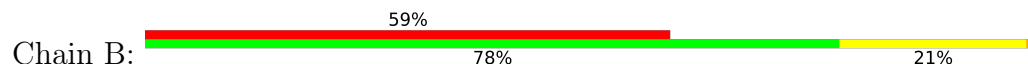
• Molecule 4: CoB-CoM heterodisulfide reductase subunit C

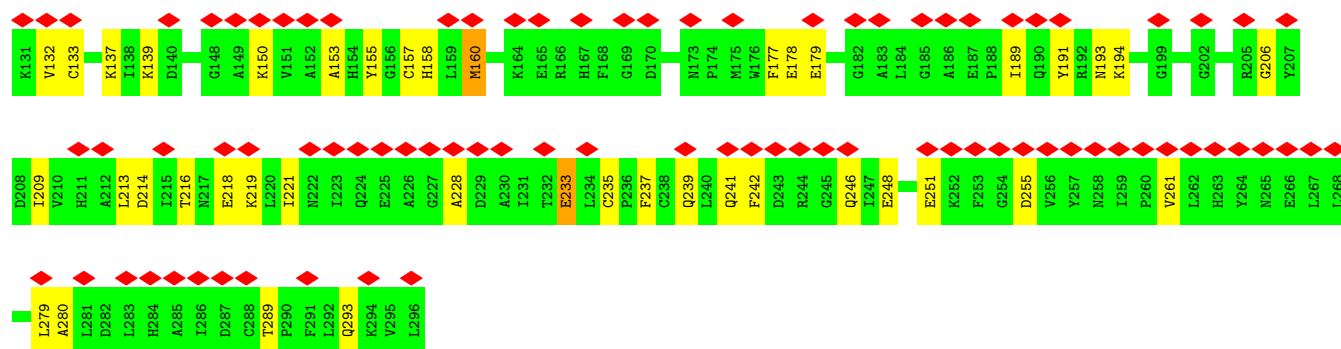


• Molecule 4: CoB-CoM heterodisulfide reductase subunit C

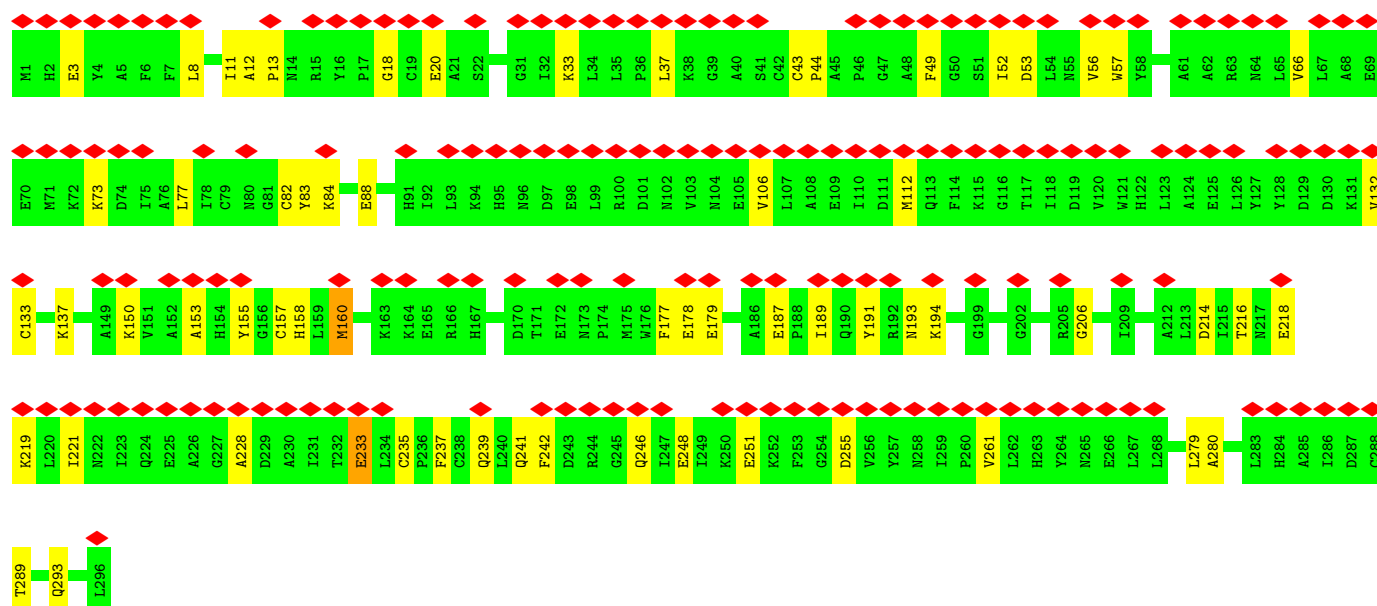
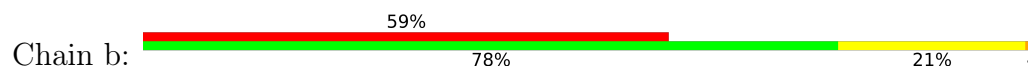


• Molecule 5: CoB-CoM heterodisulfide reductase subunit B

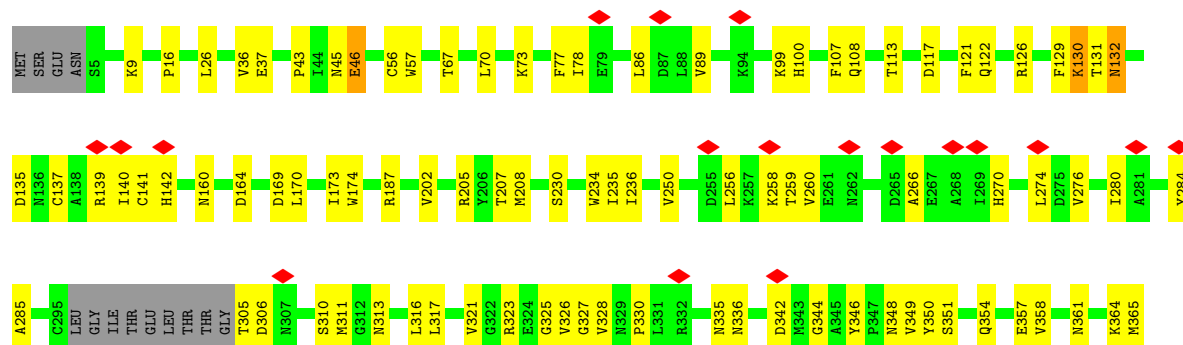


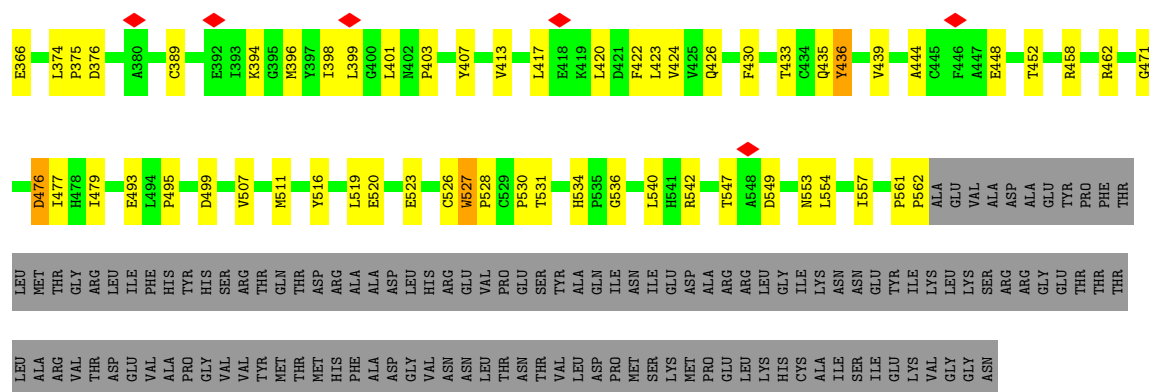


• Molecule 5: CoB–CoM heterodisulfide reductase subunit B

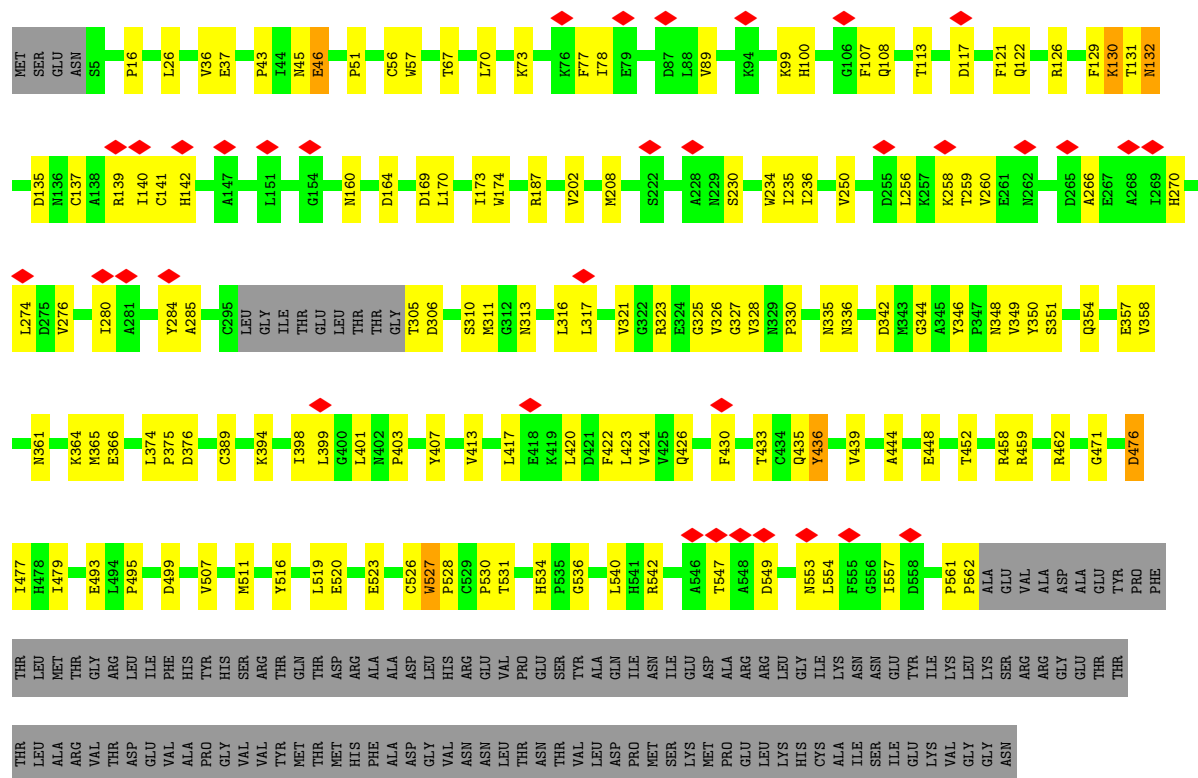


• Molecule 6: Formate dehydrogenase

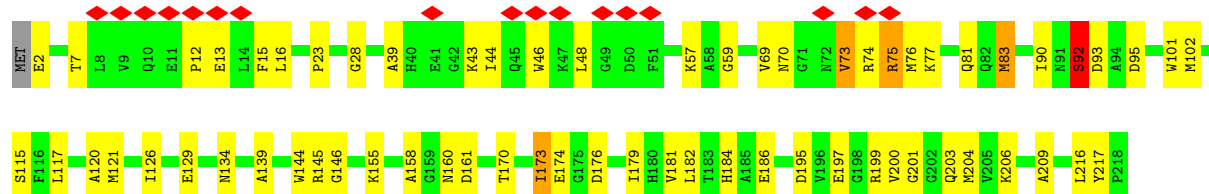


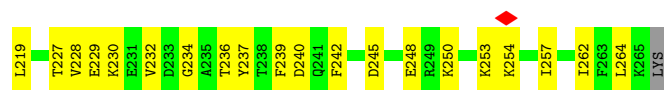


• Molecule 6: Formate dehydrogenase

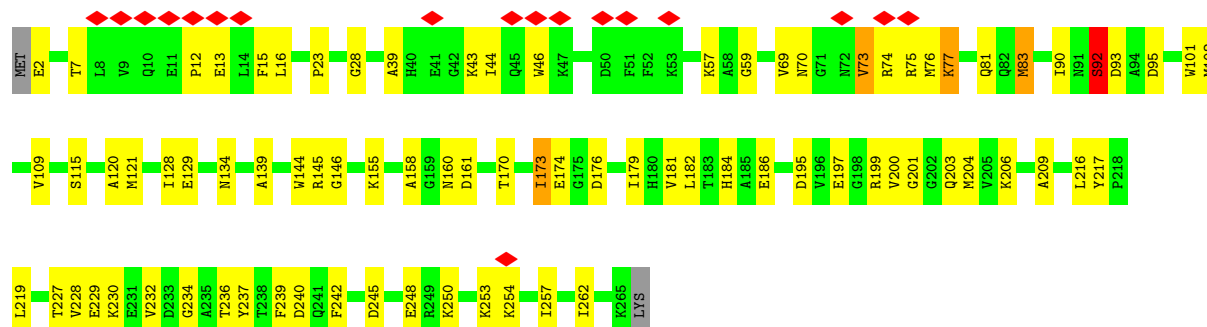


• Molecule 7: Formylmethanofuran dehydrogenase

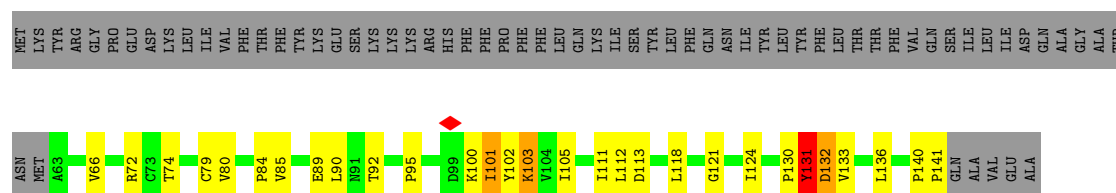
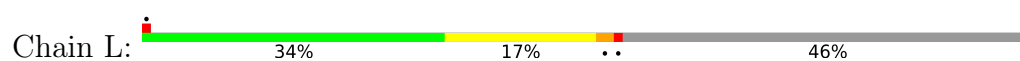




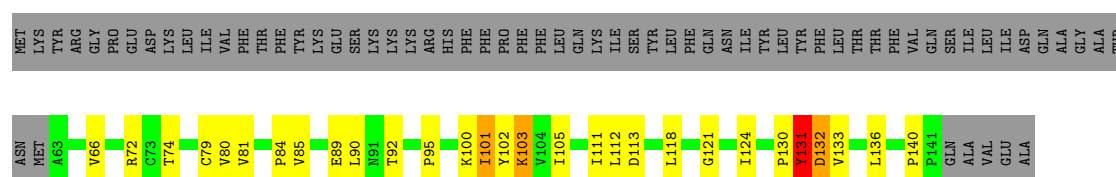
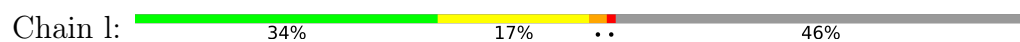
• Molecule 7: Formylmethanofuran dehydrogenase



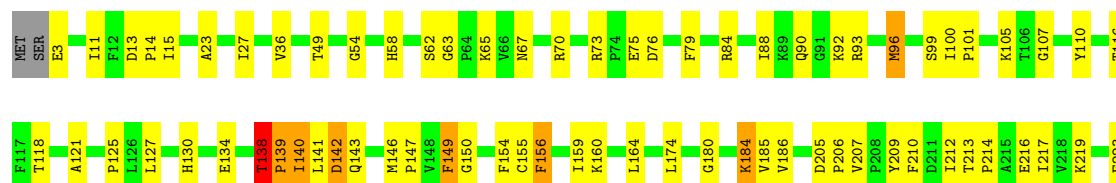
• Molecule 8: Formylmethanofuran dehydrogenase, subunit G

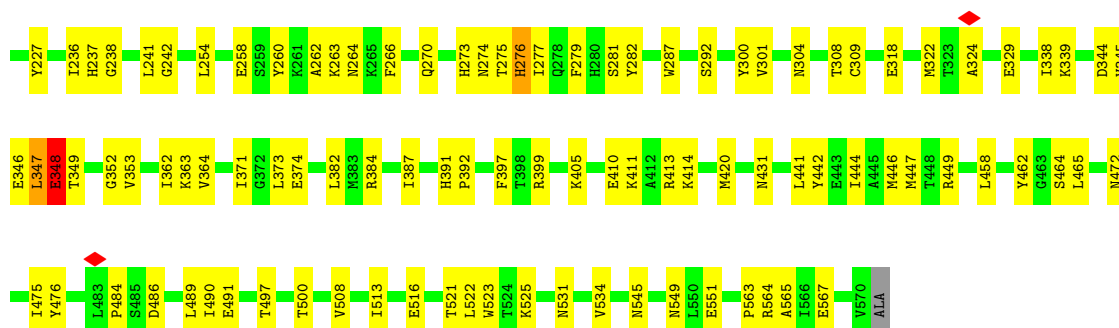


• Molecule 8: Formylmethanofuran dehydrogenase, subunit G



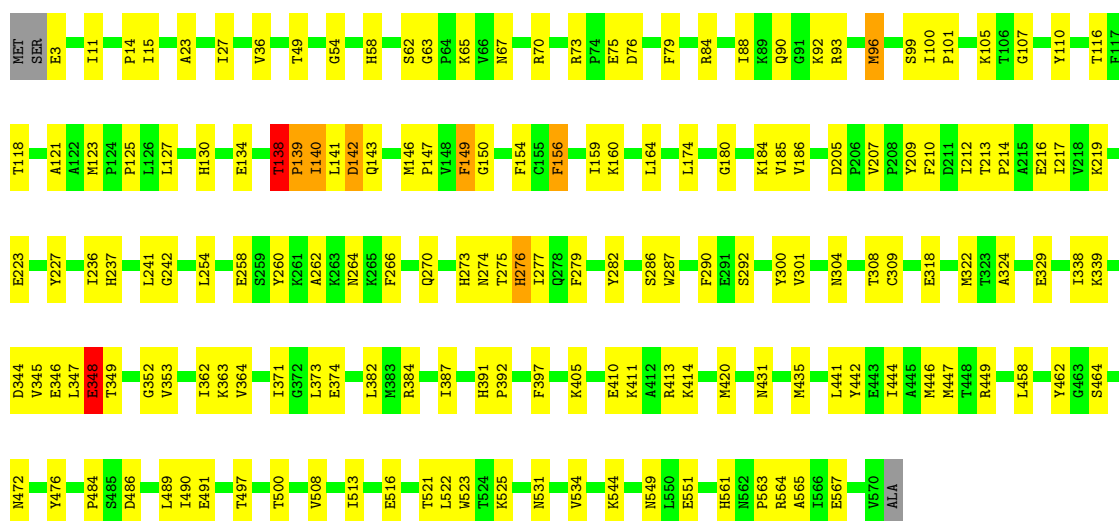
• Molecule 9: Formylmethanofuran dehydrogenase, subunit A





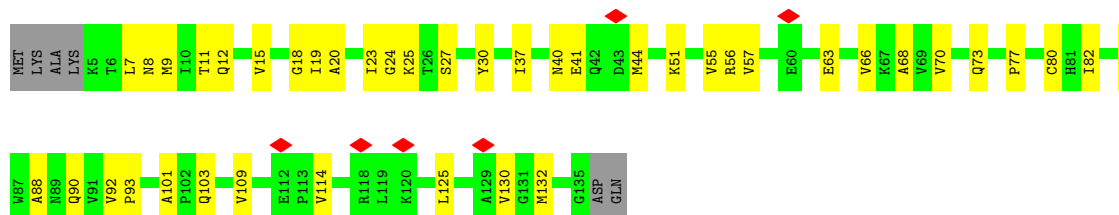
• Molecule 9: Formylmethanofuran dehydrogenase, subunit A

Chain g: 70% 28%



• Molecule 10: Formylmethanofuran dehydrogenase, subunit D

Chain J: 65% 31%



• Molecule 10: Formylmethanofuran dehydrogenase, subunit D

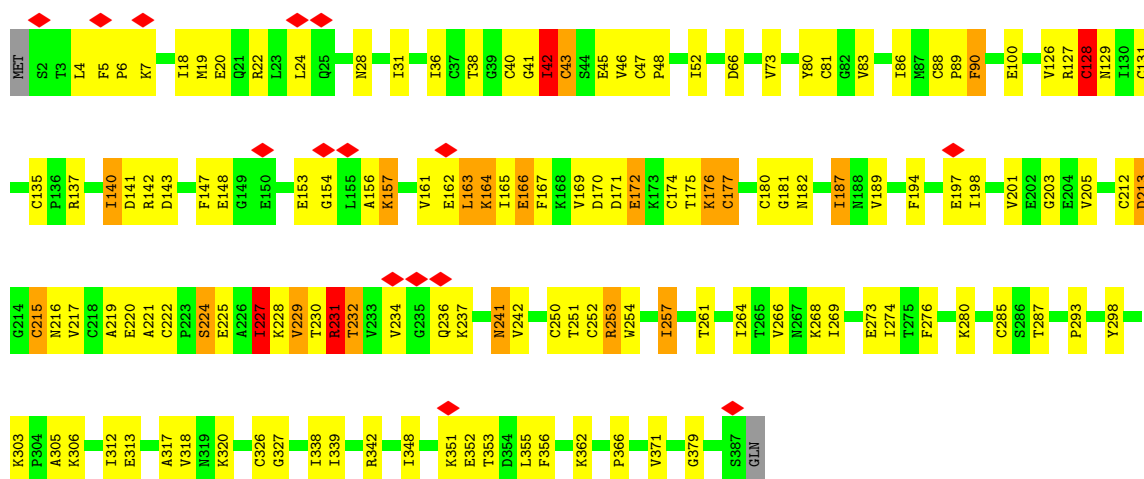
Chain j: 64% 32%





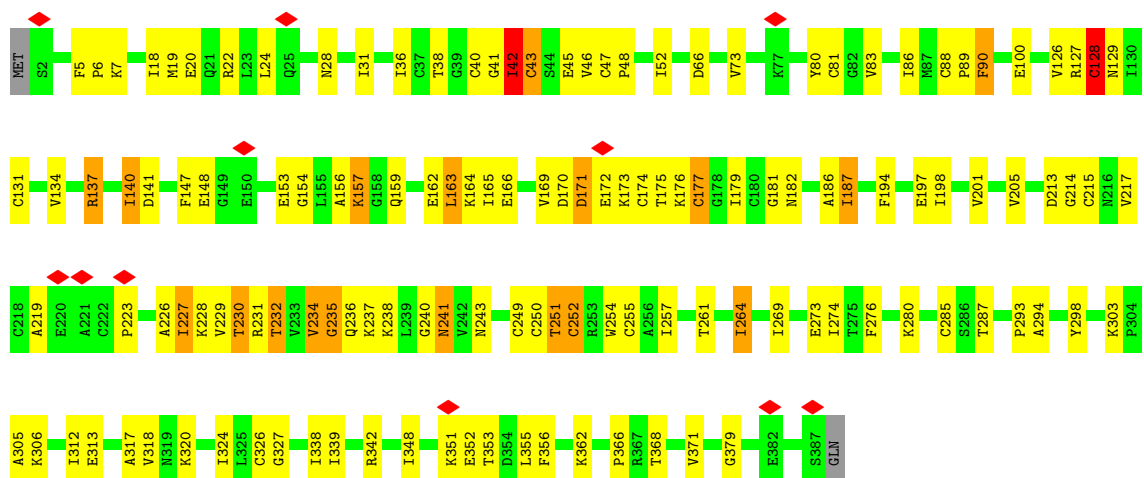
- Molecule 11: Formylmethanofuran dehydrogenase, subunit F

Chain K: 64% 30% 5% ..



- Molecule 11: Formylmethanofuran dehydrogenase, subunit F

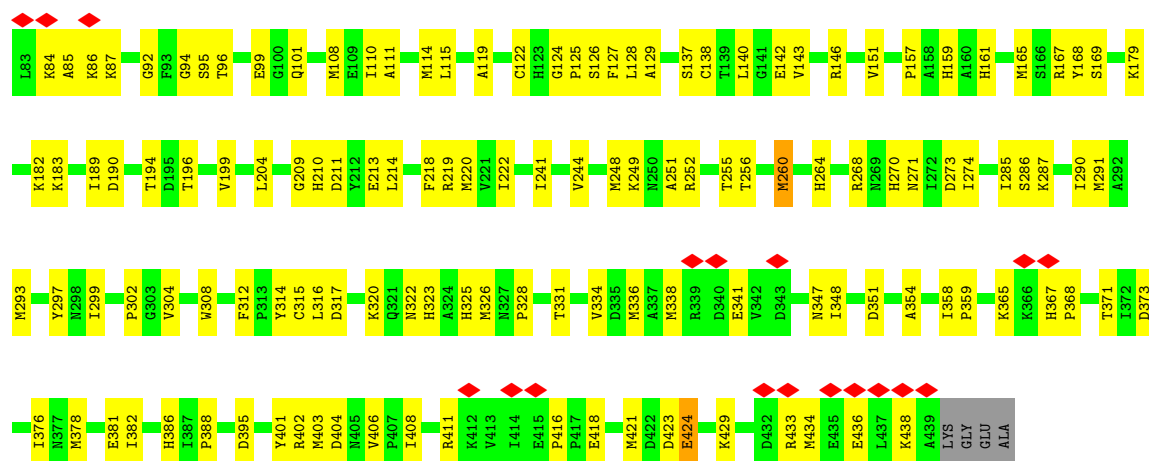
Chain k: 64% 30% 5% ..



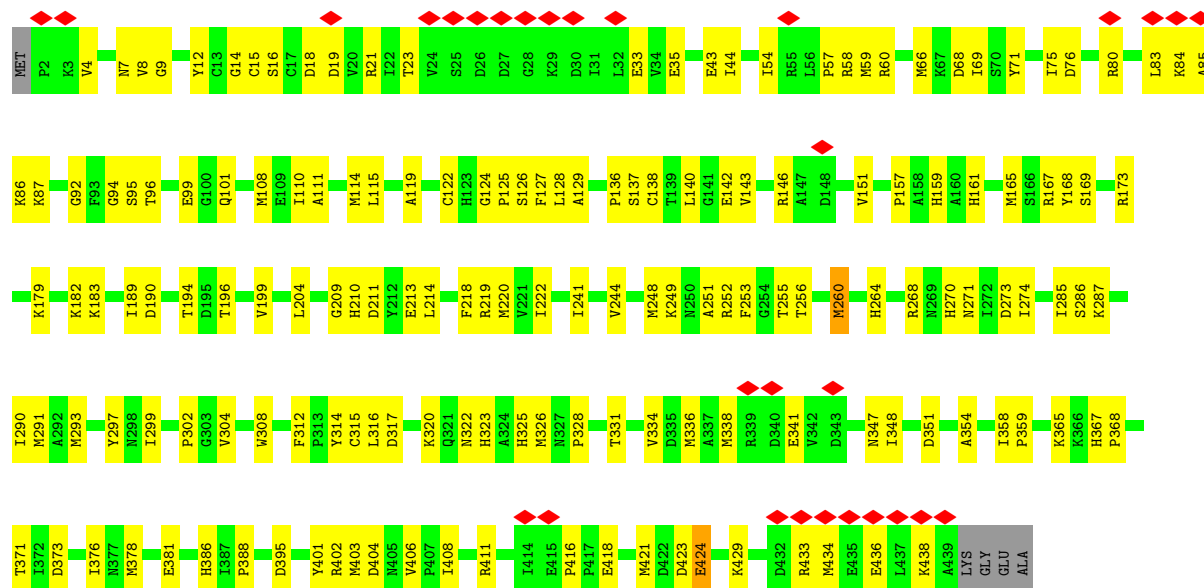
- Molecule 12: Formylmethanofuran dehydrogenase, subunit B

Chain H: 8% 63% 35% .





• Molecule 12: Formylmethanofuran dehydrogenase, subunit B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	203264	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	84.060	Depositor
Minimum map value	-31.762	Depositor
Average map value	0.047	Depositor
Map value standard deviation	1.829	Depositor
Recommended contour level	7	Depositor
Map size (Å)	537.6, 537.6, 537.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.68, 1.68, 1.68	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: SF4, ZN, FES, KCX, 9S8, MO, FAD, MGD

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	0.46	0/5115	0.65	3/6920 (0.0%)
1	a	0.47	0/5115	0.64	3/6920 (0.0%)
2	F	0.49	0/1096	0.64	1/1474 (0.1%)
2	f	0.50	0/1096	0.64	1/1474 (0.1%)
3	E	0.59	0/3208	0.75	2/4314 (0.0%)
3	e	0.59	0/3208	0.75	1/4314 (0.0%)
4	C	0.31	0/1529	0.41	0/2072
4	c	0.31	0/1529	0.41	0/2072
5	B	0.43	0/2355	0.62	2/3187 (0.1%)
5	b	0.43	0/2355	0.62	2/3187 (0.1%)
6	D	0.50	0/4345	0.70	7/5889 (0.1%)
6	d	0.50	0/4345	0.70	7/5889 (0.1%)
7	I	0.47	0/2029	0.73	1/2724 (0.0%)
7	i	0.47	0/2029	0.73	1/2724 (0.0%)
8	L	0.80	0/585	1.12	4/800 (0.5%)
8	l	0.80	0/585	1.12	3/800 (0.4%)
9	G	0.42	0/4549	0.65	10/6174 (0.2%)
9	g	0.42	0/4549	0.65	10/6174 (0.2%)
10	J	0.37	0/1023	0.58	0/1383
10	j	0.37	0/1023	0.57	0/1383
11	K	0.71	0/2952	1.04	11/3988 (0.3%)
11	k	0.70	0/2952	1.04	12/3988 (0.3%)
12	H	0.51	0/3497	0.68	1/4732 (0.0%)
12	h	0.52	0/3497	0.68	1/4732 (0.0%)
All	All	0.51	0/64566	0.72	83/87314 (0.1%)

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
11	k	0	1

There are no bond length outliers.

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	f	96	ILE	N-CA-C	-8.34	104.58	112.83
2	F	96	ILE	N-CA-C	-8.31	104.60	112.83
11	k	128	CYS	N-CA-C	8.18	120.28	111.36
11	K	128	CYS	N-CA-C	8.15	120.25	111.36
7	I	12	PRO	CB-CA-C	-7.76	102.03	111.11
7	i	12	PRO	CB-CA-C	-7.75	102.04	111.11
11	K	182	ASN	N-CA-C	-7.49	104.03	113.02
9	G	156	PHE	N-CA-C	-7.46	103.79	113.12
9	g	156	PHE	N-CA-C	-7.43	103.83	113.12
9	g	139	PRO	N-CA-C	7.38	127.67	112.47
9	G	139	PRO	N-CA-C	7.35	127.62	112.47
11	K	221	ALA	N-CA-C	-7.35	103.78	112.89
3	E	307	TYR	CB-CA-C	-7.26	99.26	111.02
3	e	307	TYR	CB-CA-C	-7.24	99.29	111.02
8	l	131	TYR	CB-CA-C	-7.05	99.90	111.68
11	K	128	CYS	CA-C-O	-7.05	112.95	120.42
11	k	128	CYS	CA-C-O	-7.01	112.99	120.42
8	L	131	TYR	CB-CA-C	-7.00	99.98	111.68
11	k	43	CYS	N-CA-C	-6.88	105.43	114.31
11	K	43	CYS	N-CA-C	-6.85	105.48	114.31
8	l	79	CYS	N-CA-C	-6.67	105.27	113.41
8	L	79	CYS	N-CA-C	-6.64	105.31	113.41
1	A	651	GLN	N-CA-C	6.63	118.50	111.28
1	a	651	GLN	N-CA-C	6.53	118.39	111.28
11	k	235	GLY	CA-C-O	-6.49	117.77	122.45
11	K	177	CYS	N-CA-C	-6.48	100.92	110.52
9	G	149	PHE	CB-CA-C	-6.38	100.68	111.02
9	g	149	PHE	CB-CA-C	-6.37	100.71	111.02
11	k	223	PRO	N-CA-C	-6.29	104.78	113.53
11	K	175	THR	N-CA-C	-6.25	105.51	113.01
9	G	142	ASP	N-CA-C	-6.11	102.30	110.55
9	g	142	ASP	N-CA-C	-6.11	102.30	110.55
11	K	80	TYR	CB-CA-C	6.07	120.34	111.73
11	k	80	TYR	CB-CA-C	6.07	120.34	111.73
6	d	530	PRO	N-CA-C	6.00	121.36	113.86
6	D	530	PRO	N-CA-C	5.95	121.30	113.86
5	B	193	ASN	CB-CA-C	5.87	120.22	111.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	b	193	ASN	CB-CA-C	5.84	120.19	111.89
6	d	37	GLU	CB-CA-C	5.77	117.55	108.84
6	D	37	GLU	CB-CA-C	5.73	117.49	108.84
6	d	45	ASN	CA-C-N	-5.70	113.53	122.08
6	d	45	ASN	C-N-CA	-5.70	113.53	122.08
6	D	45	ASN	CA-C-N	-5.66	113.59	122.08
6	D	45	ASN	C-N-CA	-5.66	113.59	122.08
1	a	193	PHE	CA-C-O	-5.60	114.71	120.87
9	g	138	THR	CB-CA-C	5.58	118.38	109.62
11	k	182	ASN	N-CA-C	-5.58	105.60	112.90
9	G	138	THR	CB-CA-C	5.56	118.36	109.62
1	A	193	PHE	CA-C-O	-5.56	114.76	120.87
6	d	46	GLU	CB-CA-C	5.53	119.68	111.88
6	D	46	GLU	CB-CA-C	5.52	119.66	111.88
6	D	45	ASN	N-CA-C	-5.51	99.45	108.76
6	d	45	ASN	N-CA-C	-5.51	99.46	108.76
9	G	154	PHE	CA-CB-CG	5.49	119.28	113.80
11	K	231	ARG	CA-C-O	-5.46	115.59	121.38
9	g	154	PHE	CA-CB-CG	5.46	119.26	113.80
8	L	85	VAL	N-CA-C	-5.39	105.86	111.58
11	K	231	ARG	N-CA-C	5.36	116.42	108.60
11	K	213	ASP	N-CA-C	-5.31	100.40	107.88
1	a	406	ARG	N-CA-C	-5.30	104.33	111.54
12	H	127	PHE	N-CA-C	-5.29	105.52	111.28
8	l	85	VAL	N-CA-C	-5.29	105.98	111.58
11	k	213	ASP	N-CA-C	-5.28	100.43	107.88
1	A	406	ARG	N-CA-C	-5.27	104.37	111.54
11	k	186	ALA	CA-C-N	-5.26	114.40	121.66
11	k	186	ALA	C-N-CA	-5.26	114.40	121.66
9	G	139	PRO	CB-CA-C	-5.26	102.88	111.56
9	g	139	PRO	CB-CA-C	-5.25	102.89	111.56
12	h	127	PHE	N-CA-C	-5.24	105.56	111.28
6	d	526	CYS	CB-CA-C	5.24	119.10	109.46
6	D	526	CYS	CB-CA-C	5.23	119.08	109.46
11	k	226	ALA	CA-C-O	-5.22	116.36	122.37
9	g	347	LEU	CA-C-O	-5.18	115.59	121.65
9	G	347	LEU	CA-C-O	-5.12	115.66	121.65
9	g	348	GLU	CA-C-N	-5.12	114.66	122.23
9	g	348	GLU	C-N-CA	-5.12	114.66	122.23
9	G	348	GLU	CA-C-N	-5.09	114.69	122.23
9	G	348	GLU	C-N-CA	-5.09	114.69	122.23
11	k	177	CYS	N-CA-C	-5.08	102.17	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	23	CYS	CA-C-O	-5.08	116.88	119.77
8	L	131	TYR	CA-C-O	-5.06	115.73	121.39
5	B	153	ALA	N-CA-C	5.05	117.85	109.46
5	b	153	ALA	N-CA-C	5.05	117.84	109.46

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	k	159	GLN	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5011	0	4967	76	0
1	a	5011	0	4967	75	0
2	F	1073	0	1082	26	0
2	f	1073	0	1082	24	0
3	E	3151	0	3162	50	0
3	e	3151	0	3162	52	0
4	C	1498	0	1495	28	0
4	c	1498	0	1495	27	0
5	B	2304	0	2272	46	0
5	b	2304	0	2272	43	0
6	D	4251	0	4204	98	0
6	d	4251	0	4204	97	0
7	I	1996	0	2001	58	0
7	i	1996	0	2001	53	0
8	L	576	0	559	18	0
8	l	576	0	559	18	0
9	G	4455	0	4380	132	0
9	g	4455	0	4380	126	0
10	J	1007	0	1022	36	0
10	j	1007	0	1022	38	0
11	K	2910	0	2894	89	0
11	k	2910	0	2894	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	H	3416	0	3354	111	0
12	h	3416	0	3354	115	0
13	A	48	0	0	2	0
13	C	16	0	0	1	0
13	D	8	0	0	0	0
13	E	32	0	0	0	0
13	H	8	0	0	0	0
13	K	64	0	0	2	0
13	L	16	0	0	0	0
13	a	48	0	0	2	0
13	c	16	0	0	1	0
13	d	8	0	0	0	0
13	e	32	0	0	0	0
13	h	8	0	0	0	0
13	k	64	0	0	2	0
13	l	16	0	0	0	0
14	A	53	0	31	0	0
14	E	53	0	31	1	0
14	a	53	0	31	0	0
14	e	53	0	31	0	0
15	F	4	0	0	0	0
15	f	4	0	0	0	0
16	B	16	0	0	1	0
16	b	16	0	0	1	0
17	G	2	0	0	0	0
17	g	2	0	0	0	0
18	H	1	0	0	0	0
18	h	1	0	0	0	0
19	H	94	0	44	8	0
19	h	94	0	44	8	0
All	All	64126	0	62996	1380	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 11.

All (1380) 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)
11:K:127:ARG:HH21	11:K:241:ASN:HA	1.23	0.99
9:g:107:GLY:HA3	9:g:139:PRO:HD2	1.49	0.94
9:G:107:GLY:HA3	9:G:139:PRO:HD2	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:11:THR:HG21	19:H:503:MGD:H191	1.34	0.92
10:j:11:THR:HG21	19:h:503:MGD:H191	1.34	0.91
7:i:74:ARG:HG3	7:i:93:ASP:HB2	1.58	0.85
7:I:74:ARG:HG3	7:I:93:ASP:HB2	1.58	0.85
11:K:251:THR:HG21	11:K:269:ILE:HG23	1.59	0.85
11:K:127:ARG:NH2	11:K:241:ASN:HA	1.93	0.83
11:K:251:THR:HB	11:K:268:LYS:HA	1.63	0.80
11:K:170:ASP:HB3	11:K:172:GLU:HG2	1.64	0.79
5:b:53:ASP:HB3	5:b:56:VAL:HG12	1.65	0.79
5:B:53:ASP:HB3	5:B:56:VAL:HG12	1.65	0.78
9:g:186:VAL:HG11	9:g:324:ALA:HB3	1.65	0.78
9:G:15:ILE:HD12	9:G:464:SER:HB2	1.66	0.78
4:C:125:PHE:HB3	5:B:52:ILE:HD11	1.65	0.77
9:G:186:VAL:HG11	9:G:324:ALA:HB3	1.65	0.77
9:G:125:PRO:HD2	9:G:348:GLU:HG2	1.67	0.77
3:e:48:LYS:HG2	3:e:73:LEU:HD21	1.66	0.77
4:c:125:PHE:HB3	5:b:52:ILE:HD11	1.65	0.77
9:g:15:ILE:HD12	9:g:464:SER:HB2	1.66	0.76
3:E:48:LYS:HG2	3:E:73:LEU:HD21	1.66	0.76
9:G:387:ILE:HG13	9:G:447:MET:HE2	1.69	0.75
9:g:387:ILE:HG13	9:g:447:MET:HE2	1.69	0.75
9:g:258:GLU:OE2	9:g:304:ASN:ND2	2.20	0.74
3:E:79:LEU:HD21	3:E:304:PRO:HG3	1.69	0.74
9:g:125:PRO:HD2	9:g:348:GLU:HG2	1.67	0.74
6:d:129:PHE:HD2	6:d:131:THR:HG23	1.54	0.73
6:D:129:PHE:HD2	6:D:131:THR:HG23	1.54	0.73
1:A:192:THR:HG23	1:A:199:SER:HB2	1.71	0.73
3:e:79:LEU:HD21	3:e:304:PRO:HG3	1.70	0.73
9:G:258:GLU:OE2	9:G:304:ASN:ND2	2.20	0.72
3:e:368:GLU:HA	3:e:371:LYS:HG2	1.72	0.72
2:F:15:ASN:OD1	2:F:40:ARG:NH1	2.23	0.72
6:D:351:SER:O	6:D:354:GLN:NE2	2.22	0.72
10:j:20:ALA:HB1	10:j:30:TYR:HA	1.72	0.72
7:i:229:GLU:HB2	7:i:236:THR:HG23	1.72	0.72
4:C:76:GLU:OE2	4:C:118:ARG:NH2	2.23	0.71
2:f:15:ASN:OD1	2:f:40:ARG:NH1	2.23	0.71
7:i:253:LYS:HG3	7:i:254:LYS:H	1.54	0.71
1:A:96:ARG:NH1	1:A:138:ASP:OD1	2.23	0.71
7:I:144:TRP:HH2	9:G:73:ARG:HH12	1.39	0.71
9:G:54:GLY:HA2	9:G:449:ARG:HG3	1.72	0.71
3:E:152:THR:HG22	3:E:167:TYR:HB2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:253:LYS:HG3	7:I:254:LYS:H	1.54	0.71
11:K:161:VAL:HA	11:K:237:LYS:HG2	1.71	0.71
12:H:59:MET:HE3	12:H:69:ILE:HD13	1.73	0.71
10:j:73:GLN:HE21	12:h:194:THR:HA	1.55	0.71
7:I:229:GLU:HB2	7:I:236:THR:HG23	1.72	0.71
1:a:96:ARG:NH1	1:a:138:ASP:OD1	2.24	0.70
2:f:82:ALA:O	2:f:86:MET:HG2	1.91	0.70
2:F:82:ALA:O	2:F:86:MET:HG2	1.91	0.70
6:d:351:SER:O	6:d:354:GLN:NE2	2.22	0.70
3:E:368:GLU:HA	3:E:371:LYS:HG2	1.72	0.70
7:I:248:GLU:OE1	12:H:219:ARG:NH2	2.25	0.70
9:G:67:ASN:OD1	9:G:130:HIS:NE2	2.24	0.70
10:J:73:GLN:HE21	12:H:194:THR:HA	1.55	0.70
9:g:54:GLY:HA2	9:g:449:ARG:HG3	1.72	0.70
10:J:20:ALA:HB1	10:J:30:TYR:HA	1.72	0.70
3:e:152:THR:HG22	3:e:167:TYR:HB2	1.73	0.70
6:d:364:LYS:NZ	6:d:507:VAL:O	2.25	0.70
4:c:76:GLU:OE2	4:c:118:ARG:NH2	2.23	0.70
7:i:144:TRP:HH2	9:g:73:ARG:HH12	1.39	0.70
7:i:248:GLU:OE1	12:h:219:ARG:NH2	2.25	0.70
12:H:354:ALA:HB2	12:H:378:MET:HG3	1.74	0.70
10:J:11:THR:HG21	19:H:503:MGD:N19	2.07	0.69
1:A:575:SER:HB2	1:a:575:SER:HB2	1.74	0.69
9:G:185:VAL:HB	9:G:236:ILE:HD12	1.73	0.69
1:a:211:GLY:HA3	1:a:297:MET:HE2	1.75	0.69
12:h:59:MET:HE3	12:h:69:ILE:HD13	1.73	0.69
12:h:114:MET:HG3	12:h:336:MET:HE1	1.74	0.69
9:g:185:VAL:HB	9:g:236:ILE:HD12	1.73	0.69
9:G:301:VAL:O	9:G:384:ARG:NH2	2.26	0.69
3:E:162:GLN:HB3	3:E:175:LYS:HE2	1.75	0.69
6:D:364:LYS:NZ	6:D:507:VAL:O	2.25	0.69
9:g:301:VAL:O	9:g:384:ARG:NH2	2.26	0.69
12:h:354:ALA:HB2	12:h:378:MET:HG3	1.73	0.69
7:I:23:PRO:HD2	7:I:83:MET:HG3	1.75	0.69
9:g:67:ASN:OD1	9:g:130:HIS:NE2	2.24	0.68
9:G:449:ARG:NH2	9:G:476:TYR:OH	2.27	0.68
12:H:19:ASP:OD2	12:H:167:ARG:NH1	2.23	0.68
3:e:162:GLN:HB3	3:e:175:LYS:HE2	1.75	0.68
12:h:19:ASP:OD2	12:h:167:ARG:NH1	2.23	0.68
12:H:114:MET:HG3	12:H:336:MET:HE1	1.74	0.68
11:k:7:LYS:HB2	11:k:22:ARG:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:7:LYS:HB2	11:K:22:ARG:HB2	1.75	0.68
9:g:344:ASP:OD1	12:h:287:LYS:NZ	2.27	0.68
1:A:211:GLY:HA3	1:A:297:MET:HE2	1.75	0.67
9:G:344:ASP:OD1	12:H:287:LYS:NZ	2.27	0.67
9:g:449:ARG:NH2	9:g:476:TYR:OH	2.27	0.67
1:a:387:ARG:HD2	1:a:503:ASP:HB3	1.77	0.67
7:i:23:PRO:HD2	7:i:83:MET:HG3	1.75	0.67
1:A:387:ARG:HD2	1:A:503:ASP:HB3	1.77	0.67
1:A:431:ILE:HD11	1:A:440:ALA:HB2	1.76	0.66
6:d:236:ILE:HD11	6:d:317:LEU:HD11	1.78	0.66
12:h:60:ARG:NH2	12:h:381:GLU:O	2.29	0.66
1:a:431:ILE:HD11	1:a:440:ALA:HB2	1.76	0.66
3:e:152:THR:HG23	3:e:168:GLU:HG3	1.78	0.66
3:E:152:THR:HG23	3:E:168:GLU:HG3	1.78	0.66
10:j:11:THR:HG21	19:h:503:MGD:N19	2.07	0.66
11:K:131:CYS:HB2	11:K:140:ILE:HD12	1.77	0.66
12:H:60:ARG:NH2	12:H:381:GLU:O	2.29	0.66
9:g:549:ASN:ND2	12:h:7:ASN:OD1	2.26	0.66
6:D:236:ILE:HD11	6:D:317:LEU:HD11	1.78	0.65
2:F:112:GLU:HB3	2:F:115:LYS:HB3	1.78	0.65
2:f:112:GLU:HB3	2:f:115:LYS:HB3	1.78	0.65
9:g:486:ASP:HB3	9:g:489:LEU:HD23	1.79	0.65
9:g:405:LYS:HD3	9:g:491:GLU:HG3	1.79	0.65
11:k:251:THR:HG21	11:k:269:ILE:HG23	1.78	0.64
6:D:122:GLN:OE1	6:D:126:ARG:NH1	2.30	0.64
9:G:405:LYS:HD3	9:G:491:GLU:HG3	1.79	0.64
9:G:549:ASN:ND2	12:H:7:ASN:OD1	2.26	0.64
12:H:137:SER:OG	12:H:138:CYS:N	2.31	0.64
9:G:486:ASP:HB3	9:G:489:LEU:HD23	1.79	0.64
9:g:65:LYS:HZ1	9:g:324:ALA:HB2	1.63	0.64
6:D:140:ILE:HD13	6:D:407:TYR:HE2	1.63	0.63
6:d:122:GLN:OE1	6:d:126:ARG:NH1	2.30	0.63
12:h:260:MET:HE3	12:h:264:HIS:CE1	2.33	0.63
3:E:123:ILE:HG12	3:E:227:LYS:HD3	1.80	0.63
9:G:287:TRP:O	9:G:363:LYS:NZ	2.31	0.63
12:H:260:MET:HE3	12:H:264:HIS:CE1	2.33	0.63
9:g:523:TRP:HE1	9:g:563:PRO:HB2	1.63	0.63
11:k:312:ILE:HG23	11:k:313:GLU:H	1.64	0.63
10:J:19:ILE:HG23	12:H:43:GLU:OE1	1.99	0.62
9:G:110:TYR:HB2	9:G:141:LEU:HD11	1.81	0.62
9:G:523:TRP:HE1	9:G:563:PRO:HB2	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:d:140:ILE:HD13	6:d:407:TYR:HE2	1.63	0.62
6:d:174:TRP:CG	6:d:311:MET:HE1	2.35	0.62
3:e:123:ILE:HG12	3:e:227:LYS:HD3	1.80	0.62
9:g:264:ASN:ND2	9:g:266:PHE:O	2.33	0.62
6:D:174:TRP:CG	6:D:311:MET:HE1	2.35	0.62
10:j:19:ILE:HG23	12:h:43:GLU:OE1	1.99	0.62
6:d:170:LEU:HD23	6:d:284:TYR:HA	1.81	0.62
9:g:110:TYR:HB2	9:g:141:LEU:HD11	1.81	0.62
11:k:41:GLY:C	11:k:43:CYS:H	2.08	0.62
1:A:429:HIS:HB2	1:A:461:ILE:HD12	1.82	0.61
11:K:41:GLY:C	11:K:43:CYS:H	2.08	0.61
3:E:118:ASN:ND2	3:E:121:ASN:OD1	2.33	0.61
11:k:166:GLU:OE2	11:k:230:THR:HB	2.01	0.61
2:F:13:ILE:HG22	2:F:66:SER:HB3	1.82	0.61
9:G:274:ASN:HD22	9:G:277:ILE:HG12	1.66	0.61
11:K:251:THR:CB	11:K:268:LYS:HA	2.30	0.61
9:g:110:TYR:HB3	9:g:141:LEU:HD21	1.81	0.61
4:C:55:PRO:O	4:C:59:ARG:NH1	2.34	0.61
6:D:170:LEU:HD23	6:D:284:TYR:HA	1.81	0.61
9:G:110:TYR:HB3	9:G:141:LEU:HD21	1.81	0.61
3:e:118:ASN:ND2	3:e:121:ASN:OD1	2.33	0.61
11:K:312:ILE:HG23	11:K:313:GLU:H	1.64	0.61
1:a:429:HIS:HB2	1:a:461:ILE:HD12	1.83	0.61
11:K:38:THR:HB	11:K:293:PRO:HG3	1.82	0.61
4:c:55:PRO:O	4:c:59:ARG:NH1	2.34	0.61
5:b:66:VAL:HG23	5:b:112:MET:HE2	1.83	0.61
1:a:161:GLN:HG2	1:a:567:VAL:HG13	1.83	0.61
6:d:235:ILE:HG12	6:d:285:ALA:HB2	1.83	0.61
9:g:287:TRP:O	9:g:363:LYS:NZ	2.31	0.61
1:A:161:GLN:HG2	1:A:567:VAL:HG13	1.82	0.61
2:f:13:ILE:HG22	2:f:66:SER:HB3	1.82	0.61
5:b:233:GLU:HG2	5:b:235:CYS:H	1.66	0.61
9:g:338:ILE:HG22	9:g:339:LYS:H	1.66	0.61
6:D:310:SER:HA	6:D:313:ASN:HD22	1.66	0.60
9:G:264:ASN:ND2	9:G:266:PHE:O	2.33	0.60
9:G:329:GLU:HG3	9:G:352:GLY:HA3	1.83	0.60
3:e:177:ASP:OD2	3:e:178:GLU:N	2.34	0.60
9:g:186:VAL:HG13	9:g:237:HIS:ND1	2.16	0.60
9:g:329:GLU:HG3	9:g:352:GLY:HA3	1.83	0.60
12:h:137:SER:OG	12:h:138:CYS:N	2.31	0.60
6:D:235:ILE:HG12	6:D:285:ALA:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:38:THR:HB	11:k:293:PRO:HG3	1.82	0.60
9:G:338:ILE:HG22	9:G:339:LYS:H	1.66	0.60
9:G:186:VAL:HG13	9:G:237:HIS:ND1	2.16	0.60
9:g:237:HIS:CD2	9:g:276:HIS:CE1	2.90	0.60
8:L:118:LEU:HD23	11:K:371:VAL:HG12	1.84	0.60
1:a:20:ILE:HG22	1:a:26:ILE:HD11	1.84	0.60
2:f:61:ASP:OD1	2:f:136:LYS:NZ	2.34	0.60
7:i:176:ASP:HB2	7:i:195:ASP:O	2.02	0.60
5:B:233:GLU:HG2	5:B:235:CYS:H	1.66	0.60
9:g:274:ASN:HD22	9:g:277:ILE:HG12	1.66	0.60
7:I:13:GLU:OE2	12:H:86:LYS:NZ	2.34	0.60
3:E:177:ASP:OD2	3:E:178:GLU:N	2.35	0.60
9:G:76:ASP:HA	9:G:84:ARG:HH22	1.67	0.59
9:G:237:HIS:CD2	9:G:276:HIS:CE1	2.90	0.59
4:C:61:SER:OG	4:C:84:ASP:OD2	2.20	0.59
7:I:176:ASP:HB2	7:I:195:ASP:O	2.02	0.59
1:A:17:GLY:O	1:A:18:THR:HG22	2.03	0.59
3:e:79:LEU:HD12	3:e:104:ASP:OD1	2.03	0.59
2:F:135:ILE:HG22	2:F:139:LYS:HE3	1.84	0.59
9:G:127:LEU:HD21	12:H:406:VAL:HG22	1.83	0.59
12:H:94:GLY:HA2	12:H:299:ILE:HD13	1.85	0.59
4:c:143:ASP:OD1	4:c:144:VAL:N	2.36	0.59
7:i:13:GLU:OE2	12:h:86:LYS:NZ	2.35	0.59
9:g:76:ASP:HA	9:g:84:ARG:HH22	1.67	0.59
11:k:305:ALA:O	11:k:306:LYS:HG2	2.02	0.59
5:B:66:VAL:HG23	5:B:112:MET:HE2	1.83	0.59
2:F:61:ASP:OD1	2:F:136:LYS:NZ	2.34	0.59
9:g:127:LEU:HD21	12:h:406:VAL:HG22	1.83	0.59
3:E:79:LEU:HD12	3:E:104:ASP:OD1	2.03	0.59
4:c:61:SER:OG	4:c:84:ASP:OD2	2.20	0.59
7:i:145:ARG:NH1	9:g:75:GLU:OE2	2.36	0.59
8:l:118:LEU:HD23	11:k:371:VAL:HG12	1.84	0.59
7:I:145:ARG:NH1	9:G:75:GLU:OE2	2.36	0.59
9:G:110:TYR:CE2	9:G:118:THR:HG21	2.38	0.59
9:G:525:LYS:HB3	9:G:567:GLU:HA	1.85	0.59
10:J:12:GLN:NE2	19:H:502:MGD:H8	2.17	0.59
11:K:305:ALA:O	11:K:306:LYS:HG2	2.02	0.59
12:H:293:MET:HA	12:H:403:MET:HE3	1.84	0.59
6:d:73:LYS:HD3	6:d:78:ILE:HD11	1.85	0.59
12:h:94:GLY:HA2	12:h:299:ILE:HD13	1.85	0.59
6:d:310:SER:HA	6:d:313:ASN:HD22	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:12:GLN:NE2	19:h:502:MGD:H8	2.17	0.58
11:k:127:ARG:HH21	11:k:241:ASN:HA	1.68	0.58
4:C:143:ASP:OD1	4:C:144:VAL:N	2.36	0.58
9:G:73:ARG:HG2	9:G:76:ASP:HB2	1.85	0.58
8:l:92:THR:HG23	11:k:280:LYS:HA	1.85	0.58
6:D:73:LYS:HD3	6:D:78:ILE:HD11	1.85	0.58
9:G:523:TRP:CE2	9:G:565:ALA:HB2	2.39	0.58
11:k:194:PHE:HE1	11:k:201:VAL:HG23	1.69	0.58
11:k:249:CYS:HA	13:k:406:SF4:S3	2.44	0.58
1:A:498:VAL:HG12	4:C:20:TYR:HB3	1.85	0.58
11:K:194:PHE:HE1	11:K:201:VAL:HG23	1.69	0.58
9:g:110:TYR:CE2	9:g:118:THR:HG21	2.38	0.58
1:A:20:ILE:HG22	1:A:26:ILE:HD11	1.84	0.58
6:D:140:ILE:HD13	6:D:407:TYR:CE2	2.38	0.58
1:a:498:VAL:HG12	4:c:20:TYR:HB3	1.85	0.58
9:g:73:ARG:NH2	9:g:318:GLU:OE1	2.37	0.58
9:G:150:GLY:HA3	9:G:185:VAL:HG13	1.85	0.58
2:f:135:ILE:HG22	2:f:139:LYS:HE3	1.84	0.58
3:e:195:MET:HE2	3:e:198:PRO:HA	1.86	0.58
6:d:140:ILE:HD13	6:d:407:TYR:CE2	2.38	0.58
11:K:180:CYS:HB2	11:K:187:ILE:HG21	1.86	0.58
4:C:10:GLU:HG2	4:C:11:LEU:HD12	1.85	0.58
12:H:256:THR:HB	12:H:290:ILE:HD12	1.85	0.57
9:g:525:LYS:HB3	9:g:567:GLU:HA	1.85	0.57
1:A:235:ASP:OD2	1:A:336:LYS:NZ	2.37	0.57
7:I:129:GLU:HA	7:I:155:LYS:HB2	1.86	0.57
9:G:65:LYS:HZ1	9:G:324:ALA:HB2	1.69	0.57
11:K:253:ARG:HB3	11:K:257:ILE:HD12	1.86	0.57
8:l:140:PRO:HA	11:k:379:GLY:HA3	1.87	0.57
12:h:256:THR:HB	12:h:290:ILE:HD12	1.85	0.57
6:D:444:ALA:HB1	6:D:448:GLU:HB2	1.86	0.57
7:I:129:GLU:HG3	7:I:155:LYS:HD3	1.87	0.57
11:K:127:ARG:HH21	11:K:241:ASN:CA	2.06	0.57
1:a:17:GLY:O	1:a:18:THR:HG22	2.03	0.57
9:G:73:ARG:NH2	9:G:318:GLU:OE1	2.37	0.57
9:g:523:TRP:CE2	9:g:565:ALA:HB2	2.39	0.57
9:G:462:TYR:OH	9:G:564:ARG:NH2	2.37	0.57
9:g:73:ARG:HG2	9:g:76:ASP:HB2	1.85	0.57
9:g:462:TYR:OH	9:g:564:ARG:NH2	2.37	0.57
12:h:128:LEU:HD21	12:h:328:PRO:HG2	1.86	0.57
12:h:293:MET:HA	12:h:403:MET:HE3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:195:MET:HE2	3:E:198:PRO:HA	1.86	0.57
9:G:138:THR:HG21	9:G:143:GLN:HE22	1.70	0.57
6:d:137:CYS:SG	6:d:401:LEU:HD21	2.45	0.57
9:g:150:GLY:HA3	9:g:185:VAL:HG13	1.85	0.57
1:a:235:ASP:OD2	1:a:336:LYS:NZ	2.38	0.57
1:A:168:SER:O	1:a:583:MET:HE2	2.04	0.56
1:A:583:MET:HE2	1:a:168:SER:O	2.05	0.56
8:L:92:THR:HG23	11:K:280:LYS:HA	1.85	0.56
8:L:140:PRO:HA	11:K:379:GLY:HA3	1.87	0.56
4:c:10:GLU:HG2	4:c:11:LEU:HD12	1.85	0.56
12:H:71:TYR:O	12:H:75:ILE:HG12	2.06	0.56
3:e:180:GLU:HG2	3:e:191:ARG:HH21	1.71	0.56
10:j:88:ALA:O	10:j:92:VAL:HG23	2.05	0.56
12:h:312:PHE:HB2	12:h:316:LEU:HD21	1.88	0.56
1:A:327:GLU:O	1:A:329:GLN:NE2	2.38	0.56
6:D:137:CYS:SG	6:D:401:LEU:HD21	2.44	0.56
7:i:129:GLU:HG3	7:i:155:LYS:HD3	1.87	0.56
9:G:277:ILE:HD12	9:G:309:CYS:HB3	1.87	0.56
12:H:128:LEU:HD21	12:H:328:PRO:HG2	1.86	0.56
6:d:444:ALA:HB1	6:d:448:GLU:HB2	1.86	0.56
11:K:298:TYR:CE1	11:K:317:ALA:HB3	2.41	0.56
10:j:9:MET:HE1	10:j:82:ILE:HD12	1.87	0.56
9:g:274:ASN:HB3	9:g:277:ILE:HD11	1.87	0.56
11:k:298:TYR:CE1	11:k:317:ALA:HB3	2.41	0.56
11:k:326:CYS:SG	11:k:327:GLY:N	2.79	0.56
9:G:274:ASN:HB3	9:G:277:ILE:HD11	1.87	0.56
1:A:282:GLY:HA3	11:K:6:PRO:HD3	1.88	0.56
6:D:107:PHE:CZ	6:D:129:PHE:HZ	2.24	0.56
10:J:9:MET:HE1	10:J:82:ILE:HD12	1.87	0.56
1:a:16:CYS:HB2	13:a:703:SF4:S4	2.45	0.56
12:h:71:TYR:O	12:h:75:ILE:HG12	2.06	0.56
12:H:14:GLY:O	12:H:403:MET:HG3	2.06	0.56
1:a:327:GLU:O	1:a:329:GLN:NE2	2.38	0.56
6:d:107:PHE:CZ	6:d:129:PHE:HZ	2.24	0.56
9:g:138:THR:HG21	9:g:143:GLN:HE22	1.70	0.56
6:D:266:ALA:HB3	6:D:270:HIS:HE2	1.70	0.55
11:K:326:CYS:SG	11:K:327:GLY:N	2.79	0.55
1:a:218:MET:HE3	1:a:298:PRO:HG3	1.88	0.55
1:A:16:CYS:HB2	13:A:703:SF4:S4	2.45	0.55
3:E:180:GLU:HG2	3:E:191:ARG:HH21	1.71	0.55
6:D:403:PRO:HB3	6:D:407:TYR:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:i:129:GLU:HA	7:i:155:LYS:HB2	1.86	0.55
9:g:387:ILE:CG1	9:g:447:MET:HE2	2.36	0.55
1:A:189:LEU:HA	1:A:372:GLU:HG2	1.89	0.55
8:L:105:ILE:HG23	12:H:35:GLU:HG2	1.88	0.55
10:J:88:ALA:O	10:J:92:VAL:HG23	2.05	0.55
12:H:312:PHE:HB2	12:H:316:LEU:HD21	1.87	0.55
7:i:253:LYS:HG3	7:i:254:LYS:N	2.22	0.55
1:a:556:VAL:HG13	1:a:560:PRO:HA	1.88	0.55
6:d:266:ALA:HB3	6:d:270:HIS:HE2	1.70	0.55
9:g:242:GLY:HA2	9:g:282:TYR:HE1	1.72	0.55
9:g:277:ILE:HD12	9:g:309:CYS:HB3	1.87	0.55
12:h:140:LEU:HG	12:h:291:MET:HE1	1.88	0.55
1:A:556:VAL:HG13	1:A:560:PRO:HA	1.88	0.55
6:D:398:ILE:HG23	6:D:401:LEU:HB2	1.88	0.55
6:D:426:GLN:NE2	6:D:479:ILE:HD12	2.22	0.55
6:d:426:GLN:NE2	6:d:479:ILE:HD12	2.22	0.55
7:i:250:LYS:HB2	7:i:257:ILE:HD11	1.88	0.55
9:g:531:ASN:HB2	9:g:534:VAL:HG22	1.88	0.55
1:a:282:GLY:HA3	11:k:6:PRO:HD3	1.88	0.55
3:e:253:ILE:O	3:e:257:VAL:HG23	2.07	0.55
1:A:218:MET:HE3	1:A:298:PRO:HG3	1.88	0.55
7:I:204:MET:O	7:I:250:LYS:NZ	2.40	0.55
9:G:531:ASN:HB2	9:G:534:VAL:HG22	1.88	0.55
11:K:167:PHE:CE2	11:K:227:ILE:HG12	2.42	0.55
11:K:342:ARG:HG3	11:K:366:PRO:HB3	1.89	0.55
6:d:403:PRO:HB3	6:d:407:TYR:CE1	2.41	0.55
8:l:105:ILE:HG23	12:h:35:GLU:HG2	1.88	0.55
1:A:225:GLU:OE2	1:A:239:ARG:NE	2.39	0.55
3:E:253:ILE:O	3:E:257:VAL:HG23	2.07	0.55
4:c:175:ILE:HG23	4:c:180:LEU:HB3	1.89	0.55
12:H:291:MET:HE3	12:H:404:ASP:HB3	1.89	0.55
7:i:242:PHE:HB2	7:i:262:ILE:HG23	1.89	0.55
12:h:291:MET:HE3	12:h:404:ASP:HB3	1.89	0.55
9:G:242:GLY:HA2	9:G:282:TYR:HE1	1.72	0.54
12:H:140:LEU:HG	12:H:291:MET:HE1	1.88	0.54
11:K:137:ARG:HG3	11:K:250:CYS:SG	2.46	0.54
7:i:204:MET:O	7:i:250:LYS:NZ	2.40	0.54
11:k:164:LYS:HB3	11:k:232:THR:HG23	1.89	0.54
7:I:250:LYS:HB2	7:I:257:ILE:HD11	1.88	0.54
1:a:225:GLU:OE2	1:a:239:ARG:NE	2.38	0.54
12:h:14:GLY:O	12:h:403:MET:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:387:ILE:CG1	9:G:447:MET:HE2	2.36	0.54
1:a:189:LEU:HA	1:a:372:GLU:HG2	1.89	0.54
9:G:149:PHE:CE2	9:G:174:LEU:HD23	2.43	0.54
11:k:351:LYS:HG3	11:k:352:GLU:H	1.72	0.54
12:H:16:SER:HB2	12:H:402:ARG:HG3	1.89	0.54
7:I:242:PHE:HB2	7:I:262:ILE:HG23	1.89	0.54
9:G:275:THR:O	9:G:276:HIS:C	2.51	0.54
9:g:159:ILE:HG22	9:g:212:ILE:HD11	1.90	0.54
11:k:255:CYS:O	11:k:264:ILE:HD12	2.07	0.54
12:h:125:PRO:HB3	12:h:268:ARG:HB3	1.90	0.54
5:B:84:LYS:NZ	5:B:88:GLU:OE1	2.41	0.54
12:h:16:SER:HB2	12:h:402:ARG:HG3	1.89	0.54
6:D:358:VAL:HG23	6:D:361:ASN:OD1	2.08	0.54
10:J:41:GLU:HG3	10:J:70:VAL:HG21	1.90	0.54
5:b:84:LYS:NZ	5:b:88:GLU:OE1	2.41	0.54
7:i:2:GLU:N	7:i:57:LYS:O	2.41	0.54
12:h:143:VAL:HG11	12:h:255:THR:HG21	1.90	0.54
4:C:175:ILE:HG23	4:C:180:LEU:HB3	1.88	0.53
11:K:147:PHE:HA	11:K:154:GLY:H	1.73	0.53
9:g:149:PHE:CE2	9:g:174:LEU:HD23	2.43	0.53
12:H:76:ASP:OD1	12:H:433:ARG:NH2	2.41	0.53
1:a:93:ASN:OD1	1:a:94:PRO:HD2	2.08	0.53
6:d:141:CYS:SG	6:d:142:HIS:N	2.81	0.53
11:k:342:ARG:HG3	11:k:366:PRO:HB3	1.89	0.53
1:A:93:ASN:OD1	1:A:94:PRO:HD2	2.08	0.53
7:I:2:GLU:N	7:I:57:LYS:O	2.41	0.53
11:K:351:LYS:HG3	11:K:352:GLU:H	1.72	0.53
4:c:152:LEU:HD21	5:b:280:ALA:HB2	1.91	0.53
6:d:398:ILE:HG23	6:d:401:LEU:HB2	1.88	0.53
10:j:8:ASN:OD1	10:j:9:MET:N	2.40	0.53
1:a:186:MET:HG2	1:a:203:LEU:HD22	1.89	0.53
6:D:335:ASN:OD1	6:D:336:ASN:N	2.42	0.53
9:G:159:ILE:HG22	9:G:212:ILE:HD11	1.90	0.53
3:E:177:ASP:O	3:E:181:GLU:HG2	2.09	0.53
4:C:152:LEU:HD21	5:B:280:ALA:HB2	1.91	0.53
10:j:103:GLN:HA	12:h:268:ARG:HH22	1.74	0.53
6:D:342:ASP:HB3	6:D:511:MET:HE1	1.90	0.53
8:L:103:LYS:HB2	8:L:112:LEU:HD11	1.90	0.53
6:d:70:LEU:HB3	6:d:77:PHE:HB3	1.90	0.53
10:j:41:GLU:HG3	10:j:70:VAL:HG21	1.90	0.53
11:k:147:PHE:HA	11:k:154:GLY:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:214:ASP:OD2	4:c:2:ALA:N	2.42	0.53
10:J:8:ASN:OD1	10:J:9:MET:N	2.40	0.53
1:a:297:MET:HB3	1:a:298:PRO:HD3	1.91	0.53
3:e:177:ASP:O	3:e:181:GLU:HG2	2.09	0.53
8:l:130:PRO:HA	12:h:199:VAL:HG23	1.90	0.53
10:J:103:GLN:HA	12:H:268:ARG:HH22	1.74	0.53
6:d:129:PHE:HD2	6:d:131:THR:CG2	2.21	0.53
6:d:323:ARG:HA	6:d:542:ARG:NH2	2.24	0.53
9:g:275:THR:O	9:g:276:HIS:C	2.51	0.53
12:h:76:ASP:OD1	12:h:433:ARG:NH2	2.41	0.53
6:D:70:LEU:HB3	6:D:77:PHE:HB3	1.90	0.52
6:D:202:VAL:HG12	6:D:202:VAL:O	2.09	0.52
7:I:253:LYS:HG3	7:I:254:LYS:N	2.22	0.52
9:G:186:VAL:HA	9:G:237:HIS:HB2	1.91	0.52
9:G:308:THR:OG1	9:G:384:ARG:O	2.21	0.52
11:K:135:CYS:SG	11:K:137:ARG:O	2.67	0.52
12:H:125:PRO:HB3	12:H:268:ARG:HB3	1.90	0.52
6:d:516:TYR:CD1	6:d:519:LEU:HD12	2.44	0.52
11:k:219:ALA:HA	11:k:227:ILE:CG2	2.39	0.52
11:K:163:LEU:HA	11:K:232:THR:O	2.09	0.52
6:d:335:ASN:OD1	6:d:336:ASN:N	2.42	0.52
9:g:67:ASN:ND2	9:g:70:ARG:HH11	2.08	0.52
1:A:297:MET:HB3	1:A:298:PRO:HD3	1.91	0.52
4:C:26:ASN:HB3	4:C:29:PHE:HB3	1.92	0.52
12:H:12:TYR:HB2	12:H:44:ILE:CD1	2.39	0.52
6:d:202:VAL:HG12	6:d:202:VAL:O	2.09	0.52
9:g:186:VAL:HA	9:g:237:HIS:HB2	1.91	0.52
12:h:320:LYS:HG3	12:h:323:HIS:NE2	2.24	0.52
1:A:186:MET:HG2	1:A:203:LEU:HD22	1.91	0.52
3:E:324:LEU:HG	6:D:208:MET:SD	2.49	0.52
4:C:2:ALA:N	5:b:214:ASP:OD2	2.43	0.52
6:D:516:TYR:CD1	6:D:519:LEU:HD12	2.44	0.52
8:L:130:PRO:HA	12:H:199:VAL:HG23	1.90	0.52
11:K:19:MET:SD	11:K:73:VAL:HB	2.49	0.52
4:c:149:ARG:NH1	5:b:20:GLU:OE2	2.42	0.52
6:d:342:ASP:HB3	6:d:511:MET:HE1	1.90	0.52
6:d:365:MET:HE1	6:d:507:VAL:HG13	1.90	0.52
6:d:407:TYR:HB2	6:d:413:VAL:HG21	1.90	0.52
7:i:39:ALA:O	7:i:46:TRP:N	2.42	0.52
5:B:233:GLU:CD	5:B:239:GLN:HB2	2.34	0.52
6:D:365:MET:HE1	6:D:507:VAL:HG13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:181:GLY:HA2	11:K:187:ILE:HB	1.91	0.52
12:H:320:LYS:HG3	12:H:323:HIS:NE2	2.24	0.52
3:e:324:LEU:HG	6:d:208:MET:SD	2.49	0.52
5:b:233:GLU:CD	5:b:239:GLN:HB2	2.35	0.52
8:l:103:LYS:HB2	8:l:112:LEU:HD11	1.90	0.52
12:h:373:ASP:HB2	12:h:386:HIS:HE1	1.75	0.52
9:G:96:MET:HE3	9:G:96:MET:HA	1.91	0.52
11:K:219:ALA:O	11:K:222:CYS:HB2	2.10	0.52
12:H:111:ALA:HB2	12:H:434:MET:HE1	1.92	0.52
4:c:26:ASN:HB3	4:c:29:PHE:HB3	1.92	0.52
7:i:28:GLY:N	7:i:59:GLY:O	2.40	0.52
9:g:96:MET:HE3	9:g:96:MET:HA	1.91	0.52
11:k:163:LEU:HD11	11:k:231:ARG:HE	1.74	0.52
8:L:103:LYS:HE3	8:L:105:ILE:HD11	1.92	0.52
10:J:40:ASN:HD22	10:J:77:PRO:HA	1.75	0.52
10:J:44:MET:HE1	10:J:51:LYS:HG2	1.92	0.52
12:H:143:VAL:HG11	12:H:255:THR:HG21	1.90	0.52
11:k:19:MET:SD	11:k:73:VAL:HB	2.49	0.52
6:D:141:CYS:SG	6:D:142:HIS:N	2.81	0.52
6:D:407:TYR:HB2	6:D:413:VAL:HG21	1.90	0.52
7:I:39:ALA:O	7:I:46:TRP:N	2.42	0.52
3:e:141:MET:HE2	3:e:184:TYR:HB3	1.92	0.52
8:l:90:LEU:O	9:g:544:LYS:NZ	2.43	0.52
10:j:90:GLN:HG3	10:j:125:LEU:HD22	1.92	0.52
11:k:276:PHE:CD2	11:k:318:VAL:HB	2.45	0.52
6:D:323:ARG:HA	6:D:542:ARG:NH2	2.24	0.52
10:J:90:GLN:HG3	10:J:125:LEU:HD22	1.92	0.52
3:e:112:ALA:HB3	3:e:381:MET:HE1	1.92	0.52
6:d:358:VAL:HG23	6:d:361:ASN:OD1	2.09	0.52
9:g:110:TYR:CD2	9:g:118:THR:HG21	2.45	0.52
9:g:110:TYR:CB	9:g:141:LEU:HD21	2.40	0.52
9:g:147:PRO:HD3	9:g:180:GLY:HA3	1.91	0.52
12:h:179:LYS:HD2	12:h:183:LYS:HG3	1.92	0.52
3:E:141:MET:HE2	3:E:184:TYR:HB3	1.92	0.52
1:A:521:ARG:HB3	1:A:534:MET:HE2	1.92	0.51
3:E:53:TYR:N	3:E:53:TYR:HD2	2.08	0.51
11:K:142:ARG:HA	11:K:242:VAL:HG22	1.92	0.51
11:K:148:GLU:OE2	11:K:157:LYS:N	2.44	0.51
11:K:236:GLN:C	11:K:237:LYS:HD3	2.35	0.51
6:d:129:PHE:CD2	6:d:131:THR:HG23	2.42	0.51
4:C:45:TYR:HE2	1:a:445:MET:SD	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:157:CYS:HB2	16:B:302:9S8:S3	2.50	0.51
6:D:323:ARG:HA	6:D:542:ARG:HH22	1.76	0.51
9:G:143:GLN:O	9:G:521:THR:HA	2.11	0.51
12:H:260:MET:SD	12:H:260:MET:N	2.83	0.51
1:a:101:ASN:O	1:a:125:GLN:NE2	2.43	0.51
9:g:160:LYS:HD3	9:g:210:PHE:O	2.10	0.51
1:A:499:ASP:HB2	4:C:19:ARG:HD3	1.93	0.51
3:E:53:TYR:N	3:E:53:TYR:CD2	2.77	0.51
3:E:112:ALA:HB3	3:E:381:MET:HE1	1.91	0.51
4:C:149:ARG:NH1	5:B:20:GLU:OE2	2.42	0.51
9:G:160:LYS:HD3	9:G:210:PHE:O	2.10	0.51
11:K:276:PHE:CD2	11:K:318:VAL:HB	2.45	0.51
1:a:110:HIS:CD2	2:f:34:PRO:HB3	2.46	0.51
1:a:521:ARG:HB3	1:a:534:MET:HE2	1.91	0.51
12:h:12:TYR:HB2	12:h:44:ILE:CD1	2.39	0.51
12:h:211:ASP:OD1	19:h:502:MGD:N1	2.43	0.51
6:D:129:PHE:HD2	6:D:131:THR:CG2	2.21	0.51
11:K:162:GLU:HB2	11:K:234:VAL:HG12	1.92	0.51
2:f:85:ARG:O	2:f:89:ILE:HG12	2.11	0.51
12:h:99:GLU:HG3	12:h:424:GLU:HG3	1.93	0.51
3:E:33:HIS:O	3:E:37:THR:HG22	2.10	0.51
6:D:234:TRP:HE1	6:D:274:LEU:HD11	1.76	0.51
9:G:67:ASN:ND2	9:G:70:ARG:HH11	2.08	0.51
9:G:110:TYR:CB	9:G:141:LEU:HD21	2.40	0.51
11:K:251:THR:O	11:K:268:LYS:HG2	2.10	0.51
5:b:155:TYR:CZ	5:b:177:PHE:HB3	2.46	0.51
9:g:205:ASP:OD1	9:g:205:ASP:N	2.44	0.51
10:j:40:ASN:HD22	10:j:77:PRO:HA	1.75	0.51
1:A:110:HIS:CD2	2:F:34:PRO:HB3	2.45	0.51
9:G:110:TYR:HD2	9:G:141:LEU:HD13	1.76	0.51
9:G:522:LEU:HD21	9:G:564:ARG:HH21	1.76	0.51
6:d:323:ARG:HA	6:d:542:ARG:HH22	1.76	0.51
2:F:85:ARG:O	2:F:89:ILE:HG12	2.11	0.51
9:G:382:LEU:HD12	9:G:447:MET:SD	2.51	0.51
12:H:211:ASP:OD1	19:H:502:MGD:N1	2.43	0.51
3:e:53:TYR:N	3:e:53:TYR:CD2	2.77	0.51
1:A:445:MET:SD	4:c:45:TYR:HE2	2.34	0.51
7:I:179:ILE:HG22	7:I:197:GLU:OE1	2.11	0.51
9:G:147:PRO:HD3	9:G:180:GLY:HA3	1.91	0.51
11:K:88:CYS:SG	11:K:90:PHE:O	2.69	0.51
11:K:148:GLU:OE1	11:K:148:GLU:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:222:CYS:HB3	11:K:224:SER:O	2.11	0.51
6:d:495:PRO:HD2	6:d:499:ASP:OD2	2.11	0.51
10:j:44:MET:HE1	10:j:51:LYS:HG2	1.92	0.51
6:D:36:VAL:HG23	6:D:57:TRP:HB3	1.93	0.51
6:D:495:PRO:HD2	6:D:499:ASP:OD2	2.11	0.51
7:I:28:GLY:N	7:I:59:GLY:O	2.40	0.51
5:b:77:LEU:HD13	5:b:83:TYR:HA	1.92	0.51
6:d:250:VAL:HG12	6:d:554:LEU:HD22	1.93	0.51
9:g:362:ILE:HG22	9:g:364:VAL:H	1.76	0.51
5:B:155:TYR:CZ	5:B:177:PHE:HB3	2.45	0.50
6:D:250:VAL:HG12	6:D:554:LEU:HD22	1.93	0.50
9:G:110:TYR:CD2	9:G:118:THR:HG21	2.45	0.50
1:a:116:ASP:OD1	1:a:116:ASP:N	2.44	0.50
3:e:53:TYR:N	3:e:53:TYR:HD2	2.08	0.50
1:A:101:ASN:O	1:A:125:GLN:NE2	2.43	0.50
1:A:281:MET:HE3	1:A:369:LEU:HD13	1.92	0.50
12:h:260:MET:SD	12:h:260:MET:N	2.83	0.50
5:B:77:LEU:HD13	5:B:83:TYR:HA	1.92	0.50
3:e:33:HIS:O	3:e:37:THR:HG22	2.10	0.50
7:i:227:THR:HA	7:i:240:ASP:HA	1.93	0.50
9:g:110:TYR:HD2	9:g:141:LEU:HD13	1.76	0.50
9:g:382:LEU:HD12	9:g:447:MET:SD	2.51	0.50
11:k:148:GLU:OE2	11:k:157:LYS:N	2.44	0.50
12:H:99:GLU:HG3	12:H:424:GLU:HG3	1.93	0.50
1:a:281:MET:HE3	1:a:369:LEU:HD13	1.92	0.50
6:d:43:PRO:HG3	6:d:523:GLU:HA	1.93	0.50
6:d:234:TRP:HE1	6:d:274:LEU:HD11	1.76	0.50
8:l:103:LYS:HE3	8:l:105:ILE:HD11	1.92	0.50
9:g:143:GLN:O	9:g:521:THR:HA	2.11	0.50
12:h:111:ALA:HB2	12:h:434:MET:HE1	1.92	0.50
6:D:43:PRO:HG3	6:D:523:GLU:HA	1.93	0.50
7:I:227:THR:HA	7:I:240:ASP:HA	1.93	0.50
6:d:36:VAL:HG23	6:d:57:TRP:HB3	1.93	0.50
6:d:250:VAL:CG1	6:d:554:LEU:HD22	2.42	0.50
11:k:214:GLY:HA3	11:k:231:ARG:HH11	1.75	0.50
5:B:289:THR:O	5:B:293:GLN:HG2	2.11	0.50
7:I:139:ALA:HB2	7:I:146:GLY:HA3	1.94	0.50
11:K:253:ARG:O	11:K:257:ILE:HB	2.11	0.50
12:H:179:LYS:HD2	12:H:183:LYS:HG3	1.92	0.50
7:i:139:ALA:HB2	7:i:146:GLY:HA3	1.94	0.50
11:k:88:CYS:SG	11:k:90:PHE:O	2.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:h:142:GLU:OE2	12:h:146:ARG:NE	2.38	0.50
1:A:332:PHE:O	1:A:333:ILE:HD13	2.12	0.50
12:H:142:GLU:OE2	12:H:146:ARG:NE	2.38	0.50
5:b:289:THR:O	5:b:293:GLN:HG2	2.11	0.50
7:i:230:LYS:HB2	7:i:239:PHE:CD2	2.46	0.50
11:K:176:LYS:HE3	11:K:203:GLY:H	1.77	0.50
11:K:276:PHE:CE1	11:K:339:ILE:HG12	2.47	0.50
12:H:314:TYR:O	12:H:326:MET:HG3	2.12	0.50
12:H:358:ILE:N	12:H:359:PRO:HD2	2.27	0.50
1:a:444:TYR:CD1	1:a:447:ILE:HG12	2.47	0.50
5:b:157:CYS:HB2	16:b:302:9S8:S3	2.50	0.50
7:i:179:ILE:HG22	7:i:197:GLU:OE1	2.11	0.50
11:k:276:PHE:CE1	11:k:339:ILE:HG12	2.47	0.50
1:A:444:TYR:CD1	1:A:447:ILE:HG12	2.47	0.50
2:F:84:LYS:HD3	3:E:389:VAL:HG22	1.93	0.50
3:E:324:LEU:O	3:E:326:THR:N	2.45	0.50
6:D:250:VAL:CG1	6:D:554:LEU:HD22	2.42	0.50
7:I:184:HIS:H	7:I:203:GLN:HB2	1.77	0.50
7:I:216:LEU:HG	7:I:217:TYR:CD2	2.47	0.50
9:G:362:ILE:HG22	9:G:364:VAL:H	1.76	0.50
12:H:373:ASP:HB2	12:H:386:HIS:HE1	1.75	0.50
1:a:499:ASP:HB2	4:c:19:ARG:HD3	1.93	0.50
6:d:256:LEU:O	6:d:260:VAL:HG22	2.12	0.50
2:F:49:MET:HE1	3:E:386:HIS:NE2	2.27	0.49
7:I:230:LYS:HB2	7:I:239:PHE:CD2	2.46	0.49
2:f:49:MET:HE1	3:e:386:HIS:NE2	2.27	0.49
5:b:216:THR:OG1	5:b:241:GLN:NE2	2.44	0.49
9:g:522:LEU:HD21	9:g:564:ARG:HH21	1.76	0.49
6:D:67:THR:HG23	6:D:471:GLY:HA3	1.94	0.49
6:D:256:LEU:O	6:D:260:VAL:HG22	2.12	0.49
6:D:516:TYR:HD1	6:D:519:LEU:HD12	1.78	0.49
2:f:84:LYS:HD3	3:e:389:VAL:HG22	1.93	0.49
6:d:174:TRP:CD2	6:d:311:MET:HE1	2.48	0.49
9:g:523:TRP:NE1	9:g:563:PRO:HB2	2.28	0.49
9:g:551:GLU:HG3	12:h:411:ARG:NH2	2.27	0.49
10:j:93:PRO:HG2	10:j:103:GLN:HB3	1.94	0.49
5:B:216:THR:OG1	5:B:241:GLN:NE2	2.43	0.49
9:G:551:GLU:HG3	12:H:411:ARG:NH2	2.27	0.49
11:K:18:ILE:HG12	11:K:31:ILE:HG12	1.94	0.49
1:a:34:LYS:HG3	1:a:42:ALA:HB3	1.95	0.49
3:e:78:LEU:HD23	3:e:78:LEU:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:i:184:HIS:H	7:i:203:GLN:HB2	1.77	0.49
7:i:216:LEU:HG	7:i:217:TYR:CD2	2.47	0.49
9:g:241:LEU:HD11	9:g:279:PHE:HB3	1.94	0.49
11:k:134:VAL:HB	11:k:254:TRP:CE3	2.47	0.49
4:C:126:LEU:O	4:C:130:GLN:HG2	2.13	0.49
9:G:237:HIS:CD2	9:G:276:HIS:HE1	2.30	0.49
11:K:41:GLY:C	11:K:43:CYS:N	2.71	0.49
1:a:93:ASN:HD22	1:a:138:ASP:HA	1.78	0.49
9:g:322:MET:HG2	9:g:353:VAL:HG13	1.95	0.49
1:A:158:ALA:HB2	1:A:566:THR:HG23	1.95	0.49
6:D:129:PHE:CD2	6:D:131:THR:HG23	2.42	0.49
6:D:323:ARG:O	6:D:326:VAL:HG12	2.12	0.49
11:K:162:GLU:HB2	11:K:234:VAL:CG1	2.43	0.49
4:c:126:LEU:O	4:c:130:GLN:HG2	2.13	0.49
6:d:113:THR:HG22	6:d:117:ASP:HB2	1.94	0.49
6:D:516:TYR:O	6:D:520:GLU:HG2	2.13	0.49
9:G:11:ILE:HG13	9:G:23:ALA:HB3	1.94	0.49
9:G:374:GLU:OE2	9:G:431:ASN:N	2.45	0.49
12:h:314:TYR:O	12:h:326:MET:HG3	2.12	0.49
6:D:113:THR:HG22	6:D:117:ASP:HB2	1.95	0.49
12:H:304:VAL:HG21	12:H:401:TYR:CE1	2.48	0.49
1:a:605:MET:HE3	1:a:642:PHE:HZ	1.78	0.49
3:e:324:LEU:O	3:e:326:THR:N	2.45	0.49
7:i:228:VAL:O	7:i:239:PHE:N	2.46	0.49
4:C:185:ASP:OD1	4:C:186:ARG:N	2.46	0.49
6:d:67:THR:HG23	6:d:471:GLY:HA3	1.94	0.49
6:d:516:TYR:O	6:d:520:GLU:HG2	2.13	0.49
12:h:358:ILE:N	12:h:359:PRO:HD2	2.27	0.49
10:J:37:ILE:HB	10:J:68:ALA:HA	1.94	0.49
11:K:252:CYS:SG	11:K:254:TRP:HB2	2.52	0.49
1:a:388:PRO:HB3	11:k:5:PHE:CZ	2.48	0.49
1:a:473:VAL:HA	1:a:489:THR:HB	1.95	0.49
6:d:436:TYR:CD1	6:d:436:TYR:N	2.81	0.49
10:j:37:ILE:HB	10:j:68:ALA:HA	1.94	0.49
12:h:421:MET:HE1	12:h:429:LYS:HE2	1.95	0.49
6:D:107:PHE:HD1	6:D:121:PHE:CZ	2.31	0.48
6:D:436:TYR:CD1	6:D:436:TYR:N	2.81	0.48
11:K:161:VAL:HA	11:K:237:LYS:CG	2.41	0.48
12:H:12:TYR:HB2	12:H:44:ILE:HD12	1.95	0.48
12:h:12:TYR:HB2	12:h:44:ILE:HD12	1.95	0.48
1:A:34:LYS:HG3	1:A:42:ALA:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:189:ILE:HD11	5:B:228:ALA:HB2	1.95	0.48
9:g:62:SER:OG	9:g:63:GLY:N	2.46	0.48
11:k:52:ILE:HG12	11:k:73:VAL:HG22	1.95	0.48
11:k:131:CYS:HB2	11:k:140:ILE:HD12	1.94	0.48
1:A:666:PHE:HZ	2:F:60:ALA:HB2	1.77	0.48
3:E:78:LEU:H	3:E:78:LEU:HD23	1.77	0.48
9:G:241:LEU:HD11	9:G:279:PHE:HB3	1.94	0.48
6:d:323:ARG:O	6:d:326:VAL:HG12	2.12	0.48
9:g:219:LYS:O	9:g:223:GLU:HG3	2.13	0.48
12:h:418:GLU:HG2	12:h:418:GLU:O	2.14	0.48
1:a:332:PHE:O	1:a:333:ILE:HD13	2.12	0.48
3:e:40:VAL:HG11	3:e:97:ALA:HB2	1.96	0.48
9:g:58:HIS:HE1	9:g:184:KCX:HE2	1.78	0.48
9:g:374:GLU:OE2	9:g:431:ASN:N	2.45	0.48
1:A:605:MET:HE3	1:A:642:PHE:HZ	1.78	0.48
5:B:255:ASP:OD2	4:c:4:LYS:NZ	2.47	0.48
6:D:174:TRP:CD2	6:D:311:MET:HE1	2.48	0.48
9:G:58:HIS:HE1	9:G:184:KCX:HE2	1.78	0.48
6:d:436:TYR:N	6:d:436:TYR:HD1	2.11	0.48
1:A:93:ASN:HD22	1:A:138:ASP:HA	1.77	0.48
1:A:116:ASP:OD1	1:A:116:ASP:N	2.44	0.48
7:I:161:ASP:OD1	12:H:270:HIS:NE2	2.43	0.48
9:G:205:ASP:OD1	9:G:205:ASP:N	2.44	0.48
3:e:159:ASP:HB3	3:e:164:ILE:HD13	1.96	0.48
5:b:133:CYS:SG	5:b:137:LYS:HB3	2.54	0.48
7:i:203:GLN:N	7:i:245:ASP:OD1	2.47	0.48
9:g:11:ILE:HG13	9:g:23:ALA:HB3	1.94	0.48
11:k:90:PHE:HB3	11:k:137:ARG:HH21	1.79	0.48
3:E:159:ASP:HB3	3:E:164:ILE:HD13	1.96	0.48
7:I:228:VAL:O	7:I:239:PHE:N	2.46	0.48
9:G:49:THR:HG21	9:G:441:LEU:HD21	1.96	0.48
9:G:273:HIS:CD2	9:G:308:THR:HG23	2.49	0.48
10:J:93:PRO:HG2	10:J:103:GLN:HB3	1.94	0.48
11:K:222:CYS:SG	11:K:227:ILE:HD12	2.54	0.48
3:e:15:ALA:O	3:e:19:LYS:HG2	2.14	0.48
9:g:237:HIS:CD2	9:g:276:HIS:HE1	2.30	0.48
3:E:15:ALA:O	3:E:19:LYS:HG2	2.14	0.48
5:B:8:LEU:HD22	5:B:13:PRO:HG3	1.96	0.48
6:D:326:VAL:HG22	6:D:327:GLY:H	1.79	0.48
7:I:182:LEU:HD12	7:I:209:ALA:HB2	1.96	0.48
9:g:273:HIS:CD2	9:g:308:THR:HG23	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:PRO:HB3	11:K:5:PHE:CZ	2.48	0.48
3:E:268:TRP:CE3	3:E:271:ARG:HD2	2.49	0.48
4:C:49:THR:HG23	1:a:474:ALA:HA	1.96	0.48
1:a:16:CYS:HA	13:a:703:SF4:S1	2.54	0.48
1:a:666:PHE:HZ	2:f:60:ALA:HB2	1.78	0.48
5:b:8:LEU:HD22	5:b:13:PRO:HG3	1.96	0.48
6:d:534:HIS:CD2	6:d:536:GLY:H	2.32	0.48
12:h:304:VAL:HG21	12:h:401:TYR:CE1	2.48	0.48
1:A:16:CYS:HA	13:A:703:SF4:S1	2.54	0.48
6:D:436:TYR:N	6:D:436:TYR:HD1	2.11	0.48
9:G:322:MET:HG2	9:G:353:VAL:HG13	1.95	0.48
9:G:373:LEU:HD13	9:G:413:ARG:HD2	1.96	0.48
12:H:114:MET:HE1	12:H:317:ASP:OD1	2.13	0.47
3:e:152:THR:CG2	3:e:168:GLU:HG3	2.43	0.47
6:d:326:VAL:HG22	6:d:327:GLY:H	1.79	0.47
6:d:344:GLY:HA3	6:d:350:TYR:O	2.14	0.47
6:d:366:GLU:HG2	6:d:374:LEU:HD23	1.96	0.47
12:h:114:MET:HE1	12:h:317:ASP:OD1	2.14	0.47
12:H:101:GLN:CD	12:H:302:PRO:HD3	2.39	0.47
12:H:421:MET:HE1	12:H:429:LYS:HE2	1.95	0.47
6:d:516:TYR:HD1	6:d:519:LEU:HD12	1.78	0.47
9:g:49:THR:HG21	9:g:441:LEU:HD21	1.95	0.47
9:g:308:THR:OG1	9:g:384:ARG:O	2.20	0.47
9:g:373:LEU:HD13	9:g:413:ARG:HD2	1.96	0.47
9:g:410:GLU:O	9:g:414:LYS:HG3	2.14	0.47
11:k:18:ILE:HG12	11:k:31:ILE:HG12	1.94	0.47
6:D:46:GLU:OE1	6:D:187:ARG:NH2	2.48	0.47
9:G:219:LYS:O	9:G:223:GLU:HG3	2.13	0.47
4:c:185:ASP:OD1	4:c:186:ARG:N	2.46	0.47
6:d:107:PHE:HD1	6:d:121:PHE:CZ	2.31	0.47
7:i:92:SER:HB2	7:i:93:ASP:H	1.54	0.47
7:i:101:TRP:CD1	7:i:120:ALA:HB3	2.50	0.47
3:E:152:THR:CG2	3:E:168:GLU:HG3	2.43	0.47
7:I:199:ARG:NH2	12:H:209:GLY:O	2.48	0.47
7:I:203:GLN:N	7:I:245:ASP:OD1	2.47	0.47
11:K:52:ILE:HG12	11:K:73:VAL:HG22	1.95	0.47
1:a:158:ALA:HB2	1:a:566:THR:HG23	1.95	0.47
1:A:474:ALA:HA	4:c:49:THR:HG23	1.97	0.47
3:E:40:VAL:HG11	3:E:97:ALA:HB2	1.96	0.47
6:D:366:GLU:HG2	6:D:374:LEU:HD23	1.96	0.47
7:I:155:LYS:HA	7:I:174:GLU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:57:VAL:HG13	10:j:109:VAL:HG21	1.96	0.47
11:k:148:GLU:OE1	11:k:148:GLU:N	2.40	0.47
10:J:57:VAL:HG13	10:J:109:VAL:HG21	1.96	0.47
11:K:303:LYS:O	12:H:252:ARG:NH1	2.48	0.47
2:f:77:GLU:HB2	2:f:80:TYR:HD2	1.80	0.47
9:g:292:SER:HB2	9:g:371:ILE:HG12	1.96	0.47
11:k:303:LYS:O	12:h:252:ARG:NH1	2.48	0.47
12:h:108:MET:HG3	12:h:115:LEU:HD13	1.96	0.47
1:A:473:VAL:HA	1:A:489:THR:HB	1.96	0.47
4:C:53:SER:HB3	4:C:97:ARG:HH11	1.80	0.47
5:B:133:CYS:SG	5:B:137:LYS:HB3	2.54	0.47
6:D:160:ASN:ND2	6:D:326:VAL:O	2.48	0.47
6:D:534:HIS:CD2	6:D:536:GLY:H	2.32	0.47
7:I:145:ARG:O	7:I:145:ARG:HG2	2.15	0.47
9:G:410:GLU:O	9:G:414:LYS:HG3	2.14	0.47
9:G:523:TRP:NE1	9:G:563:PRO:HB2	2.28	0.47
11:K:353:THR:HG22	11:K:355:LEU:H	1.79	0.47
12:H:189:ILE:HG13	12:H:204:LEU:HB2	1.97	0.47
12:H:418:GLU:O	12:H:418:GLU:HG2	2.14	0.47
1:a:380:PRO:HB2	11:k:24:LEU:HD12	1.97	0.47
3:e:100:CYS:HB2	3:e:104:ASP:HB2	1.97	0.47
5:b:189:ILE:HD11	5:b:228:ALA:HB2	1.95	0.47
6:d:108:GLN:HG3	6:d:401:LEU:HD12	1.97	0.47
7:i:199:ARG:NH2	12:h:209:GLY:O	2.48	0.47
11:k:348:ILE:HD13	11:k:356:PHE:CE2	2.50	0.47
12:h:151:VAL:HG21	12:h:248:MET:HE3	1.97	0.47
12:h:189:ILE:HG13	12:h:204:LEU:HB2	1.97	0.47
6:D:344:GLY:HA3	6:D:350:TYR:O	2.14	0.47
7:I:101:TRP:CD1	7:I:120:ALA:HB3	2.50	0.47
11:K:170:ASP:HB3	11:K:172:GLU:CG	2.40	0.47
11:K:266:VAL:HG21	13:K:406:SF4:S1	2.55	0.47
1:a:88:LYS:HE3	1:a:94:PRO:HG3	1.97	0.47
2:f:88:MET:SD	3:e:386:HIS:NE2	2.80	0.47
4:c:53:SER:HB3	4:c:97:ARG:HH11	1.80	0.47
12:h:54:ILE:HD11	12:h:376:ILE:HG12	1.97	0.47
12:h:101:GLN:CD	12:h:302:PRO:HD3	2.39	0.47
3:E:110:GLU:OE2	3:E:113:LYS:NZ	2.33	0.47
6:D:108:GLN:HG3	6:D:401:LEU:HD12	1.97	0.47
11:K:348:ILE:HD13	11:K:356:PHE:CE2	2.50	0.47
12:H:151:VAL:HG21	12:H:248:MET:HE3	1.97	0.47
12:H:214:LEU:HD11	12:H:241:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:650:MET:O	1:a:654:THR:HG22	2.15	0.47
3:e:268:TRP:CE3	3:e:271:ARG:HD2	2.49	0.47
3:e:297:TYR:O	3:e:301:GLU:HG2	2.15	0.47
12:h:214:LEU:HD11	12:h:241:ILE:HD11	1.96	0.47
2:F:77:GLU:HB2	2:F:80:TYR:HD2	1.80	0.47
3:E:100:CYS:HB2	3:E:104:ASP:HB2	1.97	0.47
8:L:131:TYR:O	8:L:132:ASP:C	2.58	0.47
12:H:119:ALA:O	12:H:124:GLY:N	2.47	0.47
1:a:417:SER:HB2	1:a:420:CYS:SG	2.55	0.47
5:b:242:PHE:O	5:b:246:GLN:HG3	2.15	0.47
6:d:160:ASN:ND2	6:d:326:VAL:O	2.48	0.47
7:i:182:LEU:HD12	7:i:209:ALA:HB2	1.96	0.47
11:k:131:CYS:HB3	13:k:405:SF4:S2	2.55	0.47
1:a:76:PRO:HB3	1:a:80:GLU:OE2	2.15	0.46
1:A:76:PRO:HB3	1:A:80:GLU:OE2	2.15	0.46
1:A:88:LYS:HE3	1:A:94:PRO:HG3	1.97	0.46
1:A:348:LEU:HD23	1:A:511:VAL:HG12	1.97	0.46
6:D:99:LYS:HG3	6:D:100:HIS:CE1	2.51	0.46
2:f:48:ASP:OD1	2:f:49:MET:N	2.48	0.46
4:c:54:CYS:HA	13:c:201:SF4:S3	2.55	0.46
4:C:54:CYS:HA	13:C:201:SF4:S3	2.55	0.46
6:D:164:ASP:OD2	6:D:325:GLY:N	2.43	0.46
9:G:292:SER:HB2	9:G:371:ILE:HG12	1.96	0.46
4:C:65:ARG:CZ	1:a:492:THR:HG23	2.45	0.46
4:C:105:THR:O	4:C:109:MET:HG2	2.16	0.46
9:G:497:THR:HG21	9:G:500:THR:OG1	2.16	0.46
11:K:131:CYS:HB3	13:K:405:SF4:S2	2.55	0.46
12:H:108:MET:HG3	12:H:115:LEU:HD13	1.97	0.46
5:b:43:CYS:SG	5:b:82:CYS:HA	2.56	0.46
6:d:46:GLU:OE1	6:d:187:ARG:NH2	2.48	0.46
9:g:497:THR:HG21	9:g:500:THR:OG1	2.16	0.46
9:G:88:ILE:CG1	9:G:90:GLN:HG3	2.46	0.46
9:G:237:HIS:HB3	9:G:238:GLY:H	1.59	0.46
11:K:42:ILE:HD12	11:K:89:PRO:HG2	1.98	0.46
11:K:276:PHE:CE2	11:K:318:VAL:HB	2.51	0.46
9:g:79:PHE:HD2	9:g:84:ARG:HD3	1.81	0.46
6:D:396:MET:HE3	6:D:396:MET:HB2	1.79	0.46
5:b:248:GLU:HA	5:b:251:GLU:HG2	1.98	0.46
6:d:130:LYS:HB3	6:d:375:PRO:HD3	1.98	0.46
7:i:145:ARG:HG2	7:i:145:ARG:O	2.15	0.46
11:k:353:THR:HG22	11:k:355:LEU:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:180:GLU:HG2	3:E:191:ARG:HD3	1.98	0.46
9:G:62:SER:OG	9:G:63:GLY:N	2.46	0.46
9:G:139:PRO:HB2	9:G:140:ILE:HG12	1.98	0.46
8:l:131:TYR:O	8:l:132:ASP:C	2.58	0.46
9:g:420:MET:HB2	9:g:420:MET:HE3	1.82	0.46
11:k:252:CYS:HB3	11:k:294:ALA:HB1	1.97	0.46
1:A:492:THR:HG23	4:c:65:ARG:CZ	2.46	0.46
3:E:297:TYR:O	3:E:301:GLU:HG2	2.15	0.46
1:a:348:LEU:HD23	1:a:511:VAL:HG12	1.97	0.46
11:k:134:VAL:HB	11:k:254:TRP:HE3	1.80	0.46
5:B:242:PHE:O	5:B:246:GLN:HG3	2.15	0.46
8:L:101:ILE:HG22	8:L:111:ILE:HG23	1.97	0.46
9:G:79:PHE:HD2	9:G:84:ARG:HD3	1.81	0.46
3:e:35:LEU:HD23	3:e:66:ILE:HD11	1.98	0.46
3:e:180:GLU:HG2	3:e:191:ARG:HD3	1.98	0.46
6:d:117:ASP:OD1	6:d:477:ILE:HG23	2.16	0.46
8:l:113:ASP:OD1	8:l:118:LEU:HD12	2.16	0.46
9:g:139:PRO:HB2	9:g:140:ILE:HG12	1.98	0.46
9:g:140:ILE:HD13	9:g:516:GLU:HG3	1.97	0.46
2:F:48:ASP:OD1	2:F:49:MET:N	2.48	0.46
12:H:18:ASP:OD1	12:H:18:ASP:N	2.44	0.46
12:H:54:ILE:HD11	12:H:376:ILE:HG12	1.97	0.46
3:e:58:THR:HG22	3:e:60:ILE:HG13	1.98	0.46
5:b:12:ALA:HB3	5:b:13:PRO:HD3	1.98	0.46
6:d:135:ASP:OD2	6:d:139:ARG:HG3	2.16	0.46
8:l:101:ILE:HG22	8:l:111:ILE:HG23	1.97	0.46
9:g:88:ILE:CG1	9:g:90:GLN:HG3	2.46	0.46
11:k:171:ASP:HA	11:k:174:CYS:HB2	1.97	0.46
1:A:417:SER:HB2	1:A:420:CYS:SG	2.55	0.45
1:A:650:MET:O	1:A:654:THR:HG22	2.15	0.45
4:C:4:LYS:NZ	5:b:255:ASP:OD2	2.49	0.45
6:D:117:ASP:OD1	6:D:477:ILE:HG23	2.16	0.45
9:G:140:ILE:HD13	9:G:516:GLU:HG3	1.97	0.45
4:c:105:THR:O	4:c:109:MET:HG2	2.16	0.45
1:A:380:PRO:HB2	11:K:24:LEU:HD12	1.97	0.45
3:E:58:THR:HG22	3:E:60:ILE:HG13	1.98	0.45
6:D:36:VAL:HG21	6:D:56:CYS:SG	2.56	0.45
8:L:113:ASP:OD1	8:L:118:LEU:HD12	2.16	0.45
11:K:66:ASP:OD1	11:K:66:ASP:N	2.50	0.45
3:e:77:THR:HG22	3:e:132:SER:OG	2.16	0.45
6:d:99:LYS:HG3	6:d:100:HIS:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:h:334:VAL:O	12:h:338:MET:HG2	2.16	0.45
2:F:95:ASN:OD1	2:F:95:ASN:N	2.50	0.45
6:d:36:VAL:HG21	6:d:56:CYS:SG	2.56	0.45
7:i:155:LYS:HA	7:i:174:GLU:HB2	1.97	0.45
9:g:458:LEU:HD13	9:g:462:TYR:HD2	1.82	0.45
12:h:94:GLY:HA2	12:h:299:ILE:CD1	2.47	0.45
6:D:89:VAL:HA	6:D:422:PHE:HZ	1.82	0.45
9:G:458:LEU:HD13	9:G:462:TYR:HD2	1.82	0.45
1:a:426:LYS:HE3	1:a:426:LYS:HB3	1.67	0.45
3:e:141:MET:CE	3:e:185:GLY:H	2.30	0.45
6:d:326:VAL:HG22	6:d:327:GLY:N	2.31	0.45
9:g:3:GLU:N	9:g:36:VAL:HG11	2.32	0.45
11:k:276:PHE:CE2	11:k:318:VAL:HB	2.51	0.45
1:A:219:MET:HE2	1:A:219:MET:HB3	1.88	0.45
5:B:12:ALA:HB3	5:B:13:PRO:HD3	1.98	0.45
5:B:160:MET:HE3	5:B:160:MET:HB3	1.67	0.45
3:E:77:THR:HG22	3:E:132:SER:OG	2.16	0.45
7:I:75:ARG:HE	7:I:75:ARG:HB3	1.43	0.45
1:a:636:CYS:SG	1:a:637:GLY:N	2.89	0.45
3:E:141:MET:CE	3:E:185:GLY:H	2.30	0.45
6:D:130:LYS:HB3	6:D:375:PRO:HD3	1.98	0.45
6:D:326:VAL:HG22	6:D:327:GLY:N	2.31	0.45
6:D:417:LEU:O	6:D:420:LEU:HB3	2.17	0.45
1:A:189:LEU:HB2	1:A:199:SER:OG	2.17	0.45
2:F:49:MET:HG2	2:F:89:ILE:HD11	1.99	0.45
3:E:93:ASP:OD1	3:E:93:ASP:N	2.50	0.45
9:G:96:MET:HA	9:G:96:MET:CE	2.47	0.45
9:G:441:LEU:O	9:G:444:ILE:HG22	2.17	0.45
11:K:83:VAL:HA	11:K:86:ILE:HD12	1.98	0.45
11:K:166:GLU:O	11:K:229:VAL:HA	2.16	0.45
2:f:95:ASN:OD1	2:f:95:ASN:N	2.50	0.45
2:f:130:LEU:HA	2:f:130:LEU:HD23	1.76	0.45
7:i:217:TYR:HE1	12:h:210:HIS:NE2	2.15	0.45
5:B:43:CYS:SG	5:B:82:CYS:HA	2.56	0.45
12:H:251:ALA:O	12:H:286:SER:OG	2.28	0.45
1:A:426:LYS:HE3	1:A:426:LYS:HB3	1.67	0.45
9:G:213:THR:OG1	9:G:216:GLU:HG3	2.17	0.45
3:e:110:GLU:OE2	3:e:113:LYS:NZ	2.33	0.45
6:d:420:LEU:HD23	6:d:423:LEU:HB2	1.99	0.45
11:k:250:CYS:SG	11:k:252:CYS:SG	3.15	0.45
6:D:9:LYS:HE3	6:D:9:LYS:HB3	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:237:LYS:HD3	11:K:237:LYS:N	2.32	0.44
6:d:89:VAL:HA	6:d:422:PHE:HZ	1.82	0.44
6:d:417:LEU:O	6:d:420:LEU:HB3	2.17	0.44
9:g:441:LEU:O	9:g:444:ILE:HG22	2.17	0.44
5:B:221:ILE:HD11	4:c:4:LYS:HD3	1.99	0.44
10:J:18:GLY:HA3	19:H:502:MGD:N19	2.33	0.44
1:a:449:SER:HB2	1:a:454:TYR:HB3	2.00	0.44
1:a:600:CYS:O	1:a:623:ARG:NH2	2.49	0.44
6:d:534:HIS:HD2	6:d:536:GLY:H	1.65	0.44
9:g:96:MET:HA	9:g:96:MET:CE	2.47	0.44
9:g:523:TRP:CH2	9:g:525:LYS:HD3	2.52	0.44
12:h:58:ARG:HG3	12:h:66:MET:SD	2.57	0.44
1:A:636:CYS:SG	1:A:637:GLY:N	2.89	0.44
6:D:26:LEU:HD23	6:D:36:VAL:HG22	1.99	0.44
9:G:138:THR:HA	9:G:139:PRO:HD3	1.89	0.44
11:k:274:ILE:O	11:k:320:LYS:NZ	2.45	0.44
3:E:35:LEU:HD23	3:E:66:ILE:HD11	1.98	0.44
5:B:248:GLU:HA	5:B:251:GLU:HG2	1.98	0.44
7:I:217:TYR:HE1	12:H:210:HIS:NE2	2.15	0.44
9:G:3:GLU:N	9:G:36:VAL:HG11	2.32	0.44
11:K:251:THR:HA	11:K:266:VAL:CG1	2.48	0.44
11:k:83:VAL:HA	11:k:86:ILE:HD12	1.99	0.44
11:k:339:ILE:O	11:k:368:THR:OG1	2.30	0.44
1:A:575:SER:OG	1:a:165:ASP:OD1	2.35	0.44
6:D:420:LEU:HD23	6:D:423:LEU:HB2	1.99	0.44
12:H:58:ARG:HG3	12:H:66:MET:SD	2.57	0.44
5:b:43:CYS:O	5:b:44:PRO:C	2.60	0.44
9:g:101:PRO:HB3	9:g:105:LYS:HD3	2.00	0.44
3:E:59:VAL:HG21	3:E:88:LEU:HD21	1.99	0.44
9:G:391:HIS:HA	9:G:392:PRO:HA	1.76	0.44
9:G:508:VAL:HG22	9:G:513:ILE:HD13	2.00	0.44
10:J:19:ILE:O	10:J:23:ILE:HG12	2.17	0.44
11:K:338:ILE:H	11:K:338:ILE:HD12	1.83	0.44
12:H:157:PRO:HD2	12:H:196:THR:HG21	2.00	0.44
12:H:334:VAL:O	12:H:338:MET:HG2	2.17	0.44
9:g:213:THR:OG1	9:g:216:GLU:HG3	2.17	0.44
9:g:508:VAL:HG22	9:g:513:ILE:HD13	2.00	0.44
10:j:18:GLY:HA3	19:h:502:MGD:N19	2.33	0.44
11:k:42:ILE:HD12	11:k:89:PRO:HG2	1.98	0.44
11:k:100:GLU:OE2	11:k:100:GLU:N	2.51	0.44
11:k:338:ILE:HD12	11:k:338:ILE:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:49:MET:HE1	3:E:386:HIS:HE2	1.81	0.44
3:E:109:TYR:CD2	3:E:381:MET:HE2	2.53	0.44
6:D:135:ASP:OD2	6:D:139:ARG:HG3	2.16	0.44
9:G:276:HIS:HB2	9:G:279:PHE:HD2	1.83	0.44
9:G:523:TRP:CH2	9:G:525:LYS:HD3	2.52	0.44
11:K:100:GLU:N	11:K:100:GLU:OE2	2.51	0.44
12:H:94:GLY:HA2	12:H:299:ILE:CD1	2.46	0.44
5:b:160:MET:HB3	5:b:160:MET:HE3	1.67	0.44
6:d:452:THR:HG22	6:d:462:ARG:HD2	2.00	0.44
6:d:528:PRO:HG2	6:d:540:LEU:CD2	2.47	0.44
7:i:161:ASP:OD1	12:h:270:HIS:NE2	2.43	0.44
9:g:276:HIS:HB2	9:g:279:PHE:HD2	1.83	0.44
10:j:7:LEU:HD21	10:j:80:CYS:HB2	2.00	0.44
1:A:600:CYS:O	1:A:623:ARG:NH2	2.49	0.44
9:G:121:ALA:O	9:G:146:MET:HB2	2.18	0.44
9:G:254:LEU:HD23	9:G:254:LEU:HA	1.82	0.44
12:H:315:CYS:HB3	12:H:331:THR:OG1	2.18	0.44
5:b:49:PHE:CE2	5:b:56:VAL:HG13	2.53	0.44
6:d:328:VAL:HG12	6:d:330:PRO:HD3	2.00	0.44
7:i:253:LYS:CG	7:i:254:LYS:H	2.29	0.44
9:g:14:PRO:HA	9:g:442:TYR:OH	2.18	0.44
9:g:99:SER:O	9:g:100:ILE:C	2.61	0.44
10:j:19:ILE:O	10:j:23:ILE:HG12	2.17	0.44
10:j:130:VAL:CG1	12:h:365:LYS:HG2	2.48	0.44
12:h:190:ASP:HB2	19:h:502:MGD:HI'	1.99	0.44
1:A:48:MET:HE3	1:A:48:MET:HB3	1.87	0.44
1:A:165:ASP:OD1	1:a:575:SER:OG	2.35	0.44
5:B:49:PHE:CE2	5:B:56:VAL:HG13	2.53	0.44
6:D:73:LYS:HD3	6:D:78:ILE:CD1	2.48	0.44
6:D:389:CYS:SG	6:D:420:LEU:HD13	2.58	0.44
9:G:223:GLU:HG2	9:G:260:TYR:CE2	2.53	0.44
5:b:150:LYS:HE3	5:b:189:ILE:HG21	2.00	0.44
6:d:164:ASP:OD2	6:d:325:GLY:N	2.43	0.44
7:i:44:ILE:HD13	12:h:86:LYS:HG2	2.00	0.44
7:i:228:VAL:N	7:i:239:PHE:O	2.44	0.44
12:h:119:ALA:O	12:h:124:GLY:N	2.47	0.44
12:h:129:ALA:HB1	12:h:273:ASP:HB3	2.00	0.44
12:H:58:ARG:HB2	12:H:66:MET:HG2	2.00	0.43
12:H:293:MET:SD	12:H:403:MET:HE1	2.58	0.43
3:e:109:TYR:CD2	3:e:381:MET:HE2	2.53	0.43
6:d:389:CYS:SG	6:d:420:LEU:HD13	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:g:121:ALA:O	9:g:146:MET:HB2	2.18	0.43
9:g:223:GLU:HG2	9:g:260:TYR:CE2	2.53	0.43
10:j:24:GLY:O	10:j:27:SER:OG	2.29	0.43
10:j:86:VAL:O	10:j:90:GLN:HG2	2.18	0.43
1:A:449:SER:HB2	1:A:454:TYR:HB3	2.00	0.43
5:B:150:LYS:HE3	5:B:189:ILE:HG21	2.00	0.43
7:I:232:VAL:C	7:I:234:GLY:H	2.26	0.43
9:G:76:ASP:HA	9:G:84:ARG:NH2	2.32	0.43
9:G:79:PHE:CB	9:G:84:ARG:HE	2.31	0.43
10:J:25:LYS:NZ	12:H:351:ASP:OD2	2.50	0.43
11:K:274:ILE:O	11:K:320:LYS:NZ	2.45	0.43
12:H:110:ILE:HG22	12:H:434:MET:HE2	1.99	0.43
5:b:3:GLU:HG2	5:b:33:LYS:HB3	2.01	0.43
6:d:26:LEU:HD23	6:d:36:VAL:HG22	1.99	0.43
7:i:181:VAL:HB	7:i:200:VAL:HG13	2.00	0.43
7:i:245:ASP:H	7:i:250:LYS:NZ	2.16	0.43
9:g:521:THR:HG23	9:g:521:THR:O	2.18	0.43
11:k:128:CYS:O	11:k:129:ASN:HB2	2.18	0.43
11:k:219:ALA:HA	11:k:227:ILE:HG21	1.99	0.43
12:h:293:MET:SD	12:h:403:MET:HE1	2.58	0.43
6:D:316:LEU:HD23	6:D:321:VAL:HG21	2.00	0.43
6:D:528:PRO:HG2	6:D:540:LEU:CD2	2.48	0.43
7:I:44:ILE:HD13	12:H:86:LYS:HG2	2.00	0.43
8:L:140:PRO:HA	8:L:141:PRO:HD3	1.89	0.43
9:G:99:SER:O	9:G:100:ILE:C	2.61	0.43
9:G:521:THR:O	9:G:521:THR:HG23	2.18	0.43
6:d:266:ALA:HB3	6:d:270:HIS:NE2	2.33	0.43
6:d:401:LEU:HD23	6:d:401:LEU:HA	1.65	0.43
6:d:403:PRO:HD2	6:d:433:THR:HG21	2.01	0.43
7:i:201:GLY:HA2	7:i:204:MET:HE3	2.00	0.43
12:h:18:ASP:OD1	12:h:18:ASP:N	2.44	0.43
1:A:174:TYR:CE2	1:A:217:GLU:HG2	2.54	0.43
5:B:3:GLU:HG2	5:B:33:LYS:HB3	2.01	0.43
6:D:452:THR:HG22	6:D:462:ARG:HD2	2.00	0.43
6:D:534:HIS:HD2	6:D:536:GLY:H	1.65	0.43
9:G:237:HIS:HD2	9:G:276:HIS:HE1	1.66	0.43
10:J:130:VAL:CG1	12:H:365:LYS:HG2	2.48	0.43
1:a:174:TYR:CE2	1:a:217:GLU:HG2	2.54	0.43
6:d:173:ILE:HD12	6:d:173:ILE:H	1.83	0.43
6:d:459:ARG:HE	6:d:459:ARG:HB2	1.54	0.43
12:h:322:ASN:N	12:h:322:ASN:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:181:VAL:HB	7:I:200:VAL:HG13	2.00	0.43
12:H:218:PHE:O	12:H:222:ILE:HG12	2.18	0.43
12:H:322:ASN:OD1	12:H:322:ASN:N	2.50	0.43
2:f:49:MET:HE1	3:e:386:HIS:HE2	1.81	0.43
5:b:8:LEU:HD21	5:b:20:GLU:HB2	2.00	0.43
6:d:89:VAL:HA	6:d:422:PHE:CZ	2.53	0.43
8:l:89:GLU:O	8:l:95:PRO:HG3	2.18	0.43
12:h:110:ILE:HG22	12:h:434:MET:HE2	1.99	0.43
2:F:88:MET:SD	3:E:386:HIS:NE2	2.80	0.43
4:C:124:ASN:HD22	5:B:206:GLY:HA3	1.83	0.43
7:I:201:GLY:HA2	7:I:204:MET:HE3	2.00	0.43
8:L:89:GLU:O	8:L:95:PRO:HG3	2.18	0.43
1:a:76:PRO:O	1:a:80:GLU:HG2	2.18	0.43
1:a:192:THR:HG23	1:a:199:SER:HB2	2.00	0.43
9:g:79:PHE:CB	9:g:84:ARG:HE	2.31	0.43
12:h:157:PRO:HD2	12:h:196:THR:HG21	2.00	0.43
12:h:218:PHE:O	12:h:222:ILE:HG12	2.18	0.43
5:B:255:ASP:CG	4:c:4:LYS:HZ1	2.27	0.43
6:D:89:VAL:HA	6:D:422:PHE:CZ	2.53	0.43
6:D:266:ALA:HB3	6:D:270:HIS:NE2	2.33	0.43
6:D:348:ASN:OD1	6:D:348:ASN:N	2.51	0.43
7:I:69:VAL:HG11	7:I:73:VAL:HG11	2.01	0.43
10:J:56:ARG:HB2	10:J:114:VAL:HG21	1.99	0.43
11:K:273:GLU:OE2	11:K:342:ARG:NH1	2.52	0.43
1:a:540:LYS:HA	1:a:540:LYS:HD2	1.84	0.43
2:f:49:MET:HG2	2:f:89:ILE:HD11	1.99	0.43
4:c:124:ASN:HD22	5:b:206:GLY:HA3	1.83	0.43
9:g:444:ILE:HD12	9:g:444:ILE:HA	1.92	0.43
11:k:153:GLU:HB2	11:k:156:ALA:HA	2.00	0.43
12:h:58:ARG:HB2	12:h:66:MET:HG2	2.00	0.43
12:h:249:LYS:HG2	12:h:285:ILE:HD11	2.01	0.43
2:F:101:ARG:HH21	2:F:130:LEU:HD21	1.84	0.43
9:G:411:LYS:HA	9:G:414:LYS:HE2	2.01	0.43
12:H:129:ALA:HB1	12:H:273:ASP:HB3	2.00	0.43
6:d:73:LYS:HD3	6:d:78:ILE:CD1	2.48	0.43
9:g:76:ASP:HA	9:g:84:ARG:NH2	2.32	0.43
12:h:299:ILE:HD12	12:h:299:ILE:HA	1.90	0.43
1:A:388:PRO:HB3	11:K:5:PHE:HZ	1.84	0.43
5:B:8:LEU:HD23	5:B:8:LEU:HA	1.82	0.43
5:B:191:TYR:CE1	5:B:194:LYS:HA	2.54	0.43
12:H:182:LYS:HA	12:H:182:LYS:HD3	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:78:LEU:HD23	1:a:79:HIS:CD2	2.53	0.43
1:a:219:MET:HE2	1:a:219:MET:HB3	1.87	0.43
2:f:32:TYR:HB2	2:f:33:PRO:HD2	2.01	0.43
3:e:59:VAL:HG21	3:e:88:LEU:HD21	1.99	0.43
5:b:49:PHE:HE2	5:b:56:VAL:HG13	1.83	0.43
6:d:316:LEU:HD23	6:d:321:VAL:HG21	2.00	0.43
2:F:32:TYR:HB2	2:F:33:PRO:HD2	2.01	0.43
6:D:306:ASP:HB3	6:D:557:ILE:HG21	2.01	0.43
11:K:164:LYS:HE3	11:K:164:LYS:HB3	1.31	0.43
12:H:54:ILE:HG22	12:H:388:PRO:HG3	2.00	0.43
1:a:43:ASP:OD1	1:a:44:GLN:N	2.48	0.43
4:c:178:TYR:OH	5:b:106:VAL:HG21	2.19	0.43
9:g:254:LEU:HB3	9:g:300:TYR:CE2	2.54	0.43
9:g:275:THR:O	9:g:277:ILE:HG13	2.19	0.43
10:j:12:GLN:HE21	19:h:502:MGD:H8	1.82	0.43
12:h:204:LEU:HD11	12:h:244:VAL:HG21	2.01	0.43
12:h:395:ASP:HB3	12:h:416:PRO:HB3	2.01	0.43
1:A:67:THR:CG2	1:A:96:ARG:HH21	2.32	0.42
1:A:76:PRO:O	1:A:80:GLU:HG2	2.19	0.42
5:B:49:PHE:HE2	5:B:56:VAL:HG13	1.83	0.42
5:B:53:ASP:HB3	5:B:56:VAL:CG1	2.42	0.42
5:B:84:LYS:HB2	5:B:158:HIS:HB3	2.01	0.42
8:L:74:THR:HG21	8:L:131:TYR:CZ	2.53	0.42
9:G:14:PRO:HA	9:G:442:TYR:OH	2.18	0.42
11:K:153:GLU:HB2	11:K:156:ALA:HA	2.00	0.42
3:e:329:MET:HE3	3:e:333:ILE:HG13	2.01	0.42
6:d:346:TYR:HB2	6:d:349:VAL:HG22	2.00	0.42
7:i:69:VAL:HG11	7:i:73:VAL:HG11	2.01	0.42
2:F:14:CYS:HB3	2:F:44:THR:HG23	2.01	0.42
6:D:476:ASP:OD1	6:D:476:ASP:N	2.53	0.42
7:I:245:ASP:H	7:I:250:LYS:NZ	2.16	0.42
9:G:254:LEU:HB3	9:G:300:TYR:CE2	2.54	0.42
10:J:103:GLN:CA	12:H:268:ARG:HH22	2.32	0.42
12:H:190:ASP:HB2	19:H:502:MGD:H1'	1.99	0.42
9:g:391:HIS:HA	9:g:392:PRO:HA	1.76	0.42
9:g:411:LYS:HA	9:g:414:LYS:HE2	2.01	0.42
10:j:56:ARG:HB2	10:j:114:VAL:HG21	2.00	0.42
11:k:273:GLU:OE2	11:k:342:ARG:NH1	2.52	0.42
12:h:315:CYS:HB3	12:h:331:THR:OG1	2.18	0.42
1:A:448:ARG:HG2	1:a:448:ARG:HG2	2.01	0.42
4:C:4:LYS:HD3	5:b:221:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:16:PRO:HA	6:D:335:ASN:HD22	1.84	0.42
7:I:240:ASP:OD1	7:I:240:ASP:N	2.46	0.42
10:J:37:ILE:HD11	10:J:57:VAL:HG21	2.02	0.42
10:J:86:VAL:O	10:J:90:GLN:HG2	2.19	0.42
12:H:365:LYS:NZ	12:H:382:ILE:O	2.40	0.42
12:H:436:GLU:O	12:H:438:LYS:HG3	2.19	0.42
1:a:67:THR:CG2	1:a:96:ARG:HH21	2.32	0.42
2:f:101:ARG:HH21	2:f:130:LEU:HD21	1.84	0.42
9:g:209:TYR:O	9:g:209:TYR:CG	2.71	0.42
12:h:87:LYS:HD2	12:h:341:GLU:O	2.20	0.42
3:E:259:LYS:HE2	3:E:259:LYS:HB3	1.88	0.42
6:D:328:VAL:HG12	6:D:330:PRO:HD3	2.00	0.42
7:I:158:ALA:HB2	7:I:173:ILE:HD12	2.01	0.42
9:G:164:LEU:HD21	9:G:227:TYR:CG	2.55	0.42
9:G:275:THR:O	9:G:277:ILE:HG13	2.19	0.42
10:J:24:GLY:O	10:J:27:SER:OG	2.29	0.42
10:J:101:ALA:O	12:H:268:ARG:NH2	2.52	0.42
11:K:45:GLU:O	11:K:362:LYS:HD2	2.19	0.42
12:H:80:ARG:O	12:H:84:LYS:HG2	2.19	0.42
3:e:93:ASP:OD1	3:e:93:ASP:N	2.50	0.42
6:d:16:PRO:HA	6:d:335:ASN:HD22	1.84	0.42
7:i:158:ALA:HB2	7:i:173:ILE:HD12	2.01	0.42
9:g:164:LEU:HD21	9:g:227:TYR:CG	2.55	0.42
5:B:11:ILE:HD12	5:B:237:PHE:HD1	1.85	0.42
6:D:173:ILE:HD12	6:D:173:ILE:H	1.83	0.42
6:D:346:TYR:HB2	6:D:349:VAL:HG22	2.00	0.42
4:c:33:ILE:HG21	4:c:71:CYS:SG	2.60	0.42
5:b:84:LYS:HB2	5:b:158:HIS:HB3	2.01	0.42
6:d:132:ASN:ND2	6:d:375:PRO:HG2	2.35	0.42
8:l:121:GLY:HA2	8:l:136:LEU:HD21	2.02	0.42
9:g:344:ASP:HB3	12:h:142:GLU:OE1	2.20	0.42
10:j:25:LYS:NZ	12:h:351:ASP:OD2	2.50	0.42
11:k:66:ASP:OD1	11:k:66:ASP:N	2.50	0.42
1:A:202:ILE:O	1:A:205:PRO:HD2	2.19	0.42
4:C:178:TYR:OH	5:B:106:VAL:HG21	2.19	0.42
6:D:493:GLU:O	6:D:495:PRO:HD3	2.19	0.42
7:I:219:LEU:HD23	12:H:213:GLU:HG3	2.02	0.42
10:J:7:LEU:HD21	10:J:80:CYS:HB2	2.00	0.42
12:H:4:VAL:HG11	12:H:21:ARG:NH1	2.34	0.42
6:d:276:VAL:O	6:d:280:ILE:HG12	2.19	0.42
8:l:74:THR:HG21	8:l:131:TYR:CZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:g:142:ASP:C	9:g:143:GLN:HG3	2.45	0.42
10:j:15:VAL:HG23	12:h:159:HIS:ND1	2.34	0.42
5:B:8:LEU:HD21	5:B:20:GLU:HB2	2.00	0.42
9:G:262:ALA:HB2	9:G:270:GLN:O	2.20	0.42
12:H:87:LYS:HD2	12:H:341:GLU:O	2.20	0.42
12:H:140:LEU:HD13	12:H:168:TYR:CD2	2.55	0.42
1:a:188:GLN:HG2	1:a:279:PHE:CE1	2.55	0.42
5:b:191:TYR:CE1	5:b:194:LYS:HA	2.54	0.42
6:d:458:ARG:HG2	6:d:527:TRP:NE1	2.35	0.42
6:d:476:ASP:OD1	6:d:476:ASP:N	2.52	0.42
7:i:237:TYR:HB2	7:i:239:PHE:CE2	2.55	0.42
12:h:4:VAL:HG11	12:h:21:ARG:NH1	2.34	0.42
12:h:436:GLU:O	12:h:438:LYS:HG3	2.20	0.42
1:A:188:GLN:HG2	1:A:279:PHE:CE1	2.55	0.42
6:D:132:ASN:ND2	6:D:375:PRO:HG2	2.35	0.42
10:J:15:VAL:HG23	12:H:159:HIS:ND1	2.34	0.42
10:J:44:MET:HE1	10:J:51:LYS:HA	2.02	0.42
6:d:493:GLU:O	6:d:495:PRO:HD3	2.19	0.42
6:d:561:PRO:HA	6:d:562:PRO:HD3	1.95	0.42
8:l:84:PRO:HB3	11:k:285:CYS:HB2	2.02	0.42
9:g:237:HIS:HD2	9:g:276:HIS:HE1	1.66	0.42
12:h:54:ILE:HG22	12:h:388:PRO:HG3	2.00	0.42
12:h:140:LEU:HD13	12:h:168:TYR:CD2	2.55	0.42
5:B:132:VAL:HG12	5:B:133:CYS:N	2.35	0.42
7:I:7:THR:HG22	7:I:70:ASN:HB2	2.02	0.42
7:I:134:ASN:HB3	7:I:160:ASN:H	1.85	0.42
7:I:219:LEU:HD23	7:I:219:LEU:HA	1.91	0.42
9:G:101:PRO:HB3	9:G:105:LYS:HD3	2.00	0.42
2:f:14:CYS:HB3	2:f:44:THR:HG23	2.01	0.42
3:e:88:LEU:HD13	3:e:88:LEU:HA	1.87	0.42
9:g:435:MET:HE3	9:g:435:MET:HB2	1.96	0.42
11:k:219:ALA:HA	11:k:227:ILE:HG22	2.00	0.42
12:h:80:ARG:O	12:h:84:LYS:HG2	2.19	0.42
1:A:203:LEU:HD12	1:A:203:LEU:HA	1.89	0.42
9:G:209:TYR:O	9:G:209:TYR:CG	2.71	0.42
2:f:49:MET:HB3	2:f:89:ILE:HD11	2.02	0.42
5:b:11:ILE:HD12	5:b:237:PHE:HD1	1.85	0.42
5:b:242:PHE:HB3	5:b:261:VAL:HG21	2.02	0.42
9:g:101:PRO:HG2	9:g:397:PHE:CZ	2.55	0.42
10:j:101:ALA:O	12:h:268:ARG:NH2	2.53	0.42
11:k:162:GLU:HB2	11:k:235:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:h:251:ALA:O	12:h:286:SER:OG	2.28	0.42
12:h:326:MET:HE2	12:h:326:MET:HB3	1.95	0.42
10:J:132:MET:HE1	12:H:60:ARG:NH2	2.35	0.41
12:H:23:THR:HB	12:H:33:GLU:HG2	2.01	0.41
12:H:317:ASP:HB3	12:H:325:HIS:HB3	2.02	0.41
1:a:8:ARG:H	1:a:67:THR:HB	1.85	0.41
2:f:49:MET:HE3	2:f:85:ARG:HG2	2.02	0.41
3:e:217:LYS:HE3	3:e:217:LYS:HB3	1.89	0.41
6:d:424:VAL:HG13	6:d:439:VAL:HB	2.02	0.41
10:j:44:MET:HE1	10:j:51:LYS:HA	2.02	0.41
11:k:45:GLU:O	11:k:362:LYS:HD2	2.20	0.41
11:k:181:GLY:HA2	11:k:187:ILE:HB	2.01	0.41
12:h:271:ASN:O	12:h:274:ILE:HG22	2.20	0.41
12:h:347:ASN:HB3	12:h:371:THR:HG23	2.02	0.41
2:F:86:MET:HB3	2:F:103:PHE:HE2	1.85	0.41
4:C:180:LEU:HD12	4:C:180:LEU:HA	1.86	0.41
6:D:403:PRO:HD2	6:D:433:THR:HG21	2.01	0.41
7:I:186:GLU:O	7:I:206:LYS:HB3	2.20	0.41
7:I:264:LEU:HD12	7:I:264:LEU:HA	1.90	0.41
9:G:344:ASP:HB3	12:H:142:GLU:OE1	2.19	0.41
1:a:188:GLN:NE2	1:a:279:PHE:O	2.54	0.41
1:a:457:PHE:O	1:a:461:ILE:HG12	2.19	0.41
3:e:213:ASP:OD1	3:e:213:ASP:N	2.53	0.41
5:b:132:VAL:HG12	5:b:133:CYS:N	2.35	0.41
6:d:306:ASP:HB3	6:d:557:ILE:HG21	2.01	0.41
9:g:236:ILE:O	9:g:275:THR:HG22	2.20	0.41
10:j:132:MET:HE1	12:h:60:ARG:NH2	2.35	0.41
11:k:197:GLU:HB2	11:k:198:ILE:HD12	2.02	0.41
12:h:15:CYS:SG	12:h:161:HIS:HB3	2.60	0.41
1:A:188:GLN:NE2	1:A:279:PHE:O	2.54	0.41
1:A:357:TRP:O	1:A:359:TYR:N	2.53	0.41
6:D:276:VAL:O	6:D:280:ILE:HG12	2.19	0.41
6:D:376:ASP:OD1	6:D:376:ASP:C	2.64	0.41
6:D:424:VAL:HG13	6:D:439:VAL:HB	2.02	0.41
7:I:43:LYS:HE2	12:H:85:ALA:O	2.19	0.41
9:G:142:ASP:C	9:G:143:GLN:HG3	2.45	0.41
9:G:475:ILE:O	9:G:497:THR:OG1	2.34	0.41
11:K:164:LYS:O	11:K:231:ARG:HA	2.20	0.41
11:K:197:GLU:HB2	11:K:198:ILE:HD12	2.02	0.41
12:H:122:CYS:SG	12:H:260:MET:HE1	2.60	0.41
7:i:43:LYS:HE2	12:h:85:ALA:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:i:232:VAL:C	7:i:234:GLY:H	2.26	0.41
10:j:132:MET:HE2	10:j:132:MET:HB3	1.88	0.41
11:k:20:GLU:HA	11:k:28:ASN:O	2.20	0.41
12:h:317:ASP:HB3	12:h:325:HIS:HB3	2.02	0.41
2:F:130:LEU:HA	2:F:130:LEU:HD23	1.76	0.41
9:G:101:PRO:HG2	9:G:397:PHE:CZ	2.55	0.41
9:G:281:SER:O	9:G:281:SER:OG	2.27	0.41
9:G:484:PRO:HD2	9:G:490:ILE:HD11	2.02	0.41
10:J:12:GLN:HE21	19:H:502:MGD:H8	1.82	0.41
11:K:128:CYS:O	11:K:129:ASN:HB2	2.18	0.41
11:K:285:CYS:C	11:K:287:THR:H	2.29	0.41
12:H:165:MET:HA	12:H:169:SER:OG	2.20	0.41
12:H:347:ASN:HB3	12:H:371:THR:HG23	2.03	0.41
1:a:234:PHE:HB2	1:a:337:VAL:HG23	2.03	0.41
5:b:73:LYS:HD3	5:b:73:LYS:HA	1.81	0.41
7:i:219:LEU:HD23	12:h:213:GLU:HG3	2.02	0.41
9:g:116:THR:HG21	9:g:472:ASN:CG	2.46	0.41
10:j:37:ILE:HD11	10:j:57:VAL:HG21	2.01	0.41
10:j:55:VAL:HG23	10:j:113:PRO:HA	2.02	0.41
11:k:127:ARG:NH2	11:k:240:GLY:O	2.53	0.41
1:A:8:ARG:H	1:A:67:THR:HB	1.85	0.41
1:A:136:LEU:HD22	1:A:652:HIS:CD2	2.56	0.41
3:E:88:LEU:HD13	3:E:88:LEU:HA	1.87	0.41
14:E:505:FAD:H9	14:E:505:FAD:H1'1	1.79	0.41
4:C:33:ILE:HG21	4:C:71:CYS:SG	2.60	0.41
6:D:430:PHE:HE2	6:D:435:GLN:HE21	1.68	0.41
7:I:216:LEU:HG	7:I:217:TYR:CE2	2.56	0.41
7:I:237:TYR:HB2	7:I:239:PHE:CE2	2.55	0.41
8:L:121:GLY:HA2	8:L:136:LEU:HD21	2.02	0.41
9:G:420:MET:HE3	9:G:420:MET:HB2	1.82	0.41
11:K:20:GLU:HA	11:K:28:ASN:O	2.20	0.41
5:b:44:PRO:HG2	5:b:57:TRP:CD1	2.56	0.41
8:l:72:ARG:HE	8:l:72:ARG:HB3	1.43	0.41
9:g:262:ALA:HB2	9:g:270:GLN:O	2.20	0.41
10:j:55:VAL:HG12	10:j:66:VAL:O	2.21	0.41
11:k:46:VAL:O	11:k:47:CYS:C	2.63	0.41
12:h:122:CYS:SG	12:h:260:MET:HE1	2.60	0.41
3:E:329:MET:HE3	3:E:333:ILE:HG13	2.02	0.41
5:B:79:CYS:HB3	5:B:82:CYS:HB2	2.02	0.41
7:I:228:VAL:N	7:I:239:PHE:O	2.44	0.41
11:K:215:CYS:SG	11:K:216:ASN:N	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:204:LEU:HD11	12:H:244:VAL:HG21	2.01	0.41
5:b:18:GLY:HA3	5:b:279:LEU:O	2.21	0.41
6:d:394:LYS:HA	6:d:420:LEU:HD12	2.03	0.41
7:i:109:VAL:HB	7:i:128:ILE:HG12	2.03	0.41
12:h:58:ARG:HA	12:h:68:ASP:HA	2.02	0.41
3:E:191:ARG:HH21	3:E:191:ARG:HD3	1.76	0.41
6:D:361:ASN:O	6:D:365:MET:HG2	2.21	0.41
7:I:13:GLU:HG3	12:H:86:LYS:HZ1	1.86	0.41
9:G:490:ILE:HD13	9:G:490:ILE:HA	1.92	0.41
11:K:220:GLU:OE1	11:K:220:GLU:N	2.51	0.41
12:H:271:ASN:O	12:H:274:ILE:HG22	2.20	0.41
1:a:136:LEU:HD22	1:a:652:HIS:CD2	2.56	0.41
3:e:46:ILE:HG21	3:e:55:ALA:HB1	2.02	0.41
6:d:376:ASP:OD1	6:d:376:ASP:C	2.64	0.41
7:i:15:PHE:CD2	12:h:341:GLU:HG3	2.56	0.41
7:i:134:ASN:HB3	7:i:160:ASN:H	1.85	0.41
7:i:186:GLU:O	7:i:206:LYS:HB3	2.20	0.41
7:i:216:LEU:HG	7:i:217:TYR:CE2	2.56	0.41
9:g:107:GLY:HA2	9:g:141:LEU:CD1	2.51	0.41
9:g:500:THR:HB	9:g:508:VAL:HB	2.03	0.41
5:B:44:PRO:HG2	5:B:57:TRP:CD1	2.56	0.41
9:G:13:ASP:CG	9:G:465:LEU:H	2.29	0.41
9:G:236:ILE:O	9:G:275:THR:HG22	2.20	0.41
9:G:347:LEU:HD11	9:G:545:ASN:HB3	2.03	0.41
10:J:55:VAL:HG12	10:J:66:VAL:O	2.21	0.41
12:H:249:LYS:HG2	12:H:285:ILE:HD11	2.01	0.41
12:H:395:ASP:HB3	12:H:416:PRO:HB3	2.01	0.41
1:a:476:VAL:CG1	1:a:485:LEU:HD12	2.51	0.41
9:g:207:VAL:HG23	9:g:212:ILE:O	2.20	0.41
11:k:285:CYS:C	11:k:287:THR:H	2.29	0.41
12:h:23:THR:HB	12:h:33:GLU:HG2	2.01	0.41
12:h:83:LEU:HA	12:h:83:LEU:HD23	1.84	0.41
12:h:165:MET:HA	12:h:169:SER:OG	2.20	0.41
1:A:476:VAL:CG1	1:A:485:LEU:HD12	2.51	0.41
2:F:49:MET:HE3	2:F:85:ARG:HG2	2.02	0.41
3:E:243:ILE:HD13	3:E:243:ILE:HA	1.90	0.41
5:B:18:GLY:HA3	5:B:279:LEU:O	2.21	0.41
5:B:209:ILE:HG13	5:B:213:LEU:HD13	2.03	0.41
5:B:242:PHE:HB3	5:B:261:VAL:HG21	2.02	0.41
7:I:15:PHE:CD2	12:H:341:GLU:HG3	2.56	0.41
8:L:84:PRO:HB3	11:K:285:CYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:67:ASN:HD21	9:G:70:ARG:HH11	1.69	0.41
9:G:155:CYS:O	9:G:159:ILE:HD13	2.21	0.41
9:G:214:PRO:HA	9:G:217:ILE:HG22	2.03	0.41
11:K:163:LEU:HG	11:K:232:THR:H	1.85	0.41
11:K:181:GLY:CA	11:K:187:ILE:HB	2.50	0.41
11:K:313:GLU:HG2	12:H:179:LYS:NZ	2.36	0.41
12:H:15:CYS:SG	12:H:161:HIS:HB3	2.60	0.41
12:H:92:GLY:HA3	12:H:348:ILE:O	2.21	0.41
1:a:357:TRP:O	1:a:359:TYR:N	2.53	0.41
2:f:86:MET:HB3	2:f:103:PHE:HE2	1.85	0.41
7:i:7:THR:HG22	7:i:70:ASN:HB2	2.02	0.41
9:g:14:PRO:HG2	9:g:446:MET:HA	2.02	0.41
9:g:92:LYS:HG3	9:g:93:ARG:HG2	2.02	0.41
9:g:286:SER:O	9:g:290:PHE:HB2	2.21	0.41
9:g:484:PRO:HD2	9:g:490:ILE:HD11	2.02	0.41
10:j:18:GLY:HA3	19:h:502:MGD:H191	1.86	0.41
11:k:41:GLY:C	11:k:43:CYS:N	2.71	0.41
12:h:136:PRO:O	12:h:290:ILE:HG22	2.21	0.41
1:A:370:GLU:OE1	11:K:4:LEU:HD23	2.21	0.41
6:D:100:HIS:HD2	6:D:394:LYS:HD2	1.86	0.41
6:D:458:ARG:HG2	6:D:527:TRP:NE1	2.35	0.41
7:I:39:ALA:HB2	7:I:48:LEU:HD13	2.03	0.41
7:I:92:SER:HB2	7:I:93:ASP:H	1.54	0.41
8:L:72:ARG:HE	8:L:72:ARG:HB3	1.43	0.41
9:G:92:LYS:HG3	9:G:93:ARG:HG2	2.01	0.41
9:G:205:ASP:HA	9:G:206:PRO:HD3	1.90	0.41
10:J:7:LEU:O	10:J:7:LEU:HD23	2.21	0.41
11:K:46:VAL:O	11:K:47:CYS:C	2.63	0.41
12:H:58:ARG:HA	12:H:68:ASP:HA	2.02	0.41
1:a:348:LEU:HD23	1:a:348:LEU:HA	1.94	0.41
3:e:276:MET:HE1	3:e:286:MET:HE2	2.03	0.41
3:e:296:CYS:HA	6:d:51:PRO:HG3	2.03	0.41
5:b:187:GLU:HG2	5:b:187:GLU:O	2.21	0.41
6:d:430:PHE:HE2	6:d:435:GLN:HE21	1.68	0.41
6:d:528:PRO:HG2	6:d:540:LEU:HD21	2.03	0.41
9:g:146:MET:HE2	9:g:184:KCX:HB3	2.03	0.41
12:h:76:ASP:CG	12:h:80:ARG:HE	2.29	0.41
12:h:92:GLY:HA3	12:h:348:ILE:O	2.21	0.41
1:A:457:PHE:O	1:A:461:ILE:HG12	2.19	0.40
2:F:11:ALA:HA	2:F:64:LEU:O	2.21	0.40
9:G:14:PRO:HG2	9:G:446:MET:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:8:VAL:HG12	12:H:9:GLY:N	2.36	0.40
12:H:76:ASP:CG	12:H:80:ARG:HE	2.29	0.40
3:e:16:GLU:HG3	3:e:67:ILE:HD11	2.03	0.40
3:e:46:ILE:HD12	3:e:78:LEU:HD21	2.04	0.40
5:b:37:LEU:HD12	5:b:37:LEU:HA	1.84	0.40
9:g:214:PRO:HA	9:g:217:ILE:HG22	2.03	0.40
5:B:43:CYS:O	5:B:44:PRO:C	2.60	0.40
5:B:139:LYS:HE3	5:B:139:LYS:HB3	1.91	0.40
6:D:205:ARG:HG3	6:D:207:THR:HG23	2.03	0.40
9:G:116:THR:HG21	9:G:472:ASN:CG	2.45	0.40
12:H:376:ILE:HD13	12:H:376:ILE:HA	1.96	0.40
5:b:53:ASP:HB3	5:b:56:VAL:CG1	2.42	0.40
9:g:521:THR:HG22	9:g:561:HIS:O	2.21	0.40
10:j:7:LEU:HD23	10:j:7:LEU:O	2.21	0.40
12:h:57:PRO:HA	12:h:388:PRO:HD3	2.03	0.40
12:h:182:LYS:HA	12:h:182:LYS:HD3	1.81	0.40
12:h:373:ASP:O	12:h:388:PRO:HA	2.22	0.40
1:A:202:ILE:HG22	1:a:541:LEU:HD12	2.04	0.40
3:E:16:GLU:HG3	3:E:67:ILE:HD11	2.03	0.40
6:D:86:LEU:HD23	6:D:86:LEU:HA	1.87	0.40
6:D:561:PRO:HA	6:D:562:PRO:HD3	1.95	0.40
7:I:182:LEU:HD23	7:I:182:LEU:HA	1.86	0.40
9:G:174:LEU:HD12	9:G:174:LEU:HA	1.80	0.40
9:G:207:VAL:HG23	9:G:212:ILE:O	2.20	0.40
9:G:263:LYS:HA	9:G:263:LYS:HE2	2.03	0.40
10:J:132:MET:HE1	12:H:60:ARG:CZ	2.51	0.40
11:K:212:CYS:SG	11:K:213:ASP:N	2.92	0.40
12:H:347:ASN:HB3	12:H:371:THR:HA	2.03	0.40
12:H:367:HIS:HB3	12:H:368:PRO:HD2	2.03	0.40
1:a:388:PRO:HB3	11:k:5:PHE:HZ	1.84	0.40
7:i:15:PHE:HB3	7:i:77:LYS:HD3	2.03	0.40
8:l:80:VAL:HG22	8:l:102:TYR:HB2	2.04	0.40
9:g:27:ILE:H	9:g:27:ILE:HD12	1.87	0.40
12:h:183:LYS:HD2	12:h:183:LYS:HA	1.87	0.40
2:F:75:TYR:O	2:F:77:GLU:N	2.54	0.40
3:E:276:MET:HE1	3:E:286:MET:HE2	2.04	0.40
7:I:117:LEU:HD11	7:I:126:ILE:HG21	2.04	0.40
8:L:89:GLU:HG2	8:L:90:LEU:HD22	2.04	0.40
9:G:27:ILE:H	9:G:27:ILE:HD12	1.87	0.40
9:G:397:PHE:C	9:G:399:ARG:H	2.29	0.40
10:J:18:GLY:HA3	19:H:502:MGD:H191	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:d:361:ASN:O	6:d:365:MET:HG2	2.21	0.40
8:l:81:VAL:O	12:h:173:ARG:NH1	2.46	0.40
9:g:123:MET:HE3	9:g:123:MET:HB2	1.95	0.40
10:j:132:MET:HE1	12:h:60:ARG:CZ	2.51	0.40
12:h:8:VAL:HG12	12:h:9:GLY:N	2.37	0.40
12:h:253:PHE:CD1	12:h:287:LYS:HG2	2.56	0.40
12:h:347:ASN:HB3	12:h:371:THR:HA	2.04	0.40
1:A:43:ASP:OD1	1:A:44:GLN:N	2.48	0.40
1:A:234:PHE:HB2	1:A:337:VAL:HG23	2.03	0.40
2:F:49:MET:HB3	2:F:89:ILE:HD11	2.03	0.40
3:E:340:ASP:HA	3:E:369:ILE:HG21	2.03	0.40
4:C:130:GLN:OE1	4:C:181:LYS:NZ	2.49	0.40
5:B:84:LYS:O	5:B:88:GLU:HB3	2.22	0.40
6:D:394:LYS:HA	6:D:420:LEU:HD12	2.03	0.40
8:L:80:VAL:HG22	8:L:102:TYR:HB2	2.04	0.40
9:G:107:GLY:HA2	9:G:141:LEU:CD1	2.51	0.40
9:G:500:THR:HB	9:G:508:VAL:HB	2.03	0.40
1:a:154:GLY:O	1:a:159:GLY:HA3	2.21	0.40
3:e:282:ARG:O	3:e:286:MET:HG3	2.21	0.40
6:d:348:ASN:OD1	6:d:348:ASN:N	2.51	0.40
9:g:138:THR:HA	9:g:139:PRO:HD3	1.89	0.40
10:j:76:TYR:HB2	10:j:77:PRO:HD2	2.04	0.40
11:k:252:CYS:HA	11:k:324:ILE:CG2	2.52	0.40
12:h:367:HIS:HB3	12:h:368:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	660/671 (98%)	625 (95%)	34 (5%)	1 (0%)	43 74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	660/671 (98%)	625 (95%)	34 (5%)	1 (0%)	43	74
2	F	135/140 (96%)	126 (93%)	9 (7%)	0	100	100
2	f	135/140 (96%)	126 (93%)	9 (7%)	0	100	100
3	E	409/414 (99%)	389 (95%)	20 (5%)	0	100	100
3	e	409/414 (99%)	389 (95%)	20 (5%)	0	100	100
4	C	187/191 (98%)	179 (96%)	8 (4%)	0	100	100
4	c	187/191 (98%)	179 (96%)	8 (4%)	0	100	100
5	B	294/296 (99%)	279 (95%)	15 (5%)	0	100	100
5	b	294/296 (99%)	279 (95%)	15 (5%)	0	100	100
6	D	545/686 (79%)	506 (93%)	39 (7%)	0	100	100
6	d	545/686 (79%)	506 (93%)	39 (7%)	0	100	100
7	I	262/266 (98%)	226 (86%)	35 (13%)	1 (0%)	30	62
7	i	262/266 (98%)	226 (86%)	35 (13%)	1 (0%)	30	62
8	L	77/146 (53%)	72 (94%)	5 (6%)	0	100	100
8	l	77/146 (53%)	72 (94%)	5 (6%)	0	100	100
9	G	565/571 (99%)	514 (91%)	49 (9%)	2 (0%)	30	62
9	g	565/571 (99%)	514 (91%)	49 (9%)	2 (0%)	30	62
10	J	129/137 (94%)	118 (92%)	11 (8%)	0	100	100
10	j	129/137 (94%)	118 (92%)	11 (8%)	0	100	100
11	K	384/388 (99%)	337 (88%)	44 (12%)	3 (1%)	16	49
11	k	384/388 (99%)	340 (88%)	41 (11%)	3 (1%)	16	49
12	H	436/443 (98%)	389 (89%)	47 (11%)	0	100	100
12	h	436/443 (98%)	389 (89%)	47 (11%)	0	100	100
All	All	8166/8698 (94%)	7523 (92%)	629 (8%)	14 (0%)	44	74

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	G	276	HIS
9	g	276	HIS
11	k	251	THR
1	A	446	ASP
11	K	42	ILE
11	K	227	ILE

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Mol	Chain	Res	Type
1	a	446	ASP
11	k	42	ILE
11	K	232	THR
7	I	92	SER
9	G	348	GLU
7	i	92	SER
9	g	348	GLU
11	k	234	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	536/543 (99%)	526 (98%)	10 (2%)	50	68
1	a	536/543 (99%)	526 (98%)	10 (2%)	50	68
2	F	112/114 (98%)	108 (96%)	4 (4%)	31	57
2	f	112/114 (98%)	108 (96%)	4 (4%)	31	57
3	E	338/341 (99%)	327 (97%)	11 (3%)	33	58
3	e	338/341 (99%)	327 (97%)	11 (3%)	33	58
4	C	168/170 (99%)	168 (100%)	0	100	100
4	c	168/170 (99%)	168 (100%)	0	100	100
5	B	245/245 (100%)	239 (98%)	6 (2%)	43	64
5	b	245/245 (100%)	239 (98%)	6 (2%)	43	64
6	D	454/571 (80%)	438 (96%)	16 (4%)	32	57
6	d	454/571 (80%)	438 (96%)	16 (4%)	32	57
7	I	202/204 (99%)	187 (93%)	15 (7%)	13	37
7	i	202/204 (99%)	187 (93%)	15 (7%)	13	37
8	L	67/128 (52%)	59 (88%)	8 (12%)	5	23
8	l	67/128 (52%)	59 (88%)	8 (12%)	5	23
9	G	472/474 (100%)	463 (98%)	9 (2%)	50	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	g	472/474 (100%)	463 (98%)	9 (2%)	50	68
10	J	111/116 (96%)	110 (99%)	1 (1%)	70	76
10	j	111/116 (96%)	110 (99%)	1 (1%)	70	76
11	K	330/332 (99%)	291 (88%)	39 (12%)	5	23
11	k	330/332 (99%)	288 (87%)	42 (13%)	4	21
12	H	370/373 (99%)	360 (97%)	10 (3%)	39	62
12	h	370/373 (99%)	360 (97%)	10 (3%)	39	62
All	All	6810/7222 (94%)	6549 (96%)	261 (4%)	30	55

All (261) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LEU
1	A	202	ILE
1	A	204	THR
1	A	405	SER
1	A	420	CYS
1	A	423	TYR
1	A	426	LYS
1	A	520	LEU
1	A	561	LYS
1	A	562	ASP
2	F	42	MET
2	F	95	ASN
2	F	98	LEU
2	F	101	ARG
3	E	28	THR
3	E	53	TYR
3	E	72	SER
3	E	88	LEU
3	E	99	THR
3	E	160	LYS
3	E	207	ASN
3	E	278	LYS
3	E	280	LYS
3	E	281	ASP
3	E	284	LYS
5	B	160	MET
5	B	178	GLU
5	B	179	GLU

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Mol	Chain	Res	Type
5	B	218	GLU
5	B	219	LYS
5	B	233	GLU
6	D	130	LYS
6	D	132	ASN
6	D	169	ASP
6	D	230	SER
6	D	258	LYS
6	D	259	THR
6	D	305	THR
6	D	357	GLU
6	D	399	LEU
6	D	436	TYR
6	D	476	ASP
6	D	527	TRP
6	D	531	THR
6	D	547	THR
6	D	549	ASP
6	D	553	ASN
7	I	16	LEU
7	I	73	VAL
7	I	75	ARG
7	I	76	MET
7	I	77	LYS
7	I	81	GLN
7	I	83	MET
7	I	90	ILE
7	I	92	SER
7	I	95	ASP
7	I	102	MET
7	I	115	SER
7	I	121	MET
7	I	170	THR
7	I	173	ILE
8	L	66	VAL
8	L	100	LYS
8	L	101	ILE
8	L	103	LYS
8	L	124	ILE
8	L	131	TYR
8	L	132	ASP
8	L	133	VAL

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Mol	Chain	Res	Type
9	G	96	MET
9	G	134	GLU
9	G	138	THR
9	G	140	ILE
9	G	156	PHE
9	G	345	VAL
9	G	346	GLU
9	G	348	GLU
9	G	349	THR
10	J	63	GLU
11	K	36	ILE
11	K	40	CYS
11	K	42	ILE
11	K	48	PRO
11	K	81	CYS
11	K	90	PHE
11	K	126	VAL
11	K	128	CYS
11	K	140	ILE
11	K	141	ASP
11	K	143	ASP
11	K	157	LYS
11	K	163	LEU
11	K	164	LYS
11	K	165	ILE
11	K	166	GLU
11	K	169	VAL
11	K	171	ASP
11	K	172	GLU
11	K	174	CYS
11	K	176	LYS
11	K	177	CYS
11	K	187	ILE
11	K	189	VAL
11	K	205	VAL
11	K	215	CYS
11	K	217	VAL
11	K	224	SER
11	K	225	GLU
11	K	227	ILE
11	K	228	LYS
11	K	229	VAL

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Mol	Chain	Res	Type
11	K	230	THR
11	K	231	ARG
11	K	241	ASN
11	K	253	ARG
11	K	257	ILE
11	K	261	THR
11	K	264	ILE
12	H	95	SER
12	H	96	THR
12	H	126	SER
12	H	220	MET
12	H	260	MET
12	H	297	TYR
12	H	308	TRP
12	H	408	ILE
12	H	423	ASP
12	H	424	GLU
1	a	78	LEU
1	a	202	ILE
1	a	204	THR
1	a	405	SER
1	a	420	CYS
1	a	423	TYR
1	a	426	LYS
1	a	520	LEU
1	a	561	LYS
1	a	562	ASP
2	f	42	MET
2	f	95	ASN
2	f	98	LEU
2	f	101	ARG
3	e	28	THR
3	e	53	TYR
3	e	72	SER
3	e	88	LEU
3	e	99	THR
3	e	160	LYS
3	e	207	ASN
3	e	278	LYS
3	e	280	LYS
3	e	281	ASP
3	e	284	LYS

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Mol	Chain	Res	Type
5	b	160	MET
5	b	178	GLU
5	b	179	GLU
5	b	218	GLU
5	b	219	LYS
5	b	233	GLU
6	d	130	LYS
6	d	132	ASN
6	d	169	ASP
6	d	230	SER
6	d	258	LYS
6	d	259	THR
6	d	305	THR
6	d	357	GLU
6	d	399	LEU
6	d	436	TYR
6	d	476	ASP
6	d	527	TRP
6	d	531	THR
6	d	547	THR
6	d	549	ASP
6	d	553	ASN
7	i	16	LEU
7	i	73	VAL
7	i	75	ARG
7	i	76	MET
7	i	77	LYS
7	i	81	GLN
7	i	83	MET
7	i	90	ILE
7	i	92	SER
7	i	95	ASP
7	i	102	MET
7	i	115	SER
7	i	121	MET
7	i	170	THR
7	i	173	ILE
8	l	66	VAL
8	l	100	LYS
8	l	101	ILE
8	l	103	LYS
8	l	124	ILE

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Mol	Chain	Res	Type
8	l	131	TYR
8	l	132	ASP
8	l	133	VAL
9	g	96	MET
9	g	134	GLU
9	g	138	THR
9	g	140	ILE
9	g	156	PHE
9	g	345	VAL
9	g	346	GLU
9	g	348	GLU
9	g	349	THR
10	j	63	GLU
11	k	36	ILE
11	k	40	CYS
11	k	42	ILE
11	k	48	PRO
11	k	81	CYS
11	k	90	PHE
11	k	126	VAL
11	k	128	CYS
11	k	137	ARG
11	k	140	ILE
11	k	141	ASP
11	k	157	LYS
11	k	163	LEU
11	k	165	ILE
11	k	169	VAL
11	k	170	ASP
11	k	171	ASP
11	k	172	GLU
11	k	173	LYS
11	k	175	THR
11	k	176	LYS
11	k	177	CYS
11	k	179	ILE
11	k	187	ILE
11	k	205	VAL
11	k	215	CYS
11	k	217	VAL
11	k	227	ILE
11	k	228	LYS

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Mol	Chain	Res	Type
11	k	229	VAL
11	k	230	THR
11	k	232	THR
11	k	234	VAL
11	k	236	GLN
11	k	237	LYS
11	k	238	LYS
11	k	241	ASN
11	k	243	ASN
11	k	252	CYS
11	k	257	ILE
11	k	261	THR
11	k	264	ILE
12	h	95	SER
12	h	96	THR
12	h	126	SER
12	h	220	MET
12	h	260	MET
12	h	297	TYR
12	h	308	TRP
12	h	408	ILE
12	h	423	ASP
12	h	424	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	GLN
1	A	361	GLN
1	A	486	HIS
1	A	512	GLN
1	A	661	GLN
2	F	31	GLN
3	E	62	ASN
3	E	118	ASN
3	E	128	ASN
4	C	21	HIS
5	B	14	ASN
5	B	136	GLN
5	B	173	ASN
5	B	190	GLN
5	B	196	GLN

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Mol	Chain	Res	Type
6	D	59	HIS
6	D	224	HIS
6	D	338	GLN
6	D	412	HIS
6	D	416	GLN
6	D	534	HIS
7	I	70	ASN
9	G	152	ASN
9	G	270	GLN
9	G	273	HIS
9	G	274	ASN
9	G	545	ASN
10	J	54	ASN
10	J	73	GLN
11	K	21	GLN
11	K	28	ASN
11	K	129	ASN
12	H	145	ASN
12	H	216	ASN
12	H	325	HIS
12	H	367	HIS
1	a	361	GLN
1	a	486	HIS
1	a	661	GLN
2	f	31	GLN
3	e	62	ASN
3	e	118	ASN
4	c	21	HIS
5	b	14	ASN
5	b	136	GLN
5	b	173	ASN
5	b	190	GLN
5	b	196	GLN
6	d	59	HIS
6	d	224	HIS
6	d	338	GLN
6	d	412	HIS
6	d	416	GLN
6	d	534	HIS
7	i	70	ASN
9	g	152	ASN
9	g	270	GLN

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Mol	Chain	Res	Type
9	g	274	ASN
9	g	545	ASN
10	j	54	ASN
10	j	73	GLN
11	k	21	GLN
11	k	28	ASN
11	k	243	ASN
11	k	277	HIS
12	h	145	ASN
12	h	325	HIS
12	h	367	HIS
12	h	386	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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$
9	KCX	g	184	9,17	10,11,12	0.36	0	6,12,14	0.45	0
9	KCX	G	184	9,17	10,11,12	2.03	1 (10%)	6,12,14	2.82	1 (16%)

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
9	KCX	g	184	9,17	-	3/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	KCX	G	184	9,17	-	3/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	184	KCX	OQ1-CX	6.13	1.32	1.21

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	184	KCX	OQ1-CX-NZ	-6.88	114.47	124.92

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	g	184	KCX	OQ1-CX-NZ-CE
9	G	184	KCX	OQ2-CX-NZ-CE
9	g	184	KCX	OQ2-CX-NZ-CE
9	G	184	KCX	N-CA-CB-CG
9	g	184	KCX	N-CA-CB-CG
9	G	184	KCX	OQ1-CX-NZ-CE

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	g	184	KCX	2	0
9	G	184	KCX	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 68 ligands modelled in this entry, 6 are monoatomic - leaving 62 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	$\# Z > 2$
19	MGD	H	503	18	47,52,52	4.89	29 (61%)	58,81,81	2.02	17 (29%)
13	SF4	l	201	8	0,12,12	-	-	-		
13	SF4	a	706	1	0,12,12	-	-	-		
13	SF4	a	704	1	0,12,12	-	-	-		
13	SF4	k	403	11	0,12,12	-	-	-		
16	9S8	b	302	5	4,10,10	6.78	2 (50%)	-		
14	FAD	a	702	-	58,58,58	0.84	3 (5%)	85,89,89	0.44	0
13	SF4	d	701	6	0,12,12	-	-	-		
13	SF4	c	201	4	0,12,12	-	-	-		
13	SF4	K	407	11	0,12,12	-	-	-		
15	FES	F	201	2	0,4,4	-	-	-		
13	SF4	e	501	3	0,12,12	-	-	-		
13	SF4	A	707	1	0,12,12	-	-	-		
13	SF4	A	701	1	0,12,12	-	-	-		
13	SF4	K	401	11	0,12,12	-	-	-		
13	SF4	a	703	1	0,12,12	-	-	-		
13	SF4	C	202	4	0,12,12	-	-	-		
13	SF4	k	407	11	0,12,12	-	-	-		
19	MGD	H	502	18	47,52,52	4.84	27 (57%)	58,81,81	2.11	15 (25%)
13	SF4	e	504	3	0,12,12	-	-	-		
13	SF4	K	403	11	0,12,12	-	-	-		
19	MGD	h	502	18	47,52,52	4.83	27 (57%)	58,81,81	2.11	15 (25%)
13	SF4	C	201	4	0,12,12	-	-	-		
13	SF4	k	401	11	0,12,12	-	-	-		
13	SF4	a	705	1	0,12,12	-	-	-		
14	FAD	A	702	-	58,58,58	0.85	3 (5%)	85,89,89	0.44	0
16	9S8	B	302	5	4,10,10	6.76	2 (50%)	-		
13	SF4	E	504	3	0,12,12	-	-	-		
13	SF4	k	405	11	0,12,12	-	-	-		
13	SF4	k	408	11	0,12,12	-	-	-		
13	SF4	A	704	1	0,12,12	-	-	-		
13	SF4	k	406	11	0,12,12	-	-	-		
13	SF4	K	406	11	0,12,12	-	-	-		
15	FES	f	201	2	0,4,4	-	-	-		
14	FAD	e	505	-	58,58,58	1.19	3 (5%)	85,89,89	0.43	0
13	SF4	K	404	11	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	9S8	B	301	5	4,10,10	6.85	2 (50%)	-		
13	SF4	a	707	1	0,12,12	-	-	-		
13	SF4	K	405	11	0,12,12	-	-	-		
13	SF4	K	402	11	0,12,12	-	-	-		
13	SF4	e	502	3	0,12,12	-	-	-		
13	SF4	c	202	4	0,12,12	-	-	-		
13	SF4	E	502	3	0,12,12	-	-	-		
13	SF4	E	503	3	0,12,12	-	-	-		
13	SF4	k	404	11	0,12,12	-	-	-		
13	SF4	A	703	1	0,12,12	-	-	-		
13	SF4	D	701	6	0,12,12	-	-	-		
13	SF4	L	201	8	0,12,12	-	-	-		
13	SF4	e	503	3	0,12,12	-	-	-		
13	SF4	l	202	8	0,12,12	-	-	-		
13	SF4	a	701	1	0,12,12	-	-	-		
13	SF4	k	402	11	0,12,12	-	-	-		
13	SF4	h	504	12	0,12,12	-	-	-		
13	SF4	A	706	1	0,12,12	-	-	-		
13	SF4	K	408	11	0,12,12	-	-	-		
13	SF4	E	501	3	0,12,12	-	-	-		
14	FAD	E	505	-	58,58,58	1.19	3 (5%)	85,89,89	0.43	0
19	MGD	h	503	18	47,52,52	4.89	29 (61%)	58,81,81	2.02	16 (27%)
13	SF4	L	202	8	0,12,12	-	-	-		
16	9S8	b	301	5	4,10,10	6.85	2 (50%)	-		
13	SF4	A	705	1	0,12,12	-	-	-		
13	SF4	H	504	12	0,12,12	-	-	-		

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
19	MGD	H	503	18	-	8/22/66/66	0/6/6/6
13	SF4	l	201	8	-	-	0/6/5/5
13	SF4	a	706	1	-	-	0/6/5/5
13	SF4	a	704	1	-	-	0/6/5/5
13	SF4	k	403	11	-	-	0/6/5/5
16	9S8	b	302	5	-	-	0/3/3/3
14	FAD	a	702	-	-	1/34/50/50	0/6/6/6
13	SF4	d	701	6	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SF4	c	201	4	-	-	0/6/5/5
13	SF4	K	407	11	-	-	0/6/5/5
15	FES	F	201	2	-	-	0/1/1/1
13	SF4	e	501	3	-	-	0/6/5/5
13	SF4	A	707	1	-	-	0/6/5/5
13	SF4	A	701	1	-	-	0/6/5/5
13	SF4	K	401	11	-	-	0/6/5/5
13	SF4	a	703	1	-	-	0/6/5/5
19	MGD	H	502	18	-	8/22/66/66	0/6/6/6
13	SF4	C	202	4	-	-	0/6/5/5
13	SF4	k	407	11	-	-	0/6/5/5
19	MGD	h	502	18	-	8/22/66/66	0/6/6/6
13	SF4	K	403	11	-	-	0/6/5/5
13	SF4	e	504	3	-	-	0/6/5/5
13	SF4	C	201	4	-	-	0/6/5/5
13	SF4	k	401	11	-	-	0/6/5/5
13	SF4	a	705	1	-	-	0/6/5/5
14	FAD	A	702	-	-	1/34/50/50	0/6/6/6
16	9S8	B	302	5	-	-	0/3/3/3
13	SF4	E	504	3	-	-	0/6/5/5
13	SF4	k	405	11	-	-	0/6/5/5
13	SF4	k	408	11	-	-	0/6/5/5
13	SF4	A	704	1	-	-	0/6/5/5
13	SF4	k	406	11	-	-	0/6/5/5
13	SF4	K	406	11	-	-	0/6/5/5
15	FES	f	201	2	-	-	0/1/1/1
14	FAD	e	505	-	-	13/34/50/50	0/6/6/6
13	SF4	K	404	11	-	-	0/6/5/5
16	9S8	B	301	5	-	-	0/3/3/3
13	SF4	a	707	1	-	-	0/6/5/5
13	SF4	K	405	11	-	-	0/6/5/5
13	SF4	K	402	11	-	-	0/6/5/5
13	SF4	e	502	3	-	-	0/6/5/5
13	SF4	c	202	4	-	-	0/6/5/5
13	SF4	E	502	3	-	-	0/6/5/5
13	SF4	E	503	3	-	-	0/6/5/5
13	SF4	k	404	11	-	-	0/6/5/5
13	SF4	A	703	1	-	-	0/6/5/5
13	SF4	D	701	6	-	-	0/6/5/5
13	SF4	L	201	8	-	-	0/6/5/5
13	SF4	e	503	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FAD	E	505	-	-	13/34/50/50	0/6/6/6
13	SF4	a	701	1	-	-	0/6/5/5
13	SF4	l	202	8	-	-	0/6/5/5
13	SF4	k	402	11	-	-	0/6/5/5
13	SF4	A	706	1	-	-	0/6/5/5
13	SF4	K	408	11	-	-	0/6/5/5
13	SF4	E	501	3	-	-	0/6/5/5
13	SF4	h	504	12	-	-	0/6/5/5
19	MGD	h	503	18	-	8/22/66/66	0/6/6/6
13	SF4	L	202	8	-	-	0/6/5/5
16	9S8	b	301	5	-	-	0/3/3/3
13	SF4	A	705	1	-	-	0/6/5/5
13	SF4	H	504	12	-	-	0/6/5/5

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	H	503	MGD	C16-C21	12.87	1.60	1.38
19	h	503	MGD	C16-C21	12.84	1.60	1.38
19	h	502	MGD	C16-C21	12.29	1.59	1.38
19	H	502	MGD	C16-C21	12.25	1.59	1.38
19	H	503	MGD	C14-N15	11.07	1.58	1.46
19	h	503	MGD	C14-N15	11.05	1.58	1.46
19	H	502	MGD	C14-N15	10.75	1.58	1.46
19	h	502	MGD	C14-N15	10.65	1.58	1.46
19	h	503	MGD	C3'-C4'	-10.37	1.26	1.53
19	H	503	MGD	C3'-C4'	-10.32	1.26	1.53
19	h	502	MGD	C3'-C4'	-10.31	1.26	1.53
19	H	502	MGD	C3'-C4'	-10.31	1.26	1.53
16	B	302	9S8	S1-FE4	-9.89	2.12	2.28
16	b	302	9S8	S1-FE4	-9.86	2.12	2.28
16	B	301	9S8	S1-FE4	-9.84	2.12	2.28
16	b	301	9S8	S1-FE4	-9.79	2.12	2.28
16	b	301	9S8	S7-FE4	-9.45	2.13	2.28
16	B	301	9S8	S7-FE4	-9.38	2.13	2.28
16	b	302	9S8	S7-FE4	-9.15	2.13	2.28
19	h	502	MGD	C2'-C1'	-9.09	1.24	1.53
19	H	502	MGD	C2'-C1'	-9.08	1.25	1.53
16	B	302	9S8	S7-FE4	-9.06	2.13	2.28
19	h	503	MGD	C23-C14	-8.74	1.46	1.53
19	H	503	MGD	C23-C14	-8.62	1.46	1.53
19	H	502	MGD	C23-C14	-8.60	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	H	503	MGD	C2'-C1'	-8.59	1.26	1.53
19	h	502	MGD	C23-C14	-8.58	1.46	1.53
19	h	503	MGD	C2'-C1'	-8.50	1.26	1.53
19	H	503	MGD	O11-C23	-8.47	1.31	1.43
19	h	503	MGD	O11-C23	-8.46	1.31	1.43
19	H	502	MGD	C23-N22	7.71	1.57	1.45
19	h	502	MGD	C23-N22	7.68	1.57	1.45
19	h	502	MGD	O11-C11	7.59	1.58	1.43
19	H	502	MGD	O11-C11	7.57	1.58	1.43
19	H	502	MGD	O11-C23	-7.52	1.32	1.43
19	h	502	MGD	O11-C23	-7.52	1.32	1.43
19	H	503	MGD	C23-N22	7.38	1.57	1.45
19	h	503	MGD	C23-N22	7.36	1.57	1.45
19	h	503	MGD	O11-C11	7.10	1.57	1.43
19	H	503	MGD	O11-C11	7.09	1.57	1.43
19	H	503	MGD	C19-N18	6.79	1.54	1.37
19	h	503	MGD	C19-N18	6.73	1.54	1.37
19	h	502	MGD	C19-N20	6.65	1.49	1.33
19	H	502	MGD	C19-N20	6.62	1.49	1.33
19	H	502	MGD	C19-N18	6.49	1.53	1.37
19	h	502	MGD	C19-N18	6.48	1.53	1.37
19	h	503	MGD	C4-N3	6.30	1.48	1.34
19	h	503	MGD	C19-N20	6.24	1.48	1.33
19	H	503	MGD	C19-N20	6.22	1.48	1.33
19	H	503	MGD	C4-N3	6.22	1.48	1.34
19	H	502	MGD	C4-N3	6.10	1.48	1.34
19	h	502	MGD	C4-N3	6.05	1.48	1.34
19	H	503	MGD	O4'-C1'	5.75	1.55	1.42
19	h	503	MGD	O4'-C1'	5.66	1.55	1.42
19	h	503	MGD	C2-N3	5.33	1.46	1.33
19	H	503	MGD	C2-N3	5.33	1.46	1.33
14	e	505	FAD	P-O3P	-5.28	1.53	1.59
14	E	505	FAD	P-O3P	-5.25	1.53	1.59
19	h	503	MGD	C17-N18	4.97	1.48	1.38
19	H	503	MGD	C17-N18	4.96	1.48	1.38
19	H	502	MGD	O4'-C1'	4.89	1.53	1.42
19	h	502	MGD	O4'-C1'	4.83	1.53	1.42
19	h	502	MGD	C17-N18	4.78	1.47	1.38
19	H	502	MGD	C17-N18	4.75	1.47	1.38
19	H	502	MGD	C2-N3	4.61	1.44	1.33
19	h	502	MGD	C2-N3	4.60	1.44	1.33
19	h	503	MGD	C2-N2	4.55	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	h	503	MGD	O4'-C4'	4.52	1.55	1.45
19	H	503	MGD	O4'-C4'	4.51	1.55	1.45
19	H	503	MGD	C2-N2	4.50	1.44	1.34
19	H	502	MGD	C2-N2	4.47	1.44	1.34
19	h	502	MGD	C21-N20	4.45	1.43	1.36
19	h	502	MGD	C2-N2	4.44	1.44	1.34
19	H	502	MGD	C21-N20	4.38	1.43	1.36
19	h	503	MGD	C19-N19	4.34	1.44	1.34
19	h	502	MGD	O4'-C4'	4.32	1.54	1.45
19	H	502	MGD	O4'-C4'	4.30	1.54	1.45
19	H	503	MGD	C19-N19	4.28	1.44	1.34
19	H	502	MGD	C19-N19	4.26	1.44	1.34
19	h	502	MGD	C19-N19	4.24	1.44	1.34
19	H	503	MGD	C2'-C3'	4.21	1.64	1.53
19	h	503	MGD	C2'-C3'	4.20	1.64	1.53
14	e	505	FAD	P-O2P	-4.06	1.36	1.55
14	E	505	FAD	P-O2P	-4.06	1.36	1.55
19	h	503	MGD	PA-O3B	4.00	1.63	1.59
19	h	502	MGD	C2'-C3'	3.97	1.64	1.53
19	H	502	MGD	C2'-C3'	3.92	1.64	1.53
19	H	502	MGD	C21-N22	3.89	1.39	1.35
19	h	502	MGD	C21-N22	3.87	1.39	1.35
19	H	503	MGD	PA-O3B	3.80	1.63	1.59
19	H	502	MGD	PA-O3B	3.72	1.63	1.59
19	h	502	MGD	PA-O3B	3.66	1.63	1.59
14	E	505	FAD	PA-O5B	-3.64	1.45	1.59
14	e	505	FAD	PA-O5B	-3.61	1.45	1.59
19	H	503	MGD	PB-O3B	3.58	1.63	1.59
19	h	503	MGD	PB-O3B	3.57	1.63	1.59
19	h	502	MGD	PB-O3B	3.53	1.63	1.59
19	H	502	MGD	PB-O3B	3.49	1.63	1.59
19	h	502	MGD	C5-N7	-3.46	1.32	1.39
19	h	503	MGD	C21-N20	3.42	1.41	1.36
19	H	502	MGD	C5-N7	-3.41	1.32	1.39
19	H	503	MGD	C21-N20	3.35	1.41	1.36
14	A	702	FAD	P-O2P	-3.22	1.40	1.55
14	a	702	FAD	P-O2P	-3.20	1.40	1.55
19	H	503	MGD	C5-N7	-3.18	1.32	1.39
19	H	502	MGD	O6-C6	-3.15	1.17	1.23
19	h	503	MGD	C5-N7	-3.13	1.32	1.39
19	h	502	MGD	O6-C6	-3.13	1.17	1.23
19	h	502	MGD	C4-N9	-3.04	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	H	502	MGD	C4-N9	-3.01	1.30	1.38
19	H	502	MGD	O17-C17	-2.98	1.17	1.23
19	h	502	MGD	O17-C17	-2.93	1.18	1.23
14	a	702	FAD	P-O3P	-2.82	1.56	1.59
19	H	503	MGD	O17-C17	-2.78	1.18	1.23
14	A	702	FAD	P-O3P	-2.76	1.56	1.59
19	h	503	MGD	O17-C17	-2.76	1.18	1.23
19	H	503	MGD	O6-C6	-2.76	1.18	1.23
19	h	503	MGD	O6-C6	-2.74	1.18	1.23
19	h	503	MGD	C21-N22	2.70	1.38	1.35
19	H	503	MGD	C21-N22	2.69	1.38	1.35
19	h	503	MGD	C16-C17	2.39	1.49	1.41
19	H	503	MGD	C16-C17	2.39	1.49	1.41
19	h	503	MGD	C2-N1	2.37	1.43	1.37
19	H	503	MGD	C2-N1	2.35	1.43	1.37
19	H	503	MGD	C5-C6	2.35	1.53	1.44
19	h	503	MGD	C5-C6	2.34	1.53	1.44
19	h	503	MGD	C4-N9	-2.22	1.32	1.38
19	H	502	MGD	C10-C11	2.21	1.54	1.51
14	A	702	FAD	C4-N3	-2.18	1.34	1.38
19	H	503	MGD	C4-N9	-2.16	1.32	1.38
19	h	502	MGD	C10-C11	2.16	1.54	1.51
14	a	702	FAD	C4-N3	-2.16	1.34	1.38

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	H	502	MGD	O11-C23-N22	-6.41	102.79	108.61
19	h	502	MGD	O11-C23-N22	-6.38	102.81	108.61
19	h	503	MGD	C23-C14-N15	5.84	113.60	107.87
19	H	503	MGD	C23-C14-N15	5.75	113.52	107.87
19	h	503	MGD	C5-C4-N3	-5.38	119.83	128.39
19	H	503	MGD	C5-C4-N3	-5.33	119.90	128.39
19	H	502	MGD	C23-C14-N15	4.72	112.50	107.87
19	h	502	MGD	C23-C14-N15	4.71	112.49	107.87
19	H	503	MGD	C2-N3-C4	4.63	120.28	112.30
19	h	503	MGD	C2-N3-C4	4.60	120.23	112.30
19	h	502	MGD	C2-N3-C4	4.12	119.40	112.30
19	H	502	MGD	C2-N3-C4	4.06	119.29	112.30
19	h	502	MGD	C19-N20-C21	4.05	120.50	113.36
19	h	502	MGD	C5-C4-N3	-4.03	121.98	128.39
19	H	502	MGD	C19-N20-C21	4.02	120.45	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	H	502	MGD	C5-C4-N3	-4.00	122.02	128.39
19	H	503	MGD	C19-N20-C21	3.84	120.13	113.36
19	h	503	MGD	C19-N20-C21	3.80	120.07	113.36
19	H	502	MGD	N9-C8-N7	-3.46	106.98	113.40
19	h	502	MGD	N9-C8-N7	-3.43	107.03	113.40
19	h	503	MGD	C2-N1-C6	-3.34	119.06	125.11
19	H	503	MGD	C2-N1-C6	-3.30	119.12	125.11
19	h	503	MGD	N19-C19-N18	3.24	123.60	116.76
19	H	503	MGD	N19-C19-N18	3.23	123.58	116.76
19	H	503	MGD	N9-C4-N3	3.23	132.40	125.95
19	H	502	MGD	O17-C17-C16	-3.22	119.49	127.26
19	H	503	MGD	N9-C8-N7	-3.21	107.45	113.40
19	h	502	MGD	O17-C17-C16	-3.20	119.55	127.26
19	h	503	MGD	N9-C8-N7	-3.19	107.48	113.40
19	h	503	MGD	N9-C4-N3	3.18	132.31	125.95
19	H	502	MGD	C4'-O4'-C1'	-3.01	102.81	109.47
19	h	502	MGD	C4'-O4'-C1'	-3.00	102.84	109.47
19	H	502	MGD	C19-N18-C17	-2.92	119.82	125.11
19	H	502	MGD	C16-C17-N18	2.90	120.08	112.13
19	h	502	MGD	C16-C17-N18	2.89	120.08	112.13
19	h	502	MGD	C19-N18-C17	-2.88	119.89	125.11
19	H	503	MGD	C5-C6-N1	2.84	120.49	113.25
19	h	503	MGD	C5-C6-N1	2.84	120.49	113.25
19	H	502	MGD	C1'-N9-C4	-2.74	118.40	126.49
19	h	502	MGD	C1'-N9-C4	-2.73	118.42	126.49
19	h	503	MGD	C16-C17-N18	2.60	119.28	112.13
19	H	503	MGD	C16-C17-N18	2.59	119.24	112.13
19	h	502	MGD	N1-C2-N3	-2.51	118.73	123.32
19	h	503	MGD	C19-N18-C17	-2.51	120.57	125.11
19	H	503	MGD	C19-N18-C17	-2.50	120.58	125.11
19	h	502	MGD	C5-C6-N1	2.47	119.55	113.25
19	H	502	MGD	N1-C2-N3	-2.47	118.80	123.32
19	H	502	MGD	C5-C6-N1	2.47	119.53	113.25
19	h	502	MGD	N9-C4-N3	2.46	130.87	125.95
19	h	503	MGD	O17-C17-C16	-2.45	121.35	127.26
19	H	502	MGD	N9-C4-N3	2.43	130.81	125.95
19	H	503	MGD	O17-C17-C16	-2.42	121.42	127.26
19	h	503	MGD	O6-C6-C5	-2.29	120.49	126.53
19	H	503	MGD	O6-C6-C5	-2.28	120.51	126.53
19	H	503	MGD	C8-N7-C5	2.22	108.22	104.26
19	H	502	MGD	O6-C6-C5	-2.21	120.69	126.53
19	h	502	MGD	O6-C6-C5	-2.20	120.72	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	h	503	MGD	C8-N7-C5	2.18	108.14	104.26
19	h	503	MGD	O4'-C1'-C2'	-2.18	101.96	106.62
19	H	503	MGD	O4'-C1'-C2'	-2.15	102.00	106.62
19	h	503	MGD	C17-C16-N15	2.11	122.02	116.27
19	H	503	MGD	C17-C16-N15	2.10	122.00	116.27
19	H	503	MGD	C4'-O4'-C1'	-2.02	105.00	109.47

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	E	505	FAD	C5B-O5B-PA-O1A
14	E	505	FAD	C5B-O5B-PA-O3P
14	E	505	FAD	C1'-C2'-C3'-O3'
14	E	505	FAD	C1'-C2'-C3'-C4'
14	E	505	FAD	O2'-C2'-C3'-O3'
14	E	505	FAD	O2'-C2'-C3'-C4'
14	E	505	FAD	C5'-O5'-P-O2P
14	E	505	FAD	C5'-O5'-P-O3P
14	e	505	FAD	C5B-O5B-PA-O1A
14	e	505	FAD	C5B-O5B-PA-O3P
14	e	505	FAD	C1'-C2'-C3'-O3'
14	e	505	FAD	C1'-C2'-C3'-C4'
14	e	505	FAD	O2'-C2'-C3'-O3'
14	e	505	FAD	O2'-C2'-C3'-C4'
14	e	505	FAD	C5'-O5'-P-O2P
14	e	505	FAD	C5'-O5'-P-O3P
19	H	502	MGD	C5'-O5'-PB-O3B
19	H	502	MGD	PB-O3B-PA-O3A
19	H	502	MGD	C10-O3A-PA-O3B
19	H	502	MGD	C10-O3A-PA-O1A
19	H	502	MGD	C10-O3A-PA-O2A
19	H	502	MGD	O3A-C10-C11-O11
19	H	502	MGD	O3A-C10-C11-C12
19	H	503	MGD	C5'-O5'-PB-O2B
19	H	503	MGD	C5'-O5'-PB-O3B
19	h	502	MGD	C5'-O5'-PB-O3B
19	h	502	MGD	PB-O3B-PA-O3A
19	h	502	MGD	C10-O3A-PA-O3B
19	h	502	MGD	C10-O3A-PA-O1A
19	h	502	MGD	C10-O3A-PA-O2A
19	h	502	MGD	O3A-C10-C11-O11

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Mol	Chain	Res	Type	Atoms
19	h	502	MGD	O3A-C10-C11-C12
19	h	503	MGD	C5'-O5'-PB-O2B
19	h	503	MGD	C5'-O5'-PB-O3B
19	H	503	MGD	C3'-C4'-C5'-O5'
19	h	503	MGD	C3'-C4'-C5'-O5'
19	H	503	MGD	O4'-C4'-C5'-O5'
19	h	503	MGD	O4'-C4'-C5'-O5'
14	E	505	FAD	C5B-O5B-PA-O2A
14	e	505	FAD	C5B-O5B-PA-O2A
19	H	503	MGD	C5'-O5'-PB-O1B
19	H	503	MGD	C10-O3A-PA-O2A
19	h	503	MGD	C5'-O5'-PB-O1B
19	h	503	MGD	C10-O3A-PA-O2A
19	H	503	MGD	PB-O3B-PA-O2A
19	h	503	MGD	PB-O3B-PA-O2A
14	E	505	FAD	C4'-C5'-O5'-P
14	e	505	FAD	C4'-C5'-O5'-P
19	H	503	MGD	PB-O3B-PA-O1A
19	h	503	MGD	PB-O3B-PA-O1A
19	H	502	MGD	O4'-C4'-C5'-O5'
19	h	502	MGD	O4'-C4'-C5'-O5'
14	E	505	FAD	C2B-C1B-N9A-C8A
14	e	505	FAD	C2B-C1B-N9A-C8A
14	E	505	FAD	N10-C1'-C2'-O2'
14	e	505	FAD	N10-C1'-C2'-O2'
14	E	505	FAD	P-O3P-PA-O2A
14	e	505	FAD	P-O3P-PA-O2A
14	A	702	FAD	O4B-C4B-C5B-O5B
14	a	702	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

15 monomers are involved in 29 short contacts:

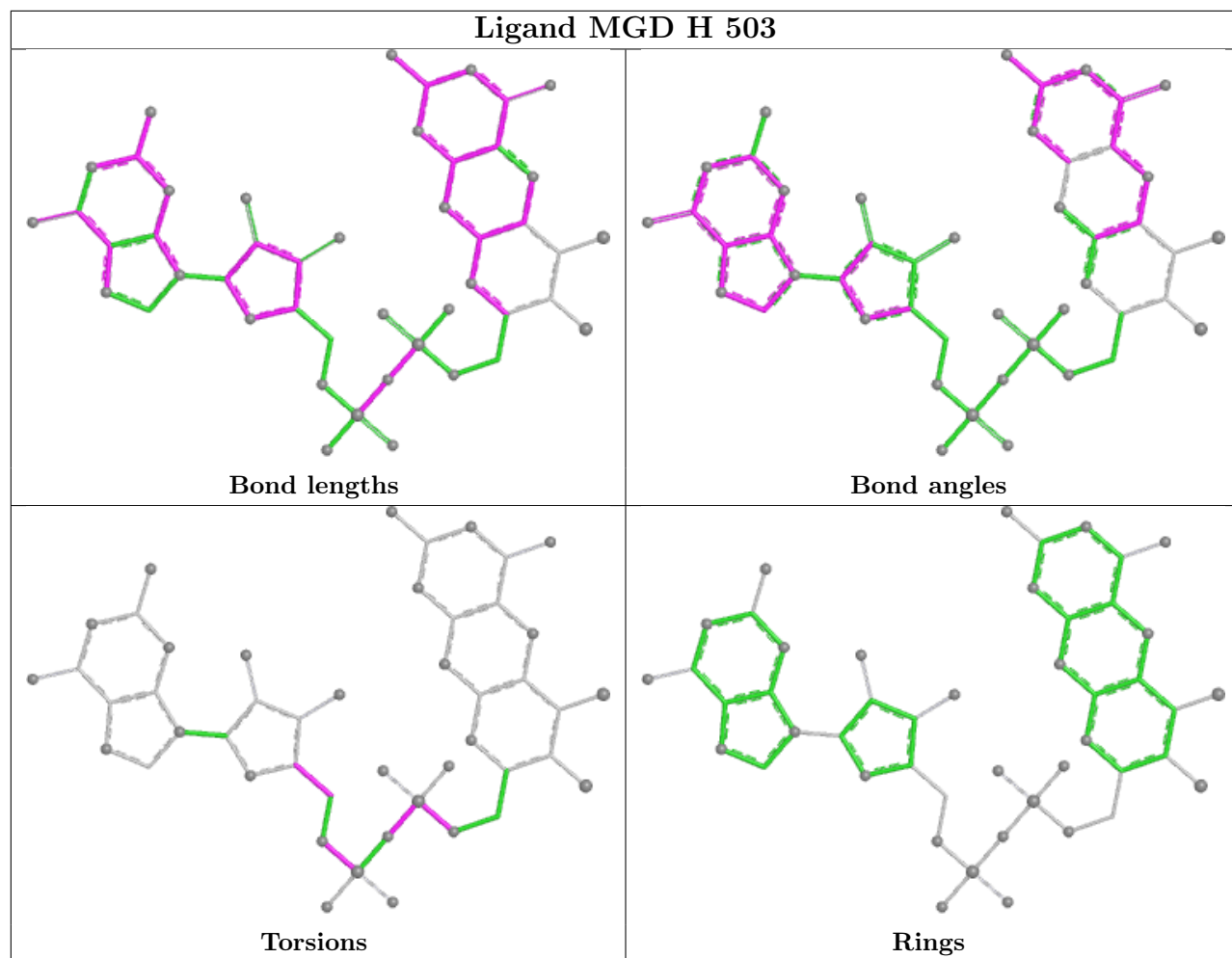
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	H	503	MGD	2	0
16	b	302	9S8	1	0
13	c	201	SF4	1	0
13	a	703	SF4	2	0
19	H	502	MGD	6	0
19	h	502	MGD	6	0
13	C	201	SF4	1	0
16	B	302	9S8	1	0

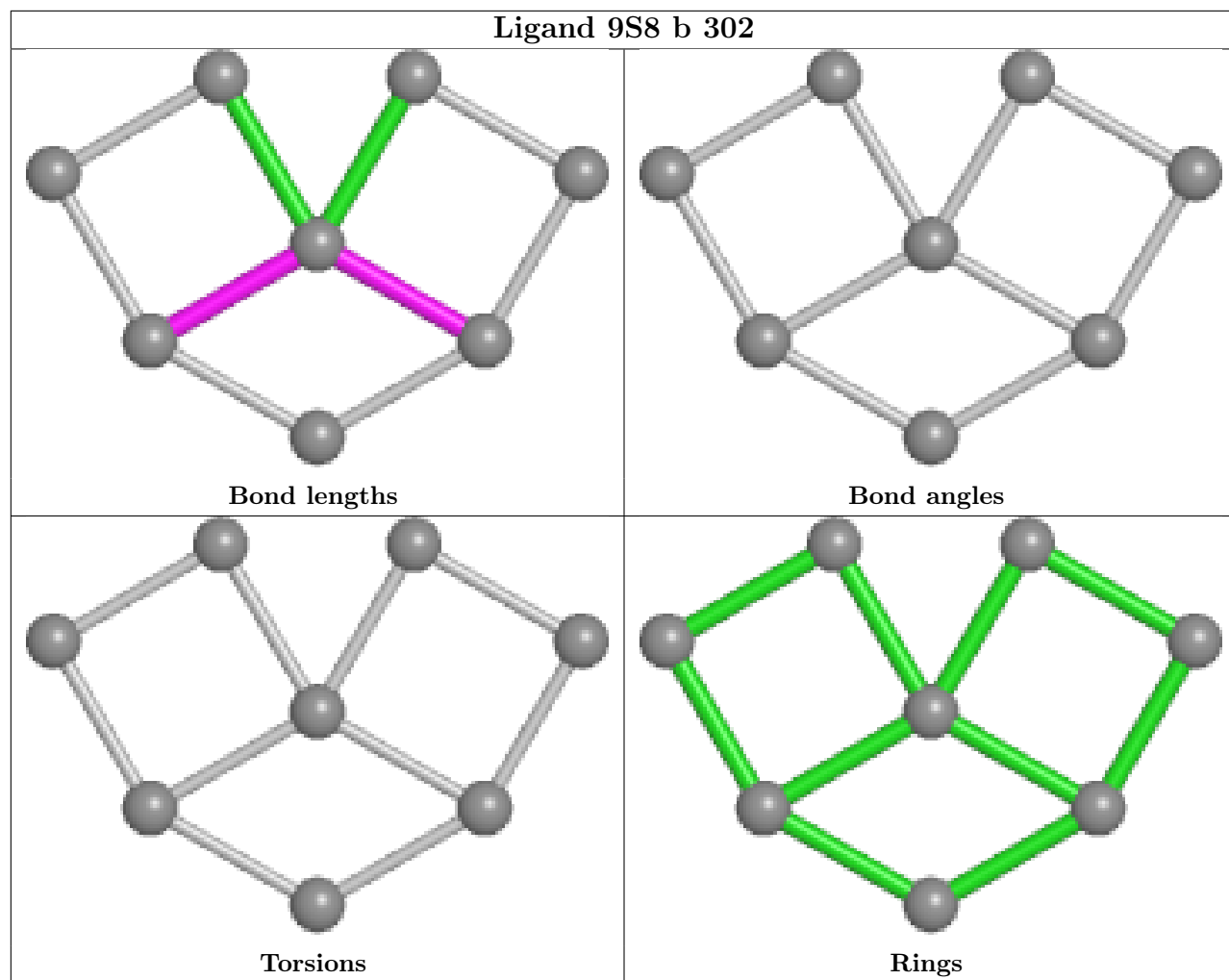
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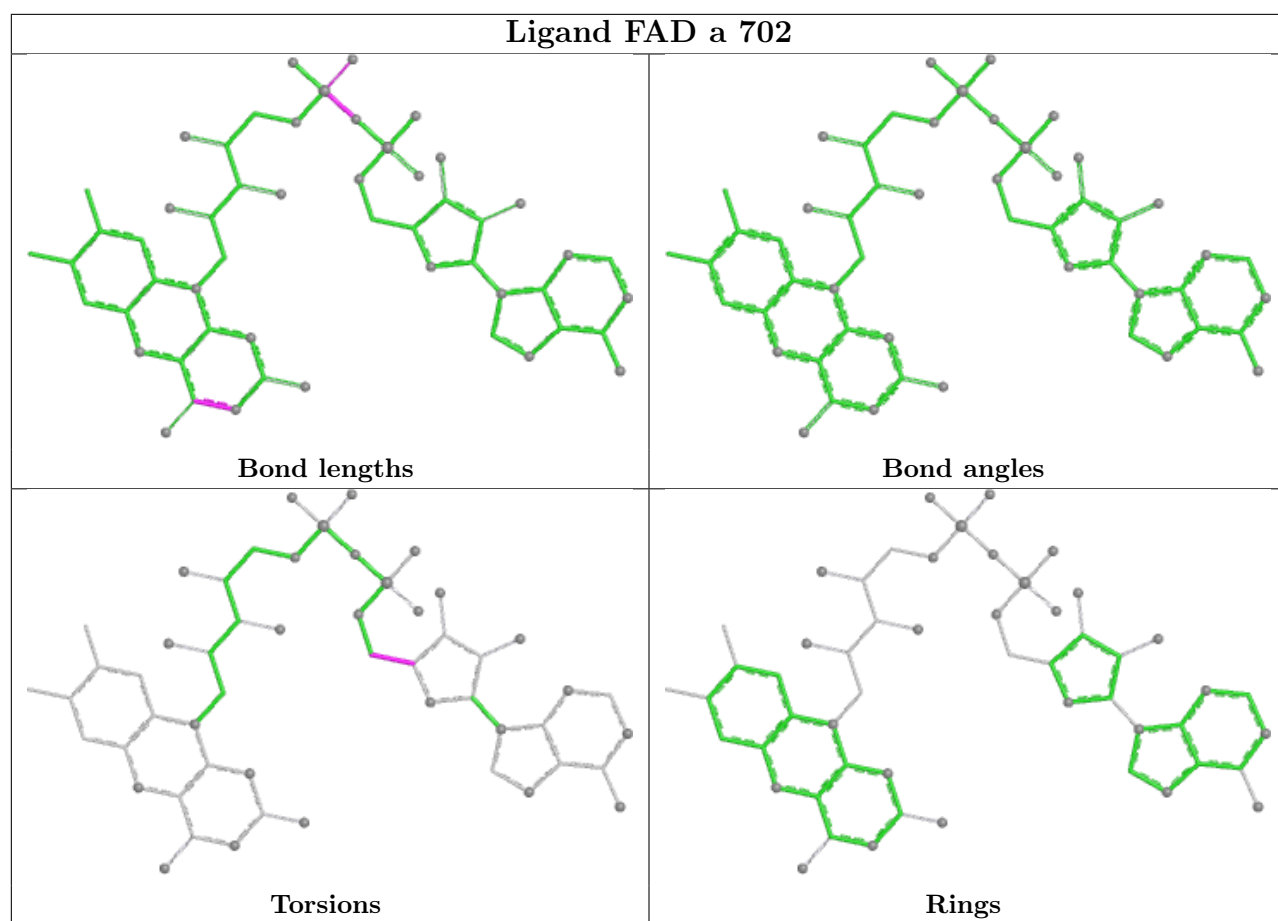
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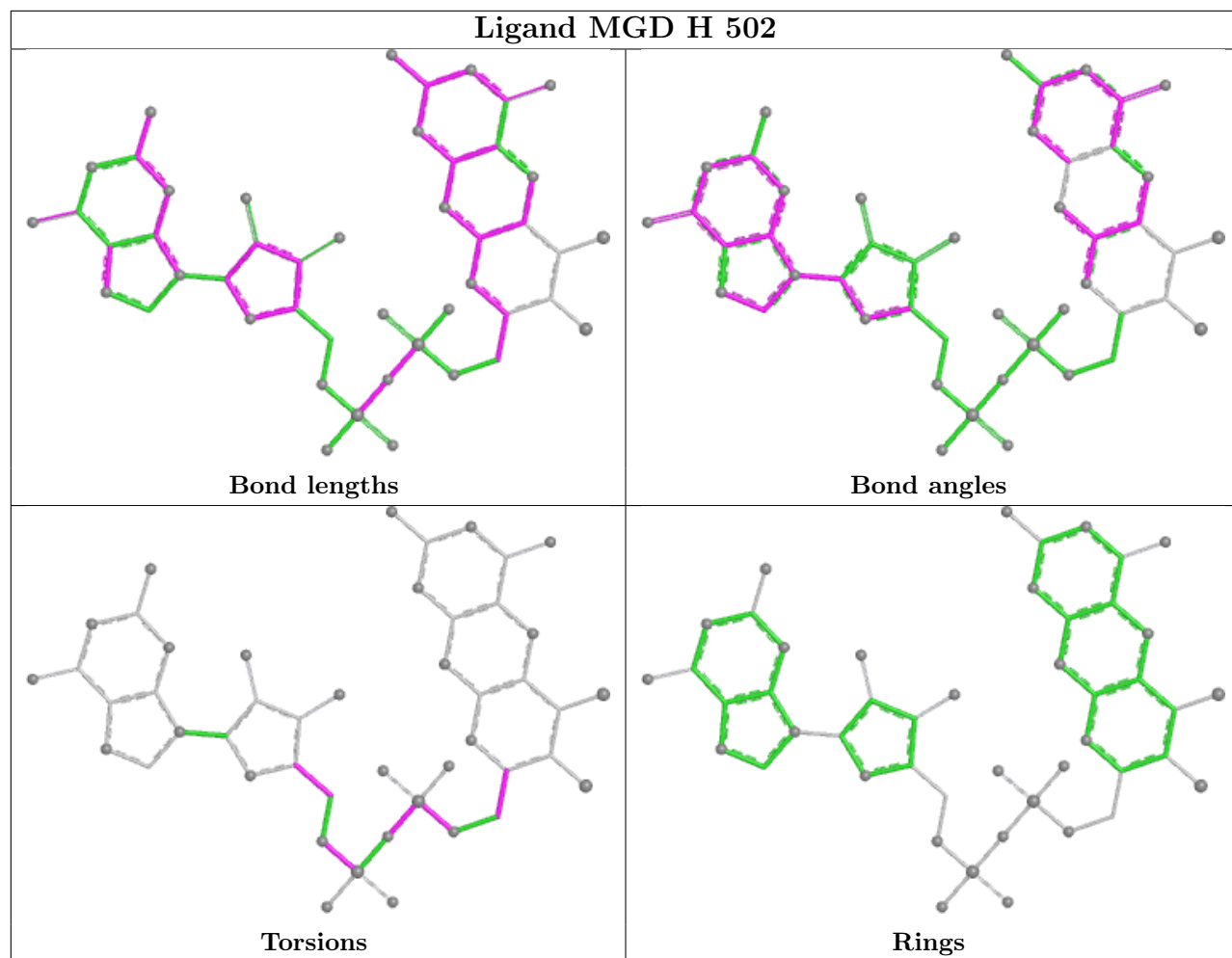
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	k	405	SF4	1	0
13	k	406	SF4	1	0
13	K	406	SF4	1	0
13	K	405	SF4	1	0
13	A	703	SF4	2	0
14	E	505	FAD	1	0
19	h	503	MGD	2	0

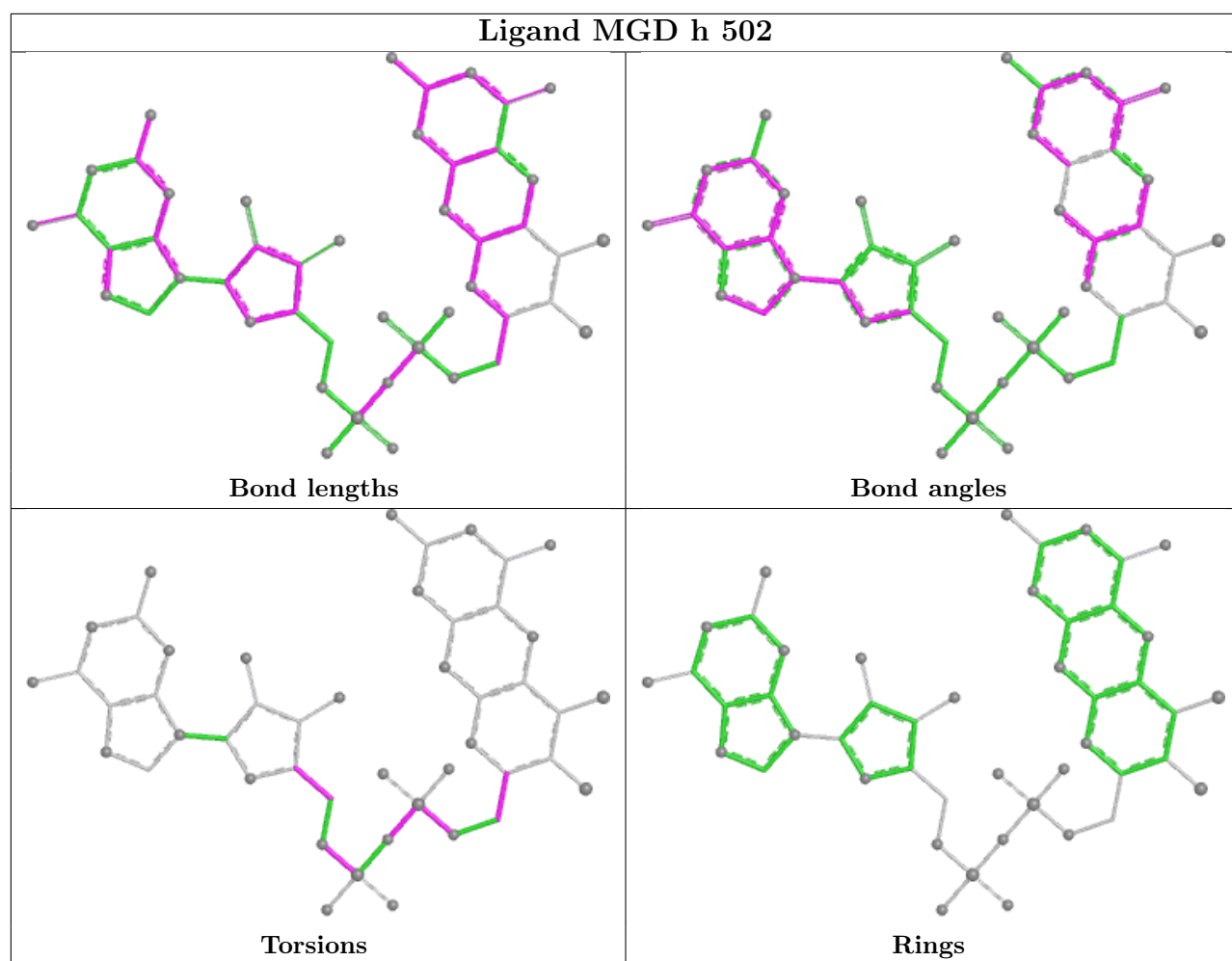
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

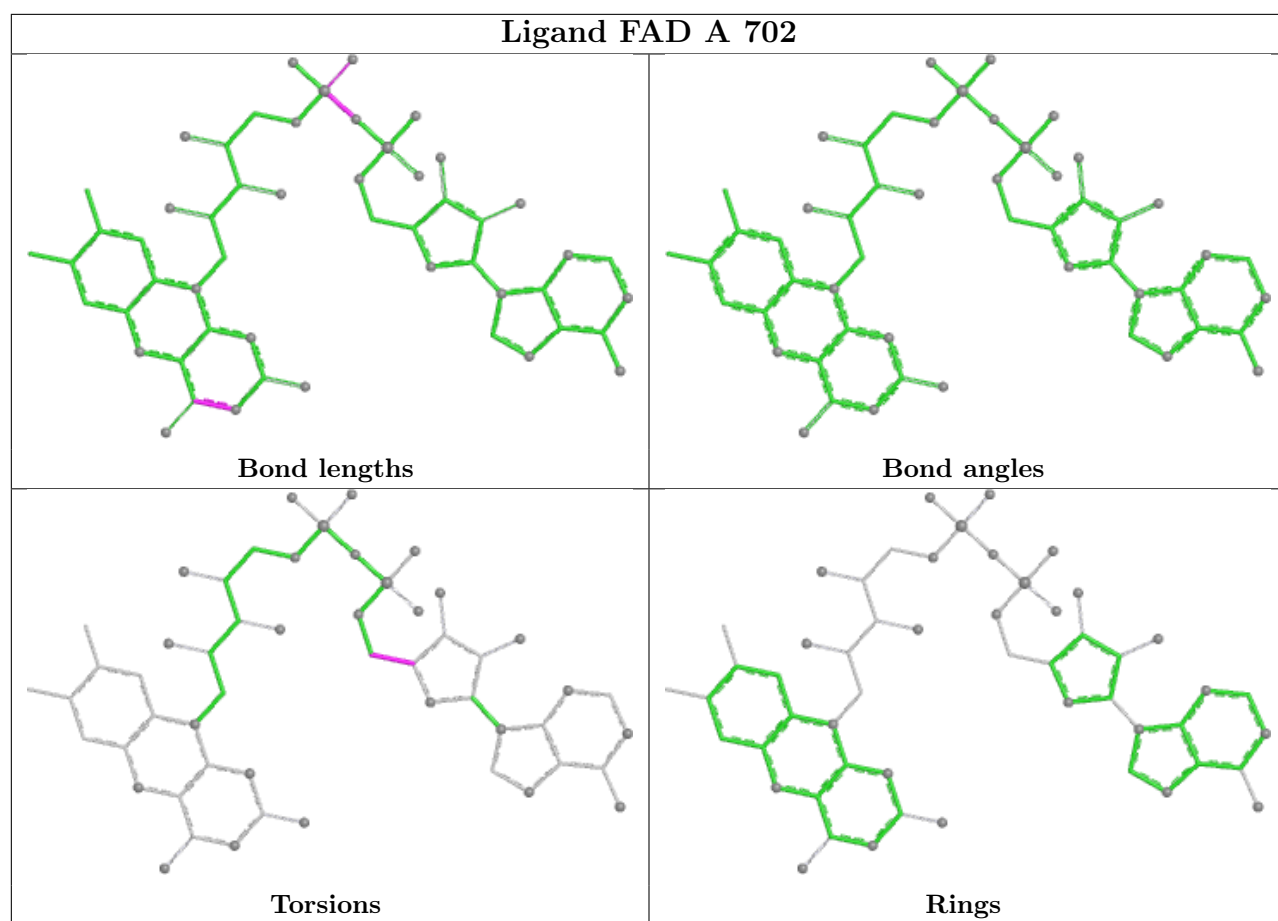


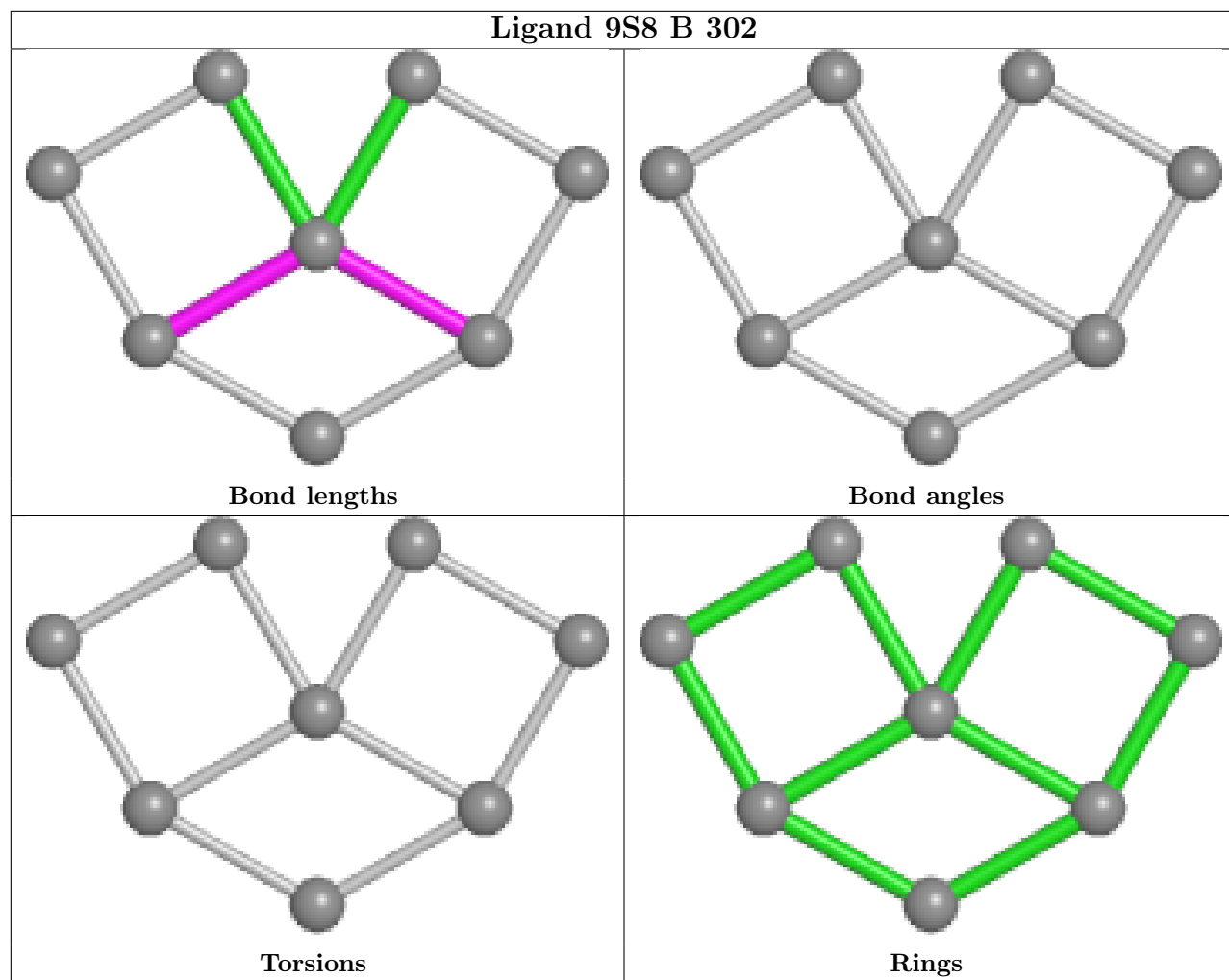


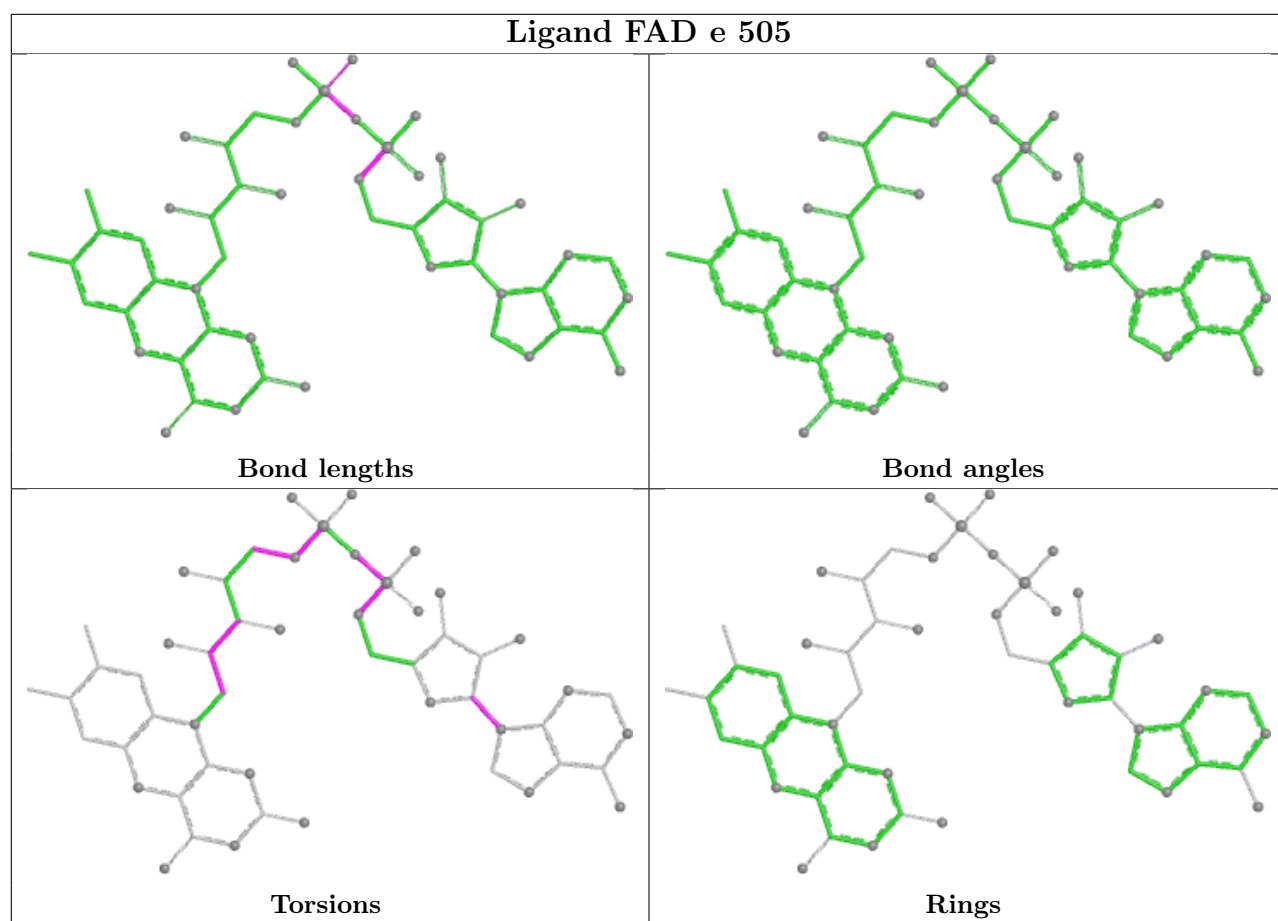


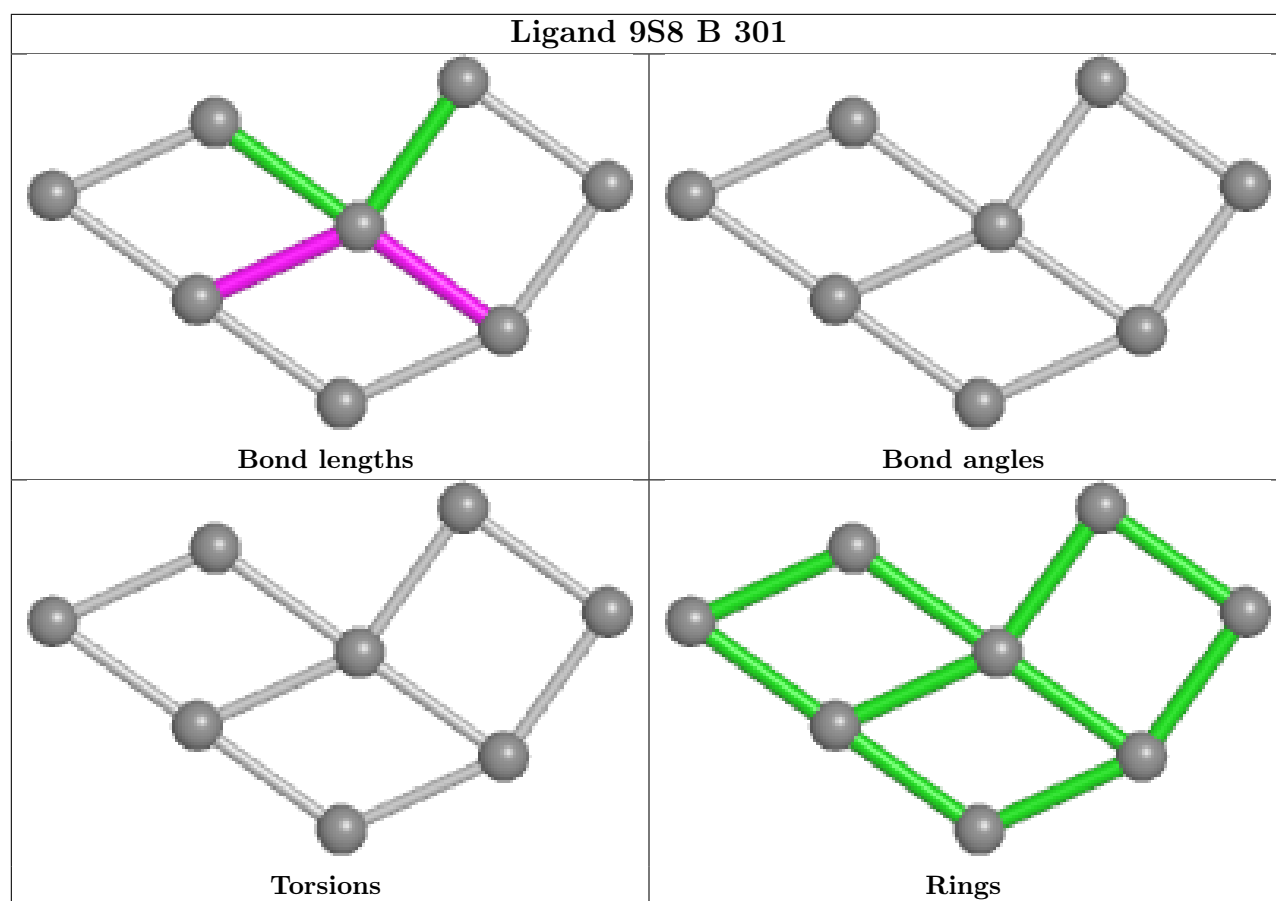


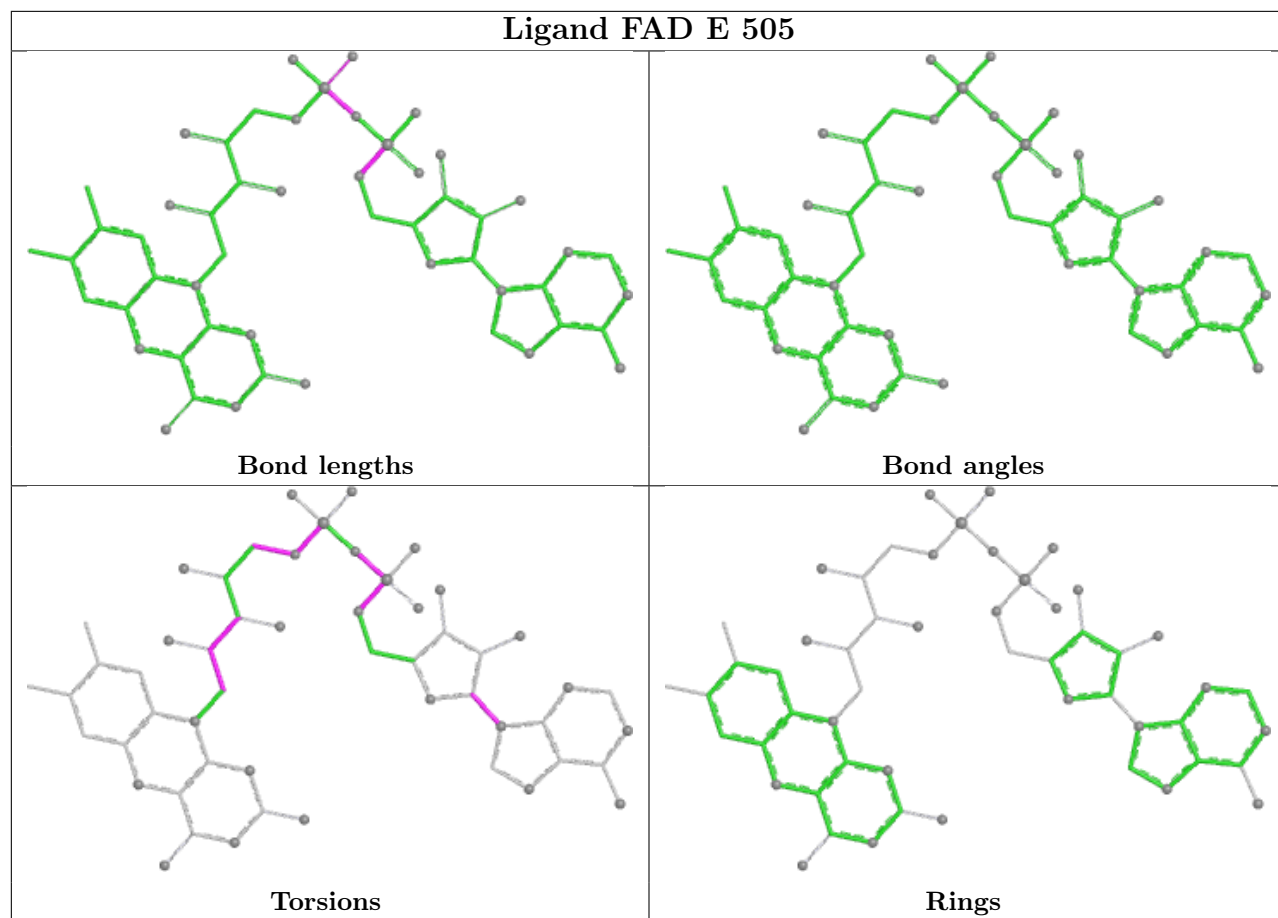


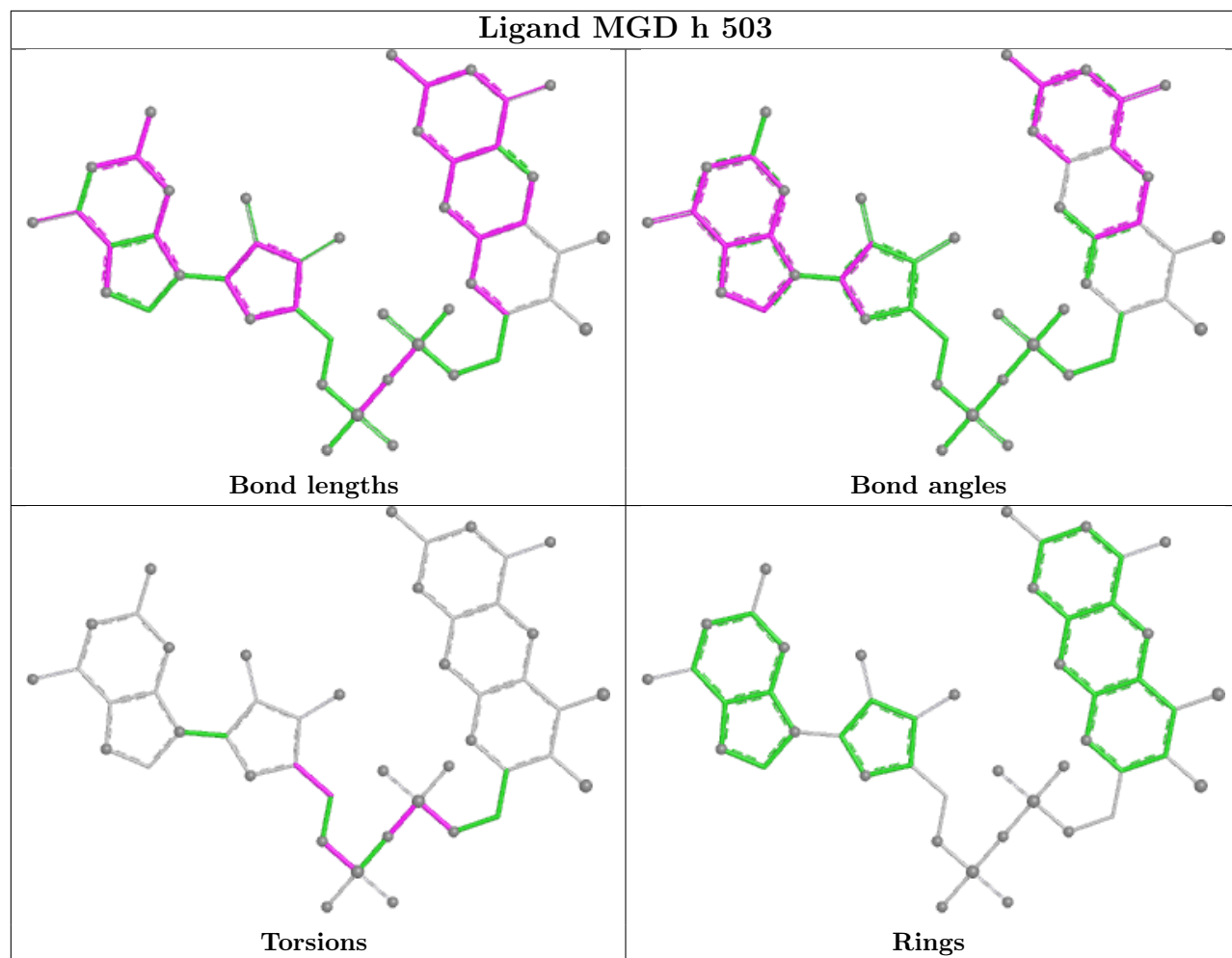


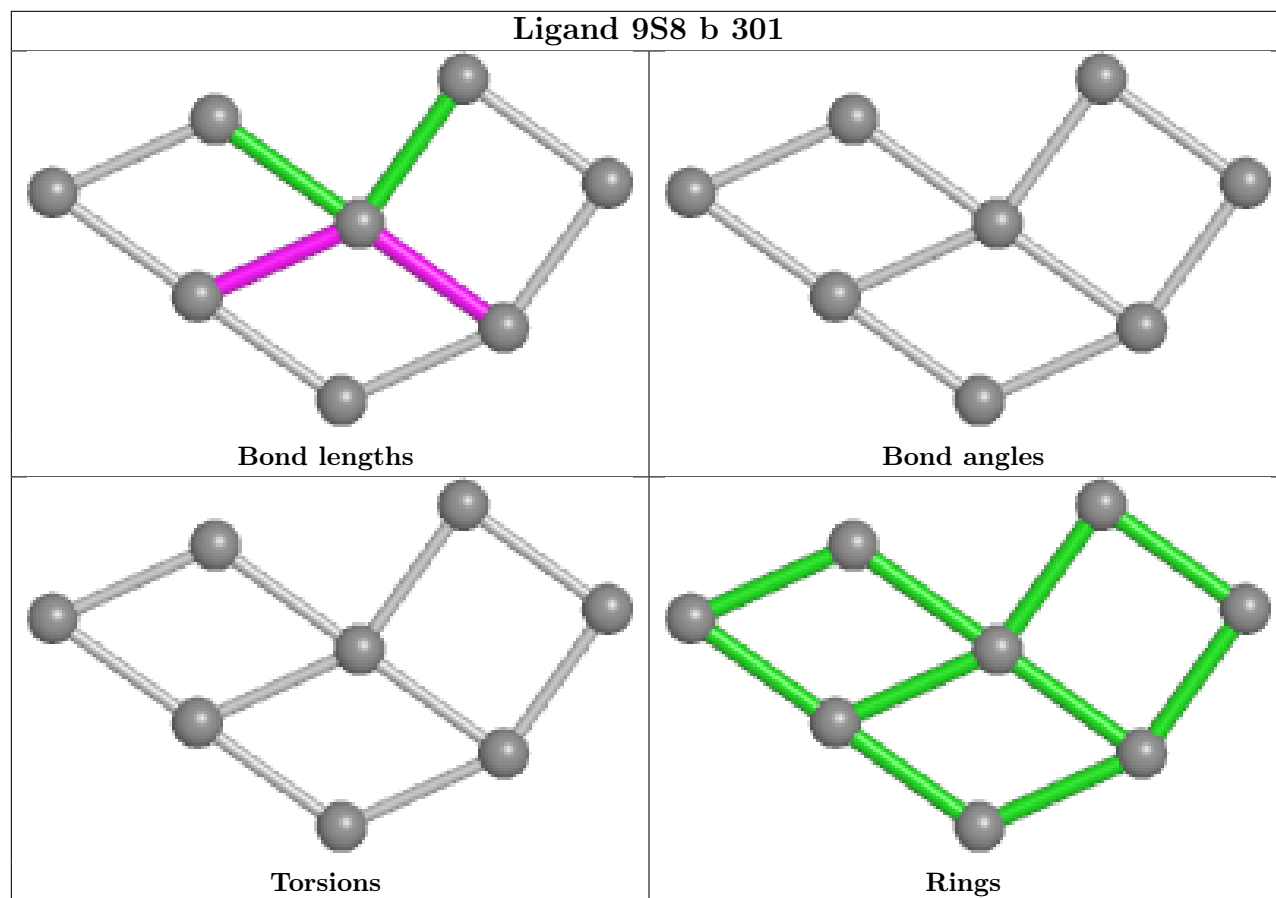












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

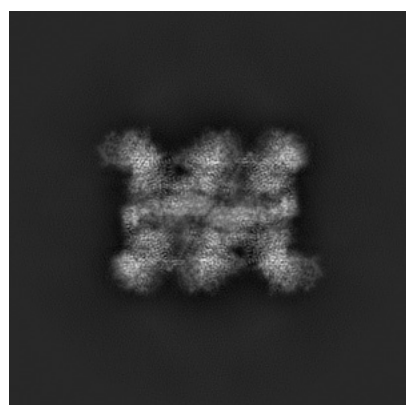
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12206. These allow visual inspection of the internal detail of the map and identification of artifacts.

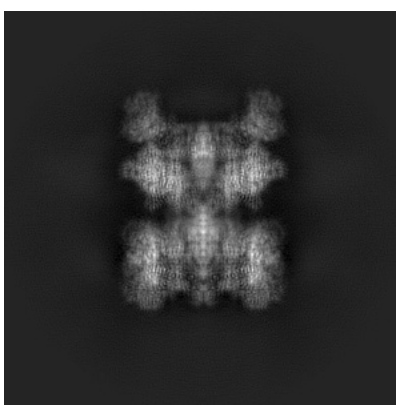
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

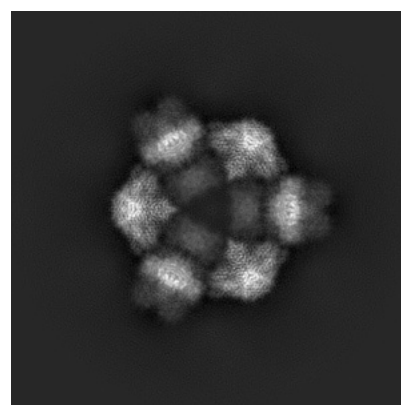
6.1.1 Primary map



X



Y

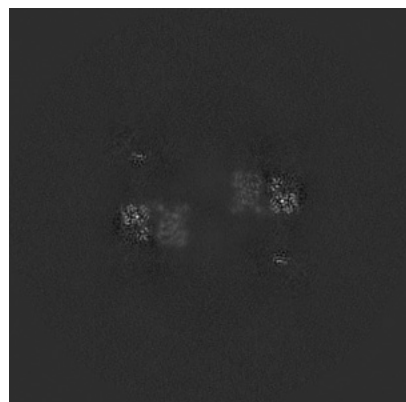


Z

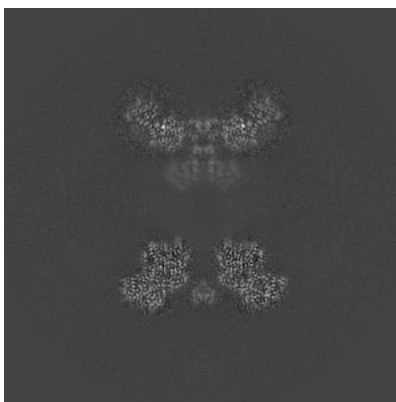
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

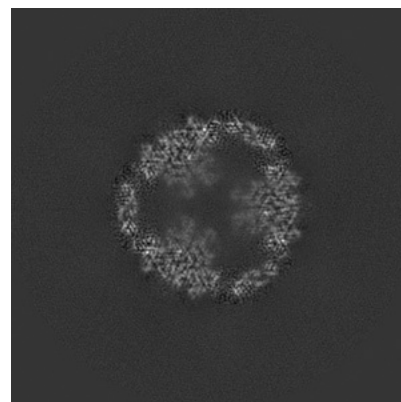
6.2.1 Primary map



X Index: 160



Y Index: 160

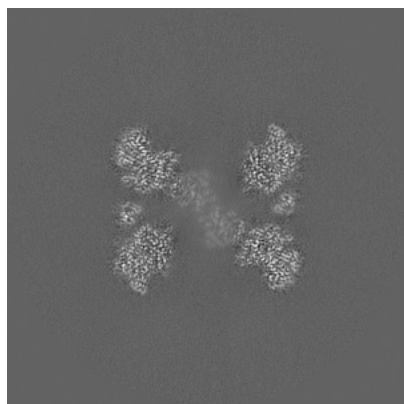


Z Index: 160

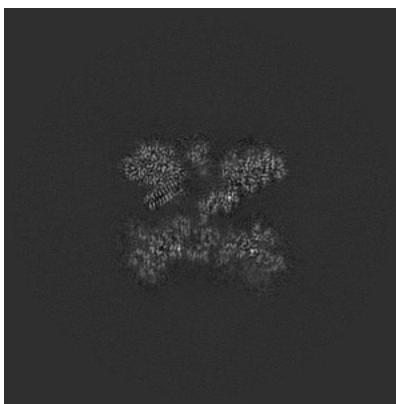
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

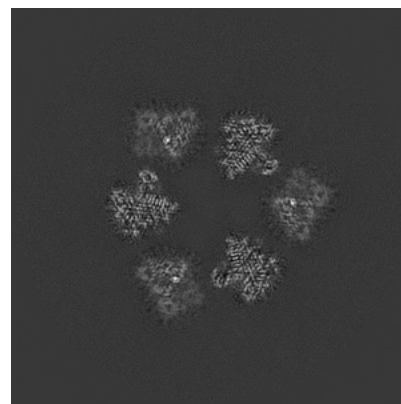
6.3.1 Primary map



X Index: 187



Y Index: 214

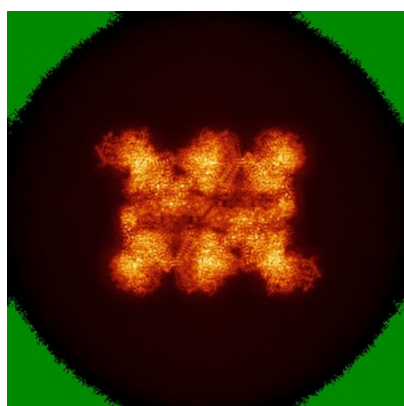


Z Index: 198

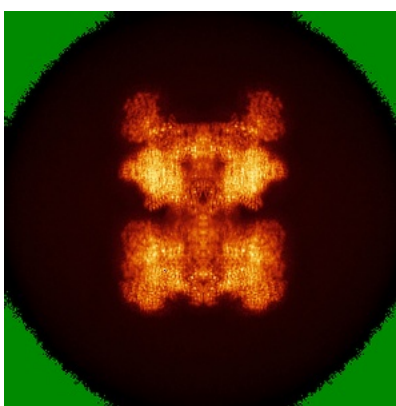
The images above show the largest variance slices of the map in three orthogonal directions.

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

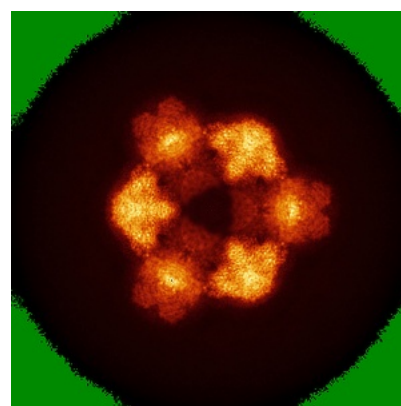
6.4.1 Primary map



X



Y

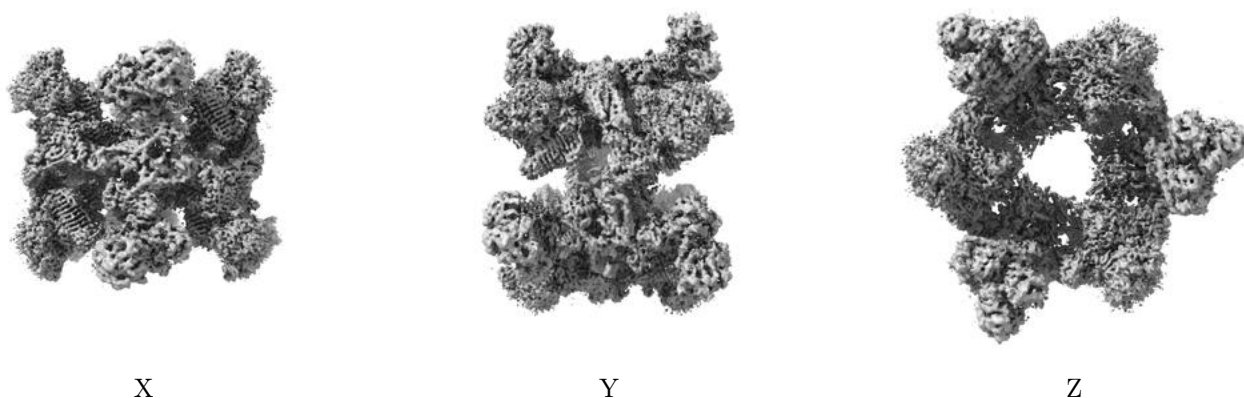


Z

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 7.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

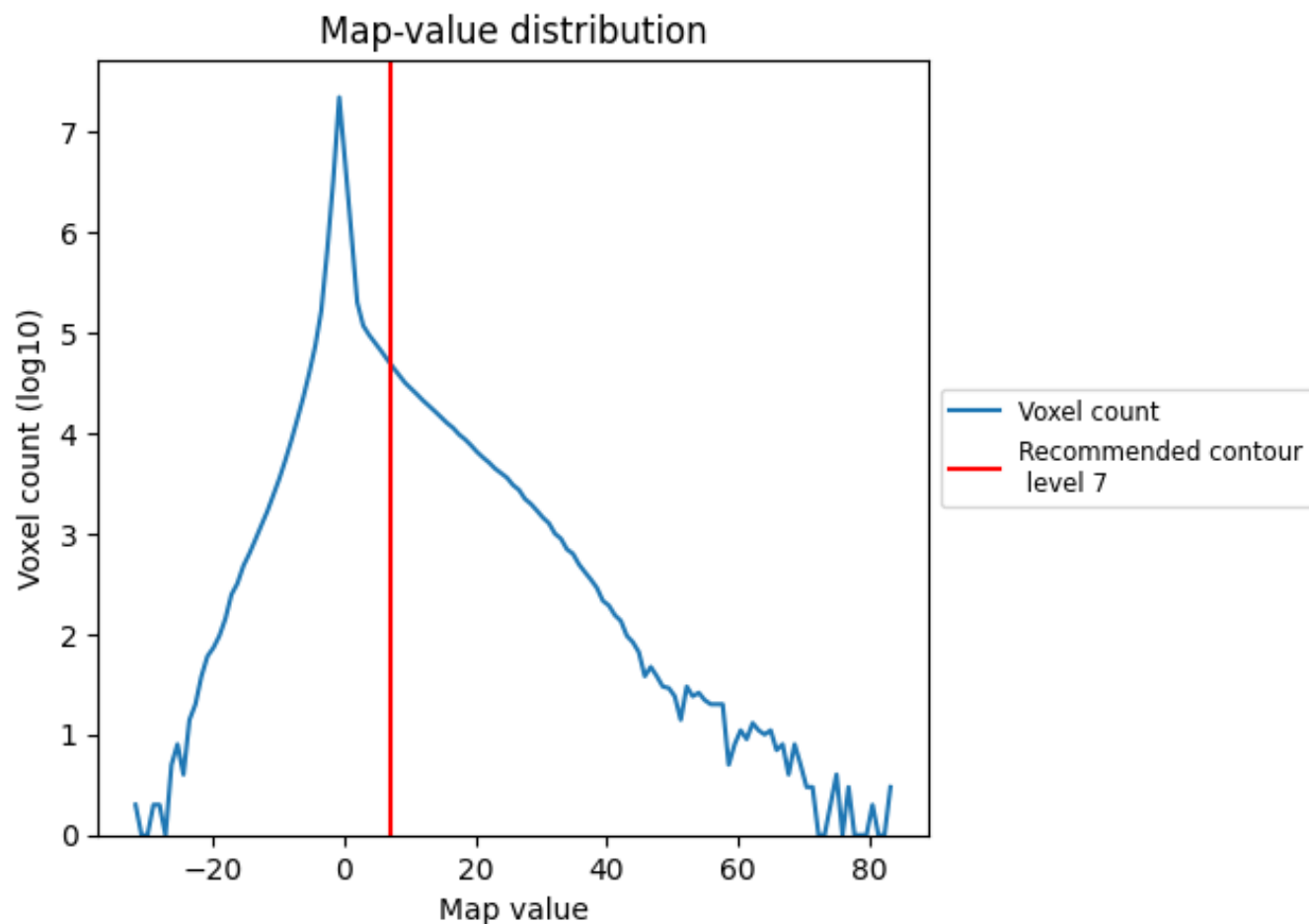
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

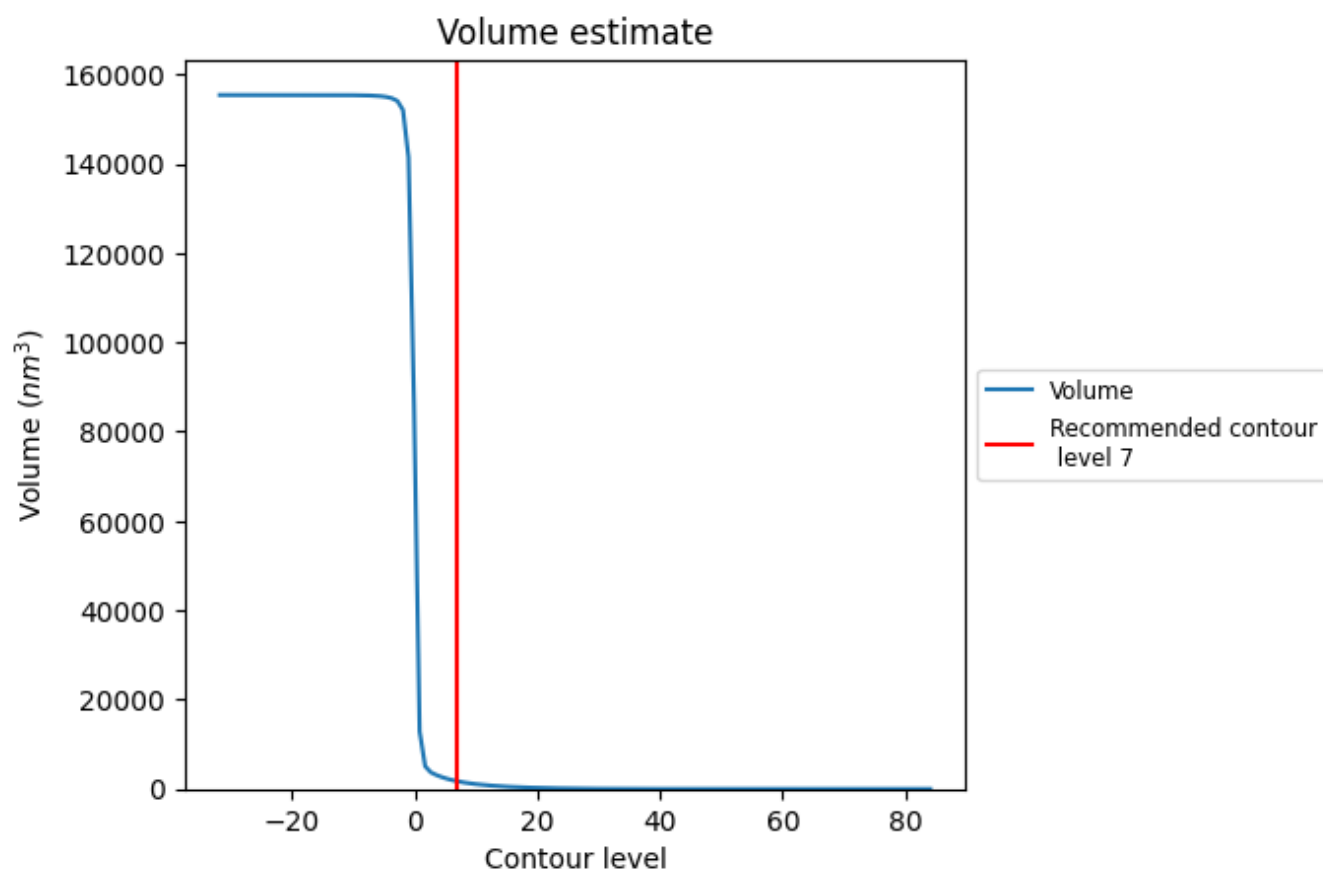
This section contains the results of statistical analysis of the map.

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.

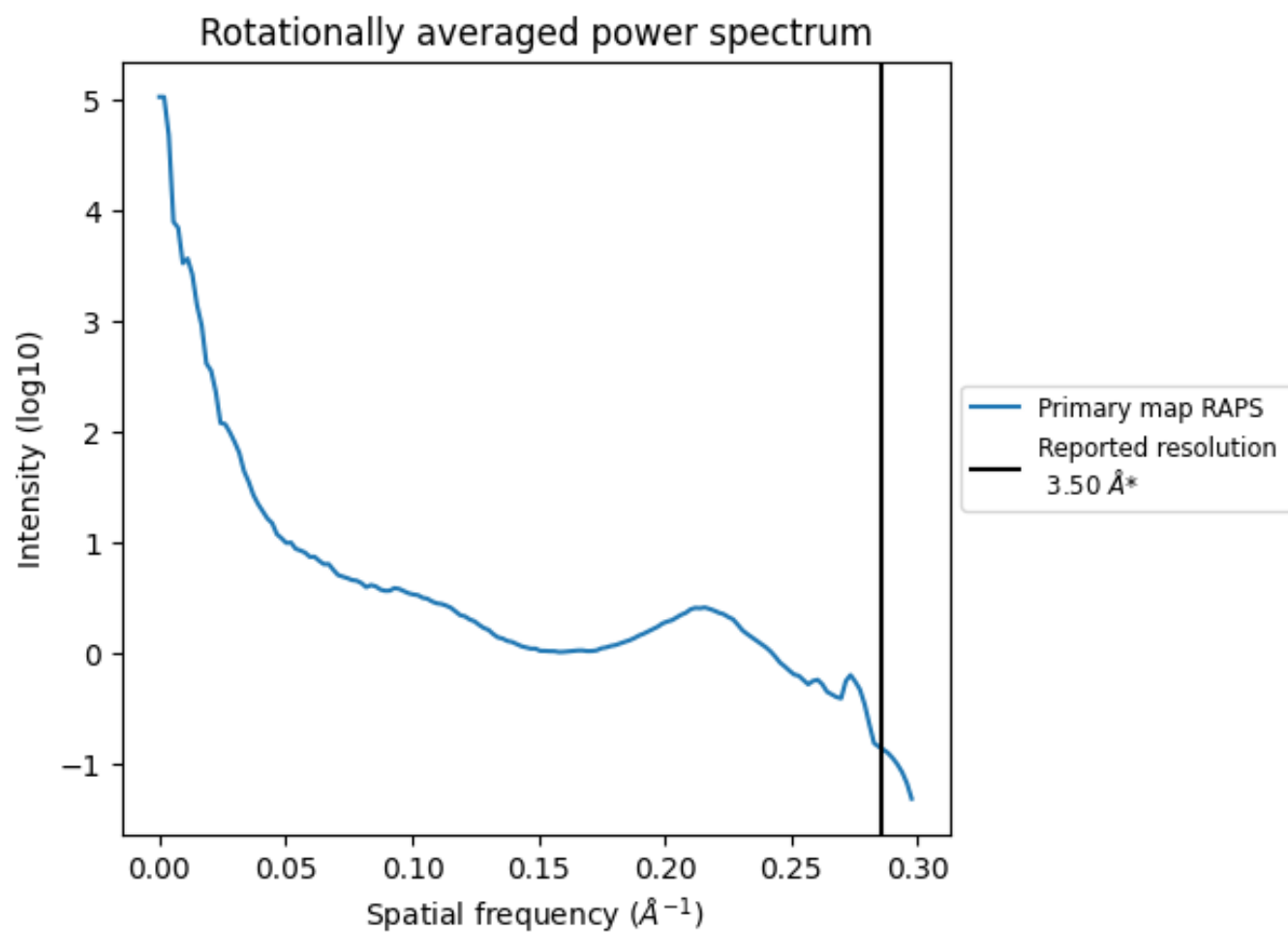
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1712 nm^3 ; this corresponds to an approximate mass of 1547 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

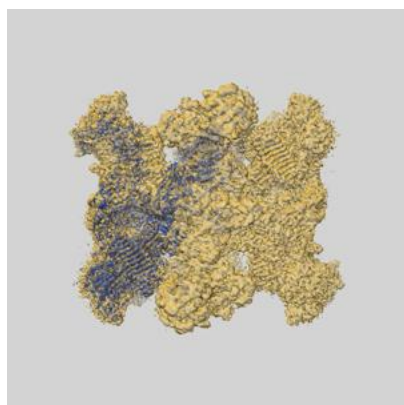
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

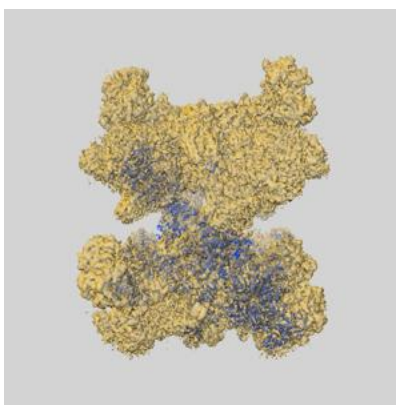
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12206 and PDB model 7BKB. Per-residue inclusion information can be found in section [3](#) on page [13](#).

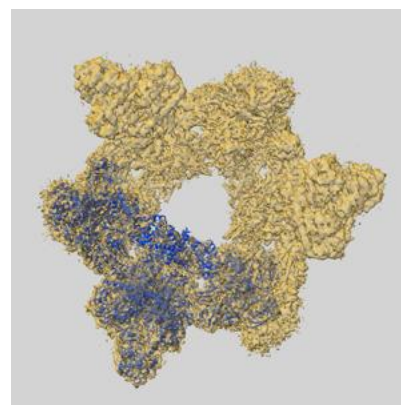
9.1 Map-model overlay [i](#)



X



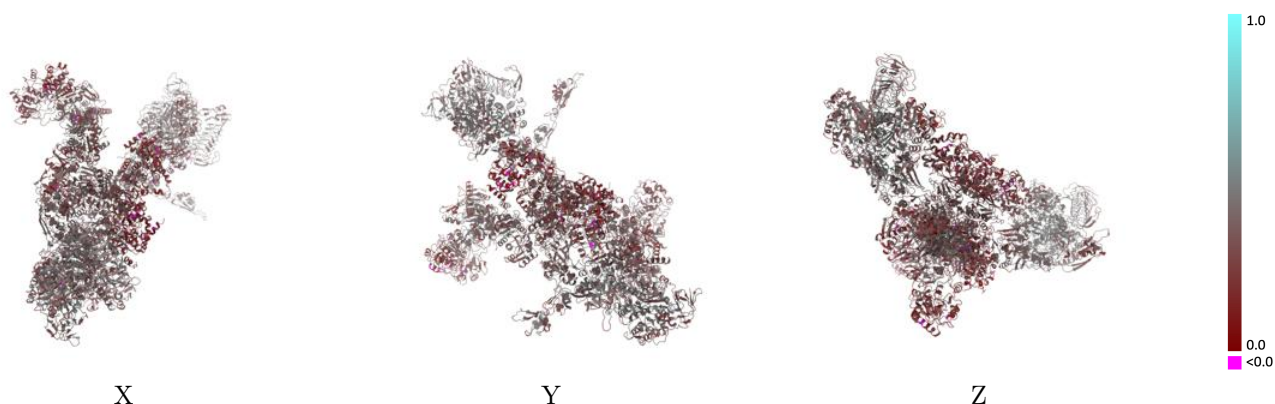
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 7.0 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](#)

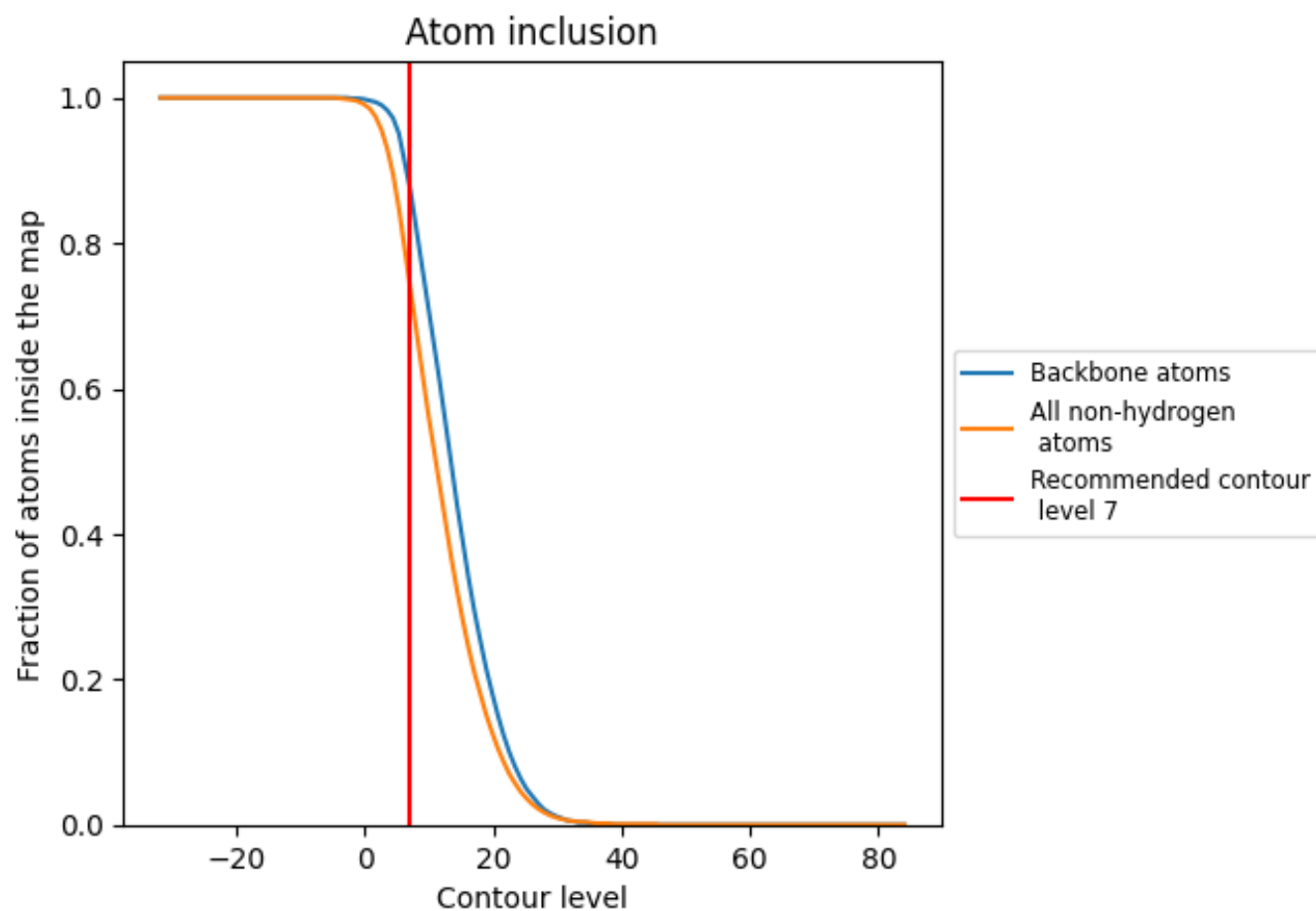


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7450	 0.3480
A	 0.7280	 0.3440
B	 0.3640	 0.2380
C	 0.4530	 0.2320
D	 0.7430	 0.2900
E	 0.8190	 0.3260
F	 0.7840	 0.3330
G	 0.8870	 0.4040
H	 0.7940	 0.3970
I	 0.7810	 0.3820
J	 0.7400	 0.3440
K	 0.8170	 0.3900
L	 0.8320	 0.4130
a	 0.7490	 0.3490
b	 0.3370	 0.2670
c	 0.3950	 0.2370
d	 0.7190	 0.2690
e	 0.8220	 0.3380
f	 0.8060	 0.3480
g	 0.8950	 0.4200
h	 0.8090	 0.4260
i	 0.7960	 0.4090
j	 0.7690	 0.3960
k	 0.8150	 0.3760
l	 0.7980	 0.3730

