



Full wwPDB EM Validation Report ⓘ

Feb 20, 2025 – 06:10 pm GMT

PDB ID : 9H1L
EMDB ID : EMD-51767
Title : Methyl-coenzyme M reductase activation complex binding to the A2 component after incubation with ATP
Authors : Ramirez-Amador, F.; Paul, S.; Kumar, A.; Schuller, J.M.
Deposited on : 2024-10-09
Resolution : 2.14 Å(reported)
Based on initial model : .

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 : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

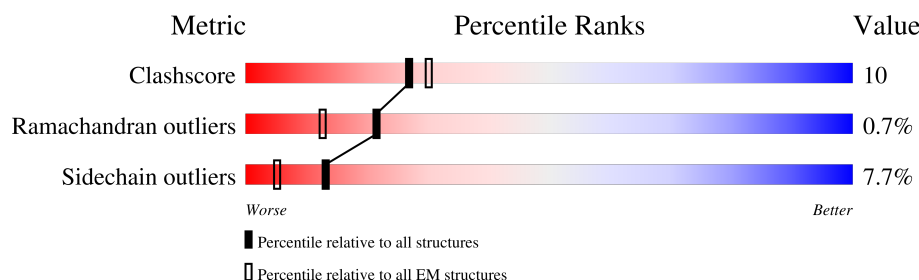
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.14 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	J	501	58% 30% 9% .
2	A	260	81% 18% .
2	B	260	81% 18%
3	D	443	84% 15% .
3	E	443	84% 15%
4	C	553	80% 18% ..
4	F	553	80% 13% . 6%
5	G	183	47% 15% 38%
6	H	304	74% 22% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	I	234	
8	K	531	
9	L	93	

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	SHT	F	602	X	-	X	-
4	GL3	C	448	-	-	X	-
4	SMC	C	455	-	-	X	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32524 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 UPF0288 protein MmarC6_0796.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	499	Total	C	N	O	S	0	0
			3962	2517	647	790	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	500	SER	LYS	variant	UNP A9A8E0

- Molecule 2 is a protein called Methyl-coenzyme M reductase subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	259	Total	C	N	O	S	0	0
			2071	1293	369	397	12		
2	B	259	Total	C	N	O	S	0	0
			2071	1293	369	397	12		

- Molecule 3 is a protein called Methyl-coenzyme M reductase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	442	Total	C	N	O	S	0	0
			3263	2066	546	630	21		
3	D	442	Total	C	N	O	S	0	0
			3263	2066	546	630	21		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	173	GLY	SER	conflict	UNP A0A2L1CBB3
D	173	GLY	SER	conflict	UNP A0A2L1CBB3

- Molecule 4 is a protein called Methyl-coenzyme M reductase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	550	Total	C	N	O	S	0	0
			4284	2707	731	826	20		
4	F	520	Total	C	N	O	S	0	0
			4039	2556	684	779	20		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	51	SER	ALA	variant	UNP A0A2L1CBB0
F	51	SER	ALA	variant	UNP A0A2L1CBB0

- Molecule 5 is a protein called Methanogenesis marker protein 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	114	Total	C	N	O	S	0	0
			931	600	152	172	7		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	109	VAL	ILE	variant	UNP G0H411
G	129	ILE	VAL	variant	UNP G0H411
G	167	GLU	GLN	variant	UNP G0H411
G	168	GLU	ASP	variant	UNP G0H411
G	171	ASN	ASP	variant	UNP G0H411

- Molecule 6 is a protein called Methanogenesis marker protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	296	Total	C	N	O	S	0	0
			2393	1530	411	440	12		

- Molecule 7 is a protein called Methyl-coenzyme M reductase operon protein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	194	Total	C	N	O	S	0	0
			1469	929	261	271	8		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-35	MET	-	initiating methionine	UNP G0H3B1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	-34	SER	-	expression tag	UNP G0H3B1
I	-33	ALA	-	expression tag	UNP G0H3B1
I	-32	TRP	-	expression tag	UNP G0H3B1
I	-31	SER	-	expression tag	UNP G0H3B1
I	-30	HIS	-	expression tag	UNP G0H3B1
I	-29	PRO	-	expression tag	UNP G0H3B1
I	-28	GLN	-	expression tag	UNP G0H3B1
I	-27	PHE	-	expression tag	UNP G0H3B1
I	-26	GLU	-	expression tag	UNP G0H3B1
I	-25	LYS	-	expression tag	UNP G0H3B1
I	-24	GLY	-	expression tag	UNP G0H3B1
I	-23	GLY	-	expression tag	UNP G0H3B1
I	-22	GLY	-	expression tag	UNP G0H3B1
I	-21	SER	-	expression tag	UNP G0H3B1
I	-20	GLY	-	expression tag	UNP G0H3B1
I	-19	GLY	-	expression tag	UNP G0H3B1
I	-18	GLY	-	expression tag	UNP G0H3B1
I	-17	SER	-	expression tag	UNP G0H3B1
I	-16	GLY	-	expression tag	UNP G0H3B1
I	-15	GLY	-	expression tag	UNP G0H3B1
I	-14	SER	-	expression tag	UNP G0H3B1
I	-13	ALA	-	expression tag	UNP G0H3B1
I	-12	TRP	-	expression tag	UNP G0H3B1
I	-11	SER	-	expression tag	UNP G0H3B1
I	-10	HIS	-	expression tag	UNP G0H3B1
I	-9	PRO	-	expression tag	UNP G0H3B1
I	-8	GLN	-	expression tag	UNP G0H3B1
I	-7	PHE	-	expression tag	UNP G0H3B1
I	-6	GLU	-	expression tag	UNP G0H3B1
I	-5	LYS	-	expression tag	UNP G0H3B1
I	-4	SER	-	expression tag	UNP G0H3B1
I	-3	ALA	-	expression tag	UNP G0H3B1
I	-2	GLY	-	expression tag	UNP G0H3B1
I	-1	SER	-	expression tag	UNP G0H3B1
I	0	GLY	-	expression tag	UNP G0H3B1

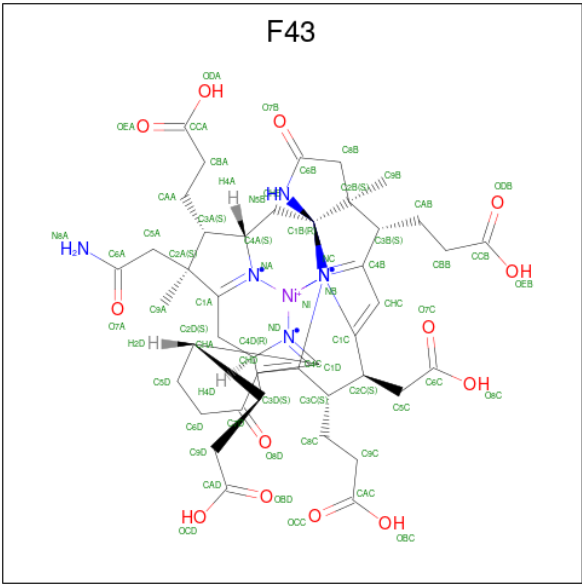
- Molecule 8 is a protein called Glycine betaine/carnitine/choline transport ATP-binding protein OpuCA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	521	Total	C	N	O	S	0	0
			4089	2598	693	774	24		

- Molecule 9 is a protein called DUF2098 domain-containing protein.

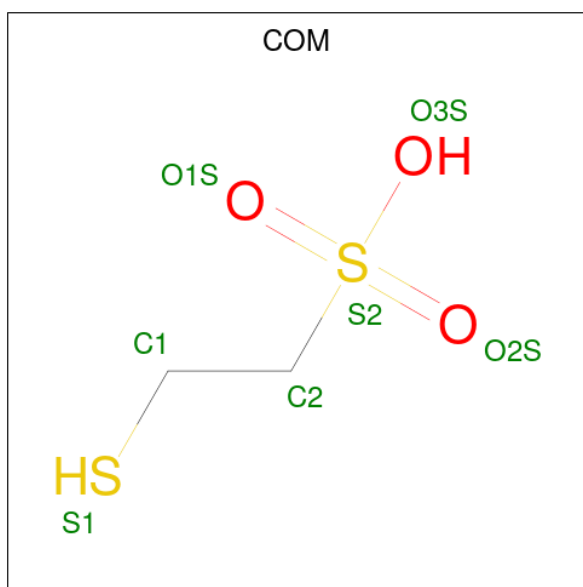
Mol	Chain	Residues	Atoms				AltConf	Trace
9	L	47	Total	C	N	O	0	0
			390	251	61	78		

- Molecule 10 is FACTOR 430 (three-letter code: F43) (formula: C₄₂H₅₁N₆NiO₁₃).



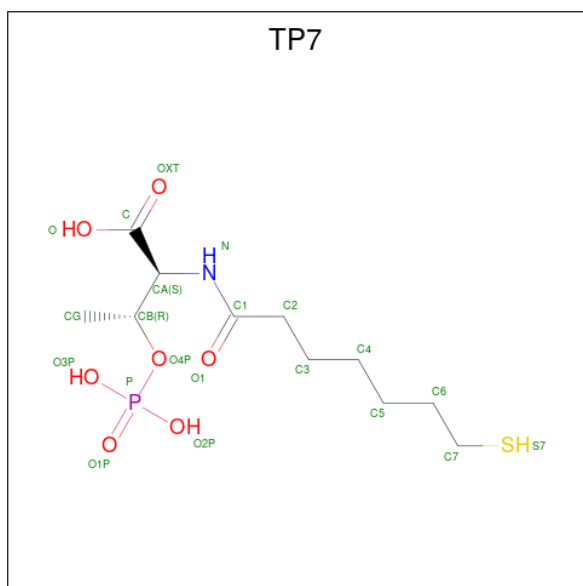
Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	Ni	O	0
			62	42	6	1	13	
10	E	1	Total	C	N	Ni	O	0
			62	42	6	1	13	

- Molecule 11 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula: C₂H₆O₃S₂).



Mol	Chain	Residues	Atoms				AltConf
11	C	1	Total	C	O	S	0
			7	2	3	2	

- Molecule 12 is Coenzyme B (three-letter code: TP7) (formula: $C_{11}H_{22}NO_7PS$).



Mol	Chain	Residues	Atoms						AltConf
12	F	1	Total	C	N	O	P	S	0
			21	11	1	7	1	1	

- Molecule 13 is O-PHOSPHONO-N-{(2E)-7-[(2-SULFOETHYL)DITHIO]HEPT-2-ENOYL}-L-THREONINE (three-letter code: SHT) (formula: $C_{13}H_{24}NO_{10}PS_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
13	F	1	Total	C	N	O	P	S	0
			28	13	1	10	1	3	

- Molecule 14 is FeFe cofactor (three-letter code: S5Q) (formula: CFe_8S_9) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
14	H	1	Total 18	C 1	Fe 8	S 9	0
14	I	1	Total 18	C 1	Fe 8	S 9	0

Continued on next page...

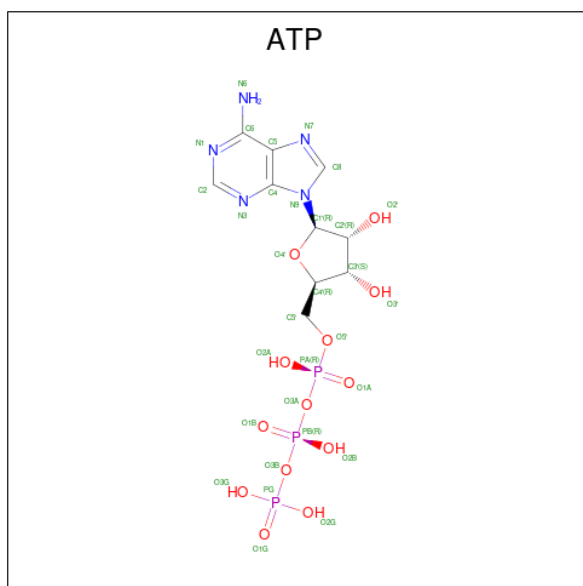
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
14	I	1	Total	C	Fe	S	0
			18	1	8	9	

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
15	K	1	Total	Zn	0
			1	1	

- Molecule 16 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
16	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
16	K	1	Total	C	N	O	P	0
			31	10	5	13	3	

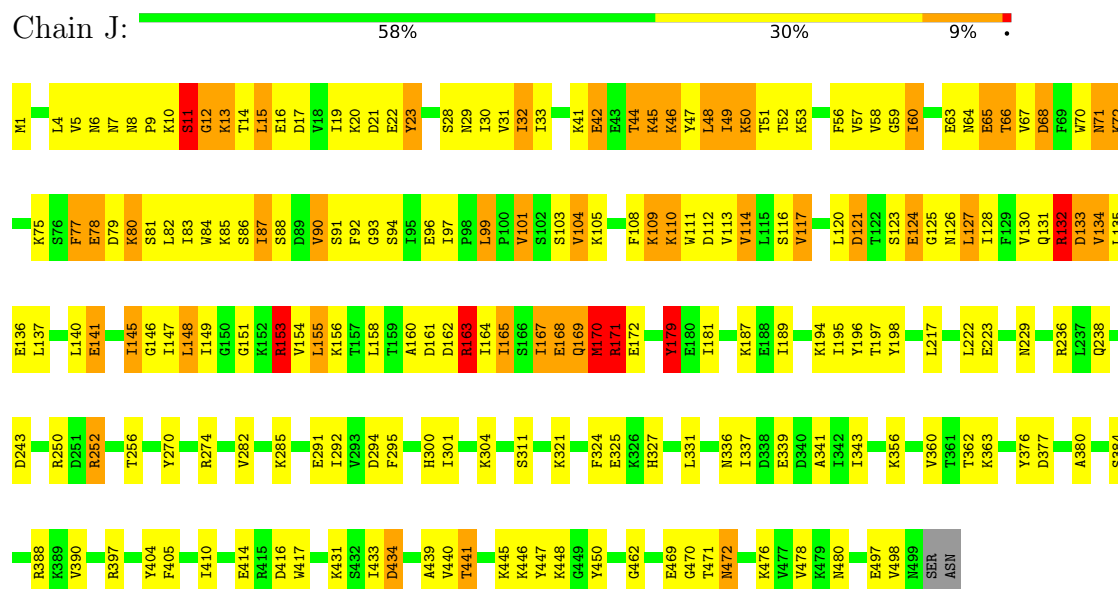
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
17	K	2	Total	Mg	0
			2	2	

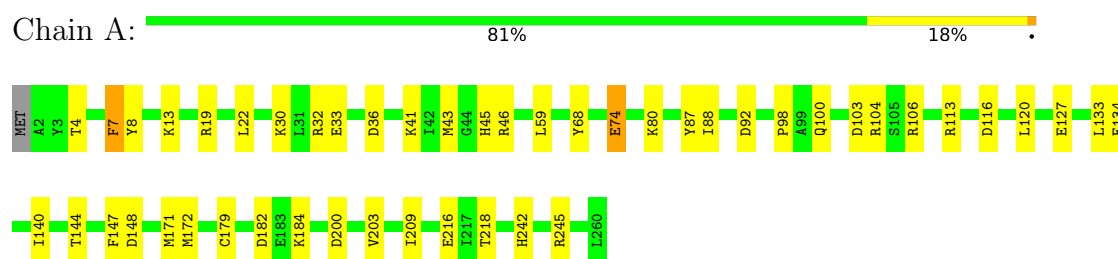
3 Residue-property plots

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. 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. 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.

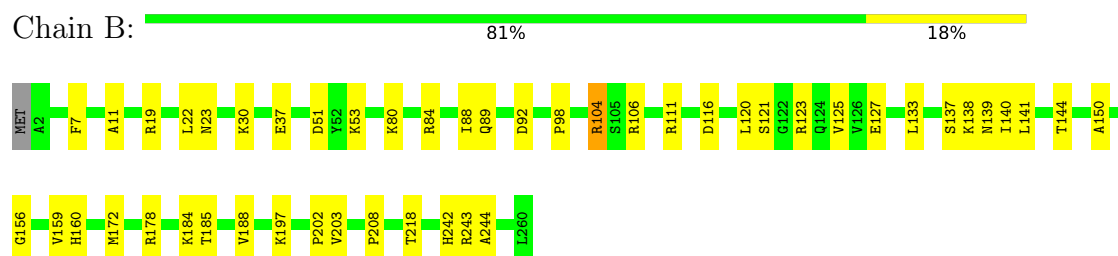
- Molecule 1: UPF0288 protein MmarC6_0796



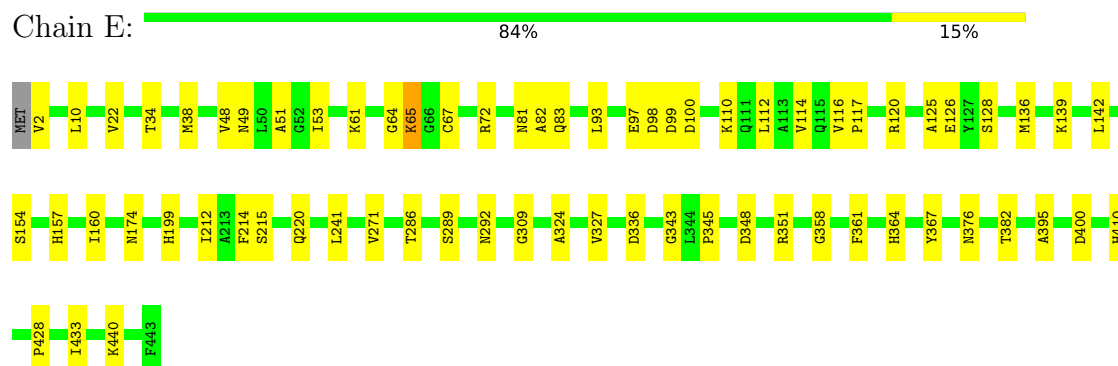
- Molecule 2: Methyl-coenzyme M reductase subunit gamma



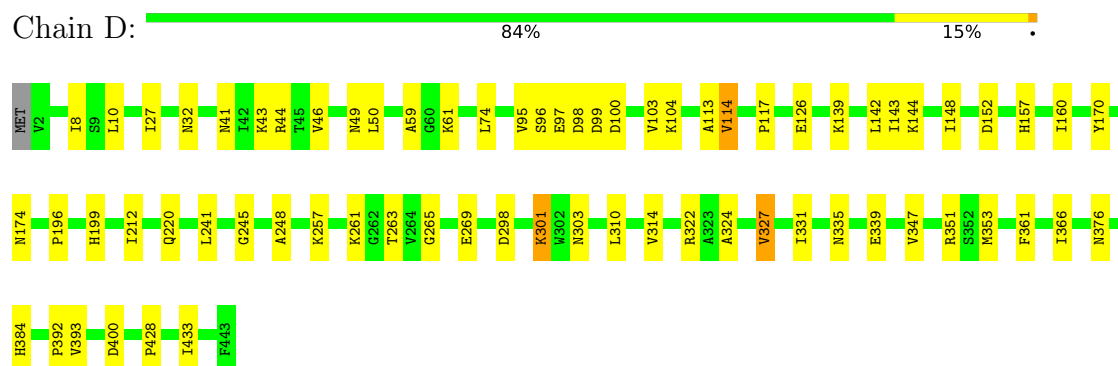
- Molecule 2: Methyl-coenzyme M reductase subunit gamma



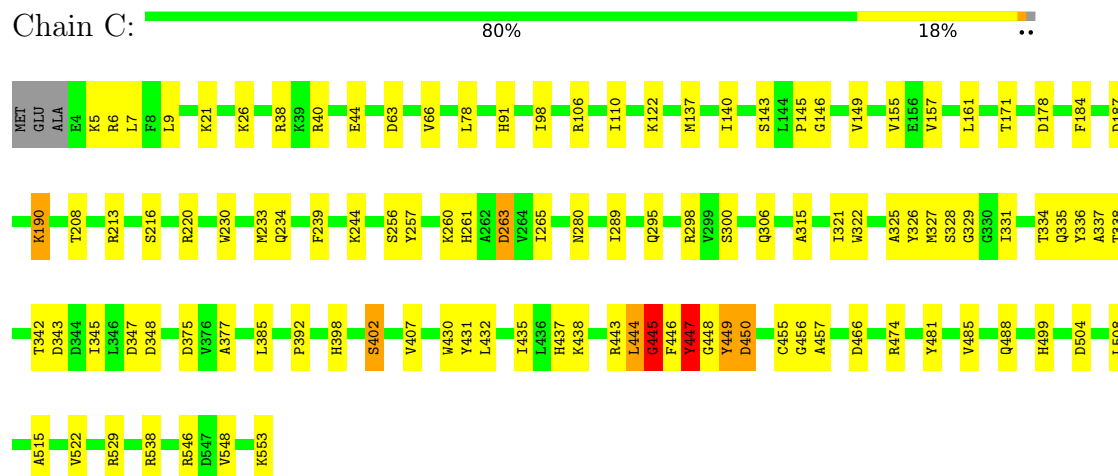
- Molecule 3: Methyl-coenzyme M reductase subunit beta



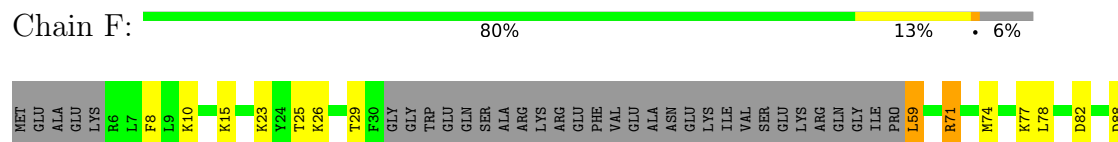
- Molecule 3: Methyl-coenzyme M reductase subunit beta

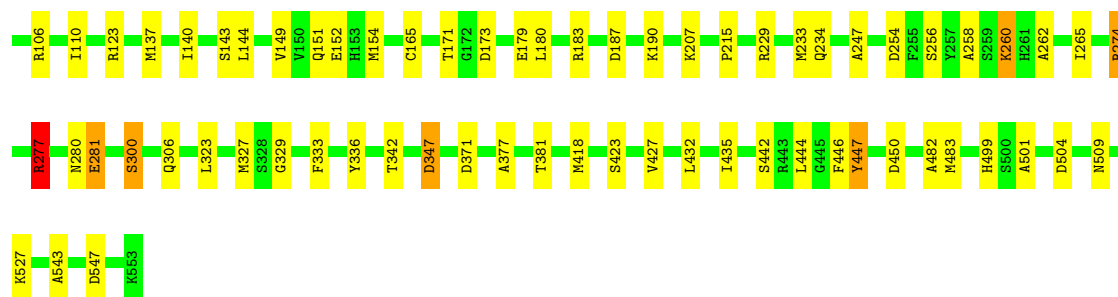


- Molecule 4: Methyl-coenzyme M reductase subunit alpha

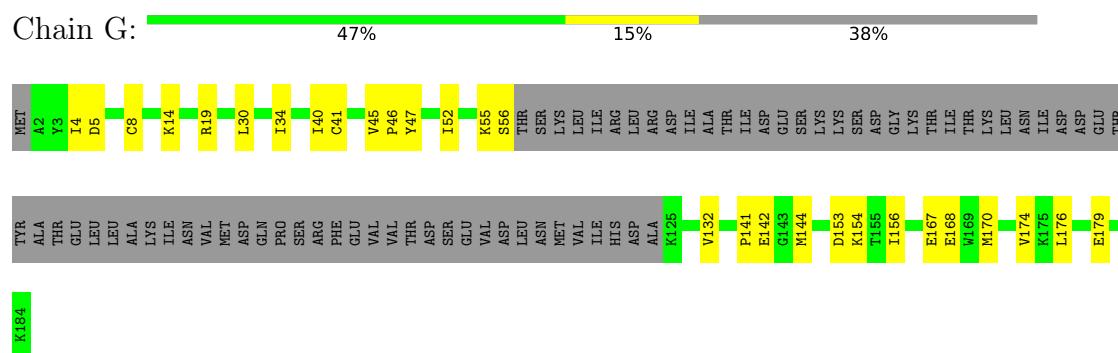


- Molecule 4: Methyl-coenzyme M reductase subunit alpha

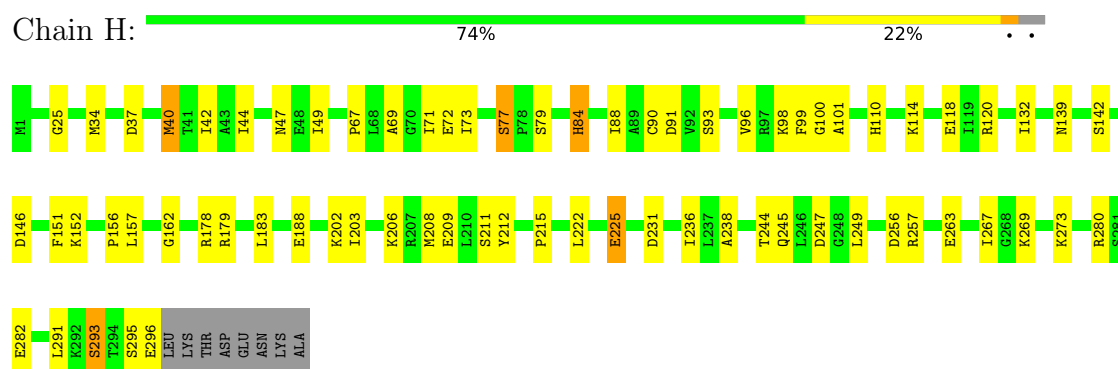




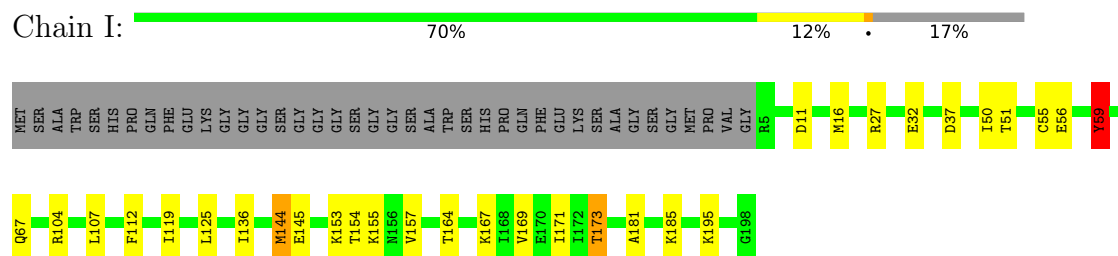
• Molecule 5: Methanogenesis marker protein 17



• Molecule 6: Methanogenesis marker protein 7

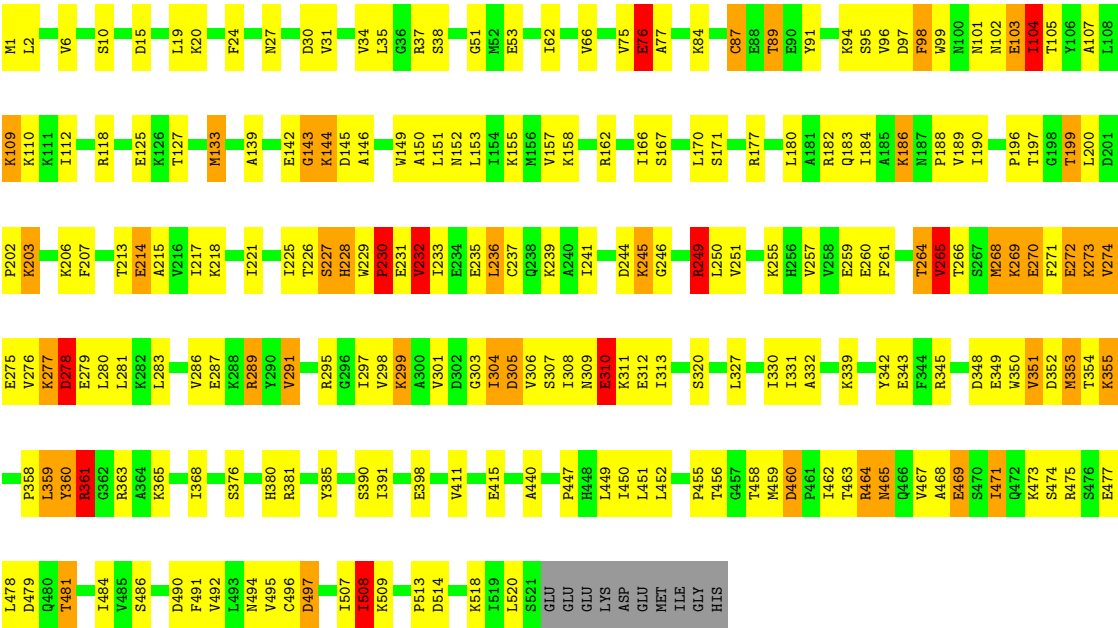


• Molecule 7: Methyl-coenzyme M reductase operon protein C



• Molecule 8: Glycine betaine/carnitine/choline transport ATP-binding protein OpuCA





● Molecule 9: DUF2098 domain-containing protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118247	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	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: AGM, SHT, MHS, TP7, MGN, GL3, MG, SMC, F43, ZN, S5Q, ATP, COM

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	J	0.41	0/4026	0.74	6/5441 (0.1%)
2	A	0.28	0/2116	0.57	2/2861 (0.1%)
2	B	0.27	0/2116	0.54	0/2861
3	D	0.29	0/3319	0.50	1/4499 (0.0%)
3	E	0.29	0/3319	0.50	1/4499 (0.0%)
4	C	0.28	0/4328	0.64	3/5856 (0.1%)
4	F	0.28	0/4078	0.50	0/5522
5	G	0.28	0/943	0.54	0/1262
6	H	0.28	0/2435	0.52	0/3280
7	I	0.27	0/1490	0.58	2/2006 (0.1%)
8	K	0.52	1/4159 (0.0%)	0.94	28/5613 (0.5%)
9	L	0.28	0/398	0.58	0/542
All	All	0.34	1/32727 (0.0%)	0.64	43/44242 (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
1	J	0	6
2	A	0	1
4	F	0	2
6	H	0	1
8	K	0	7
All	All	0	17

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	230	PRO	N-CD	11.52	1.64	1.47

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	447	TYR	CB-CA-C	-26.05	58.31	110.40
1	J	32	ILE	O-C-N	21.22	156.65	122.70
1	J	32	ILE	CA-C-N	-18.02	77.56	117.20
8	K	354	THR	N-CA-CB	-14.10	83.50	110.30
4	C	447	TYR	N-CA-C	13.90	148.54	111.00
1	J	32	ILE	C-N-CA	-13.53	87.88	121.70
8	K	230	PRO	N-CA-CB	-12.86	87.86	103.30
1	J	179	TYR	CA-C-N	-12.68	89.30	117.20
1	J	179	TYR	C-N-CA	-12.21	91.17	121.70
8	K	353	MET	CB-CA-C	-11.93	86.54	110.40
1	J	179	TYR	O-C-N	10.94	140.21	122.70
8	K	228	HIS	N-CA-C	-10.87	81.66	111.00
8	K	230	PRO	CA-N-CD	-8.87	99.08	111.50
8	K	303	GLY	N-CA-C	-8.80	91.11	113.10
8	K	227	SER	N-CA-C	-8.67	87.59	111.00
2	A	8	TYR	N-CA-CB	-7.67	96.80	110.60
7	I	144	MET	CA-CB-CG	7.50	126.06	113.30
8	K	360	TYR	N-CA-C	7.36	130.88	111.00
8	K	353	MET	N-CA-C	7.25	130.57	111.00
8	K	274	VAL	CB-CA-C	6.90	124.52	111.40
8	K	139	ALA	CB-CA-C	-6.68	100.07	110.10
8	K	264	THR	N-CA-C	-6.62	93.12	111.00
8	K	509	LYS	N-CA-CB	-6.58	98.76	110.60
8	K	275	GLU	N-CA-C	-6.47	93.53	111.00
8	K	229	TRP	N-CA-C	-6.30	93.99	111.00
4	C	445	GLY	N-CA-C	6.15	128.47	113.10
8	K	361	ARG	N-CA-C	-6.08	94.58	111.00
8	K	310	GLU	C-N-CA	-6.06	106.56	121.70
2	A	7	PHE	N-CA-C	-6.03	94.73	111.00
8	K	275	GLU	N-CA-CB	5.94	121.30	110.60
8	K	508	ILE	N-CA-C	-5.74	95.51	111.00
8	K	265	VAL	N-CA-CB	5.72	124.08	111.50
8	K	360	TYR	CB-CA-C	-5.59	99.23	110.40
3	D	97	GLU	N-CA-CB	-5.55	100.62	110.60
8	K	232	VAL	N-CA-C	-5.51	96.11	111.00
8	K	304	ILE	N-CA-CB	5.47	123.38	110.80
8	K	76	GLU	CB-CA-C	5.42	121.25	110.40
8	K	230	PRO	N-CD-CG	-5.21	95.39	103.20
3	E	343	GLY	C-N-CA	5.18	134.65	121.70
8	K	77	ALA	N-CA-CB	5.10	117.25	110.10
8	K	77	ALA	N-CA-C	-5.10	97.23	111.00
8	K	89	THR	CB-CA-C	5.09	125.35	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	59	TYR	CA-CB-CG	5.07	123.04	113.40

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	104	ARG	Sidechain
4	F	274	ARG	Sidechain
4	F	277	ARG	Sidechain
6	H	257	ARG	Sidechain
1	J	132	ARG	Sidechain
1	J	153	ARG	Sidechain
1	J	163	ARG	Sidechain
1	J	171	ARG	Sidechain
1	J	179	TYR	Mainchain
1	J	42	GLU	Mainchain
8	K	177	ARG	Sidechain
8	K	249	ARG	Sidechain
8	K	289	ARG	Sidechain
8	K	345	ARG	Sidechain
8	K	361	ARG	Sidechain
8	K	363	ARG	Sidechain
8	K	464	ARG	Sidechain

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	J	3962	0	3996	179	0
2	A	2071	0	2012	24	0
2	B	2071	0	2012	32	0
3	D	3263	0	3260	44	0
3	E	3263	0	3259	33	0
4	C	4284	0	4147	75	0
4	F	4039	0	3904	64	0
5	G	931	0	970	16	0
6	H	2393	0	2475	45	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	I	1469	0	1534	15	0
8	K	4089	0	4163	156	0
9	L	390	0	378	3	0
10	A	62	0	43	7	0
10	E	62	0	42	10	0
11	C	7	0	5	3	0
12	F	21	0	19	3	0
13	F	28	0	20	15	0
14	H	18	0	0	0	0
14	I	36	0	0	0	0
15	K	1	0	0	0	0
16	K	62	0	24	2	0
17	K	2	0	0	0	0
All	All	32524	0	32263	631	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 10.

All (631) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:179:TYR:CE1	1:J:295:PHE:HB3	1.36	1.59
3:E:367:TYR:OH	10:E:601:F43:C5A	1.67	1.40
1:J:179:TYR:CD1	1:J:295:PHE:HB3	1.61	1.33
1:J:179:TYR:CE1	1:J:295:PHE:CB	2.16	1.26
1:J:42:GLU:HA	1:J:172:GLU:HB3	1.24	1.13
8:K:196:PRO:HG3	8:K:225:ILE:HD11	1.28	1.08
1:J:96:GLU:HA	1:J:123:SER:HA	1.37	1.07
4:C:448:GL3:S	4:C:449:TYR:HA	1.98	1.03
8:K:351:VAL:HG21	8:K:360:TYR:O	1.59	1.03
1:J:117:VAL:HA	1:J:125:GLY:HA2	1.41	1.02
1:J:179:TYR:CZ	1:J:295:PHE:HB3	1.96	1.01
1:J:179:TYR:CD1	1:J:295:PHE:CB	2.40	0.97
1:J:44:THR:HG21	1:J:169:GLN:HB2	1.46	0.96
1:J:33:ILE:HG12	1:J:196:TYR:HE1	1.30	0.95
1:J:99:LEU:HG	1:J:141:GLU:OE2	1.66	0.94
1:J:170:MET:CE	1:J:172:GLU:OE1	2.15	0.93
8:K:351:VAL:CG2	8:K:360:TYR:O	2.16	0.93
4:F:446:PHE:HB2	13:F:602:SHT:OS2	1.72	0.90
1:J:170:MET:HE1	1:J:172:GLU:OE1	1.71	0.90
4:C:448:GL3:C	4:C:449:TYR:N	2.37	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:448:GL3:S	4:C:449:TYR:CA	2.60	0.88
8:K:278:ASP:O	8:K:309:ASN:O	1.92	0.88
4:F:327:MET:CE	13:F:602:SHT:O8P	2.24	0.86
8:K:35:LEU:HD11	8:K:230:PRO:HD3	1.59	0.85
1:J:42:GLU:CA	1:J:172:GLU:HB3	2.08	0.84
8:K:127:THR:O	8:K:167:SER:HB3	1.79	0.82
1:J:46:LYS:HA	1:J:59:GLY:HA2	1.61	0.82
8:K:76:GLU:O	8:K:189:VAL:HG12	1.77	0.82
1:J:170:MET:HE3	1:J:172:GLU:HB2	1.61	0.81
1:J:99:LEU:HB3	1:J:140:LEU:HD11	1.62	0.81
1:J:155:LEU:HA	1:J:158:LEU:HD12	1.62	0.80
1:J:168:GLU:HG2	1:J:171:ARG:HH12	1.45	0.80
8:K:196:PRO:HG3	8:K:225:ILE:CD1	2.11	0.80
4:F:482:ALA:O	13:F:602:SHT:P	2.40	0.80
4:F:327:MET:HE2	13:F:602:SHT:O8P	1.83	0.78
4:C:257:TYR:HA	4:C:261:MHS:HD2	1.64	0.78
8:K:283:LEU:HD23	8:K:286:VAL:HG21	1.66	0.77
8:K:281:LEU:HD12	8:K:308:ILE:HG13	1.66	0.77
8:K:76:GLU:O	8:K:189:VAL:CG1	2.32	0.76
1:J:47:TYR:HB2	1:J:58:VAL:HG22	1.68	0.76
1:J:33:ILE:HG12	1:J:196:TYR:CE1	2.18	0.75
4:C:448:GL3:S	4:C:449:TYR:C	2.65	0.75
1:J:101:VAL:HA	1:J:140:LEU:HA	1.68	0.75
1:J:84:TRP:HD1	1:J:86:SER:H	1.35	0.74
1:J:321:LYS:HD3	1:J:331:LEU:HD13	1.68	0.74
4:C:448:GL3:C	4:C:449:TYR:CA	2.66	0.74
1:J:81:SER:HA	1:J:163:ARG:HA	1.70	0.74
8:K:158:LYS:HG3	8:K:207:PHE:CD2	2.23	0.73
1:J:179:TYR:OH	1:J:181:ILE:HB	1.87	0.73
1:J:65:GLU:HG3	1:J:141:GLU:OE2	1.89	0.72
4:F:327:MET:HB2	13:F:602:SHT:HG23	1.71	0.72
3:D:96:SER:O	3:D:99:ASP:OD1	2.07	0.71
1:J:46:LYS:HB2	6:H:212:TYR:OH	1.89	0.71
1:J:179:TYR:CE1	1:J:295:PHE:HB2	2.23	0.71
8:K:301:VAL:HG13	8:K:304:ILE:HD12	1.70	0.71
1:J:179:TYR:CD1	1:J:295:PHE:CG	2.79	0.71
1:J:33:ILE:CG1	1:J:196:TYR:HE1	2.03	0.70
1:J:404:TYR:OH	4:F:15:LYS:O	2.10	0.70
8:K:278:ASP:O	8:K:309:ASN:C	2.30	0.70
3:E:367:TYR:OH	10:E:601:F43:H5A1	1.84	0.69
1:J:153:ARG:HE	1:J:154:VAL:HG23	1.57	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:230:PRO:O	8:K:232:VAL:N	2.25	0.69
1:J:82:LEU:HB3	1:J:160:ALA:HA	1.74	0.69
1:J:229:ASN:ND2	6:H:47:ASN:O	2.24	0.69
1:J:22:GLU:HB3	1:J:197:THR:HG21	1.74	0.69
8:K:268:MET:HG2	8:K:494:ASN:OD1	1.93	0.69
1:J:440:VAL:O	1:J:472:ASN:ND2	2.27	0.68
1:J:170:MET:CE	1:J:172:GLU:HB2	2.23	0.68
1:J:42:GLU:HA	1:J:172:GLU:CB	2.15	0.67
4:F:483:MET:HA	13:F:602:SHT:HCB	1.77	0.67
4:F:482:ALA:C	13:F:602:SHT:O1P	2.34	0.67
8:K:343:GLU:HB3	8:K:350:TRP:HB3	1.76	0.66
4:F:482:ALA:O	13:F:602:SHT:O1P	2.13	0.66
1:J:56:PHE:HA	1:J:151:GLY:HA3	1.77	0.65
1:J:179:TYR:CZ	1:J:181:ILE:HB	2.31	0.65
2:B:30:LYS:HA	2:B:144:THR:HA	1.78	0.65
1:J:5:VAL:H	1:J:9:PRO:HA	1.62	0.65
1:J:49:ILE:HA	1:J:168:GLU:H	1.62	0.65
8:K:34:VAL:HB	8:K:226:THR:HG22	1.79	0.65
1:J:96:GLU:CA	1:J:123:SER:HA	2.23	0.64
8:K:268:MET:SD	8:K:494:ASN:ND2	2.70	0.64
8:K:279:GLU:HA	8:K:309:ASN:HA	1.80	0.64
8:K:162:ARG:HH12	8:K:298:VAL:HG22	1.62	0.64
4:F:258:ALA:HA	4:F:262:ALA:HB3	1.79	0.64
8:K:353:MET:O	8:K:361:ARG:CD	2.45	0.64
4:C:446:PHE:CE1	4:C:448:GL3:HA1	2.33	0.64
1:J:97:ILE:HG13	1:J:125:GLY:HA3	1.80	0.63
4:F:482:ALA:O	13:F:602:SHT:O2P	2.17	0.63
1:J:222:LEU:HD23	1:J:301:ILE:HD11	1.79	0.63
8:K:281:LEU:HD21	8:K:449:LEU:HD22	1.81	0.63
4:C:213:ARG:NH2	4:C:515:ALA:O	2.32	0.63
8:K:228:HIS:HE1	8:K:458:THR:HA	1.63	0.63
1:J:149:ILE:HG21	6:H:209:GLU:OE2	1.96	0.62
1:J:23:TYR:CE2	1:J:304:LYS:HB2	2.34	0.62
1:J:149:ILE:HG21	6:H:209:GLU:HG3	1.82	0.62
8:K:84:LYS:NZ	8:K:87:CYS:O	2.32	0.62
1:J:110:LYS:HG2	1:J:132:ARG:HA	1.80	0.62
4:C:327:MET:HB3	12:F:601:TP7:H31C	1.81	0.61
4:F:327:MET:CB	13:F:602:SHT:HG23	2.29	0.61
6:H:256:ASP:OD1	6:H:280:ARG:NH2	2.33	0.61
1:J:101:VAL:HG11	1:J:120:LEU:HA	1.82	0.61
3:D:27:ILE:HA	3:D:32:ASN:HD22	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:88:ILE:HD11	6:H:179:ARG:HB2	1.83	0.61
1:J:29:ASN:OD1	1:J:300:HIS:O	2.19	0.61
8:K:19:LEU:HD23	8:K:246:GLY:HA2	1.81	0.61
2:A:13:LYS:HD2	2:A:216:GLU:HA	1.81	0.61
1:J:112:ASP:HA	1:J:147:ILE:HA	1.81	0.61
2:A:32:ARG:NH2	2:A:144:THR:O	2.34	0.60
8:K:182:ARG:O	8:K:186:LYS:NZ	2.34	0.60
1:J:78:GLU:HA	1:J:167:ILE:HG13	1.82	0.60
4:C:446:PHE:HB2	11:C:601:COM:O3S	2.01	0.60
1:J:79:ASP:HA	1:J:165:ILE:HA	1.82	0.60
4:C:448:GL3:HS	4:C:449:TYR:HA	1.64	0.60
1:J:51:THR:HG21	1:J:158:LEU:HD11	1.84	0.60
6:H:44:ILE:HD11	6:H:49:ILE:HD13	1.82	0.60
3:D:314:VAL:HG21	3:D:392:PRO:HB3	1.82	0.60
8:K:97:ASP:H	8:K:102:ASN:HD22	1.50	0.60
6:H:183:LEU:HD22	6:H:188:GLU:HB3	1.84	0.59
1:J:274:ARG:HD2	6:H:25:GLY:HA3	1.84	0.59
10:A:601:F43:HAB2	4:F:247:ALA:HB1	1.84	0.59
8:K:452:LEU:HB3	8:K:455:PRO:HG3	1.83	0.59
1:J:4:LEU:HD12	1:J:9:PRO:HB3	1.83	0.59
3:E:376:ASN:O	3:E:382:THR:OG1	2.20	0.59
2:B:156:GLY:O	2:B:178:ARG:NH2	2.35	0.59
10:E:601:F43:N8A	4:C:233:MET:SD	2.76	0.59
8:K:232:VAL:HA	8:K:235:GLU:HG2	1.85	0.59
4:F:327:MET:HE1	13:F:602:SHT:O8P	2.02	0.59
1:J:41:LYS:O	1:J:172:GLU:O	2.19	0.58
8:K:269:LYS:O	8:K:270:GLU:C	2.41	0.58
8:K:291:VAL:HB	8:K:297:ILE:HD12	1.85	0.58
1:J:33:ILE:HD11	1:J:196:TYR:OH	2.04	0.58
8:K:6:VAL:HB	8:K:24:PHE:H	1.69	0.58
4:F:377:ALA:HB3	4:F:432:LEU:HD23	1.85	0.57
4:C:155:VAL:HG13	4:F:88:ASP:HA	1.85	0.57
1:J:324:PHE:HD2	1:J:331:LEU:HD21	1.69	0.57
4:C:553:LYS:HG2	5:G:4:ILE:HD12	1.87	0.57
8:K:171:SER:HB3	16:K:603:ATP:H2'	1.86	0.57
8:K:353:MET:O	8:K:361:ARG:HD2	2.05	0.57
4:C:230:TRP:HA	4:F:329:GLY:HA3	1.87	0.57
1:J:445:LYS:NZ	1:J:469:GLU:OE2	2.37	0.57
3:D:303:ASN:ND2	3:D:347:VAL:O	2.37	0.57
5:G:142:GLU:HG3	6:H:84:HIS:CE1	2.40	0.57
2:B:202:PRO:HD3	8:K:358:PRO:HG3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:ASP:HB3	2:B:127:GLU:HB2	1.87	0.56
8:K:313:ILE:HD13	8:K:471:ILE:HD11	1.86	0.56
8:K:276:VAL:CG1	8:K:312:GLU:HB3	2.34	0.56
1:J:170:MET:HE3	1:J:172:GLU:OE1	2.03	0.56
5:G:46:PRO:HG3	6:H:114:LYS:HD3	1.88	0.56
8:K:6:VAL:HA	8:K:62:ILE:HG22	1.88	0.56
1:J:445:LYS:HE2	1:J:470:GLY:HA3	1.87	0.56
8:K:142:GLU:OE2	8:K:145:ASP:N	2.30	0.56
4:C:322:TRP:O	4:C:326:TYR:HB2	2.06	0.56
8:K:171:SER:HB2	16:K:603:ATP:O1A	2.06	0.56
4:C:438:LYS:HB2	4:C:444:LEU:HD22	1.88	0.56
4:C:91:HIS:NE2	4:C:331:ILE:O	2.37	0.55
2:B:159:VAL:HG22	10:E:601:F43:HBB2	1.88	0.55
4:C:122:LYS:O	8:K:125:GLU:HG2	2.07	0.55
1:J:179:TYR:CG	1:J:295:PHE:HB3	2.33	0.55
1:J:148:LEU:HG	1:J:155:LEU:HD22	1.87	0.55
6:H:77:SER:OG	6:H:79:SER:O	2.25	0.55
4:C:448:GL3:C	4:C:449:TYR:HA	2.32	0.55
6:H:71:ILE:HD13	6:H:203:ILE:HG13	1.88	0.55
2:B:188:VAL:HG23	2:B:208:PRO:HD3	1.88	0.55
2:A:120:LEU:HG	4:C:447:TYR:HA	1.89	0.55
1:J:22:GLU:C	1:J:23:TYR:N	2.59	0.55
8:K:353:MET:O	8:K:361:ARG:HG3	2.07	0.55
1:J:252:ARG:O	1:J:285:LYS:NZ	2.40	0.55
2:A:92:ASP:O	4:C:443:ARG:NH2	2.40	0.55
2:B:23:ASN:O	2:B:111:ARG:NH1	2.40	0.55
2:B:137:SER:HA	2:B:141:LEU:HB2	1.88	0.55
7:I:155:LYS:O	9:L:48:ARG:NH2	2.40	0.55
8:K:213:THR:O	8:K:217:ILE:HG12	2.07	0.55
8:K:112:ILE:HG22	8:K:190:ILE:HG22	1.88	0.54
2:B:150:ALA:HB2	2:B:208:PRO:HB3	1.89	0.54
10:E:601:F43:H5D2	4:F:336:TYR:CE2	2.43	0.54
1:J:49:ILE:HG13	1:J:167:ILE:HA	1.88	0.54
1:J:250:ARG:NH1	1:J:270:TYR:OH	2.39	0.54
3:E:49:ASN:HB3	3:E:174:ASN:HB3	1.89	0.54
3:D:196:PRO:HA	3:D:376:ASN:HB3	1.88	0.54
1:J:46:LYS:HE2	6:H:212:TYR:HE1	1.72	0.54
3:E:212:ILE:HD11	3:E:395:ALA:HB2	1.90	0.54
1:J:114:VAL:HG12	1:J:128:ILE:HB	1.90	0.54
1:J:390:VAL:HG23	1:J:416:ASP:HB2	1.88	0.54
3:D:212:ILE:HG22	3:D:245:GLY:HA2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:310:GLU:O	8:K:312:GLU:N	2.40	0.54
2:A:7:PHE:HB2	2:A:19:ARG:HG2	1.89	0.54
2:B:139:ASN:OD1	8:K:381:ARG:NH2	2.41	0.54
4:C:143:SER:O	4:C:234:GLN:NE2	2.38	0.54
8:K:310:GLU:O	8:K:481:THR:HB	2.07	0.54
8:K:213:THR:HA	8:K:217:ILE:HG23	1.90	0.53
2:B:7:PHE:HB2	2:B:19:ARG:HG2	1.90	0.53
8:K:261:PHE:O	8:K:264:THR:O	2.25	0.53
4:C:377:ALA:HB3	4:C:432:LEU:HD23	1.90	0.53
8:K:250:LEU:HD23	8:K:257:VAL:HG22	1.89	0.53
8:K:269:LYS:HE3	8:K:271:PHE:CE1	2.43	0.53
8:K:283:LEU:HD11	8:K:331:ILE:HD12	1.89	0.53
2:A:200:ASP:OD1	2:A:200:ASP:N	2.42	0.53
1:J:32:ILE:HD11	1:J:195:ILE:HB	1.89	0.53
1:J:336:ASN:HB3	1:J:341:ALA:HB1	1.89	0.53
1:J:388:ARG:NH1	1:J:497:GLU:OE1	2.37	0.53
2:A:43:MET:HE1	2:A:134:GLU:HG2	1.91	0.53
3:E:64:GLY:H	3:E:67:CYS:HB2	1.73	0.53
1:J:23:TYR:CE2	1:J:304:LYS:HE3	2.44	0.53
8:K:51:GLY:HA2	8:K:99:TRP:CZ2	2.44	0.53
2:B:244:ALA:HB1	3:E:345:PRO:HG3	1.91	0.52
7:I:153:LYS:HB3	7:I:167:LYS:HG3	1.92	0.52
8:K:268:MET:CE	8:K:494:ASN:HD21	2.22	0.52
8:K:490:ASP:OD1	8:K:490:ASP:N	2.42	0.52
2:A:182:ASP:OD1	2:A:182:ASP:N	2.40	0.52
10:A:601:F43:H9B1	4:F:247:ALA:HB1	1.92	0.52
2:B:140:ILE:O	2:B:144:THR:OG1	2.26	0.52
2:A:32:ARG:NH2	2:A:147:PHE:O	2.43	0.52
2:B:11:ALA:HB2	3:E:289:SER:HB3	1.92	0.52
4:F:300:SER:O	4:F:306:GLN:NE2	2.41	0.52
8:K:186:LYS:HG3	8:K:188:PRO:HG3	1.92	0.52
1:J:41:LYS:O	1:J:172:GLU:HB3	2.10	0.52
3:E:367:TYR:CZ	10:E:601:F43:C5A	2.83	0.52
1:J:32:ILE:HD13	1:J:194:LYS:O	2.10	0.52
4:F:171:THR:HG22	4:F:173:ASP:H	1.74	0.52
8:K:277:LYS:HD3	8:K:311:LYS:HE2	1.91	0.52
8:K:447:PRO:HG2	8:K:450:ILE:HG12	1.91	0.52
8:K:475:ARG:O	8:K:479:ASP:HA	2.10	0.52
8:K:492:VAL:HG12	8:K:513:PRO:HB3	1.91	0.52
1:J:149:ILE:CG2	6:H:209:GLU:OE2	2.26	0.52
4:C:171:THR:HB	4:C:208:THR:HG23	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:238:GLN:HG3	1:J:238:GLN:O	2.10	0.51
1:J:478:VAL:HG11	1:J:498:VAL:HG21	1.92	0.51
3:D:44:ARG:NH2	3:D:100:ASP:O	2.42	0.51
5:G:141:PRO:HG2	5:G:144:MET:HG2	1.92	0.51
6:H:96:VAL:HG13	6:H:101:ALA:HB3	1.92	0.51
1:J:405:PHE:CZ	4:F:8:PHE:HE1	2.27	0.51
7:I:112:PHE:HB3	7:I:119:ILE:HG12	1.92	0.51
8:K:76:GLU:O	8:K:189:VAL:HG11	2.10	0.51
1:J:111:TRP:CE3	1:J:155:LEU:HD21	2.44	0.51
3:E:214:PHE:HB2	3:E:428:PRO:HG2	1.93	0.51
3:D:49:ASN:HB3	3:D:174:ASN:HB3	1.92	0.51
3:D:351:ARG:HA	4:C:455:SMC:SG	2.50	0.51
1:J:197:THR:HG23	1:J:198:TYR:HD1	1.74	0.51
1:J:256:THR:HG22	1:J:282:VAL:HG12	1.91	0.51
1:J:324:PHE:HB2	1:J:331:LEU:HD11	1.90	0.51
2:A:30:LYS:NZ	2:A:33:GLU:OE1	2.43	0.51
3:D:324:ALA:HB2	3:D:400:ASP:HB2	1.93	0.51
4:C:161:LEU:HD13	4:C:548:VAL:HG22	1.92	0.51
8:K:353:MET:O	8:K:361:ARG:CG	2.58	0.51
8:K:31:VAL:HB	8:K:237:CYS:HA	1.93	0.51
1:J:324:PHE:HE2	1:J:360:VAL:HG11	1.75	0.51
3:E:48:VAL:HB	3:E:112:LEU:HB2	1.91	0.51
1:J:405:PHE:HZ	4:F:8:PHE:CE1	2.29	0.51
4:F:143:SER:O	4:F:234:GLN:NE2	2.42	0.51
6:H:156:PRO:HB3	6:H:202:LYS:HD3	1.93	0.51
3:E:220:GLN:HG3	3:E:241:LEU:HB2	1.92	0.51
3:E:324:ALA:HB2	3:E:400:ASP:HB2	1.93	0.51
6:H:72:GLU:OE2	6:H:245:GLN:NE2	2.43	0.51
1:J:48:LEU:HB3	1:J:168:GLU:HB3	1.92	0.51
1:J:70:TRP:HZ3	1:J:127:LEU:HD11	1.75	0.51
4:C:546:ARG:NH2	4:F:543:ALA:O	2.40	0.51
8:K:276:VAL:HG13	8:K:311:LYS:O	2.11	0.51
1:J:70:TRP:O	1:J:71:ASN:C	2.50	0.50
2:A:74:GLU:HG2	3:D:261:LYS:HG2	1.93	0.50
4:C:315:ALA:HB1	4:C:337:ALA:HB1	1.93	0.50
7:I:56:GLU:OE1	7:I:181:ALA:N	2.43	0.50
7:I:153:LYS:NZ	7:I:164:THR:O	2.43	0.50
4:C:7:LEU:HB2	4:C:348:ASP:HB2	1.92	0.50
1:J:28:SER:HA	1:J:300:HIS:CB	2.42	0.50
3:D:327:VAL:HG11	3:D:393:VAL:HA	1.93	0.50
4:F:144:LEU:HA	4:F:234:GLN:HG3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:230:PRO:O	8:K:233:ILE:N	2.44	0.50
1:J:410:ILE:HD11	8:K:398:GLU:OE1	2.12	0.50
3:D:384:HIS:HB3	4:C:455:SMC:CS	2.41	0.50
8:K:491:PHE:O	8:K:495:VAL:HB	2.11	0.50
1:J:377:ASP:OD2	1:J:388:ARG:NH2	2.31	0.50
1:J:405:PHE:CZ	4:F:8:PHE:CE1	3.00	0.50
2:A:140:ILE:O	2:A:144:THR:OG1	2.24	0.50
4:F:26:LYS:O	4:F:59:LEU:N	2.45	0.50
2:B:138:LYS:HD2	8:K:381:ARG:HH22	1.76	0.50
10:E:601:F43:H5D2	4:F:336:TYR:CZ	2.46	0.50
8:K:102:ASN:O	8:K:103:GLU:C	2.50	0.50
8:K:352:ASP:OD2	8:K:355:LYS:HD2	2.12	0.50
1:J:380:ALA:O	1:J:384:SER:OG	2.24	0.49
4:F:110:ILE:HB	4:F:265:ILE:HB	1.93	0.49
6:H:263:GLU:HB3	6:H:273:LYS:HB3	1.94	0.49
8:K:35:LEU:HD12	8:K:228:HIS:HA	1.93	0.49
3:D:103:VAL:HG13	3:D:114:VAL:HG12	1.93	0.49
8:K:127:THR:HA	8:K:166:ILE:HA	1.93	0.49
4:C:21:LYS:HA	4:C:392:PRO:HD2	1.95	0.49
1:J:111:TRP:HA	1:J:130:VAL:O	2.11	0.49
3:D:100:ASP:OD1	3:D:100:ASP:N	2.42	0.49
1:J:441:THR:OG1	1:J:447:TYR:O	2.24	0.49
2:A:245:ARG:NH2	3:D:339:GLU:OE1	2.45	0.49
8:K:107:ALA:HA	8:K:110:LYS:HE2	1.94	0.49
2:A:242:HIS:HB2	4:C:435:ILE:HD11	1.95	0.49
2:B:88:ILE:HG22	2:B:133:LEU:HD11	1.94	0.49
3:E:81:ASN:O	3:E:83:GLN:N	2.45	0.49
1:J:117:VAL:HA	1:J:125:GLY:CA	2.29	0.49
2:A:100:GLN:OE1	4:C:443:ARG:NH1	2.44	0.49
3:E:126:GLU:HG3	3:E:128:SER:H	1.76	0.49
4:F:333:PHE:HB3	4:F:336:TYR:HB2	1.94	0.49
3:E:142:LEU:HD12	3:E:160:ILE:HD11	1.94	0.49
5:G:34:ILE:HD13	5:G:52:ILE:HD12	1.95	0.49
7:I:51:THR:HA	7:I:55:CYS:HB2	1.95	0.49
1:J:66:THR:HB	1:J:145:ILE:HB	1.95	0.49
4:F:187:ASP:HB3	4:F:190:LYS:HB2	1.95	0.49
4:F:277:ARG:HG2	4:F:281:GLU:HG2	1.95	0.49
1:J:46:LYS:O	1:J:46:LYS:HG2	2.12	0.49
4:C:481:TYR:O	4:C:488:GLN:NE2	2.43	0.49
4:F:327:MET:HE2	13:F:602:SHT:P	2.53	0.49
5:G:132:VAL:HG11	5:G:156:ILE:HD12	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:23:TYR:HE2	1:J:304:LYS:HB2	1.77	0.48
8:K:281:LEU:HD12	8:K:308:ILE:CG1	2.42	0.48
4:F:229:ARG:O	4:F:233:MET:HG2	2.13	0.48
3:D:220:GLN:HG3	3:D:241:LEU:HB2	1.94	0.48
4:C:300:SER:O	4:C:306:GLN:NE2	2.46	0.48
1:J:92:PHE:HB2	1:J:127:LEU:HB3	1.95	0.48
1:J:68:ASP:OD1	1:J:68:ASP:N	2.45	0.48
10:A:601:F43:OCD	4:C:335:GLN:NE2	2.22	0.48
1:J:31:VAL:HG21	1:J:292:ILE:HA	1.96	0.48
8:K:199:THR:O	8:K:199:THR:OG1	2.27	0.48
8:K:2:LEU:HA	8:K:27:ASN:HA	1.95	0.48
8:K:245:LYS:HA	8:K:245:LYS:HD3	1.60	0.48
8:K:276:VAL:HG12	8:K:277:LYS:H	1.77	0.48
1:J:112:ASP:H	1:J:130:VAL:HB	1.79	0.48
1:J:158:LEU:HD23	1:J:162:ASP:HB2	1.95	0.48
2:A:68:TYR:OH	3:D:257:LYS:NZ	2.45	0.48
2:B:242:HIS:HB2	4:F:435:ILE:HD11	1.96	0.48
4:C:6:ARG:HB2	4:C:9:LEU:HG	1.95	0.48
4:F:23:LYS:HD2	4:F:23:LYS:HA	1.68	0.48
8:K:265:VAL:HG13	8:K:266:THR:N	2.29	0.48
8:K:465:ASN:O	8:K:468:ALA:HB3	2.13	0.48
4:C:187:ASP:HB3	4:C:190:LYS:HG2	1.94	0.47
6:H:295:SER:OG	6:H:296:GLU:OE1	2.31	0.47
1:J:91:SER:HA	1:J:128:ILE:HA	1.94	0.47
1:J:404:TYR:CZ	4:F:15:LYS:HG3	2.50	0.47
2:B:53:LYS:HB2	2:B:84:ARG:HD3	1.96	0.47
3:D:74:LEU:HD11	3:D:152:ASP:HB3	1.96	0.47
3:D:361:PHE:HB2	4:C:448:GL3:HA2	1.95	0.47
1:J:92:PHE:HZ	1:J:158:LEU:HD22	1.80	0.47
3:D:10:LEU:HD13	3:D:433:ILE:HG23	1.96	0.47
4:C:450:ASP:N	4:C:450:ASP:OD1	2.47	0.47
1:J:46:LYS:HG3	1:J:57:VAL:HG12	1.95	0.47
1:J:109:LYS:HA	1:J:109:LYS:HD3	1.47	0.47
10:A:601:F43:H9A1	4:C:331:ILE:HB	1.96	0.47
10:A:601:F43:O7B	3:D:366:ILE:HG12	2.14	0.47
3:E:117:PRO:HG2	3:E:120:ARG:HG3	1.97	0.47
3:E:286:THR:HA	3:E:292:ASN:HA	1.95	0.47
4:F:483:MET:HG2	13:F:602:SHT:OXT	2.14	0.47
8:K:180:LEU:O	8:K:184:ILE:HD12	2.15	0.47
8:K:241:ILE:HG22	8:K:251:VAL:HG13	1.95	0.47
1:J:30:ILE:HG23	1:J:195:ILE:HD11	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:215:PRO:HA	6:H:293:SER:HA	1.95	0.47
7:I:136:ILE:HB	7:I:171:ILE:HD13	1.96	0.47
8:K:109:LYS:HE2	8:K:109:LYS:HB2	1.33	0.47
8:K:235:GLU:HG3	8:K:236:LEU:HD22	1.96	0.47
3:D:104:LYS:HG3	3:D:113:ALA:HB3	1.97	0.47
2:B:51:ASP:HA	8:K:376:SER:HB3	1.96	0.47
3:D:310:LEU:HD11	3:D:331:ILE:HA	1.96	0.47
8:K:277:LYS:O	8:K:278:ASP:HB2	2.14	0.47
1:J:42:GLU:HB2	1:J:172:GLU:H	1.80	0.47
2:B:89:GLN:HE21	2:B:125:VAL:HB	1.80	0.47
8:K:276:VAL:HG12	8:K:309:ASN:O	2.15	0.47
1:J:82:LEU:HD11	1:J:90:VAL:HG22	1.96	0.46
2:B:98:PRO:HA	2:B:218:THR:HA	1.98	0.46
4:C:40:ARG:O	4:C:44:GLU:HG3	2.15	0.46
6:H:110:HIS:HB2	6:H:118:GLU:HG2	1.97	0.46
7:I:154:THR:HG22	7:I:157:VAL:H	1.80	0.46
1:J:87:ILE:H	1:J:87:ILE:HG13	1.45	0.46
1:J:405:PHE:CE1	4:F:8:PHE:HE1	2.32	0.46
2:A:113:ARG:HG2	3:D:263:THR:HG22	1.97	0.46
3:E:72:ARG:NH2	3:E:154:SER:OG	2.49	0.46
1:J:433:ILE:HD12	1:J:462:GLY:HA2	1.98	0.46
3:D:41:ASN:OD1	3:D:44:ARG:NH1	2.49	0.46
4:F:106:ARG:O	4:F:280:ASN:ND2	2.42	0.46
7:I:145:GLU:OE2	9:L:47:TYR:OH	2.32	0.46
3:E:10:LEU:HD13	3:E:433:ILE:HD12	1.98	0.46
8:K:280:LEU:HD22	8:K:481:THR:HG21	1.97	0.46
8:K:352:ASP:OD2	8:K:355:LYS:CD	2.64	0.46
1:J:33:ILE:CD1	1:J:196:TYR:OH	2.64	0.46
1:J:405:PHE:HZ	4:F:8:PHE:CZ	2.34	0.46
8:K:265:VAL:HG22	8:K:266:THR:H	1.81	0.46
1:J:13:LYS:HA	1:J:189:ILE:HG22	1.97	0.46
1:J:41:LYS:O	1:J:172:GLU:C	2.54	0.46
1:J:168:GLU:HG2	1:J:171:ARG:NH1	2.24	0.46
6:H:152:LYS:HA	6:H:152:LYS:HD3	1.69	0.46
3:E:34:THR:O	3:E:38:MET:HG3	2.15	0.46
3:D:46:VAL:HB	3:D:114:VAL:HG22	1.98	0.46
8:K:228:HIS:CE1	8:K:458:THR:HA	2.46	0.46
8:K:474:SER:O	8:K:478:LEU:HB3	2.16	0.46
3:D:384:HIS:HB3	4:C:455:SMC:HCS2	1.98	0.46
6:H:225:GLU:HG2	6:H:267:ILE:HG22	1.98	0.46
8:K:167:SER:HA	8:K:170:LEU:HG	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:121:ASP:HB2	1:J:124:GLU:HB2	1.99	0.46
2:B:22:LEU:HD21	2:B:106:ARG:HB3	1.98	0.46
8:K:102:ASN:O	8:K:104:ILE:N	2.49	0.46
1:J:45:LYS:HD2	6:H:208:MET:HE1	1.87	0.45
1:J:311:SER:O	1:J:311:SER:OG	2.33	0.45
3:E:51:ALA:HB2	3:E:110:LYS:HB2	1.98	0.45
3:D:298:ASP:HB3	3:D:301:LYS:HB2	1.98	0.45
3:D:351:ARG:HG2	4:C:455:SMC:CS	2.45	0.45
8:K:184:ILE:HG21	8:K:215:ALA:HB1	1.98	0.45
1:J:50:LYS:HD2	1:J:50:LYS:HA	1.41	0.45
1:J:217:LEU:HD21	1:J:222:LEU:HD13	1.97	0.45
2:A:116:ASP:HB3	2:A:127:GLU:HB2	1.99	0.45
3:D:99:ASP:HB2	3:D:117:PRO:HB3	1.98	0.45
1:J:48:LEU:HD23	1:J:48:LEU:HA	1.84	0.45
1:J:113:VAL:HG22	1:J:148:LEU:HD22	1.97	0.45
1:J:117:VAL:CA	1:J:125:GLY:HA2	2.30	0.45
10:E:601:F43:HHA2	13:F:602:SHT:S1	2.56	0.45
4:F:499:HIS:HB3	4:F:504:ASP:HB2	1.98	0.45
8:K:51:GLY:HA2	8:K:99:TRP:CH2	2.51	0.45
8:K:142:GLU:O	8:K:143:GLY:C	2.54	0.45
8:K:188:PRO:HD2	8:K:221:ILE:HD13	1.97	0.45
1:J:5:VAL:O	1:J:7:ASN:N	2.49	0.45
1:J:30:ILE:HG23	1:J:195:ILE:CD1	2.47	0.45
1:J:343:ILE:HG23	1:J:362:THR:HG23	1.98	0.45
1:J:447:TYR:HB3	1:J:450:TYR:HD2	1.81	0.45
8:K:279:GLU:HG2	8:K:350:TRP:HH2	1.81	0.45
1:J:79:ASP:HB3	1:J:163:ARG:HH12	1.82	0.45
5:G:168:GLU:OE1	5:G:168:GLU:N	2.40	0.45
8:K:10:SER:HA	8:K:20:LYS:HA	1.99	0.45
2:B:160:HIS:ND1	10:E:601:F43:OCC	2.38	0.45
4:C:343:ASP:HB2	4:C:345:ILE:HG13	1.98	0.45
8:K:133:MET:SD	8:K:146:ALA:HB1	2.57	0.45
1:J:60:ILE:HB	1:J:67:VAL:HG22	1.98	0.45
5:G:8:CYS:HB3	5:G:14:LYS:HG2	1.99	0.45
6:H:247:ASP:N	6:H:247:ASP:OD1	2.48	0.45
2:A:88:ILE:HG22	2:A:133:LEU:HD11	1.98	0.45
6:H:67:PRO:HD2	6:H:99:PHE:HB3	1.99	0.45
7:I:50:ILE:HD13	7:I:50:ILE:HA	1.80	0.45
3:D:335:ASN:HB3	3:D:353:MET:HE2	1.98	0.44
3:D:265:GLY:O	3:D:269:GLU:HG2	2.17	0.44
5:G:8:CYS:HB2	5:G:41:CYS:HB2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:144:MET:HB2	7:I:171:ILE:HG13	2.00	0.44
8:K:230:PRO:C	8:K:232:VAL:H	2.19	0.44
1:J:46:LYS:HB2	6:H:212:TYR:CZ	2.53	0.44
3:E:65:LYS:HD3	4:C:263:ASP:HA	1.98	0.44
4:C:5:LYS:HD2	4:C:5:LYS:HA	1.71	0.44
8:K:144:LYS:HA	8:K:144:LYS:HD2	1.35	0.44
1:J:28:SER:HA	1:J:300:HIS:HB2	1.98	0.44
1:J:97:ILE:HG22	1:J:99:LEU:HB2	1.99	0.44
3:D:139:LYS:HD3	3:D:157:HIS:HB2	1.99	0.44
12:F:601:TP7:H42C	12:F:601:TP7:H72C	1.71	0.44
6:H:69:ALA:HB2	6:H:100:GLY:HA3	1.99	0.44
6:H:222:LEU:HD22	6:H:291:LEU:HD21	1.99	0.44
3:E:139:LYS:HD3	3:E:157:HIS:HB2	1.99	0.44
8:K:236:LEU:HD13	8:K:236:LEU:HA	1.74	0.44
1:J:291:GLU:HA	1:J:294:ASP:HB2	2.00	0.44
2:B:92:ASP:OD1	2:B:104:ARG:NH1	2.51	0.44
4:C:448:GL3:CA	4:C:449:TYR:N	2.80	0.44
8:K:213:THR:O	8:K:215:ALA:N	2.51	0.44
1:J:48:LEU:HB3	1:J:168:GLU:CB	2.48	0.44
3:D:10:LEU:HD22	3:D:433:ILE:HD12	2.00	0.44
8:K:271:PHE:CE1	8:K:469:GLU:HB2	2.53	0.44
1:J:80:LYS:HD2	1:J:80:LYS:HA	1.64	0.44
1:J:108:PHE:HD2	1:J:134:VAL:HG23	1.83	0.44
1:J:223:GLU:OE2	1:J:300:HIS:NE2	2.37	0.44
10:A:601:F43:C1C	11:C:601:COM:H12	2.47	0.44
3:E:125:ALA:HA	3:D:43:LYS:HD3	1.99	0.44
4:C:328:SER:HB3	12:F:601:TP7:H52C	2.00	0.44
3:D:8:ILE:HB	3:D:248:ALA:HB1	2.00	0.44
4:C:106:ARG:O	4:C:280:ASN:ND2	2.42	0.44
4:C:446:PHE:CE2	4:C:485:VAL:HG12	2.52	0.44
4:F:123:ARG:NH1	4:F:254:ASP:OD2	2.50	0.44
8:K:507:ILE:O	8:K:508:ILE:C	2.56	0.44
3:E:22:VAL:HG22	3:E:440:LYS:HD2	1.99	0.43
4:C:466:ASP:OD1	4:C:466:ASP:N	2.40	0.43
8:K:276:VAL:HG11	8:K:312:GLU:HB3	1.99	0.43
1:J:5:VAL:HG21	1:J:10:LYS:HB2	1.99	0.43
1:J:51:THR:HB	1:J:158:LEU:HD21	2.00	0.43
4:C:38:ARG:HA	4:C:38:ARG:HD3	1.68	0.43
4:C:398:HIS:CE1	4:C:407:VAL:HG21	2.53	0.43
5:G:170:MET:O	5:G:174:VAL:HG23	2.19	0.43
6:H:98:LYS:HB2	6:H:98:LYS:HE2	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:11:ASP:N	7:I:32:GLU:O	2.49	0.43
8:K:456:THR:HG21	8:K:464:ARG:HG3	2.00	0.43
1:J:60:ILE:HA	1:J:146:GLY:HA3	2.00	0.43
1:J:93:GLY:HA3	1:J:94:SER:HA	1.57	0.43
1:J:111:TRP:HE3	1:J:155:LEU:HD21	1.82	0.43
4:C:146:GLY:HA3	4:C:157:VAL:HB	2.00	0.43
4:F:483:MET:HE2	4:F:483:MET:HB2	1.88	0.43
10:A:601:F43:CHC	11:C:601:COM:H12	2.48	0.43
6:H:206:LYS:HB2	6:H:206:LYS:HE2	1.65	0.43
8:K:157:VAL:CG1	8:K:180:LEU:HD23	2.48	0.43
4:C:499:HIS:HB3	4:C:504:ASP:HB2	2.01	0.43
4:F:71:ARG:HA	4:F:74:MET:HG3	2.01	0.43
5:G:142:GLU:HG3	6:H:84:HIS:HE1	1.83	0.43
6:H:40:MET:HB3	6:H:42:ILE:HD11	2.00	0.43
6:H:236:ILE:HG22	6:H:238:ALA:H	1.84	0.43
4:C:66:VAL:N	4:F:149:VAL:O	2.52	0.43
8:K:38:SER:N	8:K:460:ASP:OD1	2.51	0.43
7:I:173:THR:O	7:I:185:LYS:NZ	2.42	0.43
8:K:311:LYS:HG2	8:K:475:ARG:HD3	2.00	0.43
1:J:41:LYS:O	1:J:172:GLU:CB	2.67	0.43
2:A:59:LEU:HG	2:A:80:LYS:HA	1.99	0.43
3:D:142:LEU:HD12	3:D:160:ILE:HD11	2.01	0.43
4:C:456:GLY:O	4:C:457:ALA:C	2.56	0.43
4:F:10:LYS:HD2	4:F:10:LYS:HA	1.81	0.43
4:F:418:MET:HA	4:F:501:ALA:HB2	2.01	0.43
8:K:200:LEU:HD23	8:K:200:LEU:HA	1.87	0.43
8:K:276:VAL:HG12	8:K:277:LYS:N	2.33	0.43
1:J:77:PHE:HE1	1:J:93:GLY:HA3	1.83	0.43
8:K:380:HIS:CD2	8:K:380:HIS:H	2.36	0.43
2:A:22:LEU:HD21	2:A:106:ARG:HB3	2.01	0.43
8:K:244:ASP:OD2	8:K:249:ARG:NH1	2.51	0.43
1:J:32:ILE:HD13	1:J:195:ILE:HA	2.01	0.42
1:J:325:GLU:OE1	1:J:325:GLU:HA	2.19	0.42
5:G:40:ILE:HD12	5:G:176:LEU:HD22	2.01	0.42
8:K:149:TRP:O	8:K:150:ALA:C	2.57	0.42
8:K:332:ALA:HB2	8:K:451:LEU:HD13	2.02	0.42
1:J:404:TYR:HB2	1:J:414:GLU:HG2	2.01	0.42
2:A:148:ASP:HB2	2:A:209:ILE:HD12	2.00	0.42
3:D:27:ILE:H	3:D:27:ILE:HG13	1.73	0.42
4:C:256:SER:O	4:C:260:LYS:HG2	2.19	0.42
4:F:179:GLU:OE1	4:F:179:GLU:N	2.47	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:168:GLU:CG	1:J:171:ARG:HH12	2.23	0.42
1:J:376:TYR:OH	1:J:476:LYS:HD3	2.19	0.42
2:A:45:HIS:NE2	2:A:87:TYR:O	2.44	0.42
3:E:348:ASP:HB3	3:E:351:ARG:HB2	2.00	0.42
4:C:216:SER:O	4:C:220:ARG:HG2	2.19	0.42
4:F:323:LEU:HA	4:F:323:LEU:HD23	1.75	0.42
6:H:203:ILE:HD13	6:H:203:ILE:HA	1.87	0.42
8:K:299:LYS:HB2	8:K:299:LYS:HE2	1.39	0.42
8:K:518:LYS:HB2	8:K:518:LYS:HE2	1.77	0.42
4:F:547:ASP:O	5:G:55:LYS:NZ	2.41	0.42
6:H:73:ILE:HG23	6:H:132:ILE:HG23	2.00	0.42
8:K:104:ILE:O	8:K:105:THR:C	2.58	0.42
8:K:273:LYS:HA	8:K:273:LYS:HD3	1.26	0.42
8:K:276:VAL:HG13	8:K:312:GLU:HB3	2.01	0.42
3:D:59:ALA:HB3	3:D:61:LYS:HG2	2.01	0.42
4:C:448:GL3:N	4:C:449:TYR:N	2.67	0.42
8:K:149:TRP:HE3	8:K:153:LEU:HD11	1.84	0.42
1:J:153:ARG:H	1:J:153:ARG:HG3	1.43	0.42
4:F:256:SER:O	4:F:260:LYS:HB2	2.19	0.42
4:F:277:ARG:NH1	4:F:327:MET:SD	2.93	0.42
6:H:244:THR:HA	6:H:249:LEU:HD23	2.01	0.42
1:J:75:LYS:O	1:J:78:GLU:HB2	2.20	0.42
3:E:292:ASN:OD1	3:E:292:ASN:N	2.53	0.42
3:D:144:LYS:HB3	3:D:144:LYS:HE3	1.85	0.42
4:C:289:ILE:HG12	4:C:508:LEU:HD23	2.01	0.42
8:K:305:ASP:N	8:K:305:ASP:OD1	2.52	0.42
4:F:165:CYS:HB2	4:F:215:PRO:HG3	2.02	0.42
5:G:14:LYS:HB3	5:G:14:LYS:HE3	1.76	0.42
8:K:269:LYS:HE3	8:K:269:LYS:HB3	1.51	0.42
8:K:473:LYS:HG2	8:K:477:GLU:OE2	2.19	0.42
1:J:170:MET:HE3	1:J:170:MET:HB3	1.77	0.42
2:B:243:ARG:NH2	4:F:371:ASP:OD1	2.39	0.42
4:C:474:ARG:NH1	4:C:481:TYR:OH	2.53	0.42
4:C:553:LYS:HE2	5:G:4:ILE:HB	2.00	0.42
7:I:155:LYS:HE2	7:I:155:LYS:HB3	1.85	0.42
8:K:381:ARG:HB3	8:K:385:TYR:HB3	2.02	0.42
8:K:467:VAL:O	8:K:471:ILE:HG22	2.20	0.42
8:K:496:CYS:SG	8:K:497:ASP:N	2.92	0.42
4:C:110:ILE:HB	4:C:265:ILE:HB	2.02	0.42
6:H:157:LEU:HD23	6:H:157:LEU:HA	1.88	0.42
8:K:273:LYS:C	8:K:274:VAL:HG23	2.40	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:GLU:HG2	8:K:391:ILE:HA	2.02	0.41
5:G:30:LEU:HD23	5:G:30:LEU:HA	1.92	0.41
2:B:184:LYS:HE2	4:F:25:THR:HG23	2.02	0.41
3:D:50:LEU:HD23	3:D:50:LEU:HA	1.95	0.41
6:H:139:ASN:HA	6:H:162:GLY:HA3	2.02	0.41
8:K:180:LEU:O	8:K:183:GLN:N	2.53	0.41
1:J:15:LEU:O	1:J:16:GLU:C	2.59	0.41
1:J:417:TRP:HE1	2:B:185:THR:HA	1.86	0.41
6:H:263:GLU:HB3	6:H:273:LYS:HE3	2.00	0.41
8:K:468:ALA:HB2	8:K:491:PHE:CE1	2.55	0.41
1:J:44:THR:O	1:J:45:LYS:C	2.58	0.41
1:J:110:LYS:HD3	1:J:111:TRP:NE1	2.35	0.41
3:D:95:VAL:HG23	3:D:117:PRO:HG2	2.02	0.41
8:K:30:ASP:OD1	8:K:30:ASP:N	2.54	0.41
8:K:95:SER:O	8:K:96:VAL:C	2.59	0.41
1:J:103:SER:O	1:J:104:VAL:C	2.59	0.41
3:E:93:LEU:HD13	3:E:116:VAL:HG12	2.03	0.41
6:H:49:ILE:HD13	6:H:49:ILE:HA	1.90	0.41
6:H:282:GLU:H	6:H:282:GLU:HG2	1.71	0.41
1:J:19:ILE:HA	1:J:22:GLU:HB2	2.01	0.41
1:J:99:LEU:HD12	1:J:99:LEU:HA	1.73	0.41
1:J:448:LYS:HE2	1:J:448:LYS:HB3	1.89	0.41
2:A:98:PRO:HA	2:A:218:THR:HA	2.03	0.41
8:K:452:LEU:HB2	8:K:484:ILE:HD13	2.03	0.41
1:J:83:ILE:HD13	1:J:83:ILE:HA	1.88	0.41
2:B:121:SER:OG	10:E:601:F43:O7C	2.27	0.41
3:E:364:HIS:O	4:F:447:TYR:OH	2.39	0.41
4:F:180:LEU:HD23	4:F:180:LEU:HA	1.91	0.41
4:F:347:ASP:OD1	4:F:347:ASP:N	2.54	0.41
1:J:11:SER:O	1:J:12:GLY:C	2.59	0.41
1:J:63:GLU:O	1:J:64:ASN:C	2.58	0.41
1:J:72:LYS:HZ2	1:J:72:LYS:H	1.69	0.41
1:J:434:ASP:N	1:J:434:ASP:OD1	2.31	0.41
2:B:80:LYS:NZ	8:K:53:GLU:OE1	2.51	0.41
3:D:143:ILE:HD13	3:D:148:ILE:HB	2.03	0.41
4:F:137:MET:HA	4:F:140:ILE:HG22	2.03	0.41
8:K:213:THR:OG1	8:K:214:GLU:N	2.53	0.41
8:K:286:VAL:HG11	8:K:330:ILE:HG21	2.02	0.41
8:K:411:VAL:HG21	8:K:440:ALA:HB2	2.03	0.41
2:B:138:LYS:HD2	8:K:381:ARG:NH2	2.36	0.41
3:E:271:VAL:HG21	3:E:309:GLY:HA3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:98:ILE:HG22	4:C:321:ILE:HD11	2.01	0.41
7:I:56:GLU:HG2	7:I:59:TYR:OH	2.21	0.41
8:K:37:ARG:NH1	8:K:462:ILE:HD13	2.35	0.41
8:K:62:ILE:CD1	8:K:98:PHE:HB2	2.51	0.41
4:C:338:THR:HB	4:C:342:THR:HG23	2.03	0.41
4:C:447:TYR:HB3	4:C:448:GL3:N	2.35	0.41
8:K:268:MET:HG2	8:K:494:ASN:CG	2.41	0.41
8:K:520:LEU:HD23	8:K:520:LEU:HA	1.90	0.41
9:L:19:ILE:H	9:L:19:ILE:HG12	1.72	0.41
1:J:31:VAL:HG11	1:J:292:ILE:HA	2.03	0.40
1:J:81:SER:HA	1:J:163:ARG:CA	2.47	0.40
4:C:402:SER:HA	4:C:445:GLY:CA	2.51	0.40
4:C:430:TRP:HD1	4:C:431:TYR:CD1	2.40	0.40
4:F:444:LEU:HD23	4:F:450:ASP:HB3	2.04	0.40
6:H:231:ASP:OD1	6:H:231:ASP:N	2.38	0.40
8:K:203:LYS:HB2	8:K:203:LYS:HE2	1.91	0.40
8:K:272:GLU:H	8:K:272:GLU:HG2	1.49	0.40
8:K:332:ALA:HA	8:K:368:ILE:HG21	2.02	0.40
1:J:111:TRP:CE3	1:J:131:GLN:HA	2.56	0.40
1:J:250:ARG:HD2	1:J:270:TYR:CZ	2.56	0.40
3:E:358:GLY:HA2	3:E:361:PHE:CE2	2.57	0.40
4:F:327:MET:CE	13:F:602:SHT:P	3.09	0.40
8:K:359:LEU:HD13	8:K:359:LEU:HA	1.88	0.40
1:J:439:ALA:HB1	1:J:471:THR:HG23	2.02	0.40
3:E:53:ILE:HG13	3:E:174:ASN:HB2	2.03	0.40
4:C:385:LEU:HD21	4:C:437:HIS:CD2	2.57	0.40
8:K:170:LEU:HD23	8:K:170:LEU:HA	1.94	0.40
8:K:271:PHE:HE1	8:K:469:GLU:HB2	1.87	0.40
8:K:304:ILE:HD13	8:K:327:LEU:HD22	2.03	0.40
2:B:120:LEU:HB2	2:B:123:ARG:HB3	2.03	0.40
4:C:137:MET:HA	4:C:140:ILE:HG22	2.04	0.40
4:C:295:GLN:HB3	4:C:298:ARG:HD3	2.03	0.40
4:F:377:ALA:O	4:F:381:THR:OG1	2.32	0.40
6:H:114:LYS:NZ	6:H:142:SER:OG	2.42	0.40
8:K:184:ILE:HD12	8:K:184:ILE:H	1.85	0.40
8:K:232:VAL:O	8:K:233:ILE:C	2.59	0.40
4:C:325:ALA:HA	4:C:329:GLY:HA2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	493/501 (98%)	435 (88%)	47 (10%)	11 (2%)	5	1
2	A	257/260 (99%)	253 (98%)	4 (2%)	0	100	100
2	B	257/260 (99%)	252 (98%)	5 (2%)	0	100	100
3	D	440/443 (99%)	422 (96%)	18 (4%)	0	100	100
3	E	440/443 (99%)	422 (96%)	17 (4%)	1 (0%)	44	43
4	C	539/553 (98%)	515 (96%)	22 (4%)	2 (0%)	30	26
4	F	511/553 (92%)	490 (96%)	20 (4%)	1 (0%)	44	43
5	G	110/183 (60%)	107 (97%)	3 (3%)	0	100	100
6	H	294/304 (97%)	283 (96%)	11 (4%)	0	100	100
7	I	192/234 (82%)	183 (95%)	9 (5%)	0	100	100
8	K	519/531 (98%)	450 (87%)	57 (11%)	12 (2%)	5	1
9	L	45/93 (48%)	45 (100%)	0	0	100	100
All	All	4097/4358 (94%)	3857 (94%)	213 (5%)	27 (1%)	21	13

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	445	GLY
8	K	103	GLU
8	K	231	GLU
8	K	265	VAL
8	K	270	GLU
8	K	310	GLU
1	J	6	ASN
1	J	71	ASN
1	J	170	MET
1	J	133	ASP
1	J	136	GLU
1	J	165	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	K	76	GLU
8	K	348	ASP
1	J	11	SER
1	J	104	VAL
3	E	82	ALA
8	K	278	ASP
8	K	508	ILE
1	J	12	GLY
4	F	152	GLU
8	K	104	ILE
8	K	143	GLY
8	K	214	GLU
1	J	167	ILE
1	J	117	VAL
4	C	145	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	452/454 (100%)	377 (83%)	75 (17%)	2	0
2	A	223/224 (100%)	212 (95%)	11 (5%)	21	17
2	B	223/224 (100%)	219 (98%)	4 (2%)	54	57
3	D	341/342 (100%)	332 (97%)	9 (3%)	41	41
3	E	341/342 (100%)	327 (96%)	14 (4%)	26	23
4	C	437/439 (100%)	415 (95%)	22 (5%)	20	16
4	F	412/439 (94%)	389 (94%)	23 (6%)	17	13
5	G	104/168 (62%)	95 (91%)	9 (9%)	8	4
6	H	264/271 (97%)	248 (94%)	16 (6%)	15	11
7	I	160/186 (86%)	149 (93%)	11 (7%)	13	8
8	K	449/458 (98%)	378 (84%)	71 (16%)	2	0
9	L	43/81 (53%)	41 (95%)	2 (5%)	22	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3449/3628 (95%)	3182 (92%)	267 (8%)	13 5

All (267) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	1	MET
1	J	8	ASN
1	J	11	SER
1	J	13	LYS
1	J	14	THR
1	J	15	LEU
1	J	17	ASP
1	J	20	LYS
1	J	21	ASP
1	J	23	TYR
1	J	44	THR
1	J	45	LYS
1	J	46	LYS
1	J	48	LEU
1	J	49	ILE
1	J	50	LYS
1	J	52	THR
1	J	53	LYS
1	J	60	ILE
1	J	65	GLU
1	J	66	THR
1	J	68	ASP
1	J	72	LYS
1	J	77	PHE
1	J	78	GLU
1	J	80	LYS
1	J	85	LYS
1	J	87	ILE
1	J	88	SER
1	J	90	VAL
1	J	99	LEU
1	J	101	VAL
1	J	105	LYS
1	J	109	LYS
1	J	110	LYS
1	J	114	VAL
1	J	116	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	121	ASP
1	J	124	GLU
1	J	126	ASN
1	J	127	LEU
1	J	132	ARG
1	J	133	ASP
1	J	134	VAL
1	J	135	LEU
1	J	137	LEU
1	J	141	GLU
1	J	145	ILE
1	J	148	LEU
1	J	153	ARG
1	J	155	LEU
1	J	156	LYS
1	J	161	ASP
1	J	163	ARG
1	J	164	ILE
1	J	168	GLU
1	J	169	GLN
1	J	170	MET
1	J	171	ARG
1	J	187	LYS
1	J	236	ARG
1	J	243	ASP
1	J	252	ARG
1	J	327	HIS
1	J	337	ILE
1	J	339	GLU
1	J	356	LYS
1	J	363	LYS
1	J	397	ARG
1	J	431	LYS
1	J	434	ASP
1	J	441	THR
1	J	446	LYS
1	J	472	ASN
1	J	480	ASN
2	A	4	THR
2	A	36	ASP
2	A	41	LYS
2	A	46	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	74	GLU
2	A	103	ASP
2	A	171	MET
2	A	172	MET
2	A	179	CYS
2	A	184	LYS
2	A	203	VAL
2	B	104	ARG
2	B	172	MET
2	B	197	LYS
2	B	203	VAL
3	E	2	VAL
3	E	61	LYS
3	E	65	LYS
3	E	97	GLU
3	E	98	ASP
3	E	99	ASP
3	E	100	ASP
3	E	114	VAL
3	E	136	MET
3	E	199	HIS
3	E	215	SER
3	E	327	VAL
3	E	336	ASP
3	E	410	HIS
3	D	98	ASP
3	D	114	VAL
3	D	126	GLU
3	D	170	TYR
3	D	199	HIS
3	D	301	LYS
3	D	322	ARG
3	D	327	VAL
3	D	428	PRO
4	C	26	LYS
4	C	63	ASP
4	C	78	LEU
4	C	149	VAL
4	C	178	ASP
4	C	184	PHE
4	C	190	LYS
4	C	239	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	C	244	LYS
4	C	263	ASP
4	C	334	THR
4	C	336	TYR
4	C	347	ASP
4	C	375	ASP
4	C	402	SER
4	C	444	LEU
4	C	447	TYR
4	C	449	TYR
4	C	450	ASP
4	C	522	VAL
4	C	529	ARG
4	C	538	ARG
4	F	29	THR
4	F	59	LEU
4	F	71	ARG
4	F	77	LYS
4	F	78	LEU
4	F	82	ASP
4	F	151	GLN
4	F	154	MET
4	F	183	ARG
4	F	207	LYS
4	F	260	LYS
4	F	274	ARG
4	F	277	ARG
4	F	281	GLU
4	F	300	SER
4	F	342	THR
4	F	347	ASP
4	F	423	SER
4	F	427	VAL
4	F	442	SER
4	F	447	TYR
4	F	509	ASN
4	F	527	LYS
5	G	5	ASP
5	G	19	ARG
5	G	45	VAL
5	G	47	TYR
5	G	56	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	G	153	ASP
5	G	154	LYS
5	G	167	GLU
5	G	179	GLU
6	H	34	MET
6	H	37	ASP
6	H	40	MET
6	H	77	SER
6	H	84	HIS
6	H	90	CYS
6	H	91	ASP
6	H	93	SER
6	H	120	ARG
6	H	146	ASP
6	H	151	PHE
6	H	178	ARG
6	H	211	SER
6	H	225	GLU
6	H	269	LYS
6	H	293	SER
7	I	16	MET
7	I	27	ARG
7	I	37	ASP
7	I	59	TYR
7	I	67	GLN
7	I	104	ARG
7	I	107	LEU
7	I	125	LEU
7	I	169	VAL
7	I	173	THR
7	I	195	LYS
8	K	1	MET
8	K	15	ASP
8	K	66	VAL
8	K	75	VAL
8	K	76	GLU
8	K	87	CYS
8	K	89	THR
8	K	91	TYR
8	K	94	LYS
8	K	98	PHE
8	K	101	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	K	104	ILE
8	K	109	LYS
8	K	118	ARG
8	K	133	MET
8	K	144	LYS
8	K	151	LEU
8	K	152	ASN
8	K	155	LYS
8	K	186	LYS
8	K	197	THR
8	K	199	THR
8	K	202	PRO
8	K	203	LYS
8	K	206	LYS
8	K	218	LYS
8	K	227	SER
8	K	230	PRO
8	K	232	VAL
8	K	236	LEU
8	K	239	LYS
8	K	245	LYS
8	K	249	ARG
8	K	255	LYS
8	K	259	GLU
8	K	260	GLU
8	K	268	MET
8	K	269	LYS
8	K	272	GLU
8	K	273	LYS
8	K	277	LYS
8	K	278	ASP
8	K	287	GLU
8	K	289	ARG
8	K	291	VAL
8	K	295	ARG
8	K	299	LYS
8	K	305	ASP
8	K	306	VAL
8	K	307	SER
8	K	320	SER
8	K	339	LYS
8	K	342	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	K	349	GLU
8	K	351	VAL
8	K	355	LYS
8	K	359	LEU
8	K	361	ARG
8	K	365	LYS
8	K	390	SER
8	K	415	GLU
8	K	459	MET
8	K	460	ASP
8	K	463	THR
8	K	465	ASN
8	K	469	GLU
8	K	471	ILE
8	K	481	THR
8	K	486	SER
8	K	497	ASP
8	K	514	ASP
9	L	14	SER
9	L	44	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	459	ASN
8	K	102	ASN
8	K	210	ASN
8	K	228	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 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
4	MHS	C	261	4	7,11,12	0.78	0	6,14,16	1.00	0
4	MHS	F	261	4	7,11,12	0.78	0	6,14,16	0.87	0
4	MGN	C	403	-	6,9,10	0.69	0	5,12,14	0.74	0
4	AGM	F	275	4	10,11,12	0.45	0	6,13,15	0.26	0
4	MGN	F	403	4	6,9,10	0.68	0	5,12,14	0.76	0
4	GL3	F	448	4	2,3,4	0.48	0	1,2,4	0.35	0
4	SMC	F	455	4	5,6,7	0.71	0	2,6,8	0.81	0
4	GL3	C	448	-	2,3,4	1.40	0	1,2,4	0.17	0
4	AGM	C	275	3,4	10,11,12	0.36	0	6,13,15	0.69	0
4	SMC	C	455	4	5,6,7	0.80	0	2,6,8	1.69	0

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
4	MHS	C	261	4	-	2/5/6/8	0/1/1/1
4	MHS	F	261	4	-	2/5/6/8	0/1/1/1
4	MGN	C	403	-	-	1/7/9/12	-
4	AGM	F	275	4	-	6/10/11/13	-
4	MGN	F	403	4	-	0/7/9/12	-
4	GL3	F	448	4	-	1/1/1/2	-
4	SMC	F	455	4	-	2/3/5/7	-
4	GL3	C	448	-	-	1/1/1/2	-
4	AGM	C	275	3,4	-	1/10/11/13	-
4	SMC	C	455	4	-	2/3/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	261	MHS	O-C-CA-CB
4	C	448	GL3	S-C-CA-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	455	SMC	N-CA-CB-SG
4	C	455	SMC	CA-CB-SG-CS
4	F	261	MHS	N-CA-CB-CG
4	F	261	MHS	C-CA-CB-CG
4	F	275	AGM	N-CA-CB-CG
4	F	275	AGM	C-CA-CB-CG
4	F	275	AGM	NH1-CZ-NE1-CD
4	F	275	AGM	NH2-CZ-NE1-CD
4	F	448	GL3	S-C-CA-N
4	F	455	SMC	N-CA-CB-SG
4	F	455	SMC	CA-CB-SG-CS
4	F	275	AGM	CE2-CD-NE1-CZ
4	C	275	AGM	CE2-CD-NE1-CZ
4	C	261	MHS	N-CA-CB-CG
4	C	403	MGN	O-C-CA-CB2
4	F	275	AGM	NE1-CD-CG-CB

There are no ring outliers.

3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	261	MHS	1	0
4	C	448	GL3	12	0
4	C	455	SMC	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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
14	S5Q	I	202	7	18,30,30	2.61	11 (61%)	-		
11	COM	C	601	10	6,6,6	1.81	3 (50%)	7,8,8	2.81	4 (57%)
16	ATP	K	603	17	26,33,33	0.88	0	31,52,52	0.81	1 (3%)
10	F43	A	601	11,4	61,71,71	2.04	4 (6%)	64,118,118	1.11	4 (6%)
13	SHT	F	602	-	26,27,27	2.04	7 (26%)	30,36,36	2.00	6 (20%)
12	TP7	F	601	-	19,20,20	0.68	0	24,26,26	0.58	0
14	S5Q	H	401	6	18,30,30	2.60	12 (66%)	-		
16	ATP	K	602	17	26,33,33	0.97	2 (7%)	31,52,52	0.75	1 (3%)
10	F43	E	601	-	61,71,71	1.96	4 (6%)	64,118,118	1.03	5 (7%)
14	S5Q	I	201	7	18,30,30	2.59	11 (61%)	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	COM	C	601	10	-	0/4/4/4	-
16	ATP	K	603	17	-	4/18/38/38	0/3/3/3
10	F43	A	601	11,4	-	14/28/185/185	-
13	SHT	F	602	-	1/1/6/9	17/31/31/31	-
12	TP7	F	601	-	-	5/24/24/24	-
16	ATP	K	602	17	-	3/18/38/38	0/3/3/3
10	F43	E	601	-	-	9/28/185/185	-

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	601	F43	NI-NA	9.76	2.10	1.89
10	E	601	F43	NI-NA	9.38	2.09	1.89
10	A	601	F43	NI-NB	9.21	2.09	1.89
10	E	601	F43	NI-NB	9.08	2.09	1.89
10	A	601	F43	NI-ND	7.16	2.04	1.89
10	E	601	F43	NI-ND	6.82	2.04	1.89
13	F	602	SHT	CK-N	5.81	1.48	1.34
14	H	401	S5Q	S3B-FE6	-4.33	2.21	2.32
14	I	202	S5Q	S4B-FE7	-4.33	2.21	2.32
14	H	401	S5Q	S4B-FE7	-4.32	2.21	2.32
14	I	201	S5Q	S4B-FE7	-4.30	2.21	2.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	I	202	S5Q	S3B-FE6	-4.27	2.21	2.32
14	I	201	S5Q	S3B-FE6	-4.23	2.22	2.32
13	F	602	SHT	CD-SG2	3.94	1.83	1.77
13	F	602	SHT	P-O3'	3.75	1.66	1.59
14	I	201	S5Q	S1B-FE6	-3.47	2.23	2.32
14	H	401	S5Q	S1B-FE6	-3.44	2.23	2.32
13	F	602	SHT	CK1-CK	3.39	1.55	1.48
14	I	202	S5Q	S1B-FE6	-3.37	2.24	2.32
14	H	401	S5Q	S2A-FE2	-3.20	2.24	2.32
14	I	202	S5Q	S2A-FE2	-3.18	2.24	2.32
14	I	202	S5Q	S3B-FE7	-3.17	2.24	2.32
11	C	601	COM	C2-S2	3.15	1.82	1.77
14	I	201	S5Q	S3B-FE7	-3.15	2.24	2.32
14	I	201	S5Q	S2A-FE2	-3.08	2.24	2.32
14	H	401	S5Q	S3B-FE7	-3.08	2.24	2.32
14	I	201	S5Q	S2B-FE6	-3.01	2.17	2.24
14	I	201	S5Q	S4A-FE3	-2.96	2.25	2.32
14	H	401	S5Q	S2B-FE6	-2.95	2.17	2.24
14	I	202	S5Q	S2B-FE6	-2.92	2.18	2.24
14	I	202	S5Q	S4A-FE3	-2.92	2.25	2.32
14	H	401	S5Q	S4A-FE3	-2.87	2.25	2.32
13	F	602	SHT	OK-CK	-2.70	1.19	1.24
14	I	202	S5Q	S4B-FE5	-2.64	2.25	2.32
14	I	202	S5Q	S1B-FE5	-2.63	2.25	2.32
14	I	201	S5Q	S4B-FE5	-2.61	2.25	2.32
14	H	401	S5Q	S1B-FE5	-2.60	2.26	2.32
14	I	201	S5Q	S1B-FE5	-2.58	2.26	2.32
10	A	601	F43	C4C-NC	2.56	1.39	1.35
14	H	401	S5Q	S4B-FE5	-2.56	2.26	2.32
10	E	601	F43	C4C-NC	2.53	1.39	1.35
14	I	202	S5Q	S2A-FE3	-2.44	2.26	2.32
14	H	401	S5Q	S2A-FE3	-2.43	2.26	2.32
14	I	201	S5Q	S2A-FE3	-2.30	2.26	2.32
14	I	202	S5Q	S1A-FE2	-2.30	2.26	2.32
13	F	602	SHT	OS1-SG2	2.27	1.51	1.45
14	H	401	S5Q	S1A-FE2	-2.25	2.26	2.32
13	F	602	SHT	OS3-SG2	2.20	1.51	1.45
14	I	201	S5Q	S1A-FE2	-2.20	2.26	2.32
11	C	601	COM	O1S-S2	2.10	1.51	1.45
16	K	602	ATP	PG-O3G	-2.07	1.46	1.54
16	K	602	ATP	PG-O2G	-2.05	1.46	1.54
14	H	401	S5Q	S2B-FE2	-2.05	2.20	2.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	601	COM	O2S-S2	2.03	1.51	1.45

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F	602	SHT	CK3-CK2-CK1	-6.48	111.95	125.85
13	F	602	SHT	OS1-SG2-CD	4.10	111.85	106.92
11	C	601	COM	O2S-S2-C2	3.90	111.61	106.92
11	C	601	COM	O1S-S2-C2	3.80	111.49	106.92
11	C	601	COM	O2S-S2-O1S	-3.77	100.91	113.95
13	F	602	SHT	OS1-SG2-OS3	-3.64	101.36	113.95
13	F	602	SHT	OS3-SG2-CD	3.62	111.27	106.92
10	A	601	F43	C2B-C1B-NB	3.45	107.01	101.84
10	A	601	F43	C3D-C4D-ND	3.24	107.38	102.34
10	E	601	F43	C2A-C3A-C4A	-3.22	97.45	102.36
10	E	601	F43	C3D-C4D-ND	3.14	107.22	102.34
11	C	601	COM	O3S-S2-C2	3.03	110.67	105.77
13	F	602	SHT	CK1-CK-N	2.99	120.30	114.56
10	E	601	F43	C2B-C3B-C4B	-2.80	98.47	101.63
10	A	601	F43	C4B-CHC-C1C	2.69	130.24	125.84
10	A	601	F43	C2A-C3A-C4A	-2.43	98.65	102.36
10	E	601	F43	C9D-C3D-C4D	-2.38	108.39	114.67
13	F	602	SHT	OS2-SG2-CD	2.35	109.57	105.77
16	K	602	ATP	C5-C6-N6	2.24	123.76	120.35
10	E	601	F43	C3D-C2D-C1D	2.06	106.17	102.69
16	K	603	ATP	C5-C6-N6	2.05	123.47	120.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	F	602	SHT	CB

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	601	F43	C2A-C3A-CAA-CBA
10	A	601	F43	C4A-C3A-CAA-CBA
10	E	601	F43	C1A-C2A-C5A-C6A
10	E	601	F43	C9A-C2A-C5A-C6A
10	E	601	F43	C2A-C3A-CAA-CBA
13	F	602	SHT	CD-CC-S1-SK
13	F	602	SHT	CC-CD-SG2-OS3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	F	602	SHT	CC-CD-SG2-OS1
13	F	602	SHT	CC-CD-SG2-OS2
13	F	602	SHT	S1-CC-CD-SG2
13	F	602	SHT	O-C-CA-N
13	F	602	SHT	C-CA-CB-CG2
13	F	602	SHT	C-CA-CB-O3'
12	F	601	TP7	O1-C1-N-CA
12	F	601	TP7	C2-C3-C4-C5
12	F	601	TP7	C2-C1-N-CA
13	F	602	SHT	CK3-CK4-CK5-CK6
10	A	601	F43	C3C-C8C-C9C-CAC
13	F	602	SHT	CK5-CK6-SK-S1
13	F	602	SHT	CK2-CK3-CK4-CK5
12	F	601	TP7	C3-C4-C5-C6
13	F	602	SHT	OXT-C-CA-N
13	F	602	SHT	N-CA-CB-CG2
13	F	602	SHT	N-CA-CB-O3'
12	F	601	TP7	C4-C5-C6-C7
10	A	601	F43	C2C-C3C-C8C-C9C
10	A	601	F43	C3C-C2C-C5C-C6C
10	A	601	F43	C2C-C5C-C6C-O8C
16	K	602	ATP	PB-O3B-PG-O3G
16	K	602	ATP	PG-O3B-PB-O2B
13	F	602	SHT	N-CK-CK1-CK2
13	F	602	SHT	OK-CK-CK1-CK2
10	A	601	F43	C1C-C2C-C5C-C6C
10	E	601	F43	C4A-C3A-CAA-CBA
10	E	601	F43	C1C-C2C-C5C-C6C
10	A	601	F43	C2C-C5C-C6C-O7C
10	E	601	F43	C2B-C3B-CAB-CBB
16	K	603	ATP	PG-O3B-PB-O2B
10	E	601	F43	CAB-CBB-CCB-ODB
10	A	601	F43	C4C-C3C-C8C-C9C
10	A	601	F43	C8C-C9C-CAC-OCC
10	A	601	F43	C8C-C9C-CAC-OBC
16	K	602	ATP	PG-O3B-PB-O1B
10	A	601	F43	CAA-CBA-CCA-ODA
10	E	601	F43	CAB-CBB-CCB-OEB
10	A	601	F43	CAB-CBB-CCB-ODB
16	K	603	ATP	PB-O3B-PG-O2G
10	A	601	F43	CAA-CBA-CCA-OEA
13	F	602	SHT	CB-O3'-P-O2P

Continued on next page...

Continued from previous page...

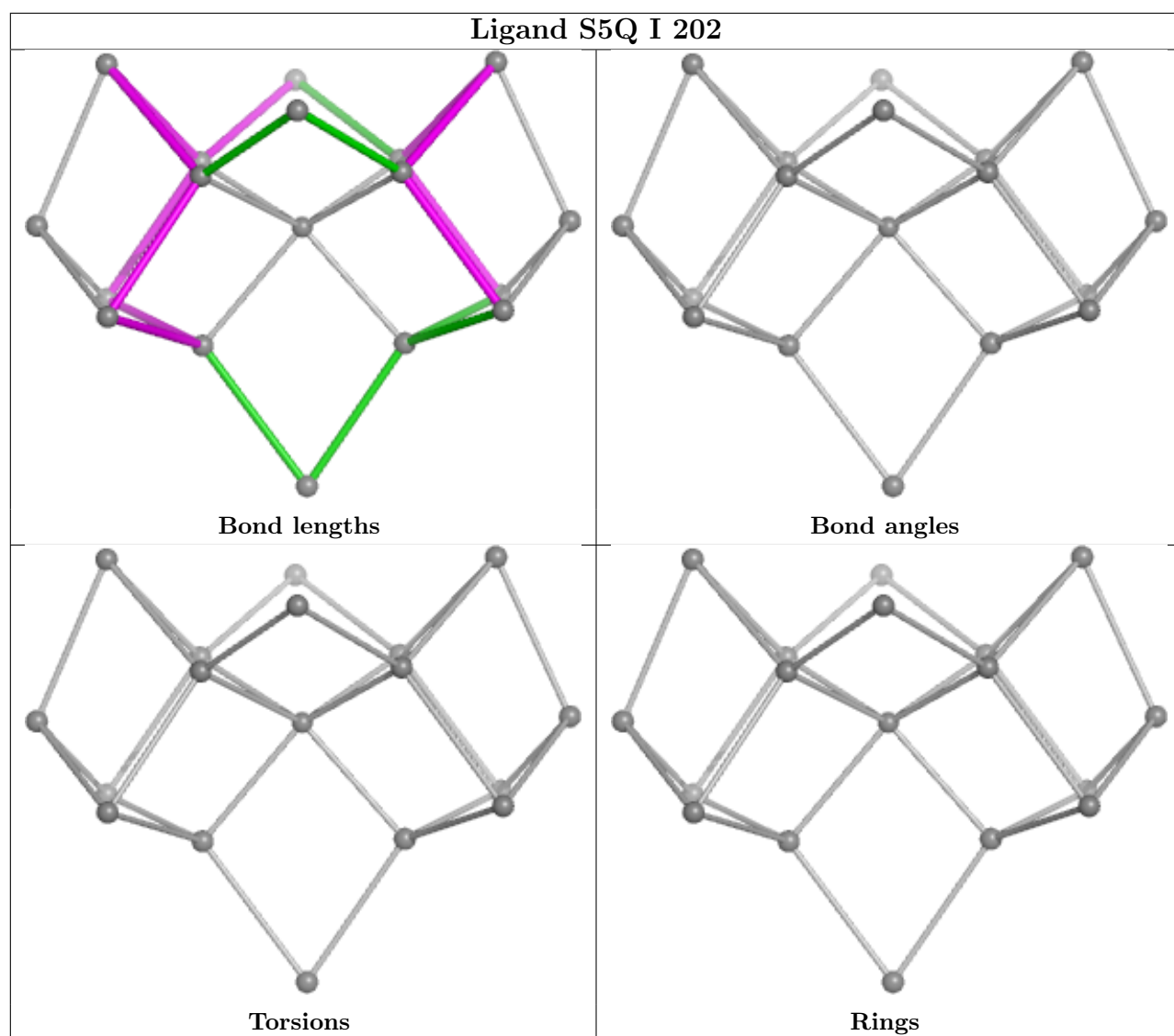
Mol	Chain	Res	Type	Atoms
16	K	603	ATP	PG-O3B-PB-O1B
16	K	603	ATP	PA-O3A-PB-O1B
10	E	601	F43	C3A-CAA-CBA-CCA

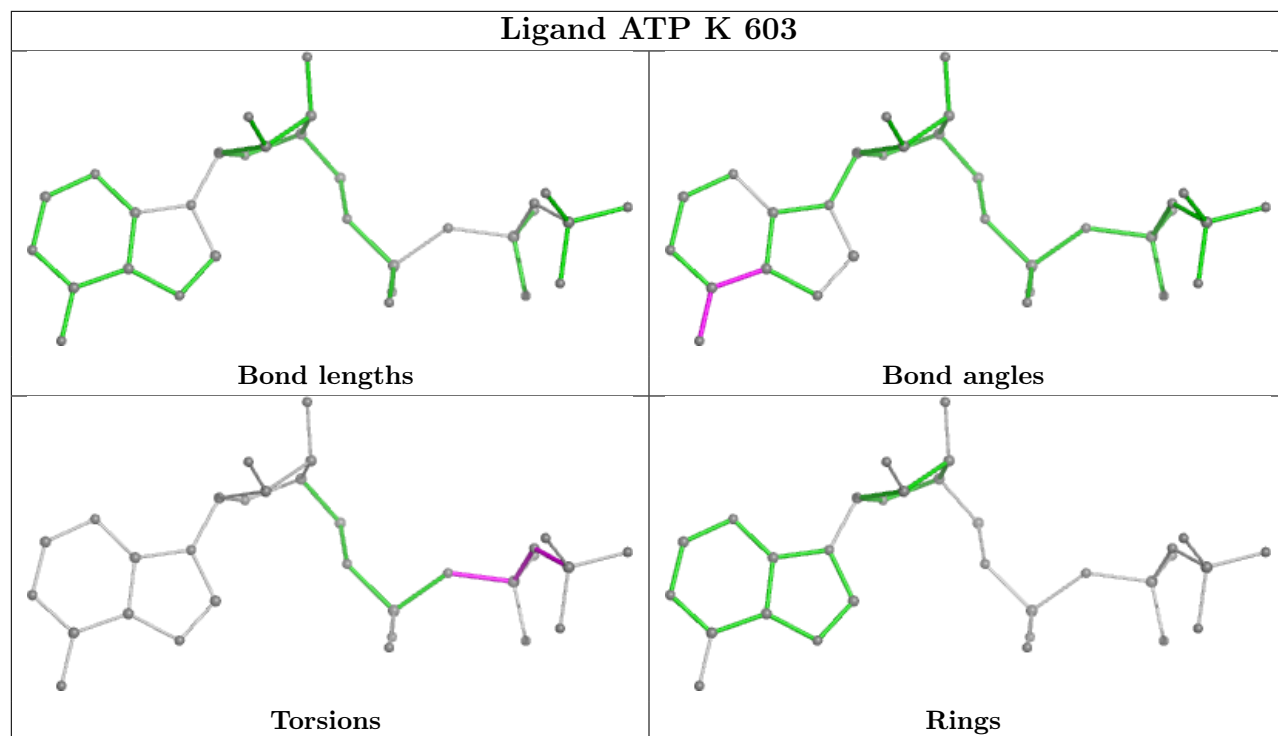
There are no ring outliers.

6 monomers are involved in 37 short contacts:

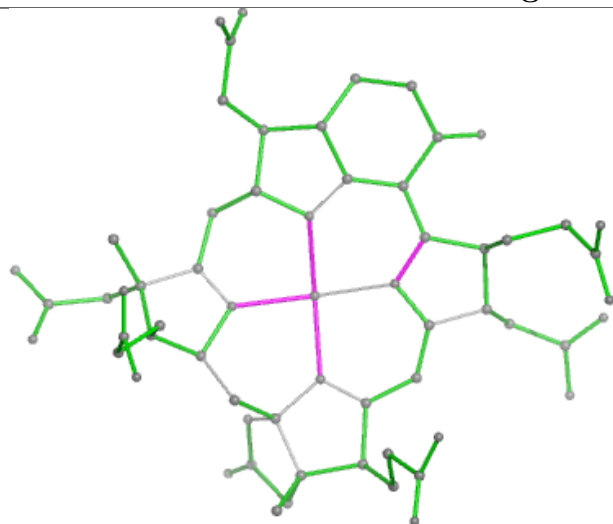
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	601	COM	3	0
16	K	603	ATP	2	0
10	A	601	F43	7	0
13	F	602	SHT	15	0
12	F	601	TP7	3	0
10	E	601	F43	10	0

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.

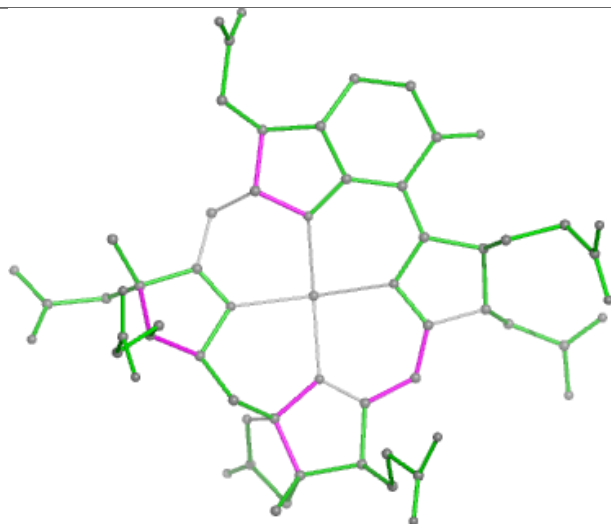




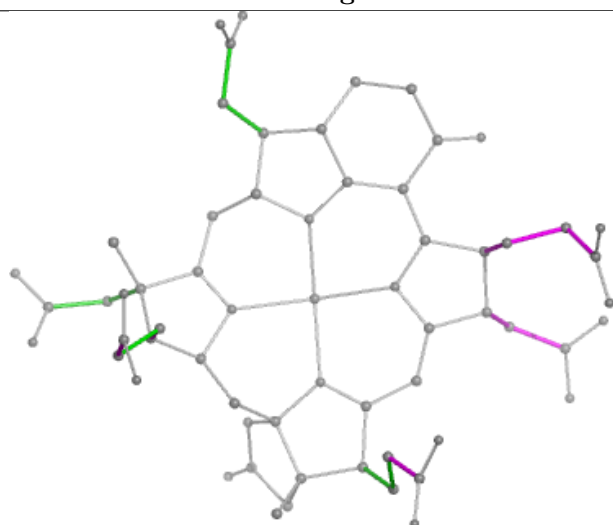
Ligand F43 A 601



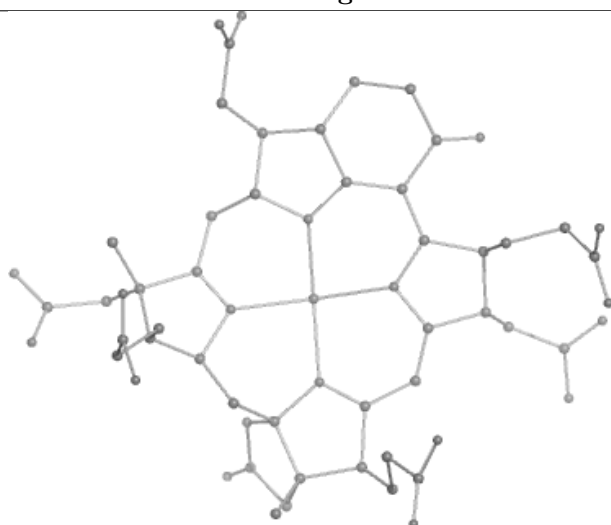
Bond lengths



Bond angles

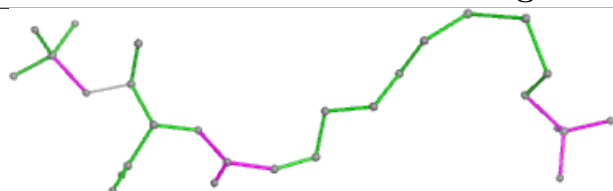


Torsions

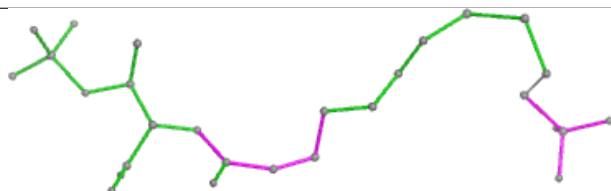


Rings

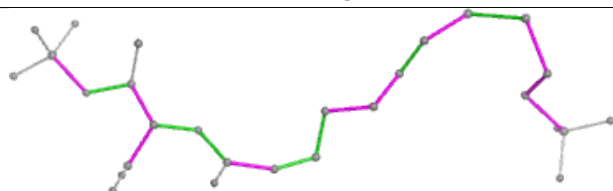
Ligand SHT F 602



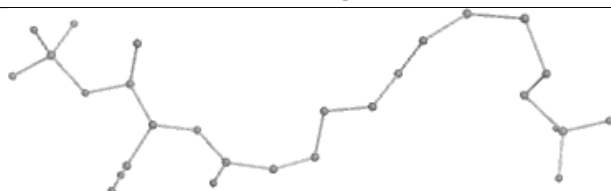
Bond lengths



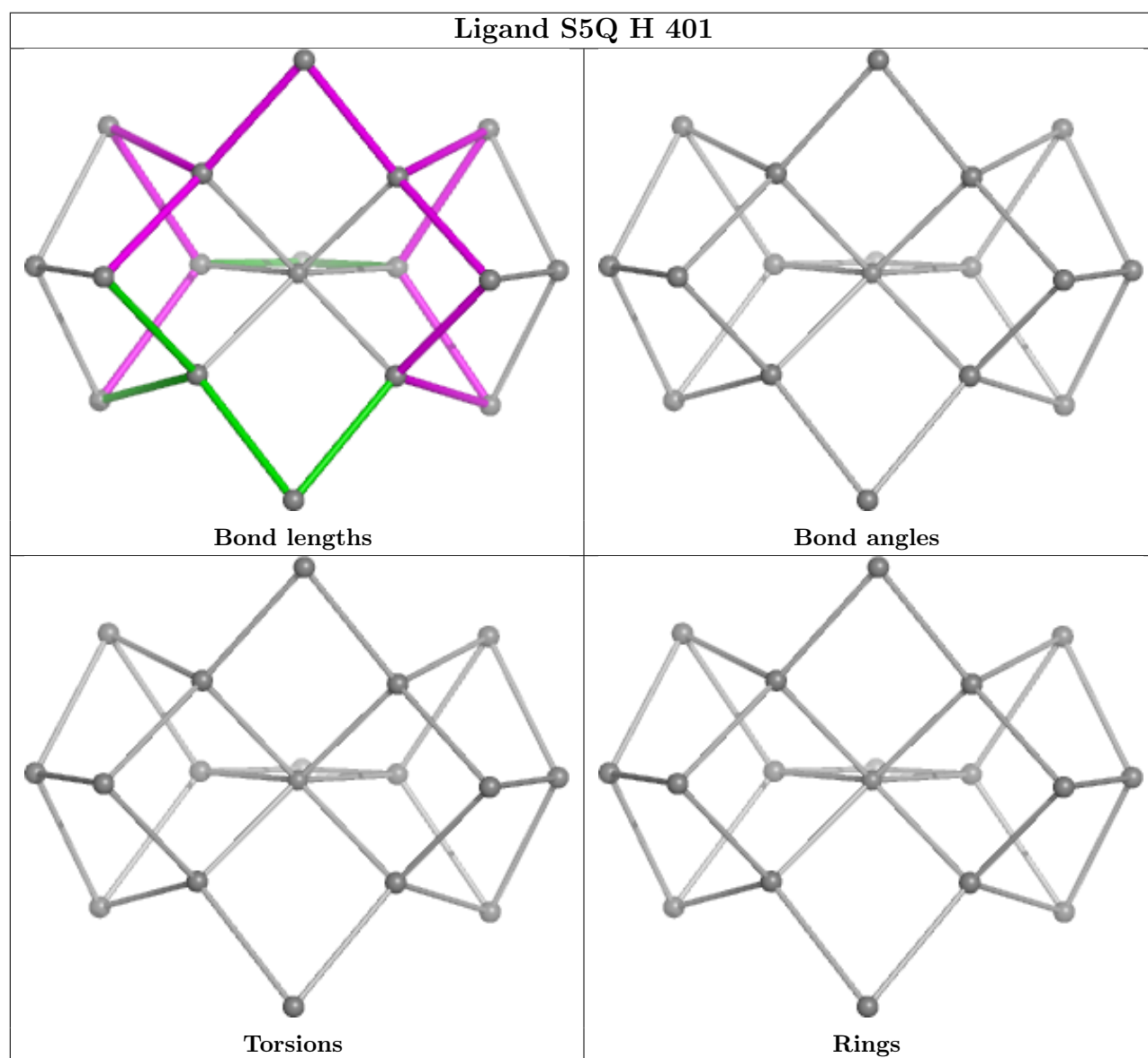
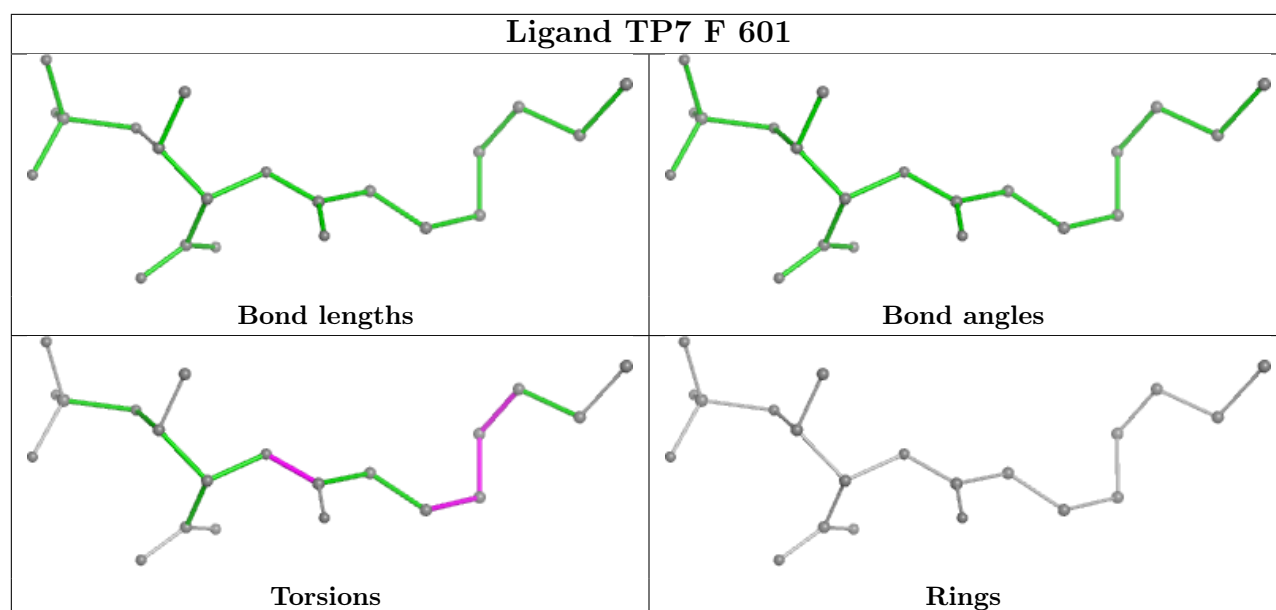
Bond angles

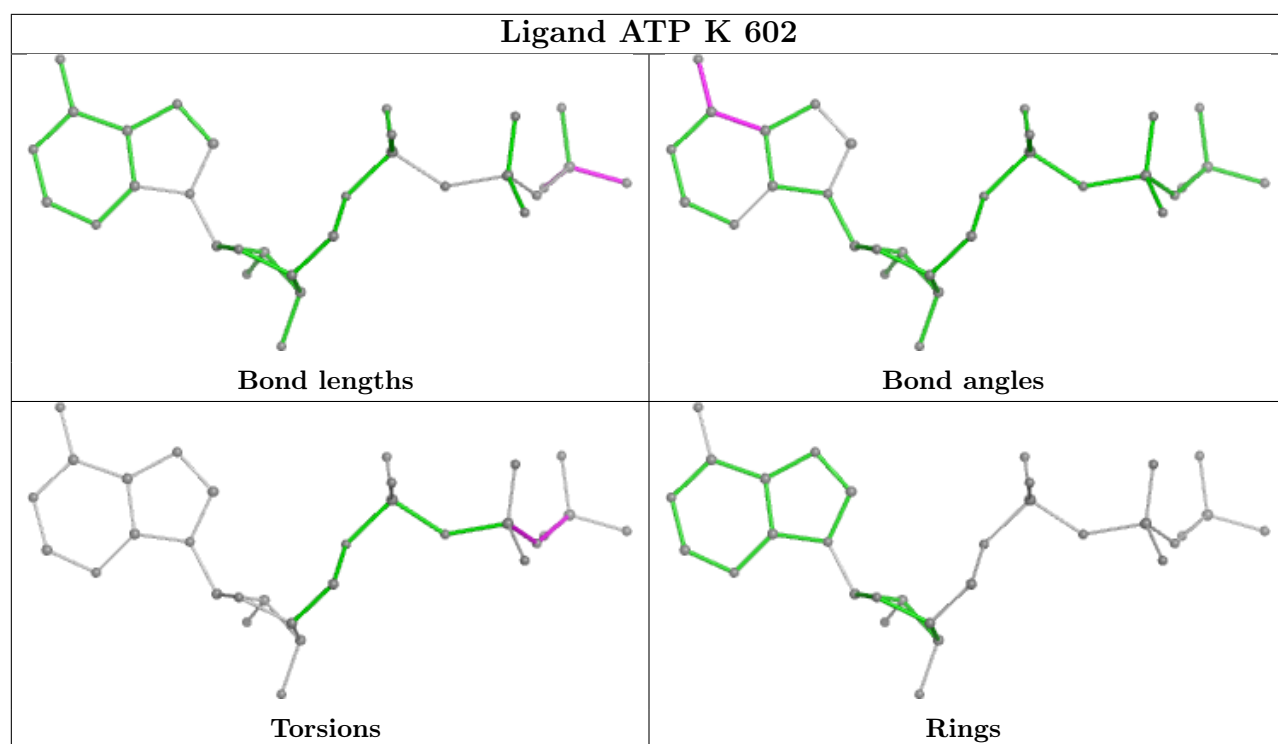


Torsions

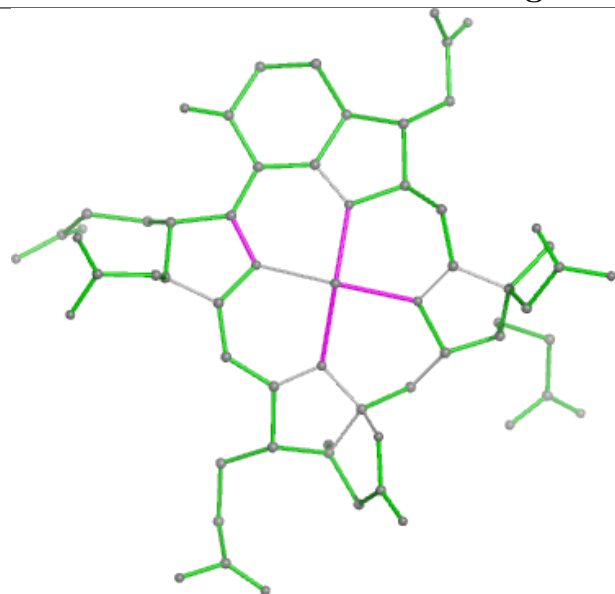


Rings

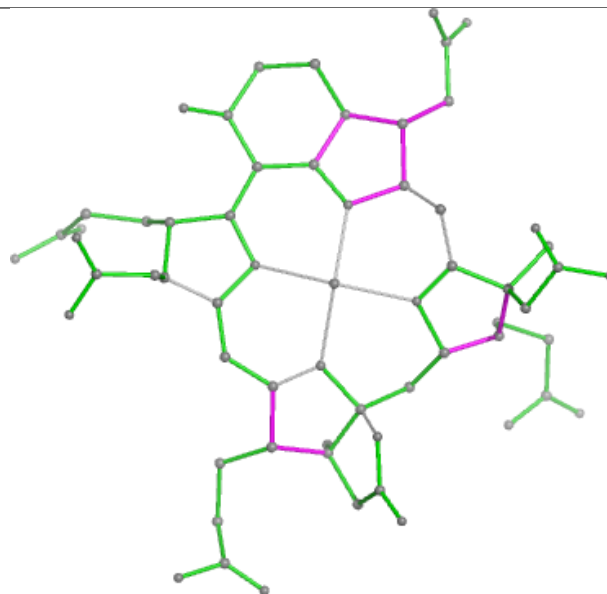




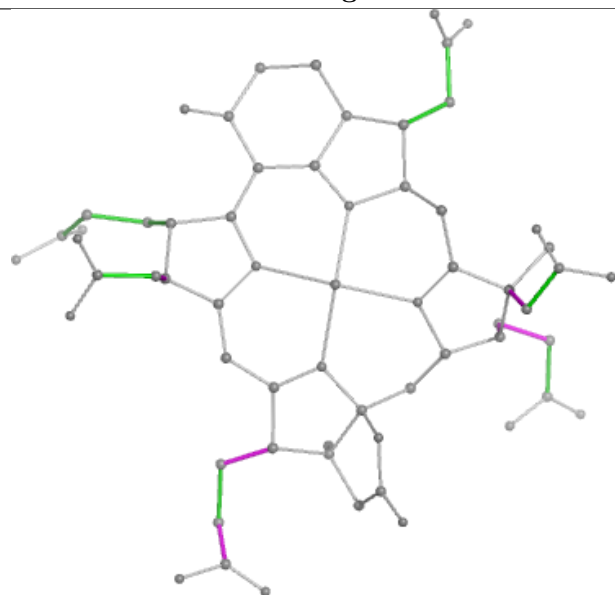
Ligand F43 E 601



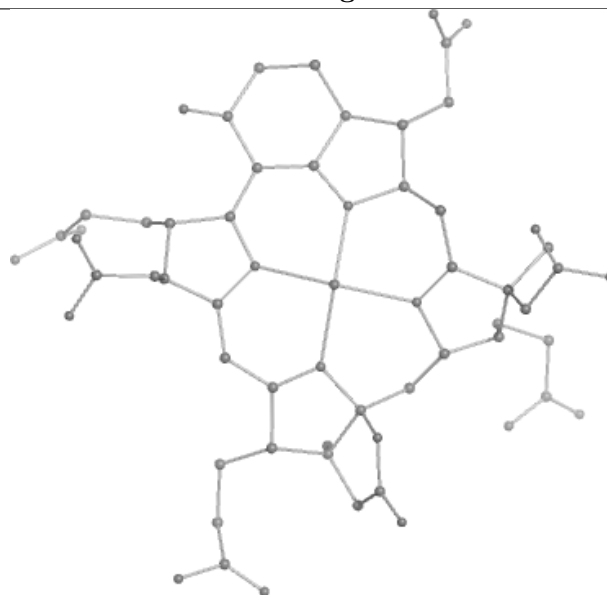
Bond lengths



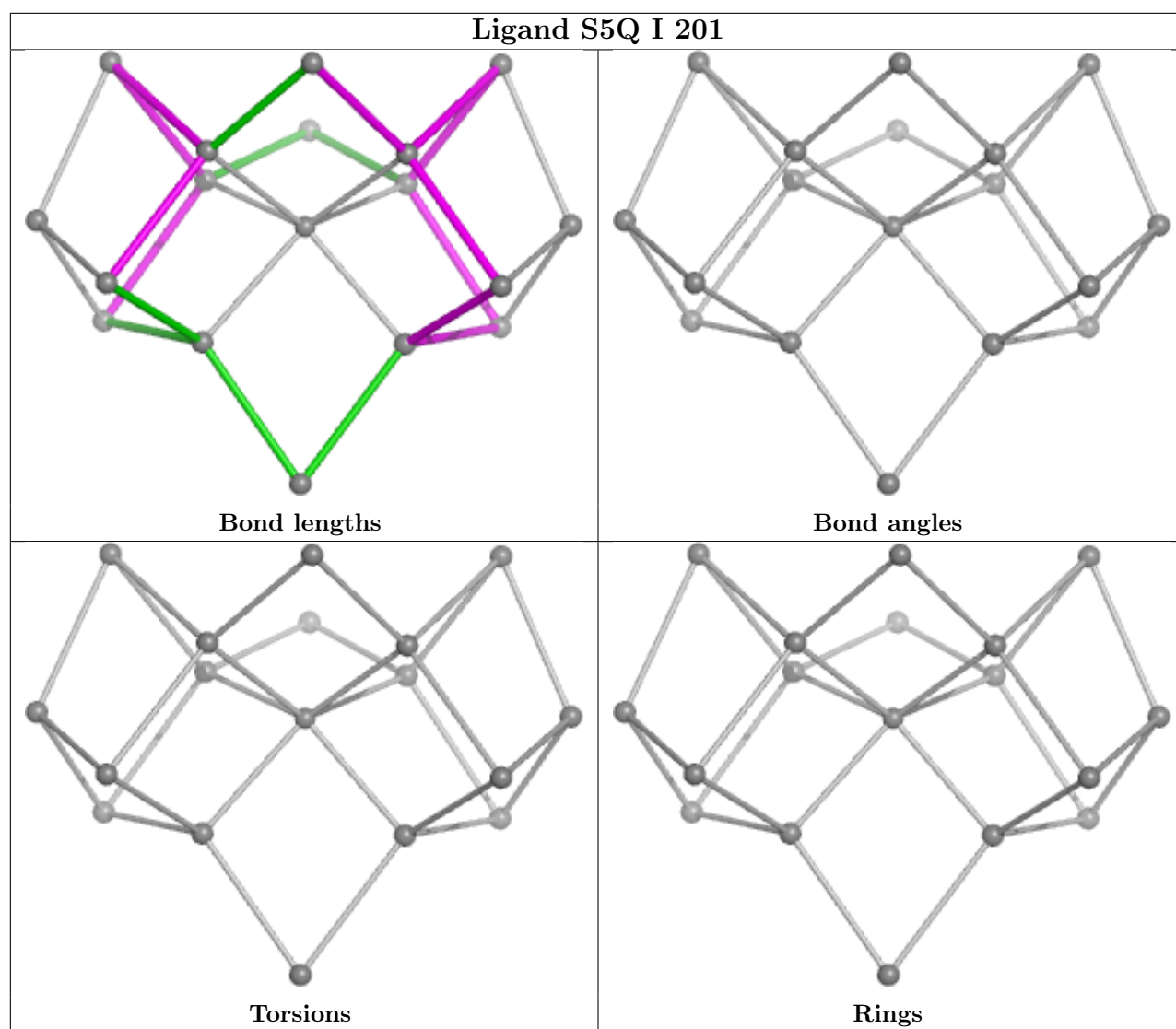
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	C	4
1	J	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	183:THR	C	184:ASN	N	3.52
1	C	402:SER	C	403:MGN	N	3.12
1	C	403:MGN	C	404:ARG	N	3.07
1	C	447:TYR	C	448:GL3	N	3.00
1	J	22:GLU	C	23:TYR	N	2.59
1	C	448:GL3	C	449:TYR	N	2.37