



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 02:55 AM UTC

PDB ID : 1ACA / pdb_00001aca
Title : THREE-DIMENSIONAL STRUCTURE OF THE COMPLEX BETWEEN
ACYL-COENZYME A BINDING PROTEIN AND PALMITOYL-
COENZYME A
Authors : Kragelund, B.B.; Andersen, K.V.; Madsen, J.C.; Knudsen, J.; Poulsen, F.M.
Deposited on : 1992-11-17

This is a Full wwPDB NMR Structure 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/NMRValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

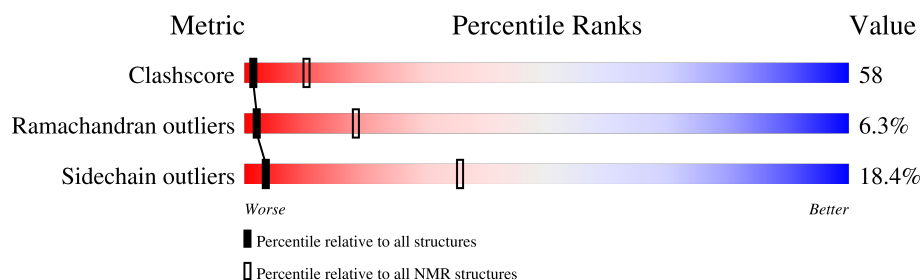
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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	A	86	7% 47% 33% 14%

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

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
2	A	COA	87	20	-

2 Ensemble composition and analysis

This entry contains 20 models. Model 19 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:4-A:41, A:51-A:86 (74)	0.58	19

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	2, 4, 6, 7, 9, 10, 13, 15, 17, 19, 20
2	5, 8, 16, 18
3	3, 11, 12, 14
Single-model clusters	1

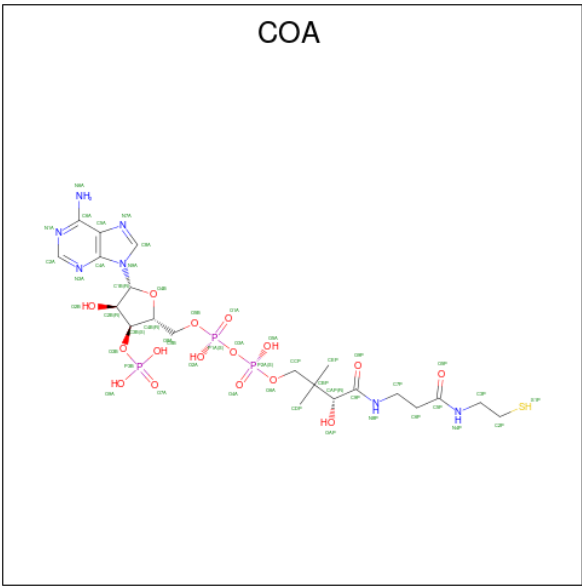
3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1518 atoms, of which 755 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ACYL-COENZYME A BINDING PROTEIN.

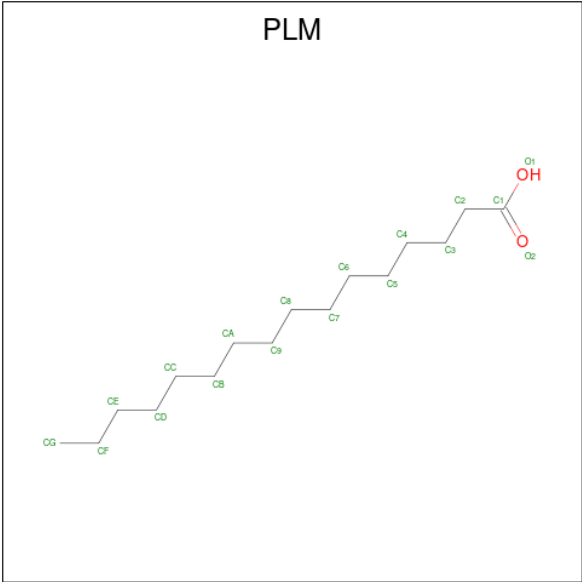
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	86	1391	445	693	114	136	3	0

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms						
			Total	C	H	N	O	P	S
2	A	1	79	21	31	7	16	3	1

- Molecule 3 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



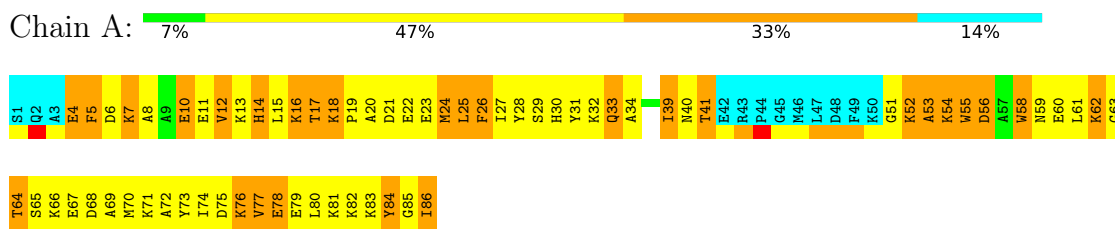
Mol	Chain	Residues	Atoms			
			Total	C	H	O
3	A	1	48	16	31	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

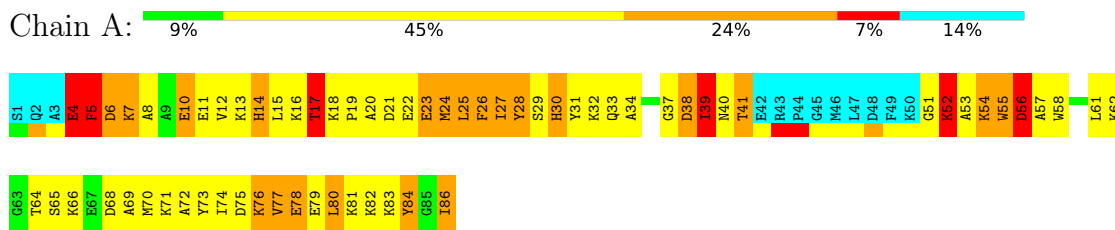


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

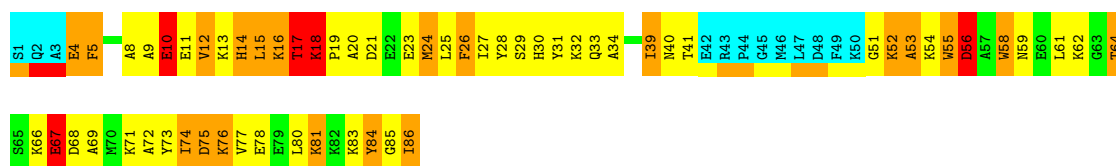
- Molecule 1: ACYL-COENZYME A BINDING PROTEIN



4.2.2 Score per residue for model 2

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

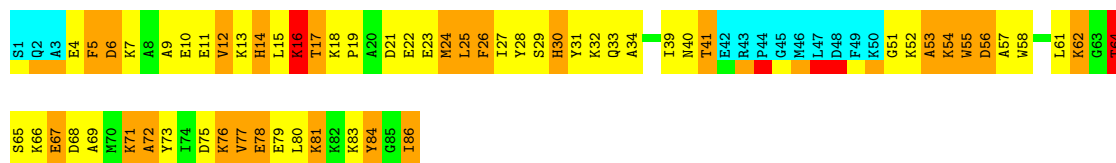




4.2.3 Score per residue for model 3

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

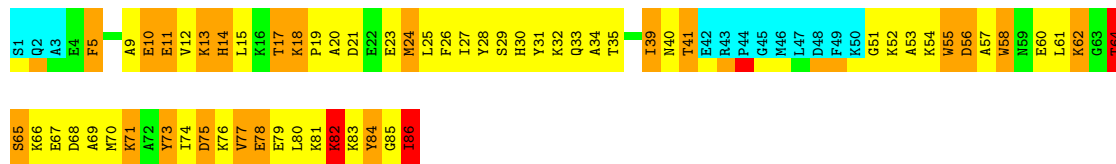
Chain A: 15% 41% 28% • 14%



4.2.4 Score per residue for model 4

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

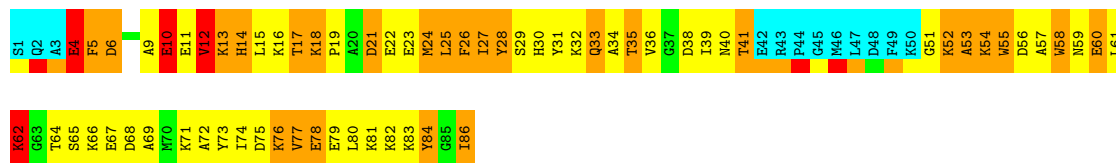
Chain A: 14% 44% 24% • 14%



4.2.5 Score per residue for model 5

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

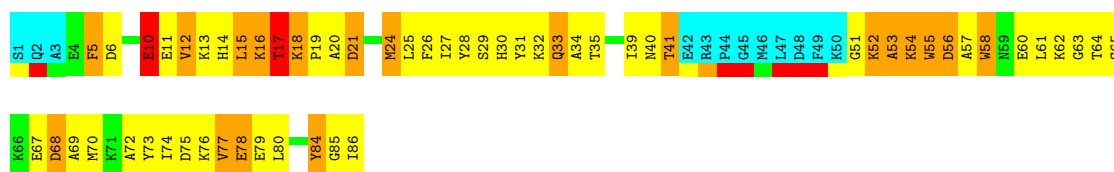
Chain A: 8% 43% 30% 5% 14%



4.2.6 Score per residue for model 6

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

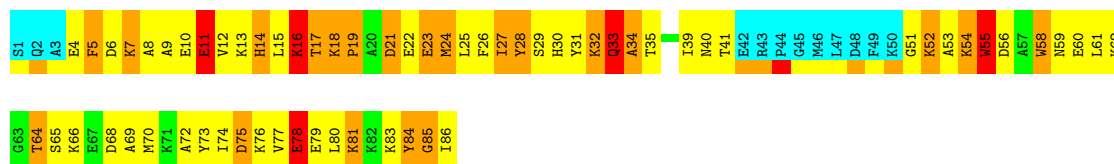
Chain A: 17% 44% 22% • 14%



4.2.7 Score per residue for model 7

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

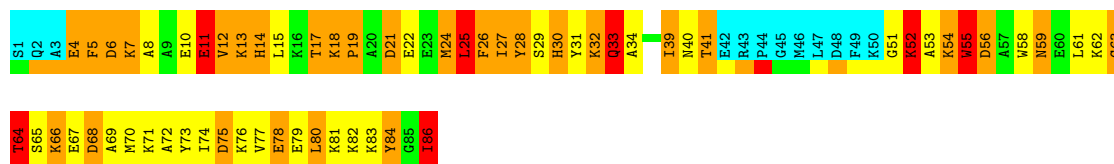
Chain A: 10% 45% 24% 6% 14%



4.2.8 Score per residue for model 8

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

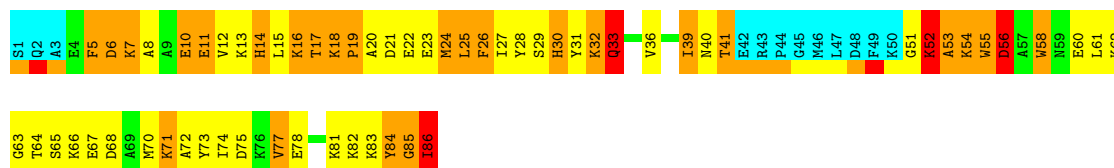
Chain A: 13% 31% 34% 8% 14%



4.2.9 Score per residue for model 9

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

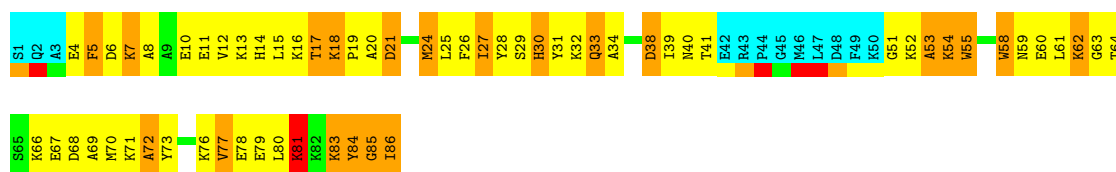
Chain A: 14% 38% 29% 5% 14%



4.2.10 Score per residue for model 10

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

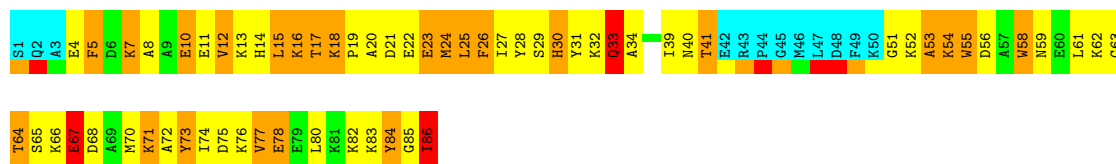
Chain A: 14% 47% 24% 14%



4.2.11 Score per residue for model 11

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

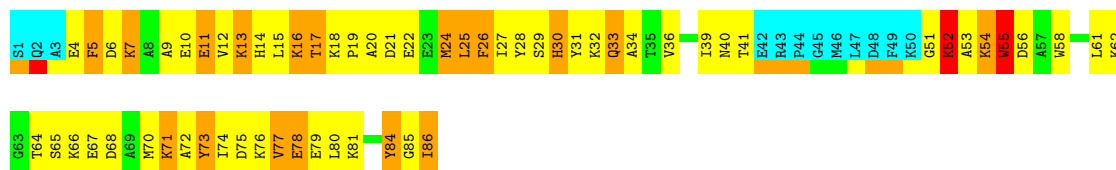
Chain A: 13% 42% 28% • 14%



4.2.12 Score per residue for model 12

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

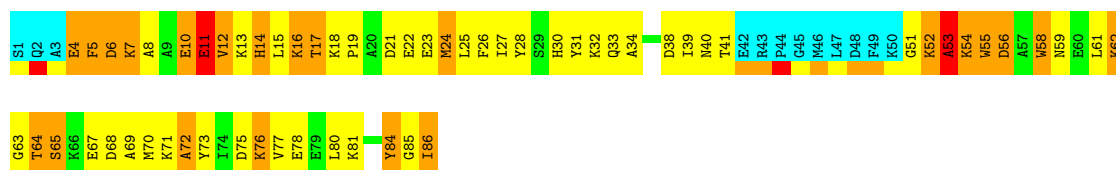
Chain A: 14% 49% 21% • 14%



4.2.13 Score per residue for model 13

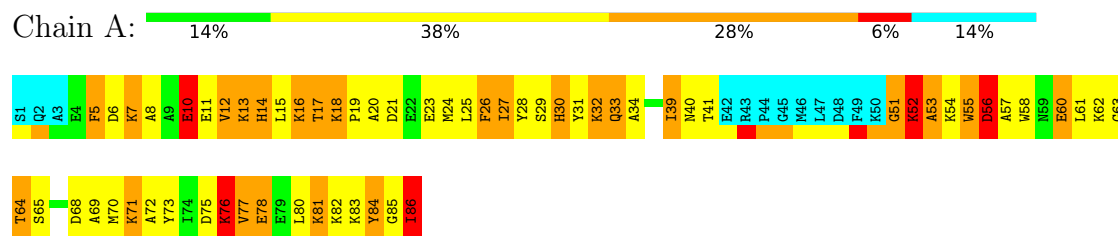
- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

Chain A: 15% 43% 26% • 14%



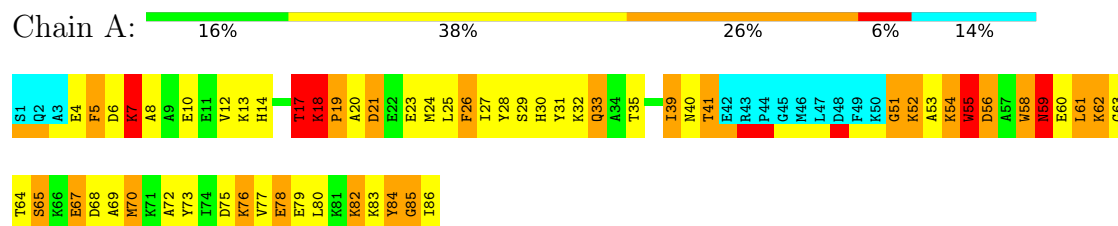
4.2.14 Score per residue for model 14

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN



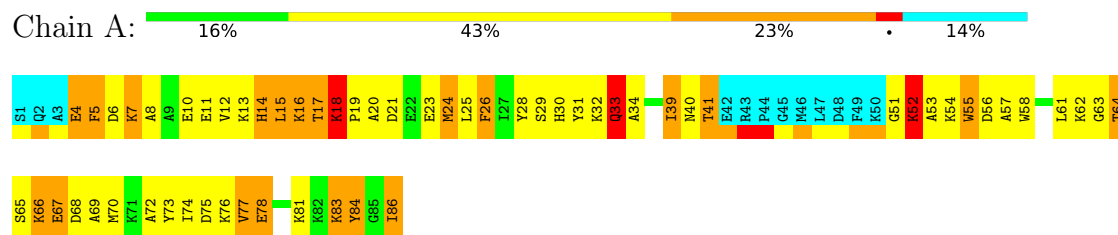
4.2.15 Score per residue for model 15

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN



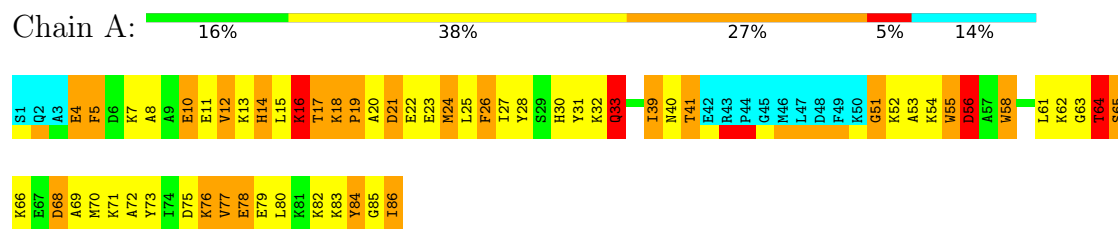
4.2.16 Score per residue for model 16

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN



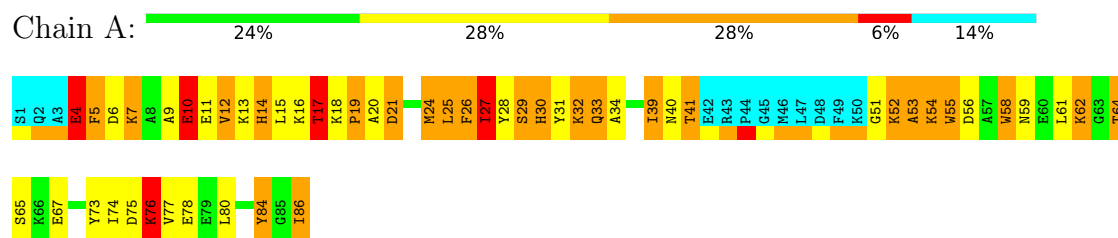
4.2.17 Score per residue for model 17

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN



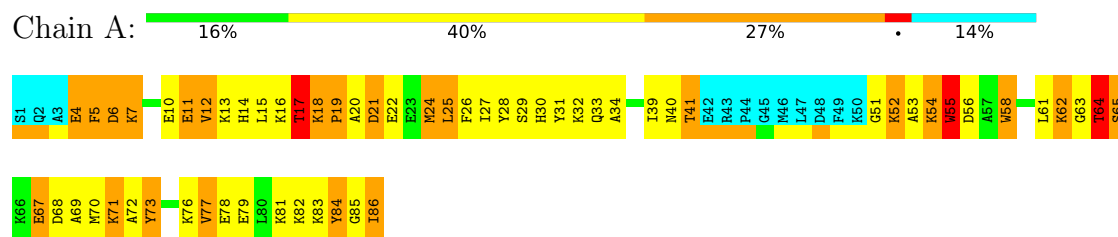
4.2.18 Score per residue for model 18

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN



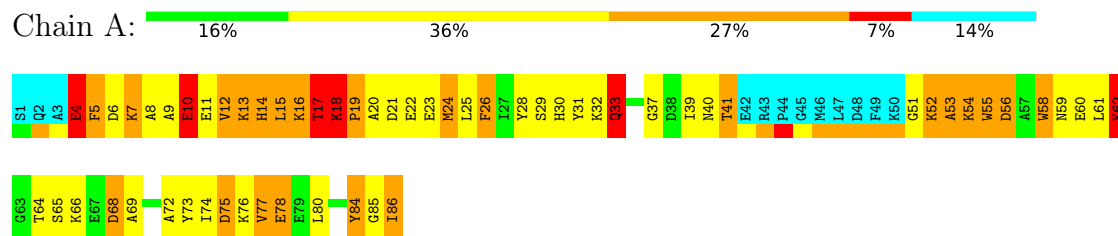
4.2.19 Score per residue for model 19 (medoid)

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN



4.2.20 Score per residue for model 20

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: ?.

Of the ? calculated structures, 20 were deposited, based on the following criterion: ?.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR	refinement	
DIANA	refinement	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: COA, PLM

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 (average) 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	1.92±0.04	7±2/615 (1.2± 0.3%)	2.25±0.06	32±5/821 (3.9± 0.6%)
All	All	1.92	149/12300 (1.2%)	2.25	648/16420 (3.9%)

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	14	HIS	CG-ND1	-9.09	1.28	1.38	2	20
1	A	30	HIS	CG-ND1	-8.90	1.28	1.38	10	20
1	A	56	ASP	CA-CB	7.81	1.65	1.53	9	1
1	A	28	TYR	N-CA	6.90	1.54	1.46	8	2
1	A	37	GLY	N-CA	6.88	1.51	1.45	1	1
1	A	52	LYS	N-CA	6.56	1.54	1.46	13	2
1	A	64	THR	N-CA	6.41	1.53	1.46	1	9
1	A	80	LEU	CA-CB	-6.32	1.43	1.53	1	2
1	A	85	GLY	N-CA	6.15	1.54	1.45	15	13
1	A	84	TYR	CA-CB	6.02	1.63	1.53	17	5
1	A	58	TRP	NE1-CE2	-5.93	1.30	1.37	17	13
1	A	62	LYS	CA-CB	-5.76	1.43	1.53	5	1
1	A	18	LYS	CA-CB	5.66	1.62	1.53	20	1
1	A	28	TYR	CA-CB	-5.62	1.44	1.53	7	2
1	A	58	TRP	CG-CD2	-5.58	1.33	1.43	5	1
1	A	58	TRP	N-CA	5.51	1.53	1.46	2	1
1	A	5	PHE	CA-CB	-5.51	1.44	1.53	9	1
1	A	55	TRP	NE1-CE2	-5.32	1.31	1.37	14	3
1	A	30	HIS	CD2-NE2	-5.30	1.32	1.37	20	17
1	A	74	ILE	CA-CB	-5.29	1.48	1.54	18	1
1	A	55	TRP	CG-CD2	-5.27	1.34	1.43	19	10
1	A	14	HIS	CD2-NE2	-5.24	1.32	1.37	16	17
1	A	10	GLU	CA-C	-5.22	1.47	1.52	20	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	53	ALA	CA-CB	5.19	1.62	1.53	13	1
1	A	52	LYS	CA-CB	-5.19	1.45	1.53	9	1
1	A	54	LYS	CA-CB	-5.07	1.45	1.53	6	1
1	A	29	SER	N-CA	5.03	1.52	1.46	16	1
1	A	63	GLY	N-CA	5.01	1.52	1.45	8	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	17	THR	N-CA-C	13.34	133.19	107.44	4	17
1	A	24	MET	N-CA-C	-11.82	98.37	111.14	9	17
1	A	30	HIS	CA-CB-CG	-11.74	102.06	113.80	5	18
1	A	10	GLU	N-CA-C	-11.21	96.15	111.96	5	18
1	A	21	ASP	CA-CB-CG	-10.14	102.46	112.60	15	12
1	A	84	TYR	CA-CB-CG	-10.06	95.80	113.90	2	18
1	A	77	VAL	N-CA-C	-9.88	100.94	110.42	5	17
1	A	56	ASP	CA-CB-CG	-9.50	103.10	112.60	13	7
1	A	5	PHE	CA-CB-CG	-9.50	104.30	113.80	13	14
1	A	59	ASN	CA-CB-CG	9.32	121.92	112.60	2	3
1	A	68	ASP	CA-CB-CG	-9.07	103.53	112.60	17	12
1	A	26	PHE	CA-CB-CG	-8.73	105.07	113.80	11	14
1	A	55	TRP	N-CA-C	-8.61	101.86	111.07	17	1
1	A	7	LYS	N-CA-C	-8.50	101.23	111.69	1	11
1	A	33	GLN	OE1-CD-NE2	-8.45	114.15	122.60	8	14
1	A	82	LYS	N-CA-CB	-8.45	97.65	110.07	15	3
1	A	27	ILE	N-CA-CB	-8.37	101.83	110.62	1	15
1	A	69	ALA	N-CA-C	-8.33	102.16	111.07	6	12
1	A	41	THR	CA-CB-OG1	-8.32	97.12	109.60	11	8
1	A	11	GLU	N-CA-CB	-8.30	97.21	109.82	19	9
1	A	33	GLN	N-CA-C	-8.27	102.27	111.28	7	3
1	A	56	ASP	N-CA-CB	-7.90	97.14	110.49	13	14
1	A	33	GLN	CG-CD-NE2	7.86	128.19	116.40	15	9
1	A	5	PHE	N-CA-C	-7.81	102.29	112.68	11	2
1	A	40	ASN	OD1-CG-ND2	-7.78	114.83	122.60	17	19
1	A	67	GLU	N-CA-CB	-7.76	98.82	110.07	10	11
1	A	59	ASN	OD1-CG-ND2	-7.71	114.89	122.60	15	3
1	A	39	ILE	N-CA-CB	-7.71	101.74	110.99	6	14
1	A	5	PHE	N-CA-CB	-7.67	98.95	110.07	4	15
1	A	52	LYS	CA-C-O	-7.42	113.01	120.80	20	3
1	A	4	GLU	N-CA-C	-7.40	101.52	111.96	18	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	52	LYS	N-CA-C	-7.37	102.93	110.97	12	6
1	A	58	TRP	CG-CD1-NE1	-7.26	100.76	110.20	14	20
1	A	6	ASP	CA-CB-CG	7.19	119.79	112.60	5	6
1	A	30	HIS	N-CA-CB	-6.93	100.02	110.07	1	12
1	A	55	TRP	CG-CD1-NE1	-6.87	101.27	110.20	10	20
1	A	60	GLU	N-CA-CB	-6.79	100.13	110.12	5	2
1	A	71	LYS	N-CA-CB	-6.78	99.52	109.82	4	1
1	A	68	ASP	N-CA-C	-6.64	103.97	111.07	1	6
1	A	23	GLU	N-CA-C	-6.63	104.13	111.36	7	7
1	A	84	TYR	CA-C-O	-6.60	111.45	118.77	10	8
1	A	75	ASP	CA-CB-CG	6.57	119.17	112.60	13	3
1	A	84	TYR	N-CA-C	-6.55	103.97	112.68	14	5
1	A	40	ASN	CA-CB-CG	-6.50	106.10	112.60	11	4
1	A	85	GLY	N-CA-C	6.49	128.55	113.18	10	2
1	A	75	ASP	N-CA-CB	-6.48	99.21	109.78	2	6
1	A	12	VAL	N-CA-CB	-6.47	103.83	110.62	5	4
1	A	6	ASP	N-CA-C	-6.46	104.16	111.07	13	3
1	A	14	HIS	N-CA-C	-6.42	105.03	112.92	9	1
1	A	84	TYR	CB-CA-C	6.34	120.84	110.24	19	7
1	A	56	ASP	CB-CA-C	6.33	121.44	110.68	9	4
1	A	32	LYS	CA-CB-CG	-6.29	101.53	114.10	8	1
1	A	61	LEU	O-C-N	6.26	129.29	122.15	15	1
1	A	68	ASP	CA-C-O	6.25	127.17	120.55	8	3
1	A	13	LYS	N-CA-C	-6.24	105.63	113.18	15	1
1	A	28	TYR	CA-CB-CG	6.23	125.11	113.90	8	1
1	A	41	THR	OG1-CB-CG2	-6.22	96.87	109.30	8	16
1	A	55	TRP	NE1-CE2-CZ2	6.20	139.40	130.10	19	13
1	A	78	GLU	N-CA-C	-6.10	103.58	111.02	3	3
1	A	54	LYS	N-CA-CB	-6.10	100.86	109.94	10	4
1	A	14	HIS	CA-CB-CG	-6.09	107.71	113.80	5	2
1	A	51	GLY	N-CA-C	-6.05	105.44	112.83	14	1
1	A	4	GLU	CA-C-O	6.05	128.60	120.13	20	3
1	A	11	GLU	CB-CA-C	6.03	120.50	110.92	19	2
1	A	76	LYS	N-CA-C	-5.99	104.72	112.68	14	2
1	A	64	THR	N-CA-C	5.98	119.41	110.14	5	1
1	A	60	GLU	N-CA-C	-5.97	104.35	111.69	14	1
1	A	38	ASP	N-CA-CB	-5.92	100.75	110.52	5	1
1	A	65	SER	N-CA-C	-5.86	99.70	109.24	5	1
1	A	6	ASP	N-CA-CB	-5.85	101.22	109.94	20	4
1	A	73	TYR	CA-CB-CG	-5.83	103.42	113.90	19	4
1	A	84	TYR	CA-C-N	-5.82	109.99	121.41	10	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	84	TYR	C-N-CA	-5.82	109.99	121.41	10	1
1	A	68	ASP	N-CA-CB	-5.79	101.38	110.06	15	4
1	A	81	LYS	N-CA-CB	-5.77	100.73	110.49	10	1
1	A	40	ASN	N-CA-CB	-5.76	103.19	111.54	8	3
1	A	58	TRP	NE1-CE2-CZ2	5.75	138.72	130.10	5	2
1	A	4	GLU	CA-C-N	5.73	128.24	120.44	2	1
1	A	4	GLU	C-N-CA	5.73	128.24	120.44	2	1
1	A	58	TRP	CA-C-N	5.73	129.85	120.63	2	2
1	A	58	TRP	C-N-CA	5.73	129.85	120.63	2	2
1	A	64	THR	CA-CB-OG1	-5.71	101.04	109.60	5	1
1	A	16	LYS	N-CA-C	-5.71	106.08	113.16	11	1
1	A	86	ILE	N-CA-CB	-5.70	101.81	111.50	10	7
1	A	80	LEU	N-CA-CB	-5.68	100.89	110.49	8	2
1	A	66	LYS	N-CA-C	5.67	122.87	110.80	1	1
1	A	64	THR	OG1-CB-CG2	-5.65	98.00	109.30	4	5
1	A	62	LYS	N-CA-CB	-5.61	101.02	110.49	20	2
1	A	72	ALA	N-CA-CB	-5.60	101.87	110.16	3	5
1	A	83	LYS	N-CA-C	5.59	117.06	110.97	16	2
1	A	70	MET	O-C-N	5.56	128.03	122.08	17	2
1	A	52	LYS	N-CA-CB	-5.56	100.99	110.33	9	2
1	A	32	LYS	N-CA-CB	-5.55	101.96	110.01	14	3
1	A	66	LYS	CA-CB-CG	-5.47	103.16	114.10	17	1
1	A	27	ILE	CB-CA-C	5.46	118.69	111.70	1	2
1	A	76	LYS	CG-CD-CE	5.44	123.81	111.30	18	1
1	A	13	LYS	CA-CB-CG	-5.42	103.26	114.10	19	1
1	A	67	GLU	CB-CA-C	5.41	119.45	110.90	4	1
1	A	15	LEU	N-CA-C	-5.41	102.87	110.50	11	1
1	A	70	MET	CB-CA-C	-5.37	102.45	110.88	4	1
1	A	66	LYS	CA-C-O	5.36	126.20	120.20	3	1
1	A	39	ILE	N-CA-C	5.35	116.02	108.36	6	3
1	A	82	LYS	CB-CA-C	5.32	119.64	110.86	15	1
1	A	30	HIS	CE1-NE2-CD2	-5.31	103.69	109.00	6	2
1	A	52	LYS	CA-CB-CG	-5.31	103.48	114.10	20	1
1	A	34	ALA	N-CA-C	5.30	117.47	111.11	7	1
1	A	62	LYS	CA-C-N	5.28	131.76	121.41	5	1
1	A	62	LYS	C-N-CA	5.28	131.76	121.41	5	1
1	A	55	TRP	CD1-NE1-CE2	5.27	118.38	108.90	11	5
1	A	23	GLU	CA-CB-CG	-5.26	103.57	114.10	1	1
1	A	38	ASP	N-CA-C	5.26	118.20	109.46	13	1
1	A	86	ILE	N-CA-C	-5.26	96.28	111.00	8	1
1	A	38	ASP	CA-CB-CG	-5.25	107.35	112.60	10	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	55	TRP	CA-CB-CG	-5.24	103.64	113.60	10	2
1	A	67	GLU	CA-CB-CG	-5.24	103.61	114.10	10	1
1	A	35	THR	CA-CB-OG1	-5.23	101.75	109.60	15	3
1	A	64	THR	CA-CB-CG2	5.20	119.34	110.50	2	3
1	A	58	TRP	CD1-NE1-CE2	5.19	118.25	108.90	1	3
1	A	59	ASN	N-CA-CB	-5.19	100.83	110.18	2	1
1	A	54	LYS	CG-CD-CE	5.19	123.24	111.30	15	1
1	A	24	MET	CA-C-N	5.18	127.49	120.65	20	1
1	A	24	MET	C-N-CA	5.18	127.49	120.65	20	1
1	A	62	LYS	O-C-N	5.17	129.47	122.59	5	1
1	A	63	GLY	N-CA-C	-5.17	108.13	115.43	16	3
1	A	7	LYS	CA-CB-CG	-5.16	103.78	114.10	20	2
1	A	11	GLU	CB-CG-CD	5.15	121.36	112.60	16	1
1	A	65	SER	CA-C-O	5.15	126.04	120.43	13	2
1	A	79	GLU	CA-CB-CG	-5.13	103.83	114.10	10	1
1	A	8	ALA	N-CA-C	-5.13	105.69	111.28	1	1
1	A	75	ASP	CB-CA-C	5.12	119.24	110.74	2	1
1	A	33	GLN	CB-CA-C	-5.11	103.10	110.96	20	1
1	A	52	LYS	CB-CA-C	5.09	119.35	110.79	1	1
1	A	27	ILE	CA-CB-CG2	-5.09	101.85	110.50	18	1
1	A	58	TRP	NE1-CE2-CD2	-5.08	100.79	107.40	5	1
1	A	66	LYS	N-CA-CB	-5.08	101.90	110.49	17	1
1	A	58	TRP	N-CA-C	-5.07	106.78	113.12	9	1
1	A	14	HIS	CE1-NE2-CD2	-5.06	103.94	109.00	10	3
1	A	81	LYS	O-C-N	5.06	129.31	122.59	14	1
1	A	82	LYS	CA-CB-CG	-5.03	104.04	114.10	19	1
1	A	71	LYS	CB-CA-C	5.02	118.90	110.92	4	1
1	A	76	LYS	CA-CB-CG	-5.01	104.08	114.10	3	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	603	598	598	68±11
2	A	48	31	31	13±4
3	A	17	31	31	14±4
All	All	13360	13200	13192	1539

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 58.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:MET:HE3	3:A:88:PLM:H32	0.88	1.43	13	7
1:A:54:LYS:HD3	1:A:54:LYS:H	0.87	1.29	13	1
1:A:24:MET:HE3	3:A:88:PLM:HD1	0.86	1.44	10	2
1:A:33:GLN:NE2	1:A:58:TRP:CD1	0.81	2.48	5	1
1:A:33:GLN:CD	1:A:58:TRP:CD1	0.81	2.58	5	1
1:A:28:TYR:CB	3:A:88:PLM:HA1	0.79	2.07	8	1
2:A:87:COA:H131	2:A:87:COA:S1P	0.79	2.17	16	3
1:A:54:LYS:H	1:A:54:LYS:CD	0.79	1.91	13	1
1:A:54:LYS:HD2	3:A:88:PLM:HD1	0.78	1.56	13	5
1:A:24:MET:HE1	3:A:88:PLM:H51	0.77	1.55	16	2
1:A:13:LYS:NZ	2:A:87:COA:S1P	0.76	2.59	20	1
1:A:24:MET:C	3:A:88:PLM:HC2	0.75	2.05	5	1
1:A:24:MET:HE2	3:A:88:PLM:HD1	0.75	1.58	18	1
1:A:28:TYR:CE1	1:A:32:LYS:HD2	0.75	2.16	8	2
2:A:87:COA:S1P	2:A:87:COA:CEP	0.75	2.74	20	1
2:A:87:COA:H141	2:A:87:COA:HN8	0.75	1.42	16	12
1:A:54:LYS:HD3	1:A:54:LYS:N	0.74	1.91	13	1
1:A:54:LYS:HD2	3:A:88:PLM:CD	0.74	2.11	13	4
1:A:53:ALA:HB3	1:A:54:LYS:HZ2	0.74	1.42	13	1
2:A:87:COA:C5B	2:A:87:COA:H133	0.74	2.13	10	6
1:A:54:LYS:CD	3:A:88:PLM:HD1	0.73	2.13	17	6
1:A:31:TYR:HB2	1:A:73:TYR:CE1	0.72	2.20	10	20
1:A:24:MET:HE3	3:A:88:PLM:C3	0.72	2.13	13	3
2:A:87:COA:CEP	2:A:87:COA:S1P	0.72	2.78	9	2
1:A:28:TYR:CD2	1:A:54:LYS:HB2	0.71	2.21	10	7
1:A:54:LYS:CE	3:A:88:PLM:HD1	0.71	2.16	14	1
2:A:87:COA:S1P	2:A:87:COA:CDP	0.70	2.79	16	1
1:A:28:TYR:CE2	1:A:54:LYS:HB3	0.70	2.22	5	2
1:A:28:TYR:CZ	1:A:32:LYS:HG3	0.70	2.22	6	12
1:A:24:MET:HE3	3:A:88:PLM:H52	0.70	1.63	18	2
1:A:5:PHE:CE2	1:A:73:TYR:CD2	0.69	2.81	14	19
1:A:26:PHE:CE1	1:A:76:LYS:HB2	0.69	2.22	19	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:MET:CE	3:A:88:PLM:HD1	0.69	2.18	10	2
1:A:52:LYS:HD3	1:A:53:ALA:N	0.68	2.03	1	1
1:A:33:GLN:NE2	1:A:61:LEU:HB3	0.68	2.04	20	1
1:A:26:PHE:CD1	1:A:76:LYS:HG3	0.68	2.23	1	2
1:A:27:ILE:HD13	1:A:76:LYS:HG2	0.68	1.65	18	1
1:A:28:TYR:HB2	3:A:88:PLM:CC	0.68	2.18	7	5
1:A:28:TYR:HB3	3:A:88:PLM:HA1	0.67	1.65	8	1
1:A:10:GLU:HG2	1:A:11:GLU:N	0.67	2.04	14	5
1:A:25:LEU:HG	3:A:88:PLM:CG	0.67	2.20	6	1
1:A:24:MET:HE2	3:A:88:PLM:CD	0.67	2.17	18	1
1:A:41:THR:HG1	1:A:55:TRP:CD1	0.67	2.07	20	12
1:A:27:ILE:HA	1:A:76:LYS:HD3	0.67	1.67	18	1
1:A:18:LYS:HG2	1:A:24:MET:SD	0.67	2.28	15	5
1:A:54:LYS:HD3	3:A:88:PLM:HD1	0.67	1.65	17	2
2:A:87:COA:N8P	2:A:87:COA:H143	0.67	2.05	5	1
1:A:24:MET:HE2	3:A:88:PLM:HC1	0.66	1.67	9	1
1:A:28:TYR:HB2	3:A:88:PLM:HC1	0.66	1.65	19	4
1:A:28:TYR:CD1	1:A:54:LYS:HB2	0.66	2.25	20	5
1:A:5:PHE:CD1	1:A:6:ASP:N	0.66	2.63	1	1
1:A:28:TYR:CE1	1:A:32:LYS:HG3	0.66	2.26	3	10
1:A:13:LYS:NZ	2:A:87:COA:O6A	0.66	2.29	11	4
1:A:16:LYS:NZ	1:A:86:ILE:C	0.65	2.54	5	3
1:A:33:GLN:CD	1:A:33:GLN:N	0.65	2.54	5	1
1:A:28:TYR:CZ	1:A:32:LYS:HD2	0.65	2.26	10	1
1:A:28:TYR:CG	1:A:54:LYS:HB2	0.65	2.26	10	6
2:A:87:COA:N3A	3:A:88:PLM:H72	0.65	2.06	7	1
1:A:5:PHE:CZ	1:A:34:ALA:HB3	0.65	2.27	1	8
1:A:28:TYR:CB	3:A:88:PLM:CA	0.65	2.74	8	1
1:A:54:LYS:HD2	1:A:54:LYS:N	0.65	2.07	9	1
1:A:54:LYS:HG2	3:A:88:PLM:HB1	0.65	1.67	4	1
1:A:19:PRO:HB3	1:A:84:TYR:CE2	0.65	2.27	13	19
1:A:25:LEU:N	3:A:88:PLM:HD2	0.64	2.07	11	5
1:A:26:PHE:CD2	1:A:76:LYS:NZ	0.64	2.66	18	1
2:A:87:COA:H131	3:A:88:PLM:H21	0.64	1.70	16	4
1:A:78:GLU:CD	1:A:82:LYS:HZ2	0.64	2.01	11	1
1:A:28:TYR:HB2	3:A:88:PLM:CB	0.63	2.23	1	6
1:A:28:TYR:CE2	1:A:54:LYS:HB2	0.63	2.28	6	4
2:A:87:COA:CDP	3:A:88:PLM:H21	0.63	2.24	16	1
1:A:28:TYR:CB	3:A:88:PLM:HC1	0.63	2.22	7	3
1:A:18:LYS:NZ	1:A:24:MET:SD	0.63	2.71	5	2
1:A:24:MET:HE3	3:A:88:PLM:C5	0.63	2.23	8	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:LYS:HD2	3:A:88:PLM:CB	0.63	2.24	12	2
1:A:24:MET:SD	3:A:88:PLM:H42	0.63	2.34	3	1
1:A:53:ALA:N	1:A:54:LYS:NZ	0.63	2.46	13	1
1:A:54:LYS:NZ	2:A:87:COA:O8A	0.63	2.30	14	7
1:A:24:MET:HB3	3:A:88:PLM:HE1	0.62	1.69	6	4
1:A:73:TYR:HA	1:A:76:LYS:CE	0.62	2.24	18	1
2:A:87:COA:CEP	2:A:87:COA:HN8	0.62	2.06	5	2
1:A:53:ALA:CB	1:A:54:LYS:HZ2	0.62	2.06	13	1
1:A:19:PRO:CG	1:A:80:LEU:HD12	0.62	2.24	8	2
1:A:33:GLN:NE2	1:A:69:ALA:HA	0.62	2.09	8	1
2:A:87:COA:HN8	2:A:87:COA:CEP	0.62	2.07	16	4
3:A:88:PLM:H41	3:A:88:PLM:H81	0.61	1.72	14	2
1:A:26:PHE:CD1	1:A:26:PHE:C	0.61	2.77	1	3
1:A:10:GLU:CG	1:A:11:GLU:N	0.61	2.62	2	6
1:A:5:PHE:CD2	1:A:73:TYR:CD2	0.61	2.87	2	17
2:A:87:COA:H131	3:A:88:PLM:C1	0.61	2.25	13	2
1:A:18:LYS:HD2	1:A:24:MET:SD	0.61	2.36	19	1
1:A:21:ASP:HB3	3:A:88:PLM:HG3	0.61	1.71	8	1
1:A:26:PHE:CZ	1:A:30:HIS:CD2	0.61	2.88	12	6
1:A:24:MET:HE1	3:A:88:PLM:C5	0.60	2.26	16	2
1:A:26:PHE:CE2	1:A:76:LYS:NZ	0.60	2.69	18	1
1:A:19:PRO:HD2	1:A:24:MET:SD	0.60	2.36	4	4
1:A:24:MET:HB3	3:A:88:PLM:HE2	0.60	1.71	17	1
2:A:87:COA:OAP	3:A:88:PLM:C1	0.60	2.49	5	1
1:A:26:PHE:CE2	1:A:76:LYS:HE2	0.60	2.32	18	1
1:A:5:PHE:C	1:A:5:PHE:CD1	0.60	2.79	17	16
1:A:28:TYR:CE2	1:A:32:LYS:NZ	0.60	2.70	4	1
1:A:54:LYS:HG2	3:A:88:PLM:CB	0.60	2.26	4	1
1:A:28:TYR:CE1	1:A:32:LYS:HE3	0.60	2.32	11	1
1:A:32:LYS:NZ	2:A:87:COA:O7A	0.60	2.35	17	5
1:A:54:LYS:HB3	3:A:88:PLM:CD	0.59	2.26	6	1
1:A:24:MET:HB3	3:A:88:PLM:HD1	0.59	1.74	16	2
1:A:28:TYR:CZ	1:A:32:LYS:CD	0.59	2.85	10	1
1:A:15:LEU:O	1:A:17:THR:N	0.59	2.36	3	14
2:A:87:COA:S1P	2:A:87:COA:H143	0.59	2.37	20	1
1:A:19:PRO:CG	1:A:80:LEU:HD22	0.59	2.28	15	7
1:A:26:PHE:CE2	1:A:76:LYS:CE	0.59	2.86	18	1
1:A:26:PHE:C	1:A:26:PHE:CD1	0.59	2.80	3	15
2:A:87:COA:N8P	2:A:87:COA:CEP	0.59	2.60	5	2
1:A:28:TYR:CE1	1:A:54:LYS:NZ	0.59	2.70	5	1
1:A:67:GLU:HA	1:A:70:MET:SD	0.59	2.37	16	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:88:PLM:C7	3:A:88:PLM:HB1	0.59	2.27	11	1
1:A:54:LYS:HB3	3:A:88:PLM:CC	0.59	2.28	3	2
1:A:28:TYR:CB	3:A:88:PLM:CC	0.59	2.81	7	2
1:A:9:ALA:HA	2:A:87:COA:H61A	0.58	1.58	4	2
1:A:52:LYS:O	1:A:53:ALA:C	0.58	2.46	1	19
2:A:87:COA:C2A	3:A:88:PLM:H82	0.58	2.27	19	1
1:A:28:TYR:HB2	3:A:88:PLM:CA	0.58	2.27	8	3
2:A:87:COA:O9P	3:A:88:PLM:C1	0.58	2.52	3	1
2:A:87:COA:P1A	2:A:87:COA:H121	0.58	2.39	16	1
1:A:54:LYS:CD	3:A:88:PLM:CD	0.58	2.82	17	1
1:A:64:THR:HG22	1:A:65:SER:N	0.58	2.13	13	8
1:A:25:LEU:HA	1:A:54:LYS:HZ3	0.58	1.57	9	1
1:A:24:MET:HE3	3:A:88:PLM:C4	0.58	2.28	6	4
3:A:88:PLM:C4	3:A:88:PLM:H81	0.57	2.28	6	3
1:A:62:LYS:HB3	1:A:62:LYS:NZ	0.57	2.13	5	1
1:A:54:LYS:NZ	2:A:87:COA:O7A	0.57	2.37	16	2
1:A:73:TYR:HA	1:A:76:LYS:HD2	0.57	1.75	18	1
1:A:33:GLN:OE1	1:A:58:TRP:NE1	0.57	2.38	5	1
1:A:58:TRP:CD1	1:A:58:TRP:C	0.57	2.80	5	4
1:A:18:LYS:CG	1:A:24:MET:SD	0.57	2.93	14	3
1:A:54:LYS:NZ	2:A:87:COA:O3B	0.57	2.37	5	2
2:A:87:COA:H131	3:A:88:PLM:C2	0.57	2.30	16	2
1:A:24:MET:O	1:A:25:LEU:C	0.57	2.48	5	5
2:A:87:COA:H141	3:A:88:PLM:H21	0.57	1.74	13	1
1:A:30:HIS:CB	1:A:76:LYS:HE3	0.57	2.30	18	1
1:A:22:GLU:O	1:A:25:LEU:HB2	0.57	2.00	8	8
1:A:32:LYS:NZ	2:A:87:COA:O9A	0.57	2.38	6	3
1:A:73:TYR:CZ	1:A:77:VAL:CG2	0.57	2.88	8	8
1:A:28:TYR:H	3:A:88:PLM:HA1	0.57	1.58	8	1
1:A:76:LYS:CE	1:A:76:LYS:HA	0.57	2.30	13	2
1:A:54:LYS:HB3	3:A:88:PLM:HC1	0.57	1.76	3	2
1:A:78:GLU:CD	1:A:82:LYS:HZ1	0.57	2.08	8	1
1:A:54:LYS:CG	1:A:55:TRP:H	0.57	2.13	20	1
2:A:87:COA:H52A	2:A:87:COA:H133	0.56	1.75	15	3
1:A:28:TYR:CD1	1:A:32:LYS:HD2	0.56	2.35	8	1
1:A:29:SER:O	1:A:33:GLN:NE2	0.56	2.37	5	1
1:A:28:TYR:CE1	1:A:32:LYS:CD	0.56	2.88	8	1
2:A:87:COA:N8P	3:A:88:PLM:H22	0.56	2.16	2	3
1:A:28:TYR:N	3:A:88:PLM:HA1	0.56	2.15	8	1
2:A:87:COA:N4P	2:A:87:COA:N8P	0.56	2.53	1	4
1:A:28:TYR:CE2	1:A:54:LYS:NZ	0.56	2.74	15	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:PHE:O	1:A:76:LYS:NZ	0.56	2.39	18	1
1:A:22:GLU:HA	1:A:25:LEU:HD12	0.56	1.78	17	6
1:A:64:THR:CG2	1:A:65:SER:N	0.56	2.69	3	14
1:A:76:LYS:HZ3	1:A:79:GLU:CD	0.56	2.08	7	2
2:A:87:COA:H22	2:A:87:COA:OAP	0.56	2.02	1	1
1:A:10:GLU:CD	1:A:13:LYS:HZ1	0.55	2.10	1	1
1:A:29:SER:HB3	1:A:57:ALA:C	0.55	2.26	1	2
1:A:17:THR:O	1:A:18:LYS:C	0.55	2.49	15	17
1:A:28:TYR:CE1	1:A:54:LYS:HB3	0.55	2.36	15	2
1:A:25:LEU:CA	3:A:88:PLM:HA2	0.55	2.31	8	1
1:A:28:TYR:CE1	1:A:54:LYS:HB2	0.55	2.36	13	2
2:A:87:COA:C9P	2:A:87:COA:HN4	0.55	2.14	2	2
1:A:54:LYS:CG	3:A:88:PLM:HB1	0.55	2.32	4	1
1:A:18:LYS:HZ1	1:A:21:ASP:CG	0.55	2.09	18	3
2:A:87:COA:H10	3:A:88:PLM:C2	0.55	2.32	6	1
1:A:19:PRO:O	1:A:20:ALA:C	0.55	2.50	9	4
3:A:88:PLM:C5	3:A:88:PLM:H91	0.55	2.32	15	1
1:A:24:MET:HE3	3:A:88:PLM:C2	0.55	2.32	1	1
1:A:25:LEU:N	3:A:88:PLM:HC2	0.55	2.16	5	1
1:A:15:LEU:HD23	1:A:86:ILE:CG2	0.54	2.32	1	6
1:A:26:PHE:CE1	1:A:30:HIS:CD2	0.54	2.94	3	2
1:A:13:LYS:CE	2:A:87:COA:H122	0.54	2.33	18	1
1:A:71:LYS:CG	1:A:72:ALA:N	0.54	2.70	13	3
1:A:13:LYS:O	2:A:87:COA:S1P	0.54	2.65	8	3
3:A:88:PLM:H71	3:A:88:PLM:CB	0.54	2.31	7	1
1:A:32:LYS:NZ	2:A:87:COA:O8A	0.54	2.39	8	2
1:A:28:TYR:HB2	3:A:88:PLM:C8	0.54	2.31	8	1
1:A:54:LYS:NZ	1:A:54:LYS:HA	0.54	2.18	9	1
1:A:54:LYS:NZ	2:A:87:COA:O9A	0.54	2.40	7	4
1:A:33:GLN:N	1:A:33:GLN:OE1	0.54	2.41	5	1
1:A:41:THR:C	1:A:55:TRP:HE1	0.54	2.09	9	13
1:A:31:TYR:CD2	2:A:87:COA:C2A	0.54	2.91	16	13
1:A:73:TYR:CZ	1:A:77:VAL:HG21	0.54	2.37	12	7
2:A:87:COA:C9P	2:A:87:COA:N4P	0.54	2.71	2	2
1:A:28:TYR:HB2	3:A:88:PLM:HA1	0.54	1.80	12	1
3:A:88:PLM:C5	3:A:88:PLM:C9	0.54	2.86	15	1
1:A:24:MET:CE	3:A:88:PLM:H51	0.54	2.33	15	5
1:A:25:LEU:HD21	1:A:53:ALA:CB	0.54	2.33	2	3
1:A:18:LYS:HB2	2:A:87:COA:H62	0.54	1.78	15	2
1:A:17:THR:HG22	1:A:17:THR:O	0.54	2.02	11	2
1:A:28:TYR:CB	3:A:88:PLM:CB	0.53	2.86	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:LYS:CD	1:A:53:ALA:N	0.53	2.71	1	2
1:A:15:LEU:HD13	1:A:19:PRO:HG2	0.53	1.80	12	3
1:A:39:ILE:HD11	1:A:55:TRP:CD1	0.53	2.39	2	12
1:A:28:TYR:CD1	3:A:88:PLM:HB2	0.53	2.39	1	2
1:A:61:LEU:O	1:A:62:LYS:C	0.53	2.50	1	13
1:A:24:MET:CE	3:A:88:PLM:H52	0.53	2.33	18	1
1:A:76:LYS:HA	1:A:76:LYS:NZ	0.53	2.19	13	3
1:A:28:TYR:CE1	1:A:54:LYS:C	0.53	2.87	16	2
1:A:28:TYR:CZ	1:A:54:LYS:HB2	0.53	2.39	1	1
1:A:26:PHE:CD1	1:A:76:LYS:HG2	0.53	2.39	4	9
1:A:5:PHE:CE2	1:A:34:ALA:CB	0.53	2.92	3	15
1:A:14:HIS:O	1:A:16:LYS:N	0.53	2.41	2	6
1:A:54:LYS:CB	3:A:88:PLM:HC1	0.53	2.33	12	3
1:A:28:TYR:H	3:A:88:PLM:CA	0.53	2.16	8	1
1:A:33:GLN:CD	1:A:61:LEU:HD13	0.53	2.29	20	2
3:A:88:PLM:H41	3:A:88:PLM:C8	0.53	2.33	20	3
1:A:54:LYS:HD2	3:A:88:PLM:HC2	0.53	1.81	20	1
1:A:54:LYS:CG	3:A:88:PLM:HD1	0.53	2.34	4	1
1:A:54:LYS:HB3	3:A:88:PLM:HD1	0.53	1.81	13	2
1:A:33:GLN:NE2	1:A:69:ALA:HB2	0.53	2.19	7	1
2:A:87:COA:N3A	3:A:88:PLM:H81	0.52	2.20	4	2
2:A:87:COA:HO1	3:A:88:PLM:C1	0.52	2.17	5	1
1:A:25:LEU:HD21	1:A:53:ALA:HB1	0.52	1.79	4	6
3:A:88:PLM:H82	3:A:88:PLM:H41	0.52	1.79	5	1
3:A:88:PLM:HE2	3:A:88:PLM:HA1	0.52	1.80	11	1
1:A:54:LYS:CD	3:A:88:PLM:HC1	0.52	2.35	12	1
1:A:54:LYS:HZ1	2:A:87:COA:P3B	0.52	2.26	15	2
1:A:5:PHE:CE1	1:A:73:TYR:CD2	0.52	2.97	9	1
1:A:28:TYR:HB2	3:A:88:PLM:HB1	0.52	1.81	11	1
1:A:19:PRO:HA	1:A:84:TYR:CZ	0.52	2.39	7	11
1:A:32:LYS:HB3	1:A:58:TRP:CD2	0.52	2.39	13	3
1:A:13:LYS:CG	2:A:87:COA:N6A	0.52	2.73	1	1
1:A:72:ALA:O	1:A:73:TYR:C	0.52	2.52	16	15
2:A:87:COA:H141	3:A:88:PLM:C2	0.52	2.34	2	2
1:A:52:LYS:O	1:A:55:TRP:N	0.52	2.43	14	10
1:A:33:GLN:CD	1:A:58:TRP:NE1	0.52	2.67	5	1
2:A:87:COA:H133	3:A:88:PLM:H52	0.52	1.81	1	1
1:A:9:ALA:O	2:A:87:COA:N6A	0.52	2.43	5	3
2:A:87:COA:H133	2:A:87:COA:H51A	0.51	1.81	12	3
1:A:7:LYS:NZ	1:A:10:GLU:OE2	0.51	2.43	18	1
1:A:27:ILE:HD13	1:A:76:LYS:CG	0.51	2.34	18	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:PRO:HB3	1:A:80:LEU:HD22	0.51	1.82	3	3
2:A:87:COA:H143	2:A:87:COA:HN8	0.51	1.64	5	1
1:A:51:GLY:N	1:A:54:LYS:HE2	0.51	2.20	13	1
1:A:73:TYR:CE2	1:A:77:VAL:HG21	0.51	2.39	8	11
1:A:24:MET:C	3:A:88:PLM:CC	0.51	2.83	5	1
1:A:53:ALA:HB3	1:A:54:LYS:NZ	0.51	2.17	13	1
1:A:5:PHE:CD1	1:A:5:PHE:C	0.51	2.88	2	3
1:A:7:LYS:NZ	1:A:11:GLU:OE2	0.51	2.44	9	4
1:A:16:LYS:NZ	1:A:85:GLY:O	0.51	2.43	9	2
1:A:18:LYS:HZ3	1:A:21:ASP:CG	0.51	2.14	19	1
1:A:28:TYR:CD1	1:A:28:TYR:C	0.51	2.88	20	1
1:A:52:LYS:HD3	1:A:52:LYS:C	0.51	2.30	1	1
1:A:28:TYR:CE2	1:A:32:LYS:HG3	0.51	2.40	16	5
1:A:5:PHE:CD2	1:A:70:MET:HG2	0.51	2.41	15	3
1:A:16:LYS:NZ	1:A:86:ILE:O	0.51	2.44	14	1
1:A:28:TYR:CB	3:A:88:PLM:HB2	0.51	2.36	8	1
1:A:24:MET:HB3	3:A:88:PLM:CD	0.51	2.36	16	2
1:A:39:ILE:HA	1:A:58:TRP:CH2	0.51	2.41	7	4
1:A:78:GLU:CD	1:A:82:LYS:NZ	0.51	2.68	8	3
1:A:51:GLY:C	1:A:54:LYS:NZ	0.51	2.69	13	1
1:A:28:TYR:CD1	1:A:32:LYS:HG3	0.51	2.40	1	4
1:A:18:LYS:CB	2:A:87:COA:H62	0.51	2.36	4	4
1:A:24:MET:O	3:A:88:PLM:HA2	0.51	2.06	5	1
1:A:67:GLU:H	1:A:67:GLU:CD	0.51	2.14	16	1
2:A:87:COA:O1A	2:A:87:COA:H132	0.50	2.05	7	1
1:A:13:LYS:NZ	2:A:87:COA:O5A	0.50	2.44	2	6
1:A:73:TYR:HA	1:A:76:LYS:CD	0.50	2.36	18	1
1:A:13:LYS:HA	2:A:87:COA:OAP	0.50	2.06	6	1
2:A:87:COA:H51A	2:A:87:COA:O6A	0.50	2.06	10	1
1:A:25:LEU:CD2	1:A:53:ALA:HB1	0.50	2.37	12	2
1:A:78:GLU:O	1:A:81:LYS:HB3	0.50	2.07	7	2
1:A:24:MET:C	3:A:88:PLM:HA1	0.50	2.32	7	1
1:A:52:LYS:C	1:A:54:LYS:HZ3	0.50	2.14	13	1
1:A:25:LEU:HD21	1:A:53:ALA:HB3	0.50	1.84	14	1
1:A:15:LEU:HD23	1:A:86:ILE:HG21	0.50	1.83	11	4
1:A:64:THR:HG22	1:A:65:SER:H	0.50	1.65	13	1
3:A:88:PLM:C9	3:A:88:PLM:H52	0.50	2.36	15	1
1:A:20:ALA:O	1:A:21:ASP:C	0.50	2.53	14	14
1:A:10:GLU:O	1:A:14:HIS:ND1	0.50	2.45	8	7
1:A:81:LYS:HZ1	1:A:86:ILE:C	0.50	2.15	4	1
1:A:79:GLU:OE1	1:A:83:LYS:NZ	0.50	2.45	15	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:LYS:O	1:A:36:VAL:N	0.50	2.44	5	2
2:A:87:COA:N4P	2:A:87:COA:O9P	0.50	2.45	16	2
1:A:25:LEU:CA	1:A:54:LYS:HZ3	0.50	2.20	9	1
1:A:29:SER:HB2	1:A:61:LEU:HD11	0.49	1.83	4	8
1:A:54:LYS:CG	1:A:55:TRP:N	0.49	2.74	20	5
1:A:17:THR:O	1:A:17:THR:HG22	0.49	2.07	17	7
2:A:87:COA:H72	2:A:87:COA:CEP	0.49	2.37	3	1
1:A:25:LEU:HD23	1:A:57:ALA:HB2	0.49	1.83	5	1
1:A:68:ASP:CG	1:A:71:LYS:HZ3	0.49	2.14	8	1
2:A:87:COA:H141	3:A:88:PLM:H22	0.49	1.84	7	2
1:A:81:LYS:HA	1:A:86:ILE:CG2	0.49	2.38	1	2
2:A:87:COA:H22	2:A:87:COA:CDP	0.49	2.37	13	4
1:A:30:HIS:HB3	1:A:73:TYR:HB2	0.49	1.84	1	1
1:A:78:GLU:O	1:A:79:GLU:C	0.49	2.54	17	5
1:A:64:THR:CG2	1:A:65:SER:H	0.49	2.20	13	2
1:A:79:GLU:CD	1:A:83:LYS:NZ	0.49	2.71	8	1
1:A:31:TYR:CE2	2:A:87:COA:C4A	0.49	2.96	9	2
1:A:78:GLU:OE1	1:A:82:LYS:NZ	0.49	2.46	1	2
2:A:87:COA:CDP	3:A:88:PLM:H22	0.49	2.36	1	1
2:A:87:COA:N3A	3:A:88:PLM:C8	0.49	2.75	19	3
2:A:87:COA:O1A	2:A:87:COA:H3B	0.49	2.08	5	1
1:A:28:TYR:CD2	1:A:28:TYR:C	0.49	2.90	6	1
1:A:33:GLN:HE21	1:A:69:ALA:HA	0.49	1.68	8	1
3:A:88:PLM:HA1	3:A:88:PLM:H62	0.49	1.84	4	1
3:A:88:PLM:H82	3:A:88:PLM:C4	0.49	2.37	5	1
1:A:7:LYS:HZ3	1:A:10:GLU:CD	0.49	2.15	8	1
3:A:88:PLM:H81	3:A:88:PLM:C4	0.49	2.37	14	1
1:A:18:LYS:HD3	1:A:24:MET:SD	0.49	2.48	18	1
1:A:28:TYR:CD2	1:A:54:LYS:CA	0.49	2.96	18	2
1:A:11:GLU:OE1	1:A:81:LYS:NZ	0.49	2.45	19	3
3:A:88:PLM:CB	3:A:88:PLM:C7	0.49	2.90	11	2
1:A:24:MET:HA	3:A:88:PLM:H61	0.49	1.83	17	1
2:A:87:COA:N8P	2:A:87:COA:H131	0.48	2.23	9	3
1:A:28:TYR:H	3:A:88:PLM:C9	0.48	2.21	8	1
1:A:14:HIS:O	1:A:15:LEU:C	0.48	2.56	1	3
1:A:18:LYS:NZ	1:A:19:PRO:O	0.48	2.46	14	2
1:A:18:LYS:HB3	3:A:88:PLM:O2	0.48	2.08	3	1
1:A:66:LYS:HB3	1:A:66:LYS:NZ	0.48	2.24	11	1
1:A:24:MET:O	1:A:27:ILE:N	0.48	2.45	5	2
2:A:87:COA:OAP	3:A:88:PLM:H22	0.48	2.09	5	1
1:A:27:ILE:HA	1:A:76:LYS:CD	0.48	2.38	18	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:ALA:HB3	3:A:88:PLM:HF2	0.48	1.84	20	1
1:A:24:MET:C	3:A:88:PLM:HD2	0.48	2.34	3	2
1:A:23:GLU:OE1	1:A:83:LYS:NZ	0.48	2.46	2	1
1:A:33:GLN:CD	1:A:64:THR:HB	0.48	2.34	12	4
1:A:24:MET:HB3	3:A:88:PLM:CA	0.48	2.39	7	1
1:A:33:GLN:HG3	1:A:61:LEU:CB	0.48	2.38	9	4
1:A:62:LYS:C	1:A:62:LYS:HD3	0.48	2.34	10	1
1:A:13:LYS:NZ	2:A:87:COA:O2A	0.48	2.47	10	4
1:A:61:LEU:O	1:A:63:GLY:N	0.48	2.47	17	8
1:A:28:TYR:O	1:A:32:LYS:CG	0.48	2.62	10	1
3:A:88:PLM:HD1	3:A:88:PLM:H92	0.48	1.86	18	1
1:A:26:PHE:CD1	1:A:76:LYS:CG	0.48	2.97	3	1
1:A:81:LYS:NZ	1:A:86:ILE:O	0.48	2.46	3	2
1:A:51:GLY:CA	1:A:54:LYS:HD3	0.48	2.39	4	2
3:A:88:PLM:H61	3:A:88:PLM:HB1	0.48	1.85	5	1
1:A:53:ALA:CB	3:A:88:PLM:HF2	0.48	2.39	20	1
2:A:87:COA:S1P	2:A:87:COA:H132	0.48	2.49	1	1
1:A:74:ILE:O	1:A:75:ASP:C	0.48	2.57	12	6
1:A:33:GLN:HG2	1:A:61:LEU:CD1	0.48	2.39	5	2
1:A:28:TYR:CD2	1:A:54:LYS:CB	0.48	2.97	6	1
1:A:15:LEU:C	1:A:17:THR:N	0.47	2.71	1	9
1:A:80:LEU:HA	1:A:83:LYS:HD2	0.47	1.86	10	1
1:A:13:LYS:HE2	2:A:87:COA:O2A	0.47	2.08	12	1
1:A:26:PHE:CE2	1:A:76:LYS:HB2	0.47	2.44	18	1
1:A:19:PRO:HG3	1:A:84:TYR:CD2	0.47	2.44	15	8
1:A:28:TYR:CZ	1:A:54:LYS:HB3	0.47	2.44	5	2
2:A:87:COA:C5P	2:A:87:COA:O9P	0.47	2.62	14	2
1:A:10:GLU:CD	1:A:13:LYS:NZ	0.47	2.72	1	1
2:A:87:COA:H62	2:A:87:COA:H10	0.47	1.85	3	1
1:A:8:ALA:HA	1:A:11:GLU:HB2	0.47	1.85	7	1
1:A:7:LYS:NZ	1:A:10:GLU:CD	0.47	2.72	8	2
1:A:26:PHE:CE2	1:A:30:HIS:CE1	0.47	3.02	9	1
1:A:39:ILE:HD11	1:A:55:TRP:CG	0.47	2.44	9	2
2:A:87:COA:H131	2:A:87:COA:C2P	0.47	2.39	16	2
1:A:5:PHE:CZ	1:A:34:ALA:CB	0.47	2.97	1	3
1:A:5:PHE:HB3	1:A:70:MET:SD	0.47	2.50	1	1
2:A:87:COA:C2A	3:A:88:PLM:H81	0.47	2.39	1	1
1:A:15:LEU:CD1	1:A:80:LEU:HD13	0.47	2.40	2	3
3:A:88:PLM:C4	3:A:88:PLM:C8	0.47	2.92	2	2
1:A:24:MET:HE1	3:A:88:PLM:H21	0.47	1.85	3	2
1:A:26:PHE:CD2	1:A:76:LYS:HB2	0.47	2.44	18	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:87:COA:H22	2:A:87:COA:CAP	0.47	2.39	18	2
1:A:8:ALA:O	1:A:11:GLU:HB2	0.47	2.09	8	2
1:A:24:MET:HE1	3:A:88:PLM:H32	0.47	1.85	10	1
1:A:15:LEU:CD1	1:A:80:LEU:HB3	0.47	2.40	8	4
1:A:71:LYS:NZ	1:A:75:ASP:CG	0.47	2.73	14	2
1:A:25:LEU:HG	3:A:88:PLM:HG2	0.47	1.86	18	6
1:A:23:GLU:OE2	1:A:83:LYS:NZ	0.47	2.48	9	4
1:A:54:LYS:HE2	2:A:87:COA:O8A	0.47	2.10	17	1
1:A:13:LYS:HG3	2:A:87:COA:N6A	0.47	2.25	13	2
1:A:61:LEU:O	1:A:64:THR:N	0.47	2.48	18	6
1:A:19:PRO:HB3	1:A:84:TYR:CE1	0.47	2.44	10	1
1:A:4:GLU:N	1:A:4:GLU:CD	0.47	2.72	16	1
1:A:13:LYS:CD	2:A:87:COA:N7A	0.47	2.78	18	1
1:A:5:PHE:HA	1:A:74:ILE:HG12	0.47	1.87	16	8
1:A:28:TYR:CE1	2:A:87:COA:O3B	0.47	2.67	1	2
1:A:28:TYR:CB	3:A:88:PLM:HC2	0.47	2.39	12	2
1:A:12:VAL:HA	1:A:15:LEU:HG	0.47	1.87	11	3
1:A:54:LYS:HZ3	2:A:87:COA:C3B	0.47	2.23	7	1
1:A:79:GLU:CD	1:A:83:LYS:HZ3	0.47	2.18	8	1
2:A:87:COA:CEP	2:A:87:COA:C7P	0.46	2.93	3	1
1:A:19:PRO:HB3	1:A:80:LEU:CD2	0.46	2.39	7	4
1:A:67:GLU:CA	1:A:70:MET:SD	0.46	3.03	16	1
2:A:87:COA:CDP	3:A:88:PLM:C2	0.46	2.93	1	1
1:A:16:LYS:CD	1:A:16:LYS:N	0.46	2.78	1	1
1:A:24:MET:HE1	3:A:88:PLM:C2	0.46	2.41	3	1
2:A:87:COA:H141	2:A:87:COA:N8P	0.46	2.25	4	5
1:A:25:LEU:CD2	1:A:53:ALA:CB	0.46	2.93	14	1
1:A:27:ILE:CD1	1:A:80:LEU:CD1	0.46	2.93	18	1
3:A:88:PLM:H41	3:A:88:PLM:H91	0.46	1.86	20	1
1:A:25:LEU:N	3:A:88:PLM:CD	0.46	2.78	8	1
2:A:87:COA:N4P	2:A:87:COA:C9P	0.46	2.78	13	1
1:A:39:ILE:O	1:A:62:LYS:NZ	0.46	2.49	1	1
2:A:87:COA:H72	2:A:87:COA:H143	0.46	1.86	3	1
1:A:35:THR:O	1:A:66:LYS:NZ	0.46	2.48	5	2
1:A:13:LYS:HA	3:A:88:PLM:O2	0.46	2.10	10	4
1:A:19:PRO:HA	1:A:84:TYR:CE2	0.46	2.46	10	1
1:A:66:LYS:C	1:A:70:MET:SD	0.46	2.99	16	1
1:A:21:ASP:HB3	3:A:88:PLM:CG	0.46	2.41	8	2
1:A:52:LYS:CD	1:A:52:LYS:C	0.46	2.89	1	2
1:A:51:GLY:HA2	1:A:54:LYS:HD3	0.46	1.86	4	2
1:A:34:ALA:HA	1:A:66:LYS:O	0.46	2.11	11	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:HIS:HB2	1:A:76:LYS:HE3	0.46	1.87	18	1
1:A:58:TRP:O	1:A:60:GLU:N	0.46	2.48	5	2
1:A:24:MET:HB3	3:A:88:PLM:HB2	0.46	1.87	11	1
1:A:76:LYS:HA	1:A:76:LYS:HZ2	0.46	1.70	13	1
1:A:41:THR:OG1	1:A:55:TRP:NE1	0.46	2.49	3	4
2:A:87:COA:H4B	2:A:87:COA:O8A	0.46	2.11	4	1
1:A:84:TYR:N	1:A:84:TYR:CD2	0.46	2.84	7	1
1:A:77:VAL:O	1:A:78:GLU:C	0.46	2.59	6	7
1:A:51:GLY:C	1:A:54:LYS:HZ1	0.46	2.19	13	1
1:A:51:GLY:O	1:A:52:LYS:C	0.46	2.59	15	1
1:A:79:GLU:OE2	1:A:82:LYS:NZ	0.45	2.49	4	2
1:A:10:GLU:O	1:A:13:LYS:N	0.45	2.49	7	1
1:A:79:GLU:HB3	1:A:83:LYS:CE	0.45	2.42	1	2
2:A:87:COA:H133	2:A:87:COA:H52A	0.45	1.88	8	2
2:A:87:COA:O4B	3:A:88:PLM:HA2	0.45	2.10	19	1
1:A:83:LYS:HB3	1:A:84:TYR:CE2	0.45	2.47	15	4
3:A:88:PLM:CB	3:A:88:PLM:H72	0.45	2.40	11	1
1:A:71:LYS:NZ	1:A:75:ASP:OD1	0.45	2.49	3	3
1:A:58:TRP:C	1:A:58:TRP:CD1	0.45	2.93	13	3
3:A:88:PLM:H81	3:A:88:PLM:H41	0.45	1.87	6	1
1:A:23:GLU:OE1	1:A:76:LYS:NZ	0.45	2.47	1	1
1:A:12:VAL:CG1	1:A:13:LYS:N	0.45	2.80	18	4
1:A:76:LYS:NZ	1:A:79:GLU:OE2	0.45	2.49	5	1
1:A:14:HIS:HB2	1:A:86:ILE:HD13	0.45	1.89	9	2
1:A:24:MET:CE	3:A:88:PLM:H21	0.45	2.42	18	1
3:A:88:PLM:H62	3:A:88:PLM:HC2	0.45	1.88	19	2
1:A:22:GLU:C	1:A:25:LEU:HB2	0.45	2.36	9	1
1:A:15:LEU:HD23	1:A:86:ILE:HG22	0.45	1.88	18	2
1:A:13:LYS:HG3	2:A:87:COA:N7A	0.45	2.27	4	1
1:A:28:TYR:CD1	1:A:54:LYS:CB	0.45	3.00	20	1
1:A:70:MET:O	1:A:71:LYS:C	0.45	2.60	10	4
1:A:54:LYS:NZ	2:A:87:COA:P3B	0.45	2.90	4	3
3:A:88:PLM:H52	3:A:88:PLM:H91	0.45	1.88	4	1
1:A:33:GLN:NE2	1:A:58:TRP:CG	0.45	2.84	5	1
1:A:80:LEU:O	1:A:81:LYS:C	0.45	2.59	10	1
1:A:67:GLU:OE1	1:A:70:MET:HE3	0.45	2.12	11	1
1:A:15:LEU:CD1	1:A:19:PRO:HG2	0.45	2.42	1	1
1:A:28:TYR:HB3	1:A:54:LYS:CE	0.45	2.42	9	1
1:A:76:LYS:NZ	1:A:79:GLU:OE1	0.44	2.50	1	2
2:A:87:COA:C2A	3:A:88:PLM:C6	0.44	2.94	1	1
1:A:19:PRO:HG2	1:A:80:LEU:HD22	0.44	1.89	11	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:TRP:C	1:A:60:GLU:N	0.44	2.74	15	5
2:A:87:COA:CDP	3:A:88:PLM:C1	0.44	2.94	1	1
1:A:67:GLU:N	1:A:67:GLU:CD	0.44	2.76	3	3
1:A:9:ALA:CA	2:A:87:COA:H61A	0.44	2.24	4	1
1:A:18:LYS:NZ	1:A:21:ASP:CG	0.44	2.76	5	3
1:A:81:LYS:HZ2	1:A:86:ILE:C	0.44	2.21	9	1
1:A:53:ALA:N	1:A:54:LYS:HZ3	0.44	2.10	13	1
1:A:29:SER:HB2	1:A:61:LEU:CD1	0.44	2.42	5	3
1:A:28:TYR:CD2	1:A:54:LYS:C	0.44	2.95	18	1
1:A:18:LYS:CB	2:A:87:COA:S1P	0.44	3.06	1	1
1:A:12:VAL:HA	1:A:15:LEU:CD1	0.44	2.43	2	1
1:A:24:MET:C	3:A:88:PLM:HA2	0.44	2.37	8	1
1:A:74:ILE:O	1:A:77:VAL:N	0.44	2.50	12	1
1:A:54:LYS:O	1:A:55:TRP:C	0.44	2.60	13	1
1:A:39:ILE:HD12	1:A:58:TRP:CE3	0.44	2.48	15	3
1:A:28:TYR:O	1:A:29:SER:C	0.44	2.59	7	2
2:A:87:COA:H51A	2:A:87:COA:O4A	0.44	2.12	9	1
1:A:24:MET:CE	3:A:88:PLM:H32	0.44	2.31	13	1
3:A:88:PLM:H41	3:A:88:PLM:C9	0.44	2.42	20	1
1:A:18:LYS:HB3	2:A:87:COA:C5P	0.44	2.43	11	2
1:A:5:PHE:O	1:A:6:ASP:C	0.44	2.61	6	3
1:A:28:TYR:CD2	1:A:54:LYS:HE3	0.44	2.48	9	1
1:A:24:MET:HE1	3:A:88:PLM:C4	0.44	2.42	16	1
1:A:25:LEU:HD23	1:A:54:LYS:NZ	0.44	2.28	9	1
2:A:87:COA:H51A	2:A:87:COA:P2A	0.44	2.53	9	1
3:A:88:PLM:C4	3:A:88:PLM:H91	0.44	2.42	17	1
1:A:33:GLN:OE1	1:A:69:ALA:CB	0.44	2.66	20	1
1:A:28:TYR:CE2	1:A:54:LYS:C	0.44	2.95	1	2
1:A:28:TYR:CD1	3:A:88:PLM:HC1	0.44	2.48	6	1
1:A:54:LYS:HD3	3:A:88:PLM:CE	0.44	2.43	9	1
1:A:71:LYS:HA	1:A:71:LYS:HE2	0.44	1.88	9	1
1:A:7:LYS:O	1:A:8:ALA:C	0.44	2.60	20	6
1:A:9:ALA:C	2:A:87:COA:H61A	0.44	2.21	12	1
1:A:54:LYS:HD2	3:A:88:PLM:CC	0.44	2.43	13	1
2:A:87:COA:H131	2:A:87:COA:H22	0.44	1.90	13	2
1:A:10:GLU:HG2	1:A:11:GLU:H	0.44	1.72	14	1
1:A:28:TYR:HB2	3:A:88:PLM:H91	0.44	1.90	18	1
1:A:15:LEU:CD1	1:A:19:PRO:CG	0.44	2.96	1	1
1:A:15:LEU:HD11	1:A:80:LEU:HB3	0.44	1.89	8	2
2:A:87:COA:N3A	3:A:88:PLM:H82	0.44	2.27	19	3
1:A:25:LEU:CD2	1:A:54:LYS:N	0.44	2.80	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:87:COA:P1A	2:A:87:COA:H8A	0.44	2.53	20	2
1:A:53:ALA:HB3	3:A:88:PLM:CF	0.43	2.43	20	1
2:A:87:COA:N4P	3:A:88:PLM:C1	0.43	2.81	2	1
1:A:30:HIS:HB3	1:A:73:TYR:CA	0.43	2.43	3	1
1:A:25:LEU:CD2	1:A:57:ALA:HB2	0.43	2.43	16	3
1:A:13:LYS:HD2	2:A:87:COA:N7A	0.43	2.28	18	2
1:A:54:LYS:CA	3:A:88:PLM:HC1	0.43	2.43	12	1
1:A:71:LYS:NZ	1:A:75:ASP:OD2	0.43	2.51	11	4
1:A:12:VAL:CG2	1:A:15:LEU:HD11	0.43	2.43	17	3
1:A:71:LYS:CG	1:A:72:ALA:H	0.43	2.26	13	1
1:A:54:LYS:HG3	3:A:88:PLM:HD1	0.43	1.90	4	1
1:A:32:LYS:C	1:A:33:GLN:OE1	0.43	2.61	5	1
1:A:79:GLU:O	1:A:80:LEU:C	0.43	2.62	6	1
2:A:87:COA:HN4	3:A:88:PLM:H21	0.43	1.72	11	1
2:A:87:COA:CEP	3:A:88:PLM:H21	0.43	2.43	13	1
1:A:58:TRP:C	1:A:60:GLU:H	0.43	2.21	15	1
1:A:33:GLN:HE21	1:A:61:LEU:HB3	0.43	1.73	20	1
1:A:76:LYS:NZ	1:A:76:LYS:HA	0.43	2.28	5	1
1:A:25:LEU:HA	1:A:54:LYS:NZ	0.43	2.26	9	1
1:A:18:LYS:O	1:A:18:LYS:CG	0.43	2.66	10	3
1:A:24:MET:HE1	3:A:88:PLM:C3	0.43	2.43	10	1
1:A:18:LYS:HD3	1:A:18:LYS:C	0.43	2.38	18	1
1:A:10:GLU:O	1:A:11:GLU:C	0.43	2.61	9	3
1:A:52:LYS:O	1:A:56:ASP:HB2	0.43	2.14	1	3
2:A:87:COA:S1P	2:A:87:COA:H141	0.43	2.51	9	1
1:A:19:PRO:HB2	1:A:24:MET:SD	0.43	2.53	16	1
1:A:6:ASP:O	1:A:7:LYS:C	0.43	2.61	10	5
1:A:84:TYR:CD2	1:A:84:TYR:N	0.43	2.87	3	2
1:A:15:LEU:O	1:A:16:LYS:C	0.43	2.61	6	1
1:A:27:ILE:CG2	3:A:88:PLM:H62	0.43	2.43	14	1
3:A:88:PLM:C9	3:A:88:PLM:HD2	0.43	2.43	14	1
2:A:87:COA:CDP	2:A:87:COA:C2P	0.43	2.96	18	2
1:A:13:LYS:CG	2:A:87:COA:H62A	0.43	2.27	20	1
2:A:87:COA:S1P	2:A:87:COA:N8P	0.43	2.92	3	1
1:A:76:LYS:NZ	1:A:79:GLU:CD	0.43	2.76	19	1
1:A:5:PHE:CE2	1:A:34:ALA:HB3	0.43	2.47	3	4
2:A:87:COA:H131	2:A:87:COA:HN8	0.43	1.73	9	1
1:A:39:ILE:HG21	1:A:59:ASN:CB	0.43	2.43	13	1
1:A:54:LYS:CE	2:A:87:COA:O8A	0.43	2.67	17	1
1:A:26:PHE:O	1:A:27:ILE:C	0.43	2.62	12	2
1:A:33:GLN:OE1	1:A:33:GLN:CA	0.43	2.67	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ASP:OD1	1:A:62:LYS:NZ	0.43	2.46	10	1
1:A:25:LEU:HD23	1:A:54:LYS:HB3	0.42	1.91	2	1
2:A:87:COA:HN4	2:A:87:COA:CAP	0.42	2.27	3	1
1:A:51:GLY:HA2	1:A:54:LYS:NZ	0.42	2.29	17	1
1:A:52:LYS:NZ	1:A:56:ASP:OD2	0.42	2.52	1	1
2:A:87:COA:C5P	3:A:88:PLM:O2	0.42	2.67	1	1
1:A:54:LYS:CD	3:A:88:PLM:HB1	0.42	2.44	4	1
1:A:24:MET:HE3	3:A:88:PLM:H41	0.42	1.91	14	2
1:A:5:PHE:CD1	1:A:73:TYR:CD2	0.42	3.07	9	1
1:A:54:LYS:HD3	3:A:88:PLM:HE1	0.42	1.89	9	1
1:A:18:LYS:N	2:A:87:COA:O5P	0.42	2.51	19	1
1:A:35:THR:C	1:A:66:LYS:HZ3	0.42	2.22	4	1
1:A:8:ALA:HB1	1:A:77:VAL:HG21	0.42	1.90	9	1
1:A:33:GLN:HG3	1:A:61:LEU:HB2	0.42	1.89	9	1
1:A:28:TYR:CE2	1:A:54:LYS:CB	0.42	3.02	12	1
1:A:71:LYS:HG3	1:A:72:ALA:N	0.42	2.29	13	1
3:A:88:PLM:H62	3:A:88:PLM:HA1	0.42	1.90	19	1
1:A:67:GLU:N	1:A:67:GLU:OE1	0.42	2.52	2	1
1:A:79:GLU:CD	1:A:82:LYS:NZ	0.42	2.77	4	1
1:A:54:LYS:HZ1	2:A:87:COA:H4B	0.42	1.74	8	1
1:A:13:LYS:CE	2:A:87:COA:N7A	0.42	2.82	11	1
2:A:87:COA:H22	2:A:87:COA:H131	0.42	1.90	17	1
2:A:87:COA:CEP	2:A:87:COA:N8P	0.42	2.83	3	1
1:A:32:LYS:NZ	2:A:87:COA:O2B	0.42	2.51	9	2
1:A:9:ALA:HA	1:A:73:TYR:OH	0.42	2.15	3	1
2:A:87:COA:O4B	3:A:88:PLM:H91	0.42	2.14	6	1
1:A:54:LYS:HA	3:A:88:PLM:HB2	0.42	1.90	8	1
1:A:78:GLU:CD	1:A:82:LYS:HZ3	0.42	2.22	9	2
1:A:27:ILE:O	1:A:28:TYR:C	0.42	2.60	10	1
2:A:87:COA:HN8	3:A:88:PLM:C2	0.42	2.27	13	1
1:A:24:MET:HE2	3:A:88:PLM:C6	0.42	2.45	19	1
1:A:13:LYS:HZ2	2:A:87:COA:H142	0.42	1.75	4	1
2:A:87:COA:O6A	2:A:87:COA:C5B	0.42	2.67	4	1
1:A:15:LEU:C	1:A:17:THR:H	0.42	2.23	1	2
1:A:24:MET:HE3	3:A:88:PLM:H22	0.42	1.92	1	1
1:A:8:ALA:C	1:A:10:GLU:H	0.42	2.23	2	1
1:A:13:LYS:CD	2:A:87:COA:N6A	0.42	2.83	3	1
1:A:76:LYS:O	1:A:79:GLU:HB2	0.42	2.15	3	1
1:A:67:GLU:O	1:A:68:ASP:C	0.42	2.62	6	1
1:A:4:GLU:OE2	1:A:7:LYS:NZ	0.42	2.51	12	1
1:A:28:TYR:CG	3:A:88:PLM:HC2	0.42	2.50	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:LEU:HD21	1:A:53:ALA:C	0.42	2.39	17	1
1:A:32:LYS:O	1:A:33:GLN:C	0.42	2.61	18	1
1:A:4:GLU:O	1:A:7:LYS:HB3	0.42	2.14	1	1
1:A:67:GLU:CD	1:A:67:GLU:N	0.42	2.78	16	1
1:A:68:ASP:O	1:A:69:ALA:C	0.42	2.62	17	1
1:A:9:ALA:CB	1:A:31:TYR:CE1	0.42	3.02	20	1
1:A:23:GLU:CD	1:A:83:LYS:HZ3	0.42	2.22	7	1
1:A:19:PRO:CB	1:A:84:TYR:CE2	0.42	3.02	14	1
1:A:18:LYS:CD	1:A:24:MET:SD	0.42	3.07	19	1
1:A:18:LYS:HB3	2:A:87:COA:C6P	0.41	2.45	4	1
2:A:87:COA:H133	2:A:87:COA:C4B	0.41	2.45	4	1
1:A:24:MET:O	3:A:88:PLM:H91	0.41	2.15	8	1
1:A:28:TYR:CZ	1:A:32:LYS:HD3	0.41	2.50	8	1
1:A:31:TYR:CD2	2:A:87:COA:N3A	0.41	2.88	9	1
1:A:13:LYS:CE	2:A:87:COA:O2A	0.41	2.68	10	2
1:A:10:GLU:OE2	1:A:13:LYS:CE	0.41	2.68	17	1
1:A:28:TYR:CE1	1:A:32:LYS:CG	0.41	3.03	1	1
1:A:13:LYS:CA	2:A:87:COA:OAP	0.41	2.68	6	1
1:A:27:ILE:HD11	1:A:76:LYS:C	0.41	2.41	7	1
1:A:25:LEU:HA	3:A:88:PLM:HC2	0.41	1.91	8	1
1:A:81:LYS:NZ	1:A:86:ILE:OXT	0.41	2.53	12	1
2:A:87:COA:HN8	3:A:88:PLM:H21	0.41	1.74	13	1
1:A:83:LYS:CB	1:A:84:TYR:CE2	0.41	3.03	19	1
1:A:13:LYS:HD3	2:A:87:COA:N7A	0.41	2.30	2	1
1:A:35:THR:C	1:A:66:LYS:NZ	0.41	2.79	4	1
1:A:12:VAL:CG1	2:A:87:COA:N1A	0.41	2.83	5	1
1:A:39:ILE:HG21	1:A:59:ASN:OD1	0.41	2.15	11	1
1:A:28:TYR:CE2	1:A:54:LYS:HE3	0.41	2.51	2	1
2:A:87:COA:O9P	2:A:87:COA:C6P	0.41	2.68	14	2
1:A:13:LYS:HZ1	2:A:87:COA:P2A	0.41	2.38	13	1
1:A:55:TRP:O	1:A:56:ASP:C	0.41	2.64	15	1
1:A:29:SER:O	1:A:33:GLN:CG	0.41	2.69	20	1
1:A:79:GLU:C	1:A:83:LYS:HD2	0.41	2.41	3	1
1:A:18:LYS:CB	2:A:87:COA:C6P	0.41	2.99	4	1
1:A:28:TYR:HB3	3:A:88:PLM:CA	0.41	2.38	8	1
3:A:88:PLM:HB1	3:A:88:PLM:HE2	0.41	1.75	19	1
1:A:52:LYS:O	1:A:56:ASP:N	0.41	2.53	1	1
1:A:76:LYS:O	1:A:77:VAL:C	0.41	2.60	1	3
1:A:4:GLU:OE1	1:A:4:GLU:HA	0.41	2.15	5	1
1:A:81:LYS:HA	1:A:86:ILE:HG22	0.41	1.91	8	1
1:A:36:VAL:O	1:A:66:LYS:NZ	0.41	2.54	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:LYS:HD3	1:A:81:LYS:C	0.41	2.40	14	1
1:A:19:PRO:CB	1:A:80:LEU:HD22	0.41	2.46	15	1
1:A:24:MET:CE	3:A:88:PLM:O2	0.41	2.69	17	1
1:A:24:MET:HB3	3:A:88:PLM:HC2	0.41	1.93	19	1
1:A:29:SER:O	1:A:33:GLN:HG2	0.41	2.14	20	1
2:A:87:COA:N3A	3:A:88:PLM:C7	0.41	2.83	7	1
1:A:19:PRO:HG2	1:A:80:LEU:HD12	0.41	1.92	8	1
1:A:33:GLN:NE2	1:A:69:ALA:CA	0.41	2.84	8	1
1:A:57:ALA:O	1:A:60:GLU:HB3	0.41	2.15	14	1
1:A:54:LYS:HG3	1:A:55:TRP:H	0.41	1.74	20	1
1:A:38:ASP:O	1:A:62:LYS:NZ	0.41	2.54	1	1
1:A:26:PHE:O	1:A:29:SER:OG	0.41	2.38	5	1
1:A:20:ALA:C	1:A:22:GLU:N	0.41	2.77	9	1
1:A:28:TYR:HA	2:A:87:COA:H2A	0.41	1.93	9	1
1:A:29:SER:OG	1:A:30:HIS:N	0.41	2.52	11	2
1:A:22:GLU:HA	1:A:25:LEU:CD1	0.41	2.46	11	1
1:A:23:GLU:OE2	1:A:83:LYS:CE	0.41	2.69	15	1
1:A:28:TYR:CD1	1:A:29:SER:N	0.41	2.89	20	1
1:A:25:LEU:CG	1:A:53:ALA:HB1	0.41	2.46	3	1
1:A:21:ASP:HA	1:A:24:MET:HB2	0.41	1.92	7	1
1:A:23:GLU:CD	1:A:83:LYS:NZ	0.41	2.79	16	1
1:A:54:LYS:HD2	3:A:88:PLM:HB1	0.40	1.92	8	1
1:A:31:TYR:CG	2:A:87:COA:C2A	0.40	3.04	10	1
1:A:18:LYS:HB2	2:A:87:COA:C6P	0.40	2.45	15	1
1:A:4:GLU:O	1:A:8:ALA:HB2	0.40	2.16	17	1
1:A:28:TYR:CE2	1:A:54:LYS:HG3	0.40	2.51	17	1
1:A:27:ILE:CD1	1:A:76:LYS:HG2	0.40	2.42	18	1
2:A:87:COA:H2A	3:A:88:PLM:H82	0.40	1.91	19	1
1:A:33:GLN:O	1:A:37:GLY:N	0.40	2.54	20	1
1:A:80:LEU:H	1:A:80:LEU:HD22	0.40	1.76	1	1
2:A:87:COA:N8P	2:A:87:COA:H141	0.40	2.30	3	1
3:A:88:PLM:H81	3:A:88:PLM:H42	0.40	1.92	6	1
1:A:51:GLY:N	1:A:54:LYS:CE	0.40	2.81	13	1
1:A:82:LYS:HG2	1:A:83:LYS:N	0.40	2.32	15	1
1:A:5:PHE:CE1	1:A:35:THR:CG2	0.40	3.04	4	1
1:A:33:GLN:HG2	1:A:61:LEU:CB	0.40	2.47	5	1
1:A:28:TYR:O	1:A:32:LYS:HG3	0.40	2.16	10	1
1:A:28:TYR:CG	1:A:54:LYS:CB	0.40	3.02	18	1
1:A:24:MET:HB3	3:A:88:PLM:HA1	0.40	1.94	7	1
1:A:30:HIS:CE1	1:A:72:ALA:HB3	0.40	2.52	10	1
1:A:29:SER:C	1:A:61:LEU:HD11	0.40	2.41	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:GLU:O	1:A:86:ILE:HG21	0.40	2.17	3	1
1:A:18:LYS:HA	2:A:87:COA:O5P	0.40	2.16	4	1
1:A:24:MET:HE1	3:A:88:PLM:C1	0.40	2.47	6	1
1:A:18:LYS:NZ	1:A:21:ASP:OD2	0.40	2.54	7	1
1:A:53:ALA:O	1:A:54:LYS:C	0.40	2.64	7	1
1:A:32:LYS:HD2	1:A:58:TRP:CZ3	0.40	2.52	13	1
1:A:25:LEU:O	1:A:26:PHE:C	0.40	2.65	14	1
1:A:68:ASP:CA	1:A:71:LYS:HZ2	0.40	2.29	17	1
1:A:29:SER:HA	1:A:58:TRP:HB2	0.40	1.92	18	1

6.3 Torsion angles [i](#)

6.3.1 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 NMR 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	73/86 (85%)	49±3 (68±4%)	19±3 (26±5%)	5±2 (6±3%)	2	18
All	All	1460/1720 (85%)	988 (68%)	380 (26%)	92 (6%)	2	18

All 20 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	18	LYS	14
1	A	16	LYS	13
1	A	62	LYS	13
1	A	53	ALA	11
1	A	19	PRO	8
1	A	59	ASN	6
1	A	15	LEU	4
1	A	66	LYS	4
1	A	81	LYS	3
1	A	85	GLY	3
1	A	74	ILE	2
1	A	25	LEU	2
1	A	51	GLY	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	38	ASP	1
1	A	39	ILE	1
1	A	9	ALA	1
1	A	56	ASP	1
1	A	71	LYS	1
1	A	55	TRP	1
1	A	29	SER	1

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR 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	62/72 (86%)	51±3 (82±4%)	11±3 (18±4%)	3	36
All	All	1240/1440 (86%)	1012 (82%)	228 (18%)	3	36

All 35 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	12	VAL	20
1	A	86	ILE	20
1	A	78	GLU	16
1	A	33	GLN	14
1	A	56	ASP	14
1	A	52	LYS	11
1	A	17	THR	10
1	A	4	GLU	9
1	A	54	LYS	9
1	A	64	THR	9
1	A	25	LEU	8
1	A	76	LYS	7
1	A	71	LYS	7
1	A	11	GLU	7
1	A	65	SER	6
1	A	75	ASP	6
1	A	10	GLU	6
1	A	13	LYS	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	16	LYS	5
1	A	55	TRP	5
1	A	18	LYS	4
1	A	29	SER	4
1	A	68	ASP	4
1	A	6	ASP	3
1	A	67	GLU	3
1	A	7	LYS	3
1	A	81	LYS	2
1	A	62	LYS	2
1	A	27	ILE	2
1	A	5	PHE	1
1	A	82	LYS	1
1	A	32	LYS	1
1	A	60	GLU	1
1	A	66	LYS	1
1	A	40	ASN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	COA	A	87	3	47,50,50	1.34±0.22	4±1 (8±2%)
3	PLM	A	88	2	15,16,17	0.85±0.13	0±0 (2±3%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	COA	A	87	3	69,75,75	1.74±0.21	13±3 (18±3%)
3	PLM	A	88	2	14,15,17	0.95±0.12	0±1 (3±4%)

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
2	COA	A	87	3	1±0,1,13,13	0±0,48,64,64	0±0,3,3,3
3	PLM	A	88	2	-	0±0,14,14,15	-

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	87	COA	CDP-CBP	8.56	1.36	1.53	5	6
2	A	87	COA	P2A-O3A	8.27	1.50	1.59	5	18
2	A	87	COA	P1A-O3A	5.52	1.53	1.59	19	18
2	A	87	COA	CCP-CBP	3.86	1.58	1.52	10	6
2	A	87	COA	C7P-N8P	3.11	1.53	1.46	18	4
2	A	87	COA	P3B-O3B	2.73	1.64	1.59	2	3
2	A	87	COA	C5B-C4B	2.62	1.59	1.51	10	6
3	A	88	PLM	CE-CD	2.52	1.39	1.51	15	1
2	A	87	COA	C7P-C6P	2.42	1.59	1.51	2	2
2	A	87	COA	P3B-O8A	2.27	1.46	1.54	9	4
3	A	88	PLM	CD-CC	2.24	1.62	1.51	14	1
3	A	88	PLM	C4-C3	2.23	1.62	1.51	18	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	87	COA	P3B-O9A	2.21	1.46	1.54	12	7
2	A	87	COA	C6P-C5P	2.13	1.55	1.51	5	1
2	A	87	COA	C5A-C4A	2.02	1.35	1.39	7	1
3	A	88	PLM	C8-C7	2.01	1.61	1.51	6	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	87	COA	CAP-C9P-N8P	10.15	97.23	116.48	6	5
2	A	87	COA	C7P-N8P-C9P	7.45	135.93	122.55	3	6
2	A	87	COA	C2P-C3P-N4P	7.17	96.03	112.31	13	19
2	A	87	COA	CDP-CBP-CCP	7.12	119.98	108.22	4	12
2	A	87	COA	CEP-CBP-CAP	7.09	120.85	108.77	4	20
2	A	87	COA	C6P-C7P-N8P	6.68	97.78	112.00	20	13
2	A	87	COA	CEP-CBP-CCP	5.95	118.04	108.22	6	7
2	A	87	COA	C6P-C5P-N4P	5.94	105.51	116.34	18	14
2	A	87	COA	C3P-N4P-C5P	5.74	133.50	122.82	5	5
2	A	87	COA	O4B-C1B-N9A	4.98	98.53	108.09	10	11
2	A	87	COA	P3B-O3B-C3B	4.78	136.20	123.43	6	2
2	A	87	COA	O9P-C9P-N8P	4.71	132.94	122.98	6	3
2	A	87	COA	O6A-CCP-CBP	4.45	117.71	110.55	8	11
2	A	87	COA	CEP-CBP-CDP	4.43	100.36	109.20	4	14
2	A	87	COA	C7P-C6P-C5P	4.14	105.50	112.39	17	9
2	A	87	COA	O9A-P3B-O8A	3.72	121.75	107.80	19	9
2	A	87	COA	O5B-C5B-C4B	3.71	121.64	108.99	2	11
2	A	87	COA	O2A-P1A-O3A	3.41	116.49	107.27	15	5
2	A	87	COA	OAP-CAP-CBP	3.33	102.47	110.18	2	11
2	A	87	COA	CDP-CBP-CAP	3.28	114.36	108.77	13	8
2	A	87	COA	O3B-P3B-O7A	3.24	97.78	109.33	19	8
2	A	87	COA	O9P-C9P-CAP	3.20	129.82	120.89	6	2
2	A	87	COA	O3A-P1A-O1A	3.14	101.25	110.70	5	3
2	A	87	COA	O4B-C4B-C3B	3.07	111.39	104.92	4	4
2	A	87	COA	OAP-CAP-C9P	3.01	121.96	109.38	1	4
2	A	87	COA	C2B-C3B-C4B	3.01	97.97	103.24	13	5
2	A	87	COA	O5P-C5P-N4P	2.95	128.81	123.03	13	5
2	A	87	COA	O9A-P3B-O3B	2.86	94.69	105.85	8	2
2	A	87	COA	O8A-P3B-O3B	2.81	94.88	105.85	9	1
3	A	88	PLM	CE-CD-CC	2.68	100.80	114.37	4	3
2	A	87	COA	C2B-C1B-N9A	2.54	119.60	113.30	10	1
3	A	88	PLM	C6-C5-C4	2.53	101.56	114.37	11	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	87	COA	C3B-C2B-C1B	2.52	105.44	99.89	1	1
2	A	87	COA	O8A-P3B-O7A	2.41	120.21	110.83	5	3
2	A	87	COA	O5A-P2A-O3A	2.38	113.72	107.27	14	2
2	A	87	COA	O9A-P3B-O7A	2.37	120.08	110.83	20	2
2	A	87	COA	C1B-N9A-C8A	2.37	132.35	127.09	7	2
3	A	88	PLM	C9-C8-C7	2.29	102.81	114.37	7	2
2	A	87	COA	O5P-C5P-C6P	2.26	126.12	122.02	18	1
2	A	87	COA	O4B-C4B-C5B	2.21	102.27	109.33	2	1
3	A	88	PLM	CC-CB-CA	2.18	103.33	114.37	7	1
2	A	87	COA	N6A-C6A-N1A	2.15	113.59	118.38	15	2
2	A	87	COA	P1A-O5B-C5B	2.14	133.62	121.35	15	2
3	A	88	PLM	C7-C6-C5	2.12	103.63	114.37	15	3
2	A	87	COA	O2A-P1A-O1A	2.11	122.26	112.44	19	1
2	A	87	COA	O3B-C3B-C2B	2.07	104.25	111.68	17	1
2	A	87	COA	C4A-N9A-C1B	2.07	121.80	126.63	7	1
2	A	87	COA	O4B-C1B-C2B	2.04	110.97	106.62	5	2
2	A	87	COA	O5A-P2A-O4A	2.02	121.84	112.44	19	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	A	87	COA	CAP	20

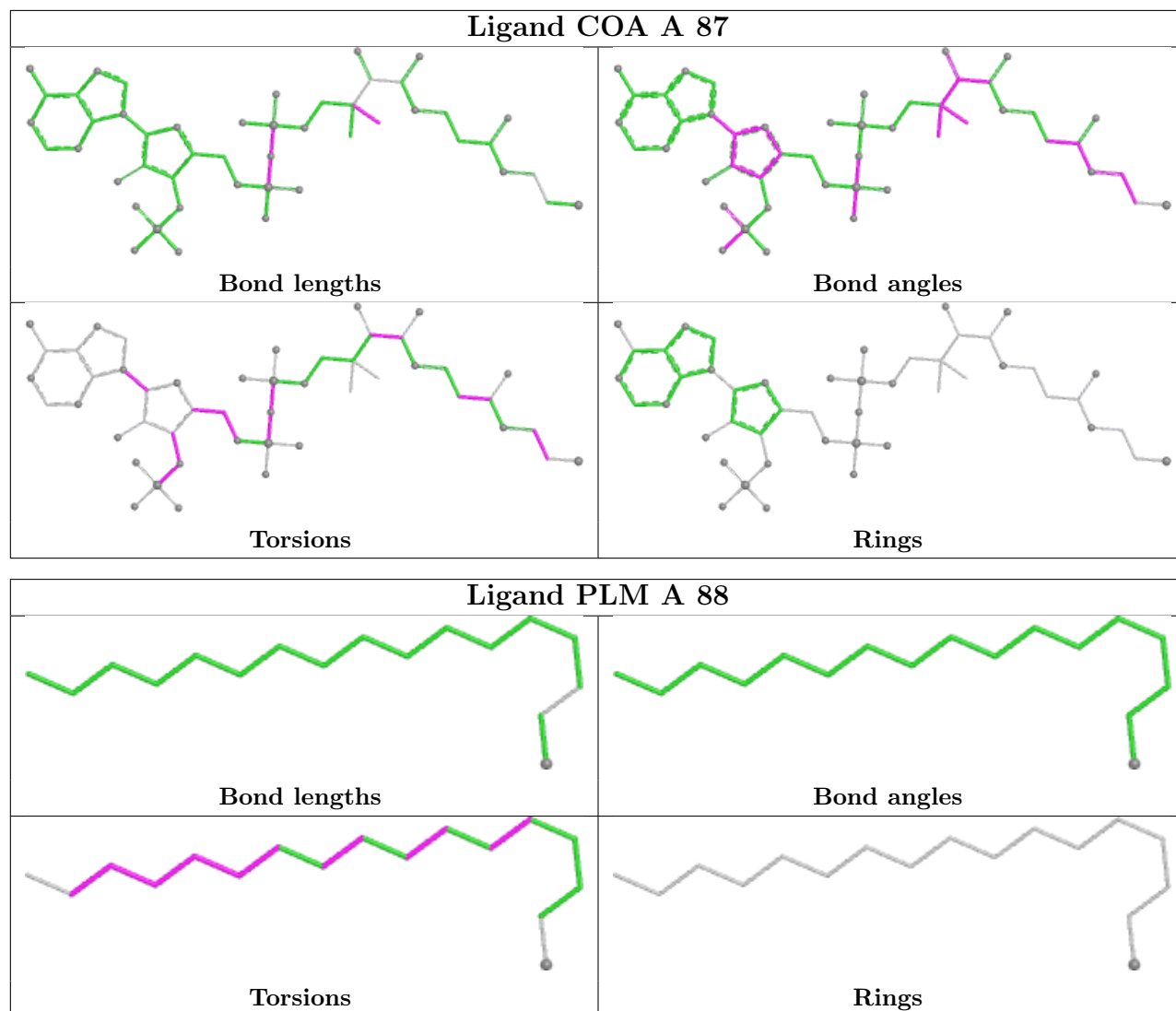
All unique torsion outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	A	87	COA	O9P-C9P-CAP-CBP	6
2	A	87	COA	N8P-C9P-CAP-CBP	5
2	A	87	COA	CAP-C9P-N8P-C7P	1

There are no ring outliers.

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.



6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided