



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 01:56 AM UTC

PDB ID : 1JTB / pdb_00001jtb
Title : LIPID TRANSFER PROTEIN COMPLEXED WITH PALMITOYL COENZYME A, NMR, 16 STRUCTURES
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Deposited on : 1996-12-03

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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

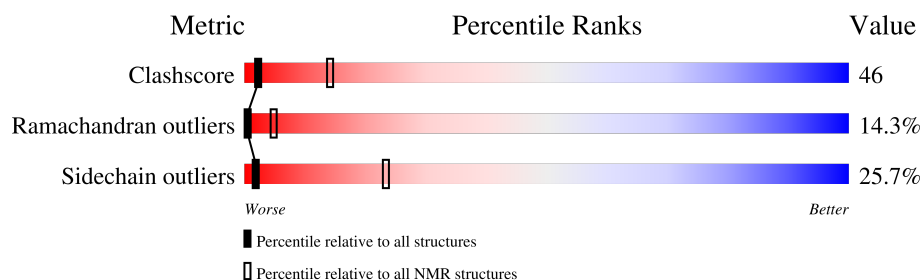
1 Overall quality at a glance

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	91	9% 55% 29% 5% •

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	92	9	-

2 Ensemble composition and analysis

This entry contains 16 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 14 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:3-A:91 (89)	1.12	14

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 2 clusters and 6 single-model clusters were found.

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

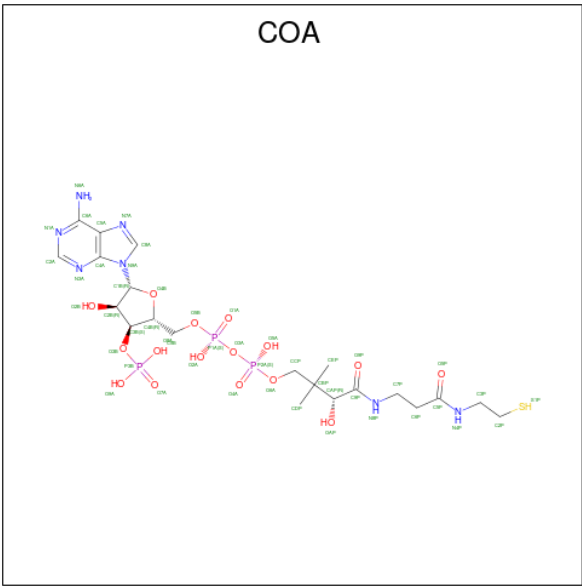
3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1449 atoms, of which 712 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called LIPID TRANSFER PROTEIN.

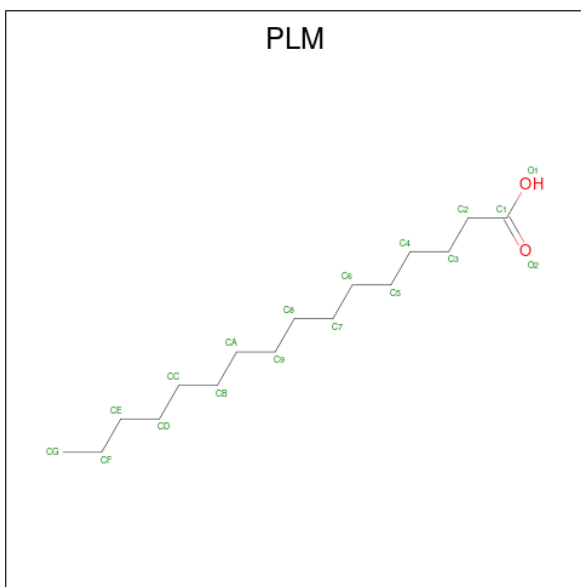
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	91	1322	404	650	126	133	9	0

- 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).



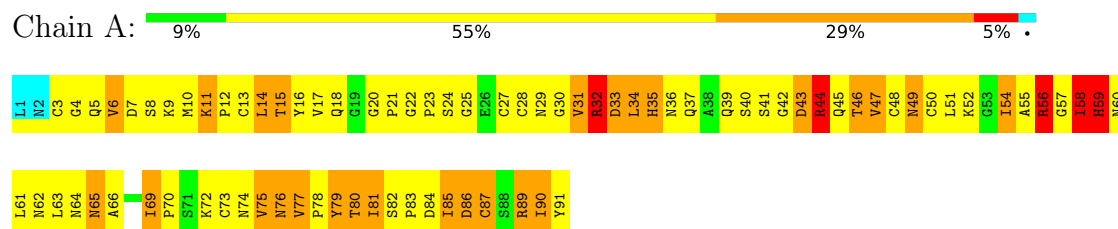
Mol	Chain	Residues	Atoms			
3	A	1	Total	C	H	O
			48	16	31	1

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: LIPID TRANSFER PROTEIN

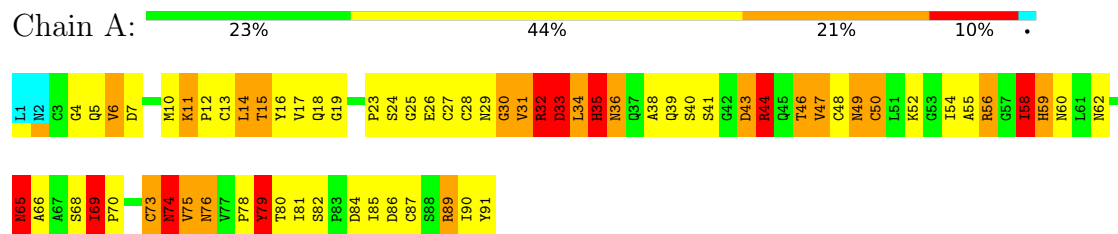


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

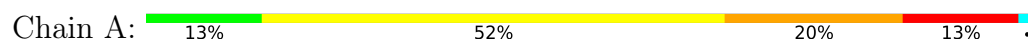
4.2.1 Score per residue for model 1

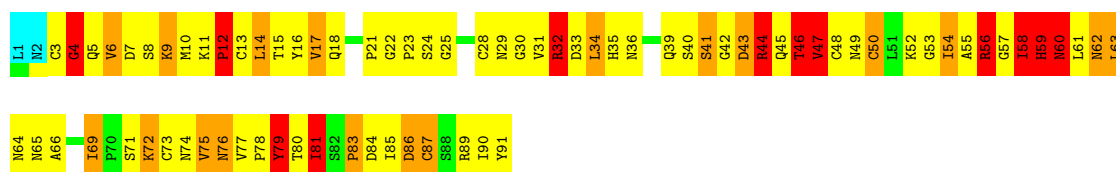
• Molecule 1: LIPID TRANSFER PROTEIN



4.2.2 Score per residue for model 2

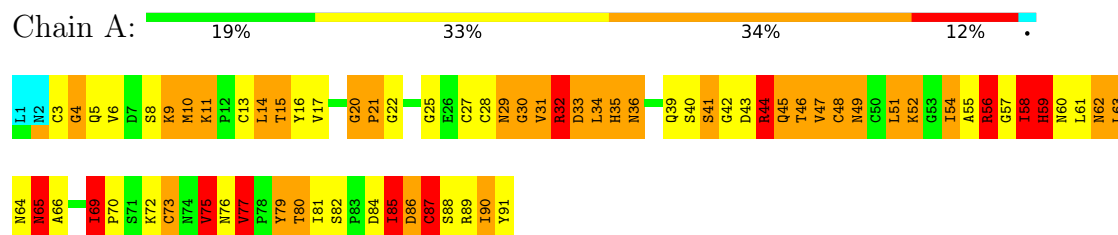
• Molecule 1: LIPID TRANSFER PROTEIN





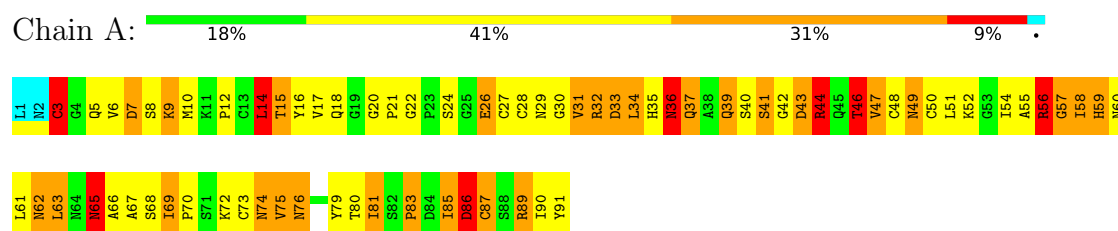
4.2.3 Score per residue for model 3

- Molecule 1: LIPID TRANSFER PROTEIN



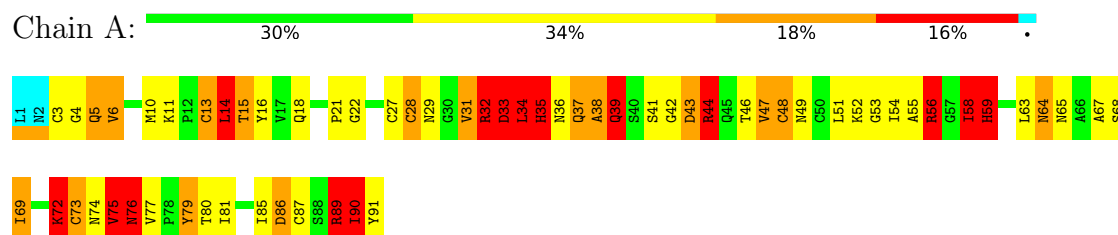
4.2.4 Score per residue for model 4

- Molecule 1: LIPID TRANSFER PROTEIN



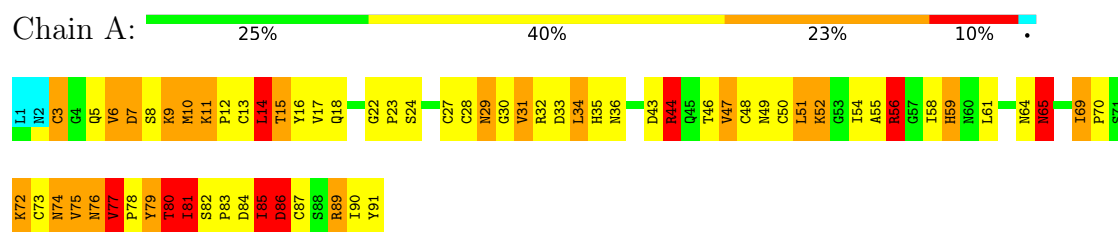
4.2.5 Score per residue for model 5

- Molecule 1: LIPID TRANSFER PROTEIN



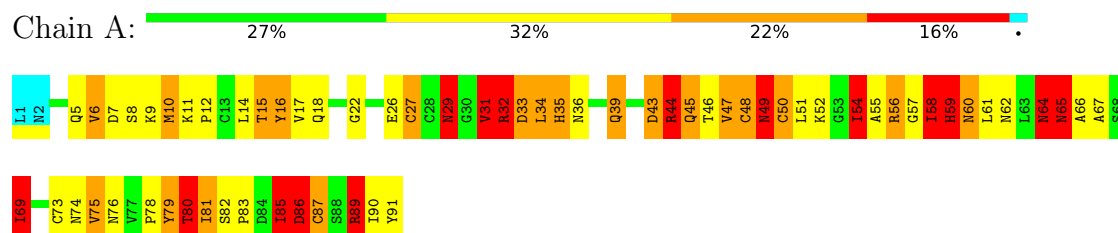
4.2.6 Score per residue for model 6

- Molecule 1: LIPID TRANSFER PROTEIN



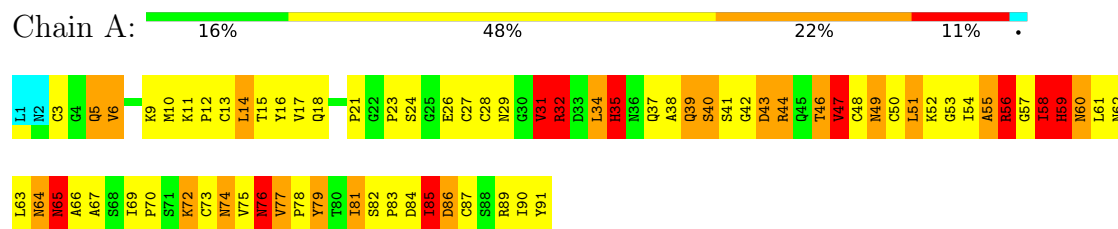
4.2.7 Score per residue for model 7

- Molecule 1: LIPID TRANSFER PROTEIN



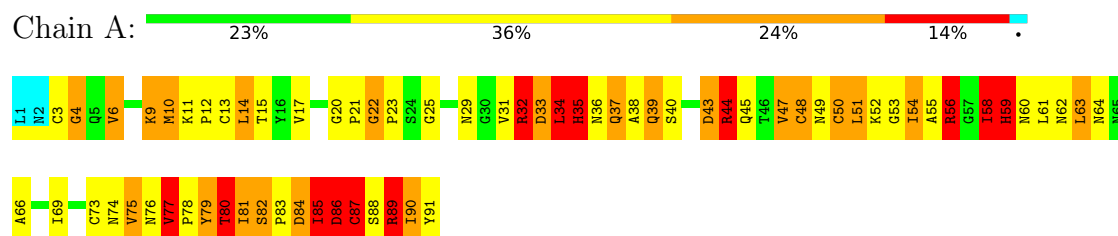
4.2.8 Score per residue for model 8

- Molecule 1: LIPID TRANSFER PROTEIN



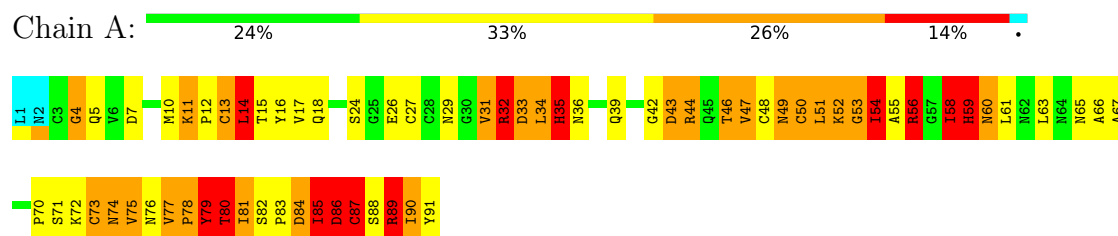
4.2.9 Score per residue for model 9

- Molecule 1: LIPID TRANSFER PROTEIN



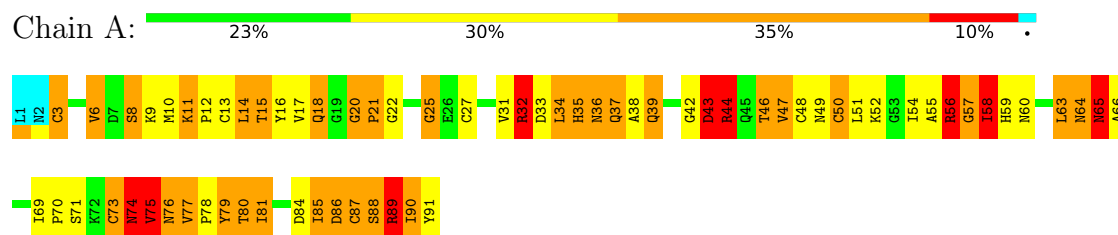
4.2.10 Score per residue for model 10

• Molecule 1: LIPID TRANSFER PROTEIN



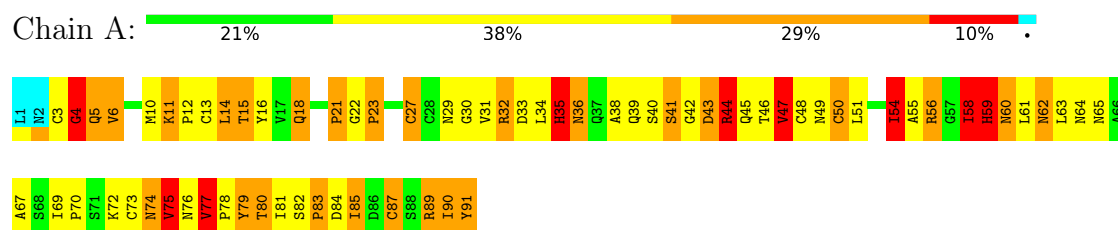
4.2.11 Score per residue for model 11

• Molecule 1: LIPID TRANSFER PROTEIN



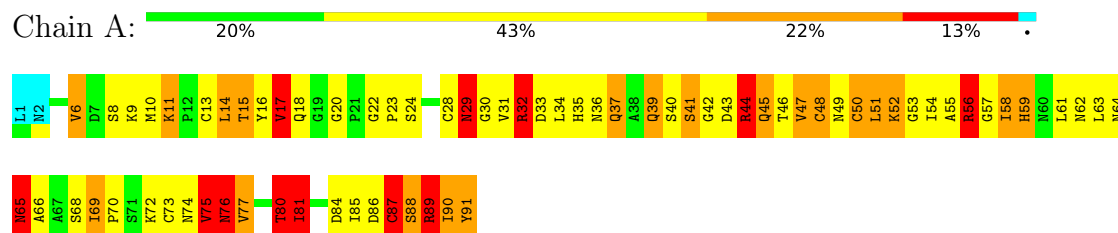
4.2.12 Score per residue for model 12

• Molecule 1: LIPID TRANSFER PROTEIN



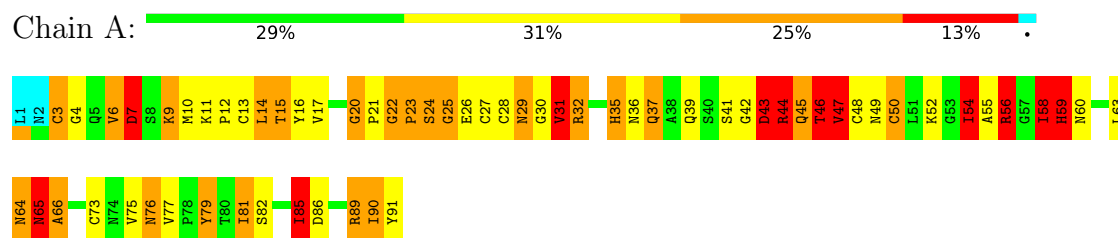
4.2.13 Score per residue for model 13

• Molecule 1: LIPID TRANSFER PROTEIN



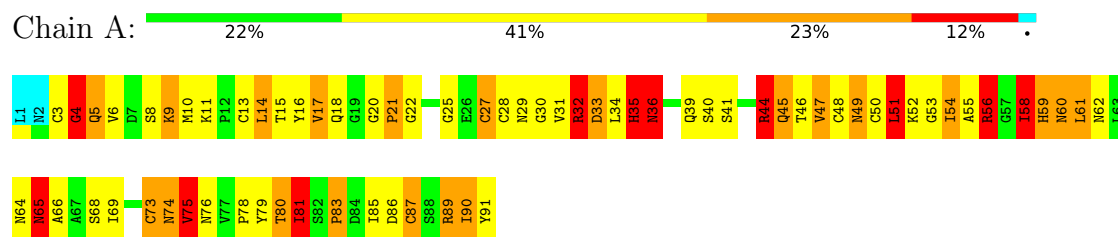
4.2.14 Score per residue for model 14 (medoid)

• Molecule 1: LIPID TRANSFER PROTEIN



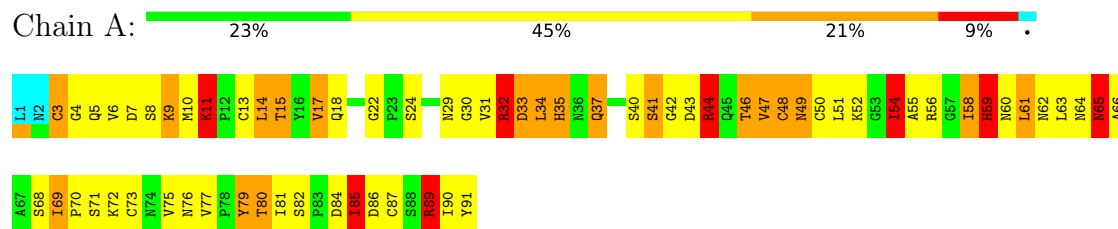
4.2.15 Score per residue for model 15

• Molecule 1: LIPID TRANSFER PROTEIN



4.2.16 Score per residue for model 16

• Molecule 1: LIPID TRANSFER PROTEIN



5 Refinement protocol and experimental data overview ⓘ

Of the 20 calculated structures, 16 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	3.1

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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	2.13±0.04	12±3/666 (1.8± 0.5%)	2.11±0.06	26±5/901 (2.9± 0.5%)
All	All	2.13	194/10656 (1.8%)	2.11	423/14416 (2.9%)

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	Planarity
1	A	0.0±0.0	4.6±0.7
All	All	0	74

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	69	ILE	CA-CB	13.83	1.61	1.54	7	8
1	A	59	HIS	CG-ND1	-8.93	1.28	1.38	5	16
1	A	35	HIS	CG-ND1	-8.67	1.28	1.38	10	16
1	A	75	VAL	CA-CB	8.56	1.66	1.54	9	9
1	A	54	ILE	CA-CB	7.88	1.62	1.54	10	1
1	A	82	SER	N-CA	7.32	1.52	1.45	1	6
1	A	75	VAL	N-CA	6.90	1.53	1.46	1	4
1	A	41	SER	N-CA	6.84	1.50	1.46	13	1
1	A	56	ARG	NE-CZ	-6.81	1.25	1.33	10	5
1	A	46	THR	N-CA	6.66	1.54	1.46	15	3
1	A	58	ILE	CA-CB	6.60	1.63	1.54	1	2
1	A	56	ARG	CZ-NH2	-6.56	1.25	1.33	13	4
1	A	15	THR	N-CA	6.39	1.53	1.46	11	7
1	A	89	ARG	CA-CB	6.08	1.60	1.53	9	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	22	GLY	N-CA	6.07	1.53	1.44	3	12
1	A	9	LYS	N-CA	5.99	1.53	1.46	6	1
1	A	51	LEU	N-CA	5.99	1.53	1.46	15	2
1	A	4	GLY	N-CA	5.95	1.54	1.45	3	7
1	A	3	CYS	CA-C	5.89	1.60	1.52	4	1
1	A	81	ILE	N-CA	5.88	1.53	1.46	7	3
1	A	32	ARG	CZ-NH2	-5.77	1.25	1.33	16	3
1	A	35	HIS	CD2-NE2	-5.77	1.31	1.37	11	14
1	A	44	ARG	NE-CZ	-5.75	1.26	1.33	4	6
1	A	41	SER	CA-C	5.74	1.55	1.52	5	1
1	A	86	ASP	CA-CB	5.73	1.61	1.52	9	1
1	A	25	GLY	N-CA	5.63	1.53	1.45	14	5
1	A	59	HIS	N-CA	5.62	1.52	1.46	16	4
1	A	44	ARG	CZ-NH2	-5.61	1.26	1.33	16	5
1	A	3	CYS	N-CA	5.59	1.52	1.46	5	1
1	A	80	THR	N-CA	5.59	1.53	1.46	16	3
1	A	20	GLY	N-CA	5.58	1.52	1.44	13	4
1	A	17	VAL	N-CA	5.58	1.53	1.46	15	1
1	A	39	GLN	CA-C	5.57	1.59	1.52	9	1
1	A	64	ASN	N-CA	5.57	1.53	1.46	7	2
1	A	77	VAL	CA-C	5.51	1.58	1.52	12	1
1	A	46	THR	CA-CB	5.49	1.61	1.53	4	1
1	A	89	ARG	CZ-NH2	-5.39	1.26	1.33	9	3
1	A	52	LYS	N-CA	5.37	1.52	1.46	10	1
1	A	59	HIS	CD2-NE2	-5.37	1.31	1.37	10	15
1	A	40	SER	N-CA	5.35	1.52	1.46	13	1
1	A	13	CYS	N-CA	5.26	1.52	1.46	10	1
1	A	55	ALA	N-CA	5.22	1.52	1.46	8	1
1	A	19	GLY	N-CA	5.21	1.51	1.44	1	1
1	A	32	ARG	N-CA	5.17	1.52	1.46	15	1
1	A	37	GLN	N-CA	5.14	1.52	1.46	14	1
1	A	76	ASN	CA-CB	5.14	1.62	1.53	13	1
1	A	44	ARG	CZ-NH1	-5.11	1.25	1.32	15	1
1	A	59	HIS	CA-C	5.07	1.56	1.52	16	1
1	A	89	ARG	N-CA	5.06	1.52	1.46	11	1
1	A	81	ILE	CA-C	5.04	1.59	1.52	7	1
1	A	47	VAL	N-CA	5.04	1.52	1.46	9	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	33	ASP	CA-CB-CG	-11.88	100.72	112.60	15	4
1	A	35	HIS	CA-CB-CG	-11.19	102.61	113.80	9	5
1	A	49	ASN	CA-CB-CG	-10.78	101.82	112.60	2	10
1	A	65	ASN	OD1-CG-ND2	-10.61	111.99	122.60	1	11
1	A	50	CYS	N-CA-C	-10.60	99.73	111.07	11	6
1	A	87	CYS	N-CA-C	-10.54	97.37	110.65	12	5
1	A	32	ARG	NE-CZ-NH2	-10.22	110.00	119.20	8	2
1	A	82	SER	N-CA-C	10.18	120.06	108.25	1	3
1	A	46	THR	N-CA-C	-9.71	99.55	111.40	2	9
1	A	47	VAL	N-CA-C	-9.63	101.18	110.42	8	3
1	A	38	ALA	N-CA-C	-9.62	90.30	110.80	5	2
1	A	41	SER	N-CA-C	-9.54	100.96	108.78	13	2
1	A	58	ILE	N-CA-C	9.38	128.85	109.34	7	10
1	A	44	ARG	NE-CZ-NH1	-9.15	112.35	121.50	12	5
1	A	60	ASN	N-CA-C	-9.05	98.09	110.68	15	2
1	A	45	GLN	N-CA-C	-8.95	100.78	112.68	15	4
1	A	14	LEU	N-CA-C	-8.89	101.28	110.97	9	15
1	A	90	ILE	N-CA-CB	-8.43	103.01	112.45	3	2
1	A	52	LYS	N-CA-CB	-8.31	97.60	110.06	13	1
1	A	59	HIS	N-CA-C	8.02	123.29	111.34	16	1
1	A	3	CYS	N-CA-CB	-7.90	97.14	110.49	4	4
1	A	68	SER	CA-C-N	-7.83	114.07	120.33	15	1
1	A	68	SER	C-N-CA	-7.83	114.07	120.33	15	1
1	A	74	ASN	OD1-CG-ND2	-7.78	114.82	122.60	9	5
1	A	55	ALA	N-CA-C	-7.78	101.53	111.02	13	1
1	A	32	ARG	NH1-CZ-NH2	7.74	129.37	119.30	8	1
1	A	21	PRO	N-CA-CB	-7.62	97.71	102.81	11	1
1	A	86	ASP	CA-CB-CG	7.53	120.13	112.60	9	2
1	A	76	ASN	OD1-CG-ND2	-7.53	115.07	122.60	13	10
1	A	3	CYS	N-CA-C	7.52	126.82	110.80	4	1
1	A	15	THR	N-CA-C	-7.51	101.85	111.02	6	5
1	A	34	LEU	N-CA-C	-7.50	101.87	111.02	4	2
1	A	73	CYS	N-CA-C	7.47	122.83	112.45	15	9
1	A	39	GLN	OE1-CD-NE2	-7.41	115.19	122.60	12	13
1	A	44	ARG	N-CA-C	-7.35	103.20	111.14	16	4
1	A	68	SER	N-CA-C	-7.12	104.85	113.97	4	5
1	A	73	CYS	N-CA-CB	-7.11	100.19	110.56	14	5
1	A	36	ASN	OD1-CG-ND2	-7.10	115.50	122.60	4	9
1	A	49	ASN	OD1-CG-ND2	-7.09	115.51	122.60	8	10
1	A	18	GLN	OE1-CD-NE2	-7.01	115.58	122.60	7	4
1	A	43	ASP	N-CA-C	6.97	119.97	110.35	9	1
1	A	33	ASP	N-CA-C	-6.96	103.39	110.97	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	86	ASP	O-C-N	6.92	129.23	122.03	8	1
1	A	81	ILE	N-CA-CB	-6.86	99.91	111.23	2	6
1	A	48	CYS	N-CA-C	-6.83	102.69	111.02	9	1
1	A	37	GLN	OE1-CD-NE2	-6.82	115.78	122.60	9	2
1	A	49	ASN	N-CA-C	-6.80	103.95	111.36	10	1
1	A	10	MET	N-CA-CB	-6.76	100.10	110.92	7	1
1	A	43	ASP	CA-CB-CG	-6.75	105.85	112.60	5	2
1	A	30	GLY	CA-C-N	6.74	128.94	120.72	1	3
1	A	30	GLY	C-N-CA	6.74	128.94	120.72	1	3
1	A	56	ARG	NH1-CZ-NH2	6.73	128.05	119.30	8	2
1	A	48	CYS	CA-CB-SG	6.70	129.81	114.40	9	1
1	A	72	LYS	N-CA-CB	-6.64	99.58	110.40	5	1
1	A	62	ASN	CA-CB-CG	-6.63	105.97	112.60	2	1
1	A	18	GLN	N-CA-C	-6.61	104.16	111.82	2	3
1	A	33	ASP	CA-C-O	-6.53	114.15	121.00	3	1
1	A	62	ASN	OD1-CG-ND2	-6.52	116.08	122.60	16	5
1	A	37	GLN	N-CA-C	-6.51	105.64	113.97	9	2
1	A	77	VAL	N-CA-CB	-6.51	102.10	111.21	9	2
1	A	84	ASP	CA-CB-CG	-6.51	106.09	112.60	11	2
1	A	11	LYS	N-CA-C	-6.50	103.91	112.75	11	1
1	A	51	LEU	N-CA-C	-6.48	103.11	111.02	6	1
1	A	80	THR	N-CA-C	6.47	124.58	110.80	6	6
1	A	60	ASN	OD1-CG-ND2	-6.46	116.14	122.60	4	9
1	A	52	LYS	CB-CA-C	6.45	121.65	110.68	13	1
1	A	7	ASP	CA-CB-CG	-6.42	106.18	112.60	1	2
1	A	89	ARG	NE-CZ-NH1	-6.41	115.09	121.50	5	2
1	A	45	GLN	OE1-CD-NE2	-6.38	116.22	122.60	15	2
1	A	44	ARG	CD-NE-CZ	-6.38	115.47	124.40	1	1
1	A	39	GLN	N-CA-C	-6.33	102.24	111.30	4	2
1	A	79	TYR	N-CA-CB	-6.31	103.28	110.35	12	1
1	A	85	ILE	N-CA-CB	-6.30	100.83	111.23	8	1
1	A	85	ILE	N-CA-C	6.29	122.43	109.34	14	2
1	A	15	THR	CA-CB-OG1	-6.28	100.17	109.60	14	1
1	A	86	ASP	N-CA-CB	-6.27	100.58	110.49	10	1
1	A	48	CYS	N-CA-CB	-6.26	100.31	109.82	9	1
1	A	46	THR	OG1-CB-CG2	-6.24	96.82	109.30	4	2
1	A	64	ASN	N-CA-C	-6.23	103.64	111.11	5	2
1	A	86	ASP	N-CA-C	6.23	119.67	110.46	7	3
1	A	32	ARG	N-CA-C	-6.21	103.66	111.11	1	1
1	A	31	VAL	N-CA-CB	-6.12	103.95	110.62	3	5
1	A	44	ARG	NH1-CZ-NH2	6.10	127.22	119.30	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	54	ILE	N-CA-C	-6.08	105.21	110.74	12	5
1	A	5	GLN	OE1-CD-NE2	-6.07	116.53	122.60	15	5
1	A	74	ASN	CA-CB-CG	-6.07	106.53	112.60	11	2
1	A	8	SER	N-CA-C	6.05	118.78	111.40	16	1
1	A	62	ASN	N-CA-CB	-6.01	103.20	110.53	12	5
1	A	56	ARG	NE-CZ-NH2	-5.99	113.81	119.20	10	2
1	A	58	ILE	CA-CB-CG2	5.97	120.64	110.50	1	1
1	A	59	HIS	CA-CB-CG	-5.95	107.85	113.80	8	2
1	A	58	ILE	CA-C-O	-5.94	113.35	120.78	10	1
1	A	31	VAL	N-CA-C	-5.93	104.14	110.36	7	1
1	A	80	THR	CA-CB-OG1	-5.91	100.74	109.60	7	1
1	A	17	VAL	N-CA-C	5.84	118.34	111.05	15	3
1	A	47	VAL	CA-C-N	5.80	128.86	120.79	9	1
1	A	47	VAL	C-N-CA	5.80	128.86	120.79	9	1
1	A	17	VAL	CA-C-O	-5.76	114.96	120.95	13	1
1	A	5	GLN	N-CA-C	-5.76	104.36	111.33	5	1
1	A	58	ILE	O-C-N	5.73	129.74	122.57	3	1
1	A	66	ALA	N-CA-C	-5.72	104.96	111.14	14	1
1	A	44	ARG	N-CA-CB	-5.71	101.49	110.06	7	1
1	A	53	GLY	N-CA-C	-5.71	105.88	112.50	10	1
1	A	43	ASP	CA-C-O	5.70	128.32	121.88	9	1
1	A	36	ASN	CA-CB-CG	-5.69	106.91	112.60	9	1
1	A	29	ASN	N-CA-C	-5.67	104.73	111.03	2	6
1	A	16	TYR	N-CA-CB	-5.67	100.54	109.78	7	1
1	A	29	ASN	OD1-CG-ND2	-5.63	116.97	122.60	16	4
1	A	45	GLN	CA-CB-CG	-5.58	102.94	114.10	3	1
1	A	84	ASP	N-CA-CB	-5.57	102.40	110.47	16	3
1	A	58	ILE	CB-CA-C	-5.57	102.16	111.29	2	1
1	A	47	VAL	N-CA-CB	-5.54	104.37	110.51	12	1
1	A	27	CYS	CB-CA-C	-5.51	102.23	110.88	7	1
1	A	35	HIS	CE1-NE2-CD2	-5.51	103.49	109.00	11	7
1	A	80	THR	OG1-CB-CG2	-5.51	98.28	109.30	5	2
1	A	40	SER	N-CA-CB	-5.51	102.19	108.96	8	1
1	A	59	HIS	N-CA-CB	-5.50	101.20	110.49	13	5
1	A	69	ILE	N-CA-C	-5.48	105.77	112.35	1	1
1	A	46	THR	CA-CB-OG1	-5.46	101.41	109.60	8	1
1	A	33	ASP	N-CA-CB	-5.44	101.84	109.94	4	1
1	A	64	ASN	CA-CB-CG	-5.43	107.17	112.60	11	1
1	A	90	ILE	N-CA-C	-5.43	101.58	109.29	13	1
1	A	15	THR	OG1-CB-CG2	-5.42	98.45	109.30	13	2
1	A	49	ASN	CB-CG-ND2	5.42	124.53	116.40	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	48	CYS	CB-CA-C	5.41	119.51	110.92	9	1
1	A	36	ASN	N-CA-CB	-5.40	102.02	110.44	1	2
1	A	79	TYR	N-CA-C	5.38	122.25	110.80	2	2
1	A	44	ARG	NE-CZ-NH2	-5.37	114.37	119.20	7	2
1	A	58	ILE	CB-CG1-CD1	-5.37	102.53	113.80	15	1
1	A	7	ASP	N-CA-CB	-5.36	102.20	110.13	1	1
1	A	4	GLY	N-CA-C	-5.36	100.48	113.18	10	1
1	A	41	SER	CA-CB-OG	-5.34	100.41	111.10	12	1
1	A	74	ASN	CB-CG-ND2	5.34	124.41	116.40	9	1
1	A	13	CYS	N-CA-C	-5.33	105.04	112.45	5	1
1	A	91	TYR	CA-CB-CG	-5.33	104.31	113.90	12	1
1	A	27	CYS	N-CA-CB	5.33	117.74	110.01	7	1
1	A	76	ASN	N-CA-C	5.29	122.08	110.80	14	2
1	A	65	ASN	N-CA-CB	-5.29	102.34	110.12	7	1
1	A	79	TYR	CB-CG-CD1	-5.27	112.89	120.80	10	1
1	A	75	VAL	N-CA-C	-5.25	98.43	109.34	2	1
1	A	42	GLY	N-CA-C	-5.24	100.76	113.18	13	1
1	A	76	ASN	CB-CG-ND2	5.24	124.26	116.40	8	1
1	A	14	LEU	CB-CA-C	5.23	119.09	110.88	5	1
1	A	50	CYS	N-CA-CB	-5.21	102.51	110.07	7	1
1	A	77	VAL	N-CA-C	5.21	120.13	108.88	3	1
1	A	59	HIS	CE1-NE2-CD2	-5.19	103.81	109.00	3	8
1	A	33	ASP	CB-CA-C	5.19	119.17	110.92	6	1
1	A	71	SER	CA-CB-OG	-5.19	100.73	111.10	2	2
1	A	28	CYS	N-CA-C	5.18	116.61	111.07	5	2
1	A	44	ARG	CB-CA-C	5.17	119.47	110.68	7	1
1	A	15	THR	CA-CB-CG2	5.17	119.29	110.50	13	1
1	A	89	ARG	CD-NE-CZ	-5.17	117.17	124.40	7	1
1	A	64	ASN	OD1-CG-ND2	-5.17	117.43	122.60	12	3
1	A	11	LYS	N-CA-CB	-5.15	101.21	110.37	16	1
1	A	84	ASP	N-CA-C	-5.14	104.17	110.65	13	1
1	A	9	LYS	N-CA-CB	-5.13	102.86	110.61	3	1
1	A	7	ASP	O-C-N	5.12	128.39	122.20	14	1
1	A	14	LEU	N-CA-CB	-5.11	102.60	110.01	5	2
1	A	90	ILE	O-C-N	5.11	127.44	122.69	5	1
1	A	21	PRO	N-CA-C	5.11	122.99	112.47	15	1
1	A	46	THR	CA-C-O	5.10	126.36	120.90	15	1
1	A	54	ILE	CA-CB-CG1	5.06	119.01	110.40	16	1
1	A	52	LYS	CA-C-O	5.02	126.54	120.92	10	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	44	ARG	Sidechain	16
1	A	56	ARG	Sidechain	16
1	A	89	ARG	Sidechain	16
1	A	32	ARG	Sidechain	15
1	A	77	VAL	Peptide	7
1	A	20	GLY	Peptide	3
1	A	82	SER	Peptide	1

6.2 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 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	656	631	631	60±6
2	A	48	31	31	11±6
3	A	17	31	31	5±4
All	All	11536	11088	11088	1039

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 46.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:MET:HB2	2:A:92:COA:S1P	0.92	2.05	7	3
1:A:10:MET:CB	2:A:92:COA:S1P	0.90	2.59	7	3
1:A:72:LYS:HZ2	1:A:72:LYS:C	0.83	1.81	2	1
1:A:28:CYS:SG	1:A:72:LYS:CE	0.83	2.67	5	5
1:A:10:MET:HE2	3:A:96:PLM:C4	0.82	2.03	5	2
1:A:14:LEU:N	2:A:92:COA:S1P	0.82	2.53	6	1
2:A:92:COA:H2B	2:A:92:COA:N3A	0.81	1.90	10	3
1:A:28:CYS:SG	1:A:72:LYS:NZ	0.81	2.53	3	6
1:A:14:LEU:HD22	2:A:92:COA:S1P	0.81	2.16	3	1
1:A:13:CYS:SG	1:A:31:VAL:HG23	0.80	2.16	16	10
1:A:13:CYS:N	1:A:27:CYS:SG	0.80	2.55	12	4
2:A:92:COA:N8P	2:A:92:COA:H131	0.77	1.92	4	3
1:A:48:CYS:SG	1:A:49:ASN:N	0.77	2.57	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:VAL:HG12	2:A:92:COA:H32	0.76	1.56	6	1
2:A:92:COA:H121	2:A:92:COA:N8P	0.75	1.96	7	1
1:A:48:CYS:SG	1:A:87:CYS:N	0.75	2.59	5	6
1:A:79:TYR:CE1	1:A:90:ILE:HD13	0.75	2.16	15	7
2:A:92:COA:CCP	2:A:92:COA:HN8	0.74	1.95	7	1
1:A:10:MET:HE1	3:A:96:PLM:HD2	0.74	1.59	15	3
1:A:14:LEU:CA	2:A:92:COA:S1P	0.74	2.76	6	1
1:A:51:LEU:HD22	2:A:92:COA:S1P	0.73	2.22	15	2
2:A:92:COA:HN8	2:A:92:COA:H131	0.72	1.45	6	3
1:A:10:MET:HE2	3:A:96:PLM:H41	0.71	1.62	5	2
2:A:92:COA:N8P	2:A:92:COA:CCP	0.71	2.51	7	1
1:A:10:MET:SD	3:A:96:PLM:H22	0.70	2.26	1	2
1:A:10:MET:HE1	1:A:31:VAL:HG22	0.70	1.61	16	4
1:A:3:CYS:SG	1:A:6:VAL:HG21	0.70	2.26	16	2
2:A:92:COA:H131	2:A:92:COA:HN8	0.70	1.46	16	1
1:A:31:VAL:CG1	1:A:75:VAL:HG11	0.70	2.16	4	9
2:A:92:COA:HN8	2:A:92:COA:H141	0.70	1.45	5	5
2:A:92:COA:H131	2:A:92:COA:N8P	0.70	2.00	6	3
1:A:14:LEU:HB2	2:A:92:COA:S1P	0.70	2.27	6	1
1:A:6:VAL:HG22	1:A:47:VAL:CG2	0.70	2.17	15	6
1:A:79:TYR:CD2	3:A:96:PLM:HD1	0.69	2.22	12	2
1:A:31:VAL:HG12	1:A:75:VAL:HG21	0.68	1.64	15	5
1:A:10:MET:HE2	3:A:96:PLM:O1	0.68	1.89	6	1
1:A:79:TYR:CE2	1:A:90:ILE:HD13	0.68	2.23	3	1
1:A:10:MET:SD	1:A:34:LEU:HG	0.68	2.29	16	5
2:A:92:COA:H133	2:A:92:COA:O3A	0.67	1.89	16	1
1:A:72:LYS:HE3	1:A:73:CYS:SG	0.67	2.29	3	4
1:A:59:HIS:CG	1:A:60:ASN:H	0.67	2.07	10	1
1:A:14:LEU:CB	2:A:92:COA:S1P	0.67	2.83	6	1
1:A:72:LYS:NZ	1:A:73:CYS:SG	0.67	2.62	2	1
1:A:13:CYS:SG	1:A:31:VAL:CG2	0.66	2.83	8	13
1:A:51:LEU:HD21	3:A:96:PLM:C1	0.65	2.21	16	2
1:A:10:MET:HB2	3:A:96:PLM:C1	0.65	2.22	7	1
1:A:48:CYS:SG	1:A:85:ILE:HG12	0.65	2.31	13	2
1:A:58:ILE:CG2	1:A:59:HIS:N	0.64	2.60	13	7
1:A:10:MET:SD	3:A:96:PLM:H41	0.64	2.32	3	1
2:A:92:COA:N8P	2:A:92:COA:CDP	0.64	2.61	4	3
1:A:48:CYS:SG	1:A:85:ILE:HG23	0.64	2.33	10	1
1:A:10:MET:SD	1:A:34:LEU:HD12	0.63	2.33	1	3
2:A:92:COA:S1P	2:A:92:COA:O5P	0.63	2.56	7	2
1:A:10:MET:SD	3:A:96:PLM:HF2	0.62	2.34	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:LEU:HD21	3:A:96:PLM:C2	0.62	2.24	13	1
1:A:47:VAL:HA	1:A:50:CYS:SG	0.62	2.34	13	5
1:A:58:ILE:HG23	1:A:59:HIS:H	0.62	1.54	1	2
1:A:10:MET:HE2	3:A:96:PLM:H42	0.62	1.70	5	3
1:A:10:MET:HE2	3:A:96:PLM:H31	0.62	1.70	13	1
1:A:58:ILE:CG2	1:A:59:HIS:H	0.61	2.08	1	2
1:A:9:LYS:HZ2	1:A:9:LYS:HB3	0.61	1.55	2	1
1:A:79:TYR:CD2	3:A:96:PLM:CD	0.61	2.83	12	1
1:A:10:MET:HB3	2:A:92:COA:S1P	0.61	2.36	7	2
1:A:51:LEU:CD2	2:A:92:COA:H61	0.61	2.26	7	1
1:A:72:LYS:CE	1:A:73:CYS:SG	0.61	2.88	3	4
1:A:79:TYR:CE1	1:A:90:ILE:CD1	0.61	2.83	15	2
1:A:7:ASP:N	2:A:92:COA:H61	0.60	2.11	10	1
1:A:90:ILE:CG2	1:A:91:TYR:N	0.60	2.64	10	11
2:A:92:COA:N8P	2:A:92:COA:H141	0.60	2.11	6	2
2:A:92:COA:N8P	2:A:92:COA:CEP	0.60	2.64	9	1
2:A:92:COA:S1P	2:A:92:COA:C5P	0.59	2.89	7	1
1:A:49:ASN:ND2	1:A:87:CYS:SG	0.59	2.75	13	5
1:A:54:ILE:CG2	1:A:55:ALA:N	0.59	2.66	10	12
1:A:14:LEU:CD1	2:A:92:COA:S1P	0.58	2.92	6	1
1:A:10:MET:CE	3:A:96:PLM:H31	0.58	2.28	13	1
1:A:10:MET:SD	1:A:34:LEU:CG	0.58	2.91	16	2
1:A:14:LEU:CD2	2:A:92:COA:H72	0.58	2.28	12	1
1:A:32:ARG:HB3	1:A:32:ARG:CZ	0.58	2.28	11	1
1:A:70:PRO:HA	1:A:75:VAL:CG1	0.58	2.28	11	5
1:A:3:CYS:SG	1:A:6:VAL:HB	0.57	2.39	9	3
1:A:29:ASN:ND2	1:A:30:GLY:N	0.57	2.52	14	2
1:A:52:LYS:HE2	1:A:85:ILE:O	0.57	1.99	11	4
1:A:35:HIS:CD2	1:A:77:VAL:HG11	0.57	2.35	9	1
1:A:44:ARG:H	1:A:44:ARG:CD	0.57	2.12	16	2
1:A:59:HIS:CG	1:A:60:ASN:N	0.57	2.69	10	1
1:A:16:TYR:C	1:A:65:ASN:HD21	0.57	2.07	14	7
1:A:51:LEU:CD2	2:A:92:COA:S1P	0.57	2.93	4	3
1:A:14:LEU:HD12	2:A:92:COA:S1P	0.57	2.40	6	1
1:A:56:ARG:NH1	2:A:92:COA:O5A	0.56	2.38	9	1
2:A:92:COA:S1P	3:A:96:PLM:H41	0.56	2.40	4	2
1:A:49:ASN:CG	1:A:87:CYS:SG	0.56	2.88	13	1
1:A:10:MET:HA	1:A:27:CYS:SG	0.56	2.40	7	1
1:A:75:VAL:O	1:A:77:VAL:N	0.56	2.38	10	4
1:A:14:LEU:HD13	2:A:92:COA:S1P	0.56	2.40	3	1
1:A:47:VAL:HG11	1:A:79:TYR:OH	0.56	2.00	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:LEU:O	1:A:54:ILE:HG22	0.56	2.01	10	2
1:A:48:CYS:SG	1:A:85:ILE:O	0.56	2.64	11	2
1:A:10:MET:HB3	3:A:96:PLM:C2	0.56	2.31	16	1
1:A:27:CYS:SG	1:A:69:ILE:HD12	0.56	2.41	3	3
1:A:77:VAL:CG2	1:A:79:TYR:HB2	0.56	2.31	8	1
1:A:83:PRO:O	1:A:85:ILE:N	0.56	2.39	9	2
1:A:90:ILE:HG22	1:A:91:TYR:N	0.56	2.16	13	2
1:A:6:VAL:CG1	2:A:92:COA:H32	0.55	2.29	6	1
2:A:92:COA:C9P	2:A:92:COA:N4P	0.55	2.70	6	1
2:A:92:COA:HN8	2:A:92:COA:CDP	0.55	2.12	15	4
1:A:78:PRO:HG2	1:A:91:TYR:CD1	0.55	2.36	1	1
1:A:33:ASP:O	1:A:34:LEU:C	0.55	2.50	3	8
1:A:3:CYS:SG	1:A:6:VAL:CB	0.55	2.95	9	2
1:A:51:LEU:HD23	2:A:92:COA:S1P	0.55	2.41	13	2
1:A:16:TYR:CD1	1:A:65:ASN:ND2	0.55	2.75	2	2
1:A:13:CYS:HB2	3:A:96:PLM:O1	0.55	2.01	6	1
2:A:92:COA:S1P	3:A:96:PLM:H52	0.55	2.42	12	1
1:A:6:VAL:HB	2:A:92:COA:C7P	0.55	2.31	15	1
1:A:6:VAL:CG1	2:A:92:COA:S1P	0.54	2.96	2	3
1:A:80:THR:HG23	1:A:85:ILE:HD12	0.54	1.78	6	1
1:A:14:LEU:HB3	2:A:92:COA:C5P	0.54	2.32	16	1
1:A:18:GLN:NE2	1:A:58:ILE:HD13	0.54	2.17	16	1
1:A:10:MET:CE	3:A:96:PLM:C4	0.54	2.86	3	2
2:A:92:COA:N8P	2:A:92:COA:N4P	0.54	2.56	16	1
1:A:14:LEU:O	1:A:15:THR:C	0.54	2.51	16	12
1:A:79:TYR:CD1	1:A:90:ILE:HG13	0.54	2.38	5	1
1:A:14:LEU:C	1:A:14:LEU:HD12	0.54	2.28	10	1
1:A:54:ILE:HD12	2:A:92:COA:H142	0.54	1.80	5	1
1:A:10:MET:HE1	3:A:96:PLM:CD	0.54	2.31	6	3
1:A:90:ILE:C	1:A:91:TYR:CD1	0.54	2.86	5	3
3:A:96:PLM:HG2	3:A:96:PLM:CC	0.54	2.33	12	1
1:A:32:ARG:HH22	1:A:33:ASP:CG	0.53	2.11	15	1
1:A:6:VAL:HG12	2:A:92:COA:H31	0.53	1.80	16	1
1:A:80:THR:CG2	1:A:85:ILE:HD12	0.53	2.33	6	1
2:A:92:COA:HN4	2:A:92:COA:H143	0.53	1.63	7	1
1:A:55:ALA:HA	1:A:58:ILE:CG1	0.53	2.33	14	1
1:A:6:VAL:CG2	1:A:47:VAL:CG2	0.53	2.86	15	1
1:A:86:ASP:O	1:A:88:SER:N	0.53	2.42	11	5
1:A:26:GLU:HG3	1:A:27:CYS:N	0.53	2.18	8	2
1:A:27:CYS:SG	1:A:31:VAL:HG23	0.53	2.44	10	1
1:A:35:HIS:CD2	1:A:36:ASN:HD22	0.53	2.22	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:LEU:HD12	2:A:92:COA:C5P	0.53	2.34	15	1
1:A:52:LYS:CE	1:A:85:ILE:O	0.53	2.57	16	1
1:A:54:ILE:HD13	1:A:55:ALA:N	0.53	2.19	16	1
1:A:11:LYS:NZ	2:A:92:COA:O5A	0.53	2.39	7	1
1:A:58:ILE:HG22	1:A:59:HIS:N	0.53	2.18	8	8
1:A:51:LEU:CD2	3:A:96:PLM:H21	0.53	2.34	13	1
1:A:69:ILE:N	1:A:70:PRO:HD2	0.52	2.19	4	3
1:A:12:PRO:HG2	1:A:27:CYS:SG	0.52	2.44	12	1
1:A:58:ILE:O	1:A:59:HIS:CB	0.52	2.58	10	4
1:A:79:TYR:CD1	1:A:90:ILE:CG1	0.52	2.92	5	1
1:A:90:ILE:HG23	1:A:91:TYR:N	0.52	2.20	10	3
1:A:64:ASN:ND2	1:A:64:ASN:H	0.52	2.02	7	2
1:A:6:VAL:CG1	2:A:92:COA:H22	0.52	2.35	12	3
1:A:32:ARG:O	1:A:33:ASP:C	0.52	2.53	7	5
1:A:65:ASN:OD1	1:A:65:ASN:C	0.52	2.52	6	7
1:A:3:CYS:HB3	1:A:6:VAL:CG2	0.52	2.35	6	2
3:A:96:PLM:HA1	3:A:96:PLM:HE1	0.52	1.81	5	1
1:A:11:LYS:HB3	1:A:12:PRO:HD2	0.52	1.81	7	3
1:A:48:CYS:SG	1:A:85:ILE:HD11	0.52	2.44	9	1
1:A:6:VAL:CG1	2:A:92:COA:H21	0.52	2.35	4	1
1:A:80:THR:HG1	1:A:90:ILE:HG12	0.52	1.65	9	1
2:A:92:COA:C5A	2:A:92:COA:CEP	0.52	2.88	6	1
1:A:84:ASP:O	1:A:85:ILE:C	0.52	2.52	10	2
1:A:3:CYS:O	1:A:5:GLN:N	0.52	2.43	3	2
1:A:9:LYS:HB2	1:A:34:LEU:CD2	0.51	2.35	3	1
1:A:58:ILE:O	1:A:59:HIS:HB2	0.51	2.06	14	4
1:A:7:ASP:HB2	2:A:92:COA:H143	0.51	1.81	4	1
1:A:50:CYS:HA	2:A:92:COA:O4A	0.51	2.05	13	1
1:A:65:ASN:OD1	1:A:66:ALA:N	0.51	2.44	1	10
1:A:6:VAL:CG1	2:A:92:COA:C2P	0.51	2.88	4	2
1:A:17:VAL:HG11	1:A:66:ALA:HB2	0.51	1.82	10	2
1:A:9:LYS:HB3	1:A:30:GLY:HA2	0.51	1.82	3	2
1:A:44:ARG:HG2	1:A:44:ARG:NH1	0.51	2.18	16	1
1:A:35:HIS:CD2	1:A:35:HIS:C	0.51	2.89	10	5
1:A:44:ARG:CB	1:A:90:ILE:HG21	0.51	2.35	2	3
1:A:26:GLU:HA	1:A:29:ASN:ND2	0.51	2.21	4	3
2:A:92:COA:C5A	2:A:92:COA:H143	0.51	2.34	6	1
1:A:63:LEU:C	1:A:63:LEU:HD13	0.51	2.30	9	3
1:A:51:LEU:CD2	2:A:92:COA:H21	0.51	2.35	16	3
1:A:10:MET:O	1:A:11:LYS:C	0.51	2.53	6	7
1:A:53:GLY:O	1:A:56:ARG:CB	0.51	2.59	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:HIS:CD2	1:A:60:ASN:HD22	0.51	2.24	1	1
1:A:69:ILE:N	1:A:70:PRO:CD	0.51	2.74	1	2
1:A:33:ASP:O	1:A:36:ASN:N	0.51	2.44	12	6
1:A:35:HIS:N	3:A:96:PLM:HG1	0.51	2.21	15	2
1:A:16:TYR:CD1	1:A:23:PRO:HD3	0.51	2.41	13	2
1:A:11:LYS:HB3	1:A:12:PRO:CD	0.50	2.36	10	6
1:A:17:VAL:CG1	1:A:66:ALA:HB2	0.50	2.36	2	6
1:A:55:ALA:HA	1:A:58:ILE:HG12	0.50	1.83	14	2
1:A:44:ARG:HB2	1:A:90:ILE:HG21	0.50	1.83	6	4
2:A:92:COA:N4P	2:A:92:COA:C9P	0.50	2.74	16	1
1:A:56:ARG:NH2	2:A:92:COA:O2A	0.50	2.43	9	1
1:A:79:TYR:CE2	3:A:96:PLM:HA2	0.50	2.42	9	1
1:A:67:ALA:HA	1:A:81:ILE:CG2	0.50	2.37	4	6
1:A:45:GLN:HE21	1:A:45:GLN:HA	0.50	1.66	15	1
1:A:35:HIS:CE1	1:A:44:ARG:HD3	0.50	2.41	9	1
1:A:81:ILE:HD13	3:A:96:PLM:HA1	0.50	1.84	9	1
2:A:92:COA:H2B	2:A:92:COA:OAP	0.50	2.07	13	1
1:A:8:SER:C	1:A:9:LYS:HD3	0.50	2.32	3	4
1:A:41:SER:O	1:A:44:ARG:NH1	0.50	2.45	13	1
1:A:51:LEU:HD21	3:A:96:PLM:H21	0.50	1.82	13	1
1:A:47:VAL:HG12	1:A:48:CYS:N	0.50	2.22	13	9
1:A:43:ASP:O	1:A:44:ARG:C	0.50	2.54	3	7
3:A:96:PLM:H22	3:A:96:PLM:C6	0.50	2.36	3	1
1:A:26:GLU:CG	1:A:27:CYS:N	0.50	2.75	8	1
1:A:14:LEU:HD22	2:A:92:COA:C5P	0.50	2.37	11	1
1:A:10:MET:HE2	3:A:96:PLM:H22	0.49	1.84	10	2
1:A:44:ARG:HH21	1:A:91:TYR:C	0.49	2.15	7	1
1:A:44:ARG:NH2	1:A:91:TYR:C	0.49	2.69	11	1
1:A:12:PRO:C	1:A:27:CYS:SG	0.49	2.95	12	1
1:A:27:CYS:SG	1:A:69:ILE:CD1	0.49	3.00	3	1
1:A:79:TYR:O	1:A:79:TYR:CG	0.49	2.64	5	1
1:A:32:ARG:HB3	1:A:32:ARG:NH1	0.49	2.22	15	1
1:A:56:ARG:NH2	2:A:92:COA:O9A	0.49	2.45	13	1
1:A:7:ASP:CB	2:A:92:COA:H10	0.49	2.38	6	1
1:A:50:CYS:CB	2:A:92:COA:O9P	0.49	2.61	7	1
1:A:14:LEU:HD22	2:A:92:COA:CDP	0.49	2.37	6	1
1:A:79:TYR:O	1:A:81:ILE:N	0.49	2.45	2	5
1:A:16:TYR:O	1:A:65:ASN:ND2	0.49	2.45	12	2
1:A:40:SER:O	1:A:41:SER:CB	0.49	2.60	4	1
1:A:79:TYR:CE2	1:A:90:ILE:HD12	0.49	2.43	14	1
1:A:32:ARG:NH2	1:A:33:ASP:N	0.49	2.60	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:ILE:HG12	2:A:92:COA:CEP	0.49	2.38	9	1
1:A:85:ILE:HD13	1:A:87:CYS:N	0.48	2.23	3	1
1:A:7:ASP:O	1:A:11:LYS:CB	0.48	2.61	16	2
1:A:80:THR:HG23	1:A:85:ILE:CD1	0.48	2.38	6	1
1:A:6:VAL:HG13	2:A:92:COA:H22	0.48	1.85	12	1
1:A:86:ASP:HB3	1:A:89:ARG:NE	0.48	2.22	10	1
1:A:11:LYS:NZ	1:A:15:THR:HG23	0.48	2.22	12	1
1:A:10:MET:SD	1:A:31:VAL:HA	0.48	2.49	2	2
1:A:70:PRO:HA	1:A:75:VAL:HG13	0.48	1.85	13	4
1:A:23:PRO:HB3	1:A:27:CYS:SG	0.48	2.48	6	1
1:A:71:SER:OG	1:A:72:LYS:N	0.48	2.46	10	2
1:A:53:GLY:O	1:A:56:ARG:HB3	0.48	2.08	9	5
2:A:92:COA:H10	2:A:92:COA:C5A	0.48	2.38	10	1
1:A:40:SER:OG	1:A:41:SER:N	0.48	2.45	16	7
1:A:16:TYR:CZ	1:A:65:ASN:OD1	0.48	2.66	10	3
1:A:54:ILE:HG21	2:A:92:COA:C7P	0.48	2.38	7	1
1:A:9:LYS:CG	1:A:34:LEU:HD23	0.48	2.39	9	1
1:A:77:VAL:O	1:A:79:TYR:N	0.48	2.46	9	1
2:A:92:COA:H51A	2:A:92:COA:H122	0.48	1.84	10	1
1:A:13:CYS:SG	1:A:31:VAL:HG21	0.48	2.47	6	2
1:A:44:ARG:HE	1:A:91:TYR:C	0.48	2.17	4	3
1:A:14:LEU:HB2	2:A:92:COA:H22	0.48	1.85	6	1
3:A:96:PLM:H61	3:A:96:PLM:CE	0.48	2.39	12	1
1:A:16:TYR:CE1	1:A:65:ASN:ND2	0.48	2.82	2	1
1:A:43:ASP:O	1:A:46:THR:HB	0.48	2.09	13	3
1:A:73:CYS:O	1:A:74:ASN:CB	0.48	2.61	4	2
2:A:92:COA:S1P	3:A:96:PLM:C4	0.48	3.02	15	2
1:A:90:ILE:O	1:A:91:TYR:CG	0.48	2.66	15	1
1:A:6:VAL:HG22	1:A:47:VAL:HG23	0.47	1.83	2	3
1:A:44:ARG:CD	1:A:44:ARG:H	0.47	2.21	2	1
1:A:7:ASP:OD2	2:A:92:COA:H132	0.47	2.08	4	1
1:A:51:LEU:O	1:A:52:LYS:C	0.47	2.56	10	2
1:A:47:VAL:CG1	1:A:79:TYR:OH	0.47	2.62	8	3
1:A:53:GLY:O	1:A:54:ILE:C	0.47	2.56	15	3
1:A:50:CYS:O	1:A:51:LEU:C	0.47	2.57	6	7
1:A:38:ALA:HB1	1:A:43:ASP:HA	0.47	1.85	9	1
1:A:38:ALA:CB	3:A:96:PLM:H92	0.47	2.39	12	1
1:A:3:CYS:O	1:A:4:GLY:C	0.47	2.57	15	2
1:A:52:LYS:HG3	1:A:87:CYS:SG	0.47	2.50	3	1
1:A:54:ILE:O	1:A:55:ALA:C	0.47	2.57	8	6
2:A:92:COA:C6A	2:A:92:COA:CDP	0.47	2.92	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:LEU:O	1:A:18:GLN:HG2	0.47	2.10	6	6
1:A:28:CYS:SG	1:A:72:LYS:HE3	0.47	2.47	5	1
1:A:34:LEU:O	1:A:35:HIS:C	0.47	2.58	5	2
1:A:9:LYS:HB3	1:A:30:GLY:CA	0.47	2.40	3	2
1:A:12:PRO:HG3	1:A:26:GLU:CD	0.47	2.35	4	1
1:A:37:GLN:C	1:A:39:GLN:H	0.47	2.17	4	3
2:A:92:COA:C6A	2:A:92:COA:H131	0.47	2.39	7	1
1:A:42:GLY:O	1:A:43:ASP:C	0.47	2.57	8	3
1:A:79:TYR:CD1	1:A:80:THR:N	0.47	2.83	9	1
1:A:51:LEU:HD12	1:A:85:ILE:HG21	0.47	1.87	10	2
1:A:83:PRO:O	1:A:84:ASP:C	0.47	2.58	10	1
1:A:6:VAL:HG13	2:A:92:COA:N4P	0.47	2.24	11	1
1:A:44:ARG:HD2	1:A:44:ARG:H	0.47	1.70	12	1
1:A:6:VAL:HG11	2:A:92:COA:S1P	0.47	2.50	16	1
1:A:14:LEU:HD22	2:A:92:COA:N4P	0.47	2.25	8	2
1:A:54:ILE:C	1:A:56:ARG:N	0.47	2.71	11	3
1:A:48:CYS:SG	1:A:86:ASP:C	0.47	2.98	7	1
1:A:51:LEU:O	1:A:54:ILE:N	0.47	2.48	10	1
1:A:14:LEU:HD22	2:A:92:COA:H72	0.47	1.87	12	1
2:A:92:COA:HN8	2:A:92:COA:CEP	0.47	2.22	10	3
2:A:92:COA:H141	2:A:92:COA:O5P	0.47	2.10	12	2
1:A:36:ASN:HA	1:A:39:GLN:NE2	0.47	2.25	1	1
1:A:10:MET:CE	3:A:96:PLM:H22	0.47	2.40	4	2
1:A:63:LEU:O	1:A:64:ASN:C	0.47	2.57	11	3
1:A:54:ILE:HD12	2:A:92:COA:C2P	0.47	2.40	10	1
1:A:42:GLY:O	1:A:46:THR:N	0.47	2.48	16	1
2:A:92:COA:H143	2:A:92:COA:C8A	0.46	2.40	10	1
1:A:11:LYS:CB	1:A:12:PRO:CD	0.46	2.94	10	3
1:A:81:ILE:HG22	1:A:81:ILE:O	0.46	2.09	13	7
1:A:45:GLN:NE2	1:A:87:CYS:O	0.46	2.49	12	2
1:A:51:LEU:HD23	2:A:92:COA:H21	0.46	1.86	12	1
1:A:81:ILE:CD1	3:A:96:PLM:HA2	0.46	2.40	1	1
3:A:96:PLM:H22	3:A:96:PLM:H61	0.46	1.86	3	1
1:A:9:LYS:O	1:A:30:GLY:C	0.46	2.59	6	1
1:A:78:PRO:O	1:A:80:THR:N	0.46	2.49	1	1
2:A:92:COA:H141	2:A:92:COA:N8P	0.46	2.26	14	2
1:A:79:TYR:CE2	3:A:96:PLM:HD1	0.46	2.46	12	2
1:A:11:LYS:HB3	1:A:12:PRO:HD3	0.46	1.86	2	1
1:A:34:LEU:HB3	3:A:96:PLM:HG2	0.46	1.87	10	2
1:A:86:ASP:OD1	1:A:86:ASP:N	0.46	2.48	6	1
1:A:48:CYS:SG	1:A:85:ILE:CG1	0.46	3.03	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:PRO:CB	1:A:26:GLU:HG2	0.46	2.41	1	1
1:A:16:TYR:CZ	1:A:65:ASN:CG	0.46	2.94	5	1
1:A:54:ILE:HG21	2:A:92:COA:N8P	0.46	2.25	7	1
1:A:7:ASP:O	1:A:8:SER:C	0.46	2.59	4	2
1:A:51:LEU:HD23	1:A:51:LEU:N	0.46	2.25	10	2
1:A:80:THR:O	1:A:82:SER:N	0.46	2.49	3	1
1:A:44:ARG:NH1	1:A:91:TYR:HA	0.46	2.26	12	1
1:A:50:CYS:SG	2:A:92:COA:H133	0.46	2.51	14	1
1:A:73:CYS:O	1:A:74:ASN:C	0.46	2.58	1	5
1:A:56:ARG:NE	2:A:92:COA:O7A	0.46	2.48	5	2
1:A:52:LYS:NZ	1:A:86:ASP:O	0.46	2.48	8	1
1:A:10:MET:SD	3:A:96:PLM:H21	0.46	2.50	14	1
1:A:47:VAL:O	1:A:50:CYS:N	0.46	2.49	2	4
1:A:11:LYS:NZ	2:A:92:COA:O8A	0.46	2.49	16	1
1:A:75:VAL:O	1:A:76:ASN:C	0.46	2.58	8	1
1:A:79:TYR:CD1	1:A:79:TYR:C	0.45	2.94	3	3
1:A:85:ILE:HD13	1:A:86:ASP:N	0.45	2.26	3	1
1:A:15:THR:OG1	1:A:16:TYR:N	0.45	2.49	5	2
1:A:69:ILE:HD13	3:A:96:PLM:H51	0.45	1.88	9	1
1:A:36:ASN:HD22	1:A:36:ASN:N	0.45	2.09	4	1
1:A:27:CYS:O	1:A:28:CYS:C	0.45	2.59	15	3
1:A:55:ALA:O	1:A:56:ARG:C	0.45	2.59	2	6
1:A:33:ASP:O	1:A:37:GLN:HG2	0.45	2.11	11	1
1:A:31:VAL:CG1	3:A:96:PLM:HE1	0.45	2.42	7	1
1:A:42:GLY:O	1:A:44:ARG:N	0.45	2.49	11	2
1:A:86:ASP:HB3	1:A:89:ARG:CD	0.45	2.41	10	1
1:A:6:VAL:CG1	2:A:92:COA:H31	0.45	2.41	16	1
1:A:38:ALA:HB1	1:A:43:ASP:HB2	0.45	1.89	1	1
1:A:6:VAL:HG11	2:A:92:COA:H22	0.45	1.89	2	1
1:A:91:TYR:N	1:A:91:TYR:CD1	0.45	2.84	3	1
1:A:6:VAL:CG2	2:A:92:COA:H22	0.45	2.42	11	1
1:A:44:ARG:N	1:A:44:ARG:CD	0.45	2.79	12	1
3:A:96:PLM:H42	3:A:96:PLM:H81	0.45	1.89	13	1
1:A:32:ARG:NH1	1:A:33:ASP:HA	0.45	2.26	16	1
1:A:20:GLY:O	1:A:22:GLY:N	0.45	2.50	4	2
1:A:45:GLN:O	1:A:46:THR:C	0.45	2.58	14	3
1:A:81:ILE:CD1	3:A:96:PLM:H91	0.45	2.42	14	1
1:A:53:GLY:O	1:A:56:ARG:N	0.45	2.50	15	1
1:A:51:LEU:CD1	1:A:85:ILE:HG21	0.45	2.41	16	1
1:A:58:ILE:O	1:A:59:HIS:ND1	0.45	2.50	8	1
1:A:62:ASN:O	1:A:63:LEU:C	0.45	2.59	2	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:THR:OG1	1:A:90:ILE:HG12	0.45	2.11	7	1
1:A:22:GLY:CA	1:A:23:PRO:C	0.45	2.90	14	1
1:A:6:VAL:HG12	2:A:92:COA:S1P	0.45	2.51	14	2
1:A:29:ASN:O	1:A:30:GLY:C	0.45	2.59	12	5
1:A:34:LEU:CD2	1:A:34:LEU:N	0.45	2.80	7	1
1:A:34:LEU:HD12	3:A:96:PLM:H81	0.45	1.89	12	1
1:A:86:ASP:N	1:A:86:ASP:OD1	0.45	2.50	4	2
3:A:96:PLM:HB2	3:A:96:PLM:C6	0.45	2.42	9	1
1:A:44:ARG:N	1:A:44:ARG:HD2	0.44	2.27	1	1
1:A:10:MET:HB3	3:A:96:PLM:C3	0.44	2.42	13	1
1:A:54:ILE:HG23	1:A:55:ALA:N	0.44	2.27	3	2
1:A:54:ILE:HG21	2:A:92:COA:H31	0.44	1.89	5	1
1:A:14:LEU:HB2	2:A:92:COA:C2P	0.44	2.42	6	1
1:A:3:CYS:HA	1:A:6:VAL:HB	0.44	1.87	11	1
1:A:89:ARG:H	1:A:89:ARG:HD2	0.44	1.71	13	2
1:A:47:VAL:O	1:A:48:CYS:C	0.44	2.59	15	4
2:A:92:COA:C5A	2:A:92:COA:OAP	0.44	2.65	3	1
1:A:80:THR:HA	1:A:89:ARG:NH2	0.44	2.28	4	1
1:A:48:CYS:SG	1:A:85:ILE:HG13	0.44	2.53	14	2
2:A:92:COA:H141	2:A:92:COA:HN8	0.44	1.71	12	1
1:A:56:ARG:HH22	2:A:92:COA:P3B	0.44	2.36	13	1
1:A:11:LYS:N	1:A:12:PRO:HD2	0.44	2.27	1	2
1:A:9:LYS:CB	1:A:9:LYS:NZ	0.44	2.81	2	1
1:A:5:GLN:H	1:A:5:GLN:CD	0.44	2.21	7	1
1:A:79:TYR:CG	3:A:96:PLM:HD1	0.44	2.47	12	1
1:A:32:ARG:O	1:A:35:HIS:HB3	0.44	2.13	7	1
1:A:62:ASN:O	1:A:64:ASN:ND2	0.44	2.51	7	1
1:A:75:VAL:O	1:A:75:VAL:HG22	0.44	2.11	15	3
1:A:54:ILE:CG1	2:A:92:COA:CEP	0.44	2.95	9	1
1:A:10:MET:SD	3:A:96:PLM:H31	0.44	2.53	13	1
1:A:80:THR:OG1	1:A:89:ARG:CD	0.44	2.66	13	1
1:A:35:HIS:N	3:A:96:PLM:CG	0.44	2.81	15	1
1:A:72:LYS:HZ2	1:A:73:CYS:N	0.44	2.11	2	1
1:A:79:TYR:CE2	1:A:90:ILE:CD1	0.44	3.01	14	1
1:A:91:TYR:CD1	1:A:91:TYR:N	0.44	2.86	5	1
1:A:10:MET:CB	3:A:96:PLM:C1	0.44	2.94	7	1
1:A:56:ARG:NH1	2:A:92:COA:O2A	0.44	2.51	9	1
1:A:6:VAL:HG13	2:A:92:COA:C2P	0.44	2.43	11	1
1:A:41:SER:OG	1:A:42:GLY:N	0.43	2.51	12	2
2:A:92:COA:H122	2:A:92:COA:C5B	0.43	2.43	10	1
1:A:7:ASP:HB2	2:A:92:COA:CEP	0.43	2.43	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:ARG:HH12	1:A:91:TYR:C	0.43	2.21	15	1
1:A:6:VAL:HG21	1:A:50:CYS:SG	0.43	2.53	1	2
1:A:14:LEU:CD2	2:A:92:COA:S1P	0.43	3.01	3	1
1:A:31:VAL:HG11	1:A:75:VAL:HG11	0.43	1.90	4	1
1:A:44:ARG:HB3	1:A:90:ILE:CG2	0.43	2.43	8	1
1:A:11:LYS:HE2	2:A:92:COA:H71	0.43	1.89	9	1
1:A:35:HIS:NE2	1:A:77:VAL:CG1	0.43	2.81	9	1
1:A:46:THR:O	1:A:47:VAL:C	0.43	2.61	11	2
1:A:59:HIS:CD2	1:A:60:ASN:H	0.43	2.30	10	1
2:A:92:COA:O8A	2:A:92:COA:H72	0.43	2.12	16	1
1:A:52:LYS:NZ	1:A:84:ASP:O	0.43	2.48	6	3
1:A:33:ASP:C	1:A:37:GLN:CD	0.43	2.86	4	1
1:A:80:THR:O	1:A:81:ILE:C	0.43	2.61	4	2
1:A:49:ASN:O	1:A:50:CYS:C	0.43	2.61	10	1
1:A:35:HIS:CE1	1:A:76:ASN:ND2	0.43	2.86	11	1
1:A:45:GLN:O	1:A:48:CYS:HB3	0.43	2.14	14	1
1:A:44:ARG:CD	1:A:44:ARG:N	0.43	2.81	16	1
1:A:54:ILE:CG2	1:A:55:ALA:H	0.43	2.26	10	1
1:A:54:ILE:O	1:A:58:ILE:HG13	0.43	2.13	15	2
2:A:92:COA:HN4	2:A:92:COA:H141	0.43	1.73	16	1
1:A:23:PRO:O	1:A:25:GLY:N	0.43	2.51	2	1
1:A:86:ASP:CG	1:A:89:ARG:NE	0.43	2.76	10	1
1:A:10:MET:HE3	1:A:31:VAL:CG2	0.43	2.44	11	1
1:A:47:VAL:HG11	3:A:96:PLM:H62	0.43	1.91	12	1
1:A:6:VAL:HB	2:A:92:COA:H71	0.43	1.89	15	1
1:A:5:GLN:O	1:A:6:VAL:C	0.43	2.61	2	4
1:A:13:CYS:O	1:A:14:LEU:C	0.43	2.58	11	5
1:A:15:THR:N	2:A:92:COA:O4A	0.43	2.52	6	1
1:A:17:VAL:HA	1:A:65:ASN:ND2	0.43	2.28	6	2
1:A:79:TYR:O	1:A:79:TYR:CD2	0.43	2.71	5	1
1:A:12:PRO:HG2	1:A:27:CYS:CB	0.43	2.44	10	1
1:A:55:ALA:O	1:A:57:GLY:N	0.43	2.52	8	3
1:A:60:ASN:CG	1:A:61:LEU:N	0.43	2.77	2	1
1:A:77:VAL:HG11	3:A:96:PLM:CC	0.43	2.44	2	1
1:A:39:GLN:HB2	1:A:43:ASP:CG	0.43	2.38	5	1
1:A:10:MET:O	2:A:92:COA:S1P	0.43	2.76	7	1
1:A:16:TYR:CE1	1:A:69:ILE:HG12	0.43	2.49	7	1
1:A:54:ILE:C	1:A:58:ILE:HG12	0.43	2.39	11	1
1:A:86:ASP:HB3	1:A:89:ARG:CZ	0.43	2.44	11	1
1:A:8:SER:C	1:A:9:LYS:HD2	0.43	2.39	15	3
3:A:96:PLM:H51	3:A:96:PLM:HA1	0.43	1.91	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:ASN:O	1:A:62:ASN:N	0.43	2.51	8	2
1:A:62:ASN:O	1:A:64:ASN:N	0.43	2.52	3	1
1:A:35:HIS:CE1	1:A:77:VAL:HB	0.43	2.49	5	1
2:A:92:COA:H51A	2:A:92:COA:N3A	0.43	2.28	12	1
3:A:96:PLM:H82	3:A:96:PLM:HC2	0.43	1.90	12	1
1:A:6:VAL:HG22	1:A:47:VAL:HG22	0.43	1.87	15	1
1:A:52:LYS:NZ	1:A:86:ASP:OD1	0.42	2.52	5	2
1:A:15:THR:O	1:A:16:TYR:C	0.42	2.61	11	4
1:A:52:LYS:NZ	1:A:84:ASP:CG	0.42	2.77	10	1
1:A:4:GLY:O	1:A:5:GLN:C	0.42	2.62	12	2
1:A:52:LYS:NZ	1:A:86:ASP:OD2	0.42	2.49	2	1
1:A:57:GLY:O	1:A:59:HIS:N	0.42	2.52	7	2
2:A:92:COA:H10	2:A:92:COA:C6A	0.42	2.43	10	1
1:A:9:LYS:N	1:A:9:LYS:CD	0.42	2.82	14	1
1:A:47:VAL:HG12	1:A:79:TYR:OH	0.42	2.13	15	1
1:A:48:CYS:O	1:A:52:LYS:HG3	0.42	2.14	1	1
1:A:14:LEU:HA	3:A:96:PLM:O1	0.42	2.13	5	1
2:A:92:COA:C9P	2:A:92:COA:C5P	0.42	2.96	6	1
1:A:79:TYR:O	1:A:81:ILE:HG12	0.42	2.13	7	1
1:A:52:LYS:NZ	1:A:84:ASP:OD2	0.42	2.52	10	1
1:A:86:ASP:CG	1:A:89:ARG:HE	0.42	2.22	10	1
1:A:47:VAL:CG1	1:A:48:CYS:N	0.42	2.82	4	2
1:A:56:ARG:NH1	2:A:92:COA:P2A	0.42	2.93	9	1
1:A:89:ARG:H	1:A:89:ARG:CD	0.42	2.27	13	1
1:A:9:LYS:HZ2	1:A:9:LYS:CB	0.42	2.25	2	1
1:A:53:GLY:O	1:A:56:ARG:CZ	0.42	2.67	2	1
1:A:10:MET:SD	3:A:96:PLM:C4	0.42	3.07	3	1
1:A:33:ASP:O	1:A:37:GLN:N	0.42	2.53	5	1
1:A:14:LEU:C	1:A:14:LEU:HD13	0.42	2.40	9	1
1:A:35:HIS:N	3:A:96:PLM:HG2	0.42	2.30	16	2
1:A:53:GLY:O	1:A:56:ARG:NH2	0.42	2.52	2	1
2:A:92:COA:OAP	2:A:92:COA:C4A	0.42	2.67	3	1
1:A:11:LYS:CE	2:A:92:COA:H71	0.42	2.45	9	1
1:A:81:ILE:CD1	3:A:96:PLM:CA	0.42	2.97	10	1
1:A:34:LEU:HB3	3:A:96:PLM:CG	0.42	2.45	3	1
1:A:57:GLY:O	1:A:58:ILE:C	0.42	2.62	3	1
1:A:29:ASN:ND2	1:A:29:ASN:C	0.42	2.78	6	1
1:A:29:ASN:OD1	1:A:30:GLY:N	0.42	2.53	3	2
1:A:35:HIS:O	1:A:44:ARG:NH1	0.42	2.52	3	1
1:A:69:ILE:O	1:A:70:PRO:C	0.42	2.62	13	2
1:A:12:PRO:HA	1:A:15:THR:OG1	0.42	2.14	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:MET:HB3	3:A:96:PLM:C1	0.42	2.44	6	1
1:A:15:THR:HA	1:A:18:GLN:CG	0.42	2.45	12	1
1:A:11:LYS:NZ	2:A:92:COA:O7A	0.42	2.52	16	1
1:A:32:ARG:HD2	1:A:32:ARG:C	0.42	2.39	3	1
1:A:54:ILE:CG2	2:A:92:COA:H31	0.42	2.45	5	1
1:A:5:GLN:O	1:A:9:LYS:HG2	0.42	2.15	7	1
2:A:92:COA:HN4	2:A:92:COA:CEP	0.42	2.26	7	1
1:A:10:MET:CG	1:A:34:LEU:HG	0.42	2.45	12	1
1:A:15:THR:HA	1:A:18:GLN:OE1	0.42	2.14	12	1
1:A:40:SER:O	1:A:42:GLY:N	0.41	2.53	3	1
1:A:7:ASP:OD2	2:A:92:COA:H143	0.41	2.14	4	1
1:A:40:SER:N	1:A:43:ASP:OD1	0.41	2.53	9	1
1:A:63:LEU:O	1:A:66:ALA:HB3	0.41	2.15	11	1
1:A:10:MET:CE	3:A:96:PLM:H21	0.41	2.45	14	1
1:A:7:ASP:O	1:A:11:LYS:HB2	0.41	2.13	16	1
1:A:44:ARG:HB2	1:A:90:ILE:CG2	0.41	2.45	6	1
1:A:78:PRO:O	1:A:79:TYR:C	0.41	2.62	10	1
1:A:86:ASP:CG	1:A:89:ARG:HH21	0.41	2.23	10	2
1:A:56:ARG:HH21	2:A:92:COA:P3B	0.41	2.38	5	1
1:A:17:VAL:HA	1:A:65:ASN:OD1	0.41	2.16	6	1
1:A:50:CYS:SG	2:A:92:COA:CDP	0.41	3.08	14	1
1:A:74:ASN:O	1:A:74:ASN:CG	0.41	2.63	2	1
1:A:10:MET:CE	3:A:96:PLM:H41	0.41	2.45	3	1
1:A:32:ARG:CD	1:A:32:ARG:C	0.41	2.94	12	1
3:A:96:PLM:CC	3:A:96:PLM:CG	0.41	2.97	12	1
1:A:51:LEU:HD21	2:A:92:COA:S1P	0.41	2.56	16	1
1:A:77:VAL:HG11	3:A:96:PLM:HC1	0.41	1.92	2	1
1:A:79:TYR:CD1	1:A:79:TYR:O	0.41	2.74	3	1
1:A:38:ALA:O	1:A:39:GLN:HG3	0.41	2.15	5	1
1:A:16:TYR:CE2	1:A:69:ILE:HG13	0.41	2.51	6	1
1:A:3:CYS:SG	1:A:6:VAL:HG11	0.41	2.56	9	1
1:A:86:ASP:CG	1:A:89:ARG:HH22	0.41	2.24	9	1
1:A:50:CYS:HB3	2:A:92:COA:O5P	0.41	2.15	10	1
1:A:16:TYR:CE1	1:A:69:ILE:HD11	0.41	2.49	2	1
1:A:55:ALA:HA	1:A:58:ILE:HG13	0.41	1.93	9	1
1:A:70:PRO:HG2	1:A:81:ILE:CD1	0.41	2.46	10	1
1:A:44:ARG:NH2	1:A:91:TYR:O	0.41	2.53	11	1
1:A:13:CYS:O	1:A:16:TYR:HB3	0.41	2.15	3	1
1:A:72:LYS:NZ	1:A:72:LYS:CB	0.41	2.84	6	1
1:A:77:VAL:C	1:A:79:TYR:N	0.41	2.78	6	1
1:A:54:ILE:O	1:A:57:GLY:N	0.41	2.54	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:ARG:CB	1:A:90:ILE:CG2	0.41	2.98	14	1
1:A:44:ARG:O	1:A:47:VAL:N	0.41	2.54	3	1
1:A:12:PRO:HG2	1:A:27:CYS:HB2	0.41	1.93	4	1
1:A:80:THR:HG22	1:A:81:ILE:N	0.41	2.30	6	1
1:A:4:GLY:N	2:A:92:COA:O8A	0.41	2.54	1	1
1:A:77:VAL:O	1:A:77:VAL:HG13	0.41	2.16	3	1
1:A:55:ALA:C	1:A:57:GLY:N	0.41	2.77	4	1
2:A:92:COA:H121	2:A:92:COA:N4P	0.41	2.31	7	1
1:A:35:HIS:CB	1:A:75:VAL:HG23	0.41	2.46	11	1
1:A:16:TYR:CZ	1:A:72:LYS:HE3	0.41	2.51	12	1
1:A:29:ASN:CG	1:A:30:GLY:N	0.41	2.79	13	1
1:A:23:PRO:O	1:A:24:SER:CB	0.41	2.68	14	1
1:A:11:LYS:CB	1:A:12:PRO:HD2	0.41	2.46	7	1
1:A:48:CYS:SG	1:A:85:ILE:CD1	0.41	3.09	9	1
1:A:35:HIS:HB2	1:A:75:VAL:HG23	0.41	1.93	14	1
1:A:44:ARG:NH1	1:A:44:ARG:CG	0.41	2.84	16	1
1:A:70:PRO:HG3	3:A:96:PLM:HA2	0.40	1.92	3	1
1:A:44:ARG:HB3	1:A:90:ILE:HG21	0.40	1.92	8	1
1:A:77:VAL:CB	1:A:79:TYR:HB2	0.40	2.46	8	1
2:A:92:COA:CDP	2:A:92:COA:O3A	0.40	2.69	11	1
1:A:44:ARG:N	1:A:44:ARG:HD3	0.40	2.31	16	1
1:A:45:GLN:HA	1:A:87:CYS:HB3	0.40	1.93	2	1
1:A:3:CYS:CB	1:A:6:VAL:CG2	0.40	2.98	6	1
1:A:70:PRO:HB3	1:A:77:VAL:HG23	0.40	1.92	6	1
1:A:5:GLN:CD	1:A:5:GLN:N	0.40	2.79	7	1
1:A:14:LEU:HB2	2:A:92:COA:H32	0.40	1.91	7	1
1:A:13:CYS:HB3	1:A:69:ILE:HD13	0.40	1.92	9	1
1:A:86:ASP:HB3	1:A:89:ARG:HE	0.40	1.76	10	1
1:A:63:LEU:HD13	1:A:63:LEU:C	0.40	2.40	11	1
3:A:96:PLM:H41	3:A:96:PLM:C9	0.40	2.46	11	1
1:A:44:ARG:HD2	1:A:44:ARG:N	0.40	2.31	13	1
2:A:92:COA:C5A	2:A:92:COA:CCP	0.40	3.00	13	1
1:A:59:HIS:C	1:A:61:LEU:H	0.40	2.24	15	1
1:A:51:LEU:CA	1:A:54:ILE:HG23	0.40	2.46	16	1
1:A:31:VAL:CG1	1:A:75:VAL:HG21	0.40	2.47	13	1
1:A:46:THR:O	1:A:50:CYS:SG	0.40	2.79	4	1
1:A:67:ALA:HA	1:A:81:ILE:HG23	0.40	1.94	5	1
2:A:92:COA:H143	2:A:92:COA:C6A	0.40	2.46	6	1
1:A:9:LYS:NZ	1:A:33:ASP:OD2	0.40	2.54	7	1
1:A:54:ILE:O	1:A:56:ARG:N	0.40	2.54	11	1
1:A:6:VAL:HG13	2:A:92:COA:S1P	0.40	2.55	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:GLU:HA	1:A:29:ASN:OD1	0.40	2.16	14	1
1:A:10:MET:HB3	3:A:96:PLM:H22	0.40	1.93	16	1
1:A:10:MET:HE1	1:A:31:VAL:CG2	0.40	2.43	8	1
1:A:89:ARG:O	1:A:91:TYR:CE1	0.40	2.75	9	1
1:A:16:TYR:N	1:A:20:GLY:HA3	0.40	2.32	11	1
1:A:9:LYS:HD3	1:A:9:LYS:N	0.40	2.31	13	1
1:A:6:VAL:O	1:A:7:ASP:C	0.40	2.64	14	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	88/91 (97%)	53±4 (60±4%)	22±3 (25±3%)	13±3 (14±3%)	0	5
All	All	1408/1456 (97%)	848 (60%)	358 (25%)	202 (14%)	0	5

All 36 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	58	ILE	14
1	A	85	ILE	14
1	A	56	ARG	12
1	A	76	ASN	11
1	A	80	THR	11
1	A	61	LEU	11
1	A	6	VAL	10
1	A	24	SER	9
1	A	21	PRO	9
1	A	59	HIS	9
1	A	43	ASP	8
1	A	74	ASN	7
1	A	81	ILE	7
1	A	87	CYS	7
1	A	78	PRO	7

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Mol	Chain	Res	Type	Models (Total)
1	A	79	TYR	6
1	A	4	GLY	6
1	A	83	PRO	6
1	A	63	LEU	5
1	A	41	SER	4
1	A	25	GLY	3
1	A	77	VAL	3
1	A	31	VAL	3
1	A	84	ASP	3
1	A	33	ASP	2
1	A	42	GLY	2
1	A	60	ASN	2
1	A	3	CYS	2
1	A	57	GLY	2
1	A	12	PRO	1
1	A	64	ASN	1
1	A	45	GLN	1
1	A	34	LEU	1
1	A	39	GLN	1
1	A	8	SER	1
1	A	23	PRO	1

6.3.2 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 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	76/78 (97%)	56±3 (74±4%)	20±3 (26±4%)	2	23
All	All	1216/1248 (97%)	904 (74%)	312 (26%)	2	23

All 62 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	47	VAL	16
1	A	32	ARG	15
1	A	34	LEU	12
1	A	58	ILE	11

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Mol	Chain	Res	Type	Models (Total)
1	A	65	ASN	11
1	A	44	ARG	10
1	A	89	ARG	10
1	A	75	VAL	10
1	A	86	ASP	10
1	A	11	LYS	9
1	A	17	VAL	8
1	A	54	ILE	8
1	A	35	HIS	7
1	A	9	LYS	7
1	A	52	LYS	7
1	A	85	ILE	7
1	A	33	ASP	6
1	A	69	ILE	6
1	A	87	CYS	6
1	A	51	LEU	6
1	A	56	ARG	6
1	A	79	TYR	6
1	A	37	GLN	6
1	A	90	ILE	6
1	A	64	ASN	6
1	A	46	THR	5
1	A	43	ASP	5
1	A	48	CYS	5
1	A	76	ASN	5
1	A	23	PRO	4
1	A	59	HIS	4
1	A	72	LYS	4
1	A	83	PRO	4
1	A	14	LEU	4
1	A	29	ASN	4
1	A	60	ASN	4
1	A	10	MET	3
1	A	21	PRO	3
1	A	63	LEU	3
1	A	77	VAL	3
1	A	5	GLN	3
1	A	31	VAL	3
1	A	36	ASN	3
1	A	7	ASP	3
1	A	39	GLN	3
1	A	49	ASN	3

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Mol	Chain	Res	Type	Models (Total)
1	A	50	CYS	2
1	A	78	PRO	2
1	A	6	VAL	2
1	A	81	ILE	2
1	A	88	SER	2
1	A	27	CYS	2
1	A	12	PRO	1
1	A	3	CYS	1
1	A	18	GLN	1
1	A	26	GLU	1
1	A	82	SER	1
1	A	80	THR	1
1	A	15	THR	1
1	A	74	ASN	1
1	A	91	TYR	1
1	A	61	LEU	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	92	3	47,50,50	1.35±0.20	4±1 (7±2%)
3	PLM	A	96	2	16,16,17	1.11±0.22	1±0 (5±2%)

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	92	3	69,75,75	1.44±0.31	9±4 (13±5%)
3	PLM	A	96	2	15,15,17	0.84±0.09	0±0 (0±1%)

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	92	3	-	0±0,48,64,64	0±0,3,3,3
3	PLM	A	96	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	92	COA	P2A-O3A	7.01	1.51	1.59	7	15
2	A	92	COA	CDP-CBP	6.91	1.39	1.53	7	2
2	A	92	COA	P1A-O3A	5.41	1.53	1.59	7	12
2	A	92	COA	CEP-CBP	5.39	1.42	1.53	6	3
2	A	92	COA	CCP-CBP	4.87	1.60	1.52	9	8
3	A	96	PLM	O1-C1	4.21	1.20	1.42	6	14
2	A	92	COA	C5B-C4B	4.19	1.64	1.51	4	4
2	A	92	COA	P3B-O3B	3.06	1.64	1.59	2	7
2	A	92	COA	C1B-N9A	2.71	1.53	1.46	8	2
2	A	92	COA	C3P-N4P	2.46	1.51	1.46	4	1
2	A	92	COA	C7P-N8P	2.12	1.50	1.46	2	1
2	A	92	COA	C9P-N8P	2.12	1.28	1.33	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	92	COA	C5P-N4P	2.09	1.28	1.33	5	1
2	A	92	COA	C7P-C6P	2.04	1.58	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	92	COA	CDP-CBP-CCP	8.85	122.84	108.22	9	6
2	A	92	COA	C7P-C6P-C5P	8.47	98.28	112.39	16	9
2	A	92	COA	CEP-CBP-CAP	8.34	122.99	108.77	10	7
2	A	92	COA	C6P-C7P-N8P	6.12	98.97	112.00	10	7
2	A	92	COA	O6A-CCP-CBP	5.39	119.22	110.55	10	11
2	A	92	COA	C2P-C3P-N4P	5.39	100.08	112.31	8	14
2	A	92	COA	CEP-CBP-CDP	4.97	99.30	109.20	9	5
2	A	92	COA	CAP-C9P-N8P	4.69	107.59	116.48	9	5
2	A	92	COA	P3B-O3B-C3B	4.56	135.62	123.43	4	7
2	A	92	COA	O5B-C5B-C4B	4.30	123.65	108.99	4	8
2	A	92	COA	C3B-C2B-C1B	3.95	108.57	99.89	10	6
2	A	92	COA	C5B-C4B-C3B	3.70	126.69	114.38	4	2
2	A	92	COA	OAP-CAP-CBP	3.59	101.86	110.18	3	9
2	A	92	COA	CDP-CBP-CAP	3.53	114.79	108.77	12	3
2	A	92	COA	O3B-P3B-O7A	3.45	97.05	109.33	9	4
2	A	92	COA	C7P-N8P-C9P	3.40	128.65	122.55	7	3
2	A	92	COA	C6P-C5P-N4P	3.06	110.78	116.34	11	3
2	A	92	COA	OAP-CAP-C9P	3.03	122.03	109.38	9	4
2	A	92	COA	CEP-CBP-CCP	2.93	103.39	108.22	16	5
2	A	92	COA	O5P-C5P-C6P	2.91	116.75	122.02	4	2
2	A	92	COA	P1A-O5B-C5B	2.90	137.98	121.35	7	1
2	A	92	COA	O9A-P3B-O8A	2.69	117.90	107.80	9	7
2	A	92	COA	O9P-C9P-CAP	2.68	128.38	120.89	7	2
2	A	92	COA	O3A-P1A-O1A	2.63	102.80	110.70	7	3
2	A	92	COA	O4B-C4B-C5B	2.51	101.28	109.33	4	1
2	A	92	COA	O2B-C2B-C1B	2.45	118.55	110.10	10	1
3	A	96	PLM	C5-C4-C3	2.44	102.02	114.37	14	1
2	A	92	COA	O5A-P2A-O4A	2.22	122.76	112.44	6	2
2	A	92	COA	O4B-C1B-C2B	2.20	111.33	106.62	8	1
2	A	92	COA	C3P-N4P-C5P	2.17	118.79	122.82	16	2
2	A	92	COA	O5A-P2A-O3A	2.17	113.13	107.27	9	1
2	A	92	COA	C4A-N9A-C1B	2.16	131.68	126.63	12	1
2	A	92	COA	O5P-C5P-N4P	2.12	127.19	123.03	7	1
2	A	92	COA	O2A-P1A-O3A	2.03	101.78	107.27	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	92	COA	O9A-P3B-O7A	2.02	118.71	110.83	14	1
2	A	92	COA	O2A-P1A-O1A	2.01	121.78	112.44	16	1

All unique chiral outliers are listed below.

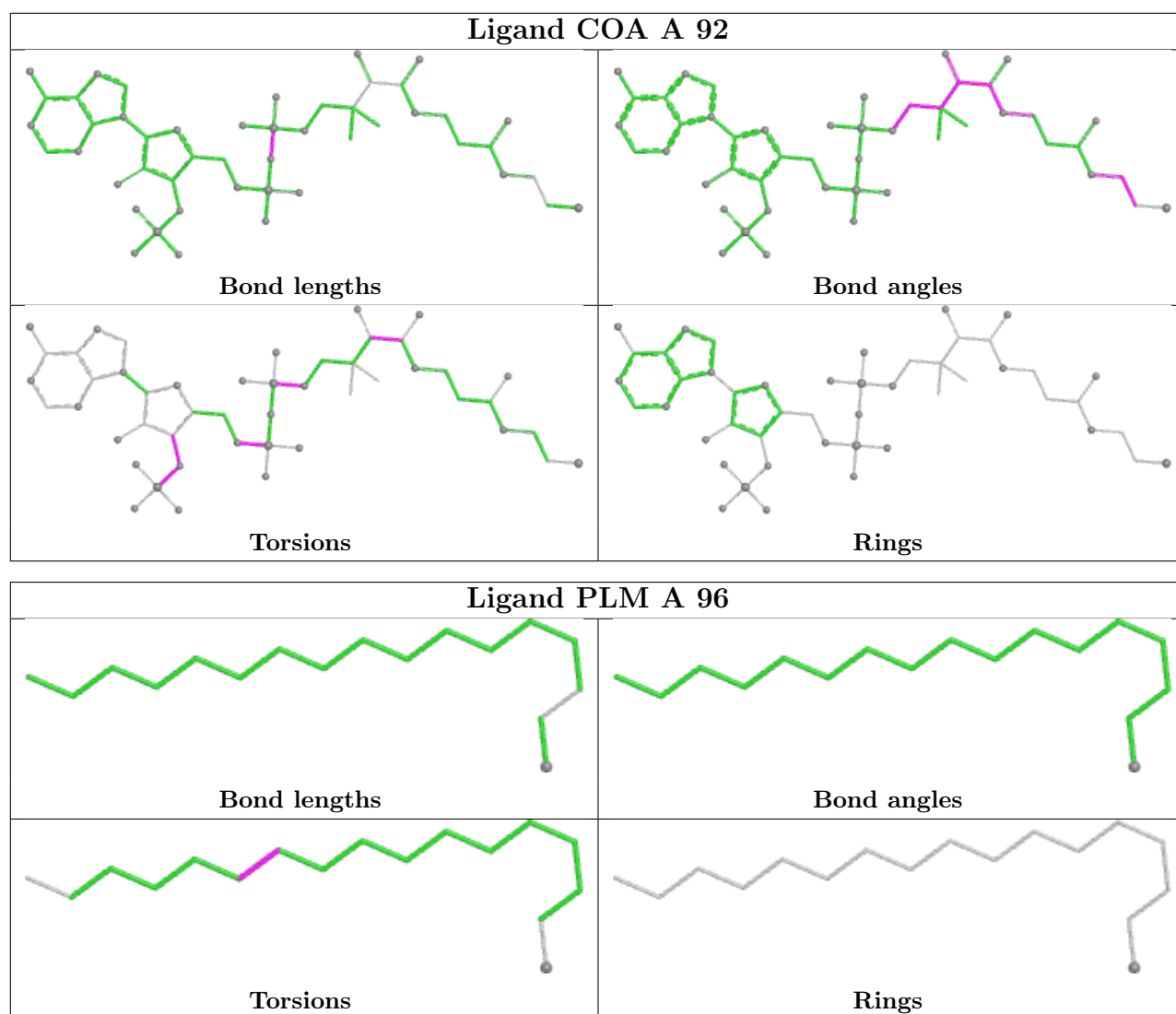
Mol	Chain	Res	Type	Atoms	Models (Total)
2	A	92	COA	CAP	9

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	92	COA	O9P-C9P-CAP-CBP	3
2	A	92	COA	N8P-C9P-CAP-CBP	3

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