



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:10 PM UTC

PDB ID : 6UIA / pdb_00006uia
EMDB ID : EMD-20784
Title : Structure of ATP citrate lyase with CoA in a partially open conformation
Authors : Wei, X.; Marmorstein, R.
Deposited on : 2019-09-30
Resolution : 4.30 Å (reported)
Based on initial model : 3MWD

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

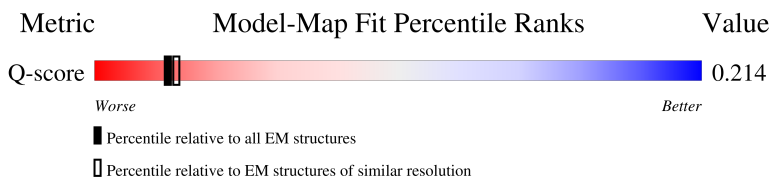
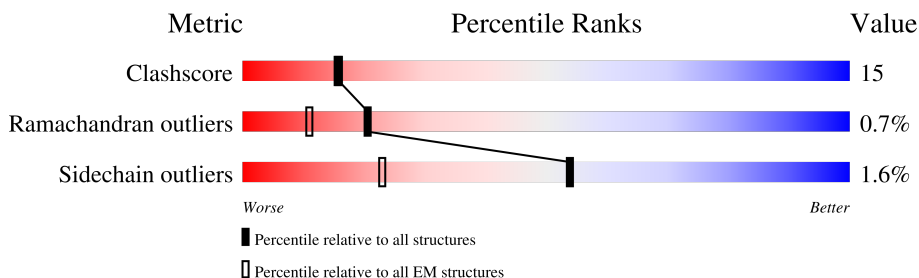
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

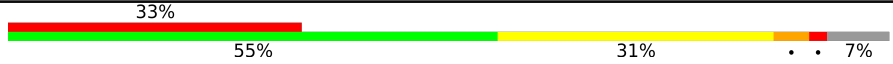
The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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

Mol	Chain	Length	Quality of chain
1	A	1101	
1	B	1101	
1	C	1101	
1	D	1101	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	COA	B	1201	-	-	X	-

2 Entry composition [i](#)

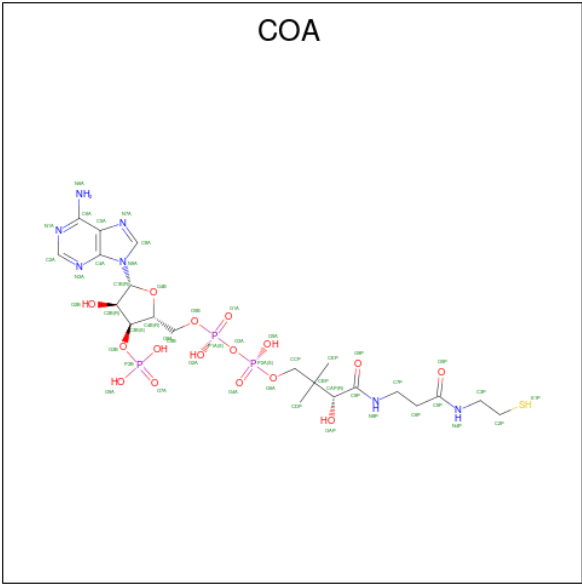
There are 2 unique types of molecules in this entry. The entry contains 31720 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP-citrate synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	1021	Total 7906	5064	1340	1458	44	2	0
1	D	1021	Total 7906	5064	1340	1458	44	2	0
1	A	1021	Total 7906	5064	1340	1458	44	2	0
1	B	1021	Total 7906	5064	1340	1458	44	2	0

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S) (labeled as "Ligand of Interest" by depositor).

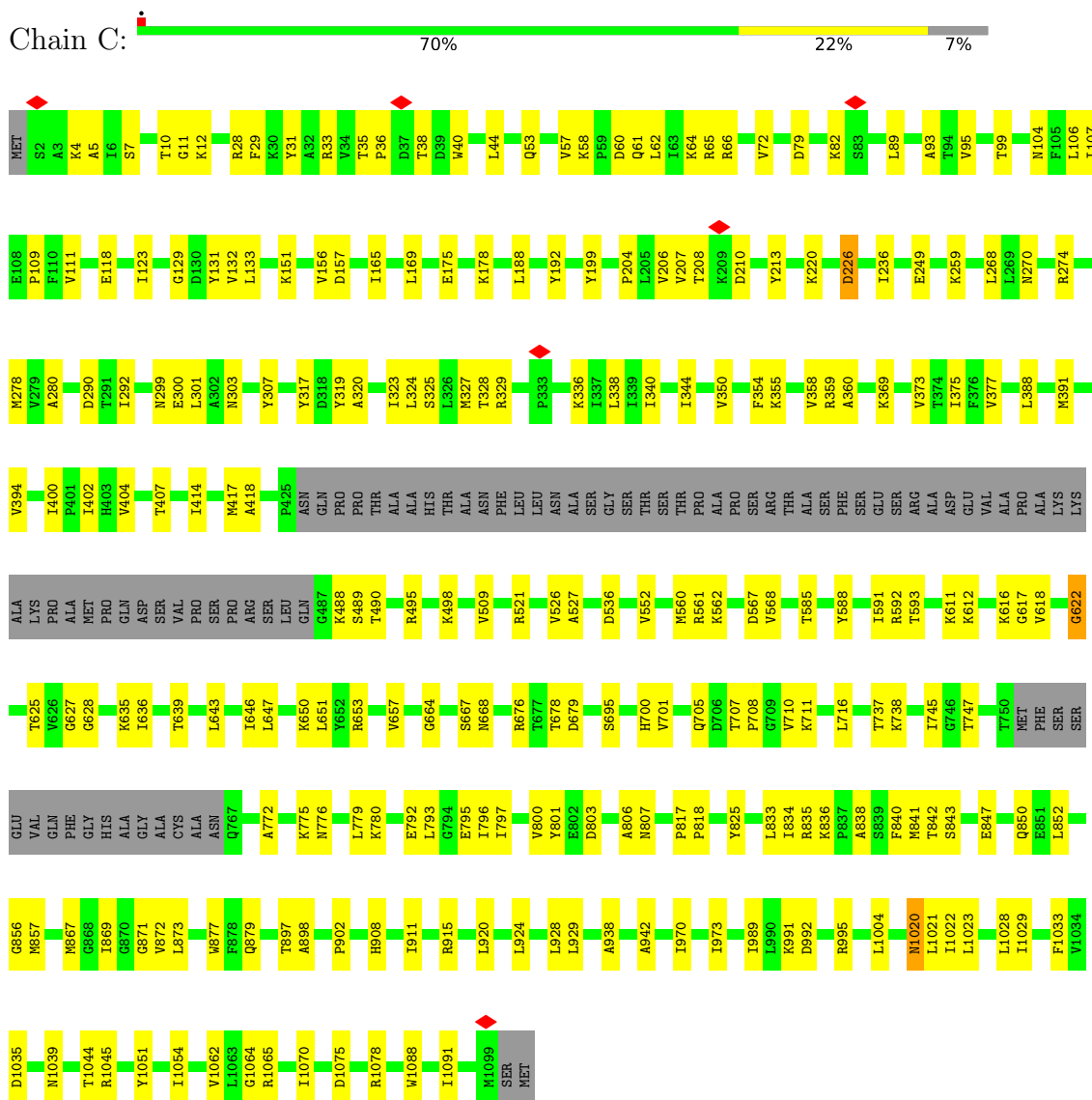


Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
2	A	1	Total 48	21	7	16	3	1	0
2	B	1	Total 48	21	7	16	3	1	0

3 Residue-property plots [i](#)

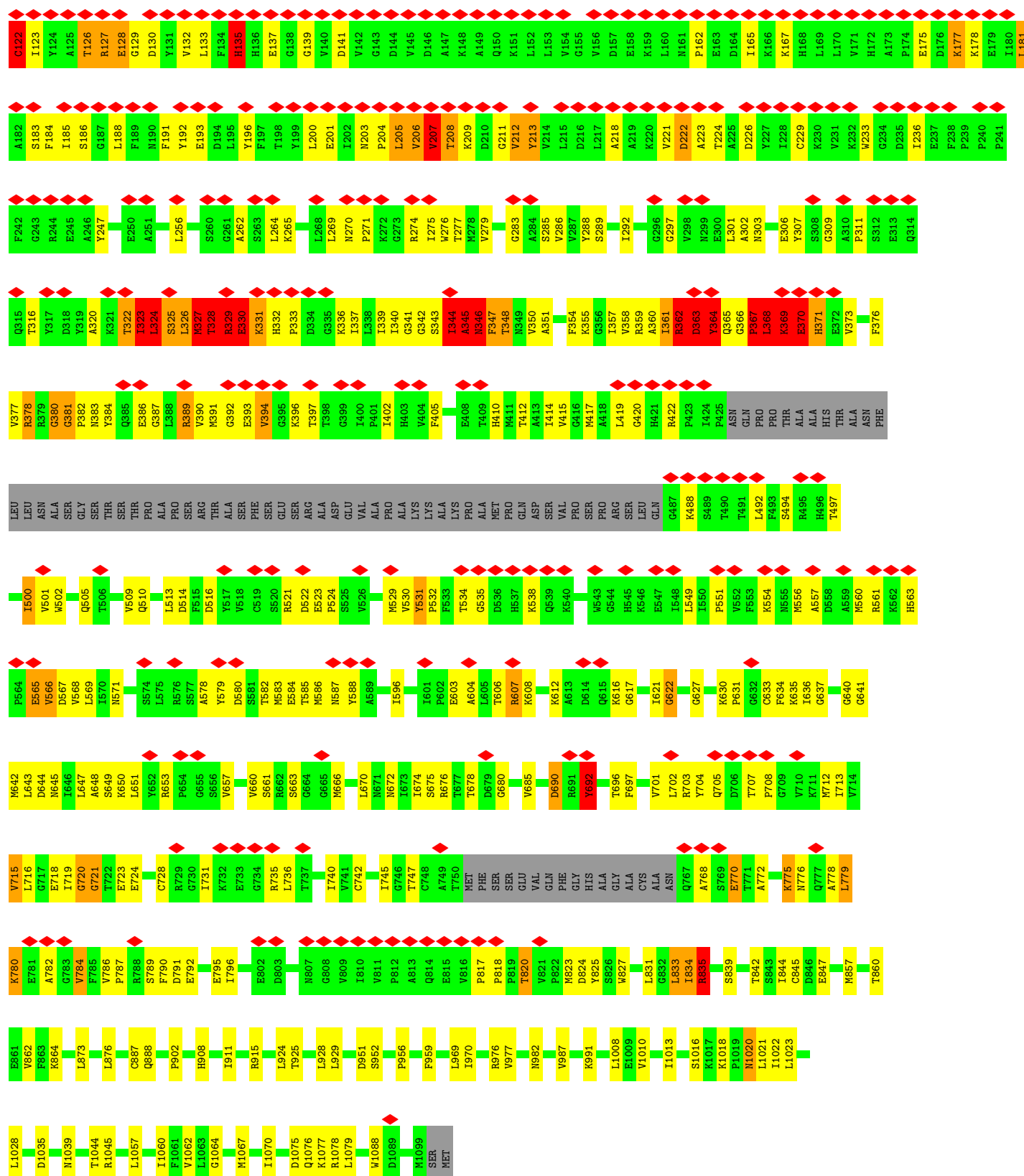
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

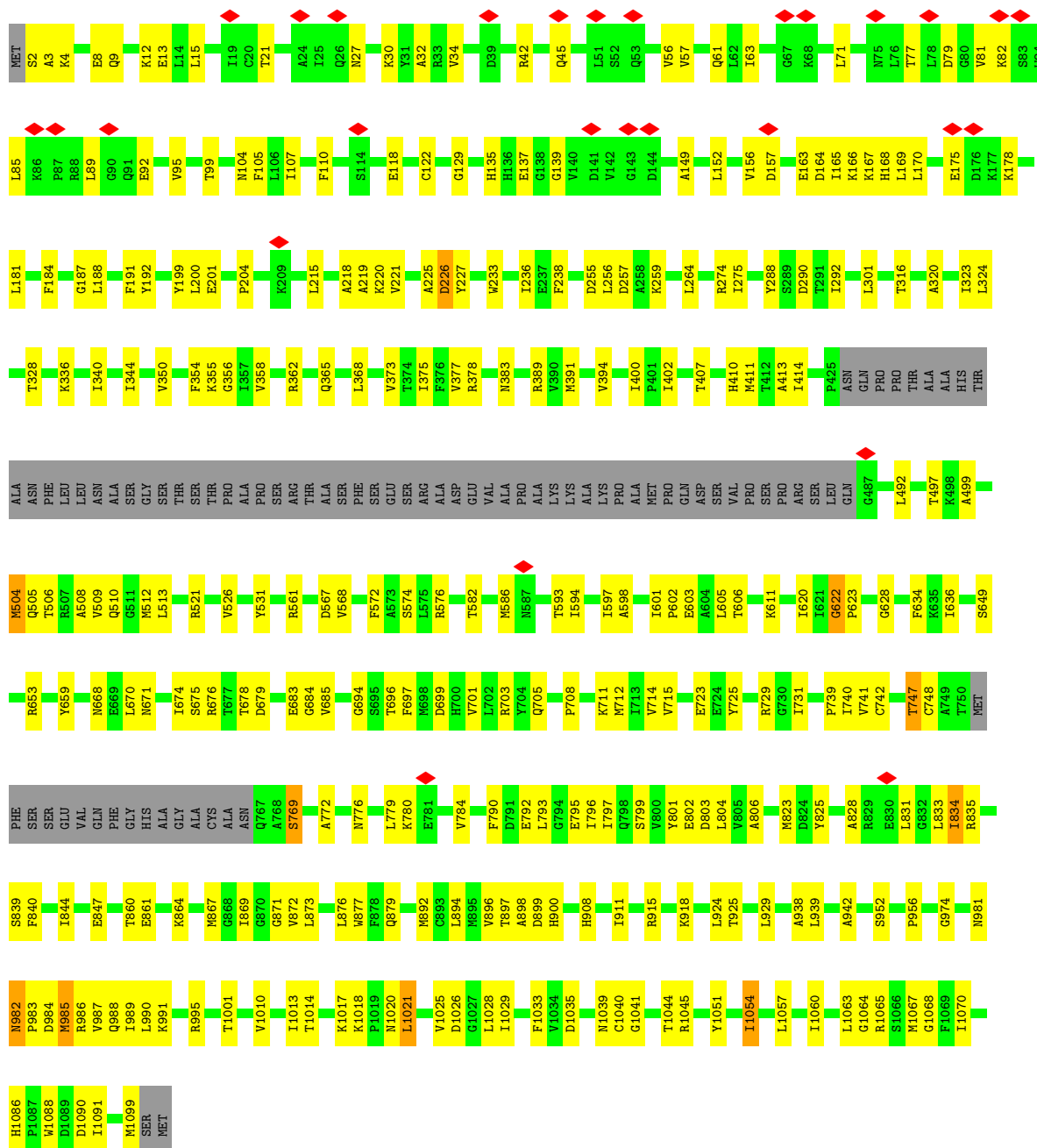
- Molecule 1: ATP-citrate synthase



- Molecule 1: ATP-citrate synthase







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	73969	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.045	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	191.4, 191.4, 191.4	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86999995, 0.86999995, 0.86999995	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.61	39/8082 (0.5%)	1.40	106/10939 (1.0%)
1	B	0.38	0/8083	0.82	8/10942 (0.1%)
1	C	0.43	2/8083 (0.0%)	0.76	6/10942 (0.1%)
1	D	0.67	11/8083 (0.1%)	0.93	36/10942 (0.3%)
All	All	0.92	52/32331 (0.2%)	1.01	156/43765 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	41
1	B	0	5
1	C	0	2
1	D	0	13
All	All	0	61

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	692	TYR	CD1-CE1	66.84	3.39	1.38
1	A	692	TYR	CD2-CE2	52.55	2.96	1.38
1	A	127	ARG	C-N	41.17	1.84	1.33
1	A	692	TYR	CE1-CZ	40.23	2.34	1.38
1	A	692	TYR	CE2-CZ	38.00	2.29	1.38
1	A	692	TYR	CG-CD1	35.28	2.13	1.39
1	A	692	TYR	CG-CD2	34.72	2.12	1.39
1	A	128	GLU	N-CA	24.15	1.72	1.46
1	D	73	GLY	C-N	19.74	1.62	1.33
1	C	817	PRO	CA-C	19.02	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	73	GLY	N-CA	18.64	1.72	1.45
1	D	56	VAL	C-N	18.47	1.58	1.33
1	D	72	VAL	C-N	17.51	1.59	1.33
1	A	328	THR	CA-C	17.04	1.72	1.52
1	A	368	LEU	CA-C	17.04	1.69	1.52
1	D	57	VAL	CA-C	14.94	1.71	1.52
1	A	328	THR	C-N	14.86	1.54	1.33
1	A	327	MET	CA-C	14.44	1.72	1.52
1	D	57	VAL	N-CA	14.38	1.64	1.46
1	A	329	ARG	N-CA	12.89	1.62	1.46
1	A	326	LEU	CA-C	12.54	1.69	1.52
1	A	368	LEU	C-N	12.27	1.52	1.33
1	D	73	GLY	CA-C	11.51	1.68	1.51
1	A	118	GLU	CA-C	10.29	1.66	1.52
1	A	326	LEU	N-CA	9.64	1.58	1.46
1	D	74	VAL	N-CA	9.08	1.57	1.46
1	A	206	VAL	N-CA	8.78	1.56	1.46
1	A	119	PHE	N-CA	8.67	1.57	1.46
1	A	369	LYS	N-CA	7.94	1.56	1.45
1	A	368	LEU	CA-CB	7.47	1.66	1.54
1	A	206	VAL	CA-C	7.34	1.61	1.52
1	D	72	VAL	CA-C	7.19	1.61	1.52
1	C	817	PRO	C-O	-7.13	1.18	1.24
1	A	327	MET	N-CA	7.11	1.55	1.46
1	A	127	ARG	CA-C	6.83	1.61	1.52
1	A	369	LYS	C-N	6.82	1.43	1.33
1	A	86	LYS	C-N	6.78	1.39	1.33
1	A	326	LEU	C-N	6.41	1.42	1.33
1	A	367	PRO	CA-C	6.18	1.61	1.52
1	A	371	HIS	CA-C	6.09	1.60	1.53
1	A	118	GLU	C-N	5.77	1.41	1.33
1	A	380	GLY	C-N	5.76	1.42	1.33
1	A	345	ALA	C-N	5.73	1.41	1.33
1	A	346	ASN	N-CA	5.63	1.53	1.46
1	A	345	ALA	N-CA	5.61	1.53	1.45
1	D	56	VAL	N-CA	5.39	1.53	1.46
1	A	212	VAL	C-N	5.36	1.41	1.33
1	A	368	LEU	CB-CG	5.23	1.64	1.53
1	D	71	LEU	C-N	5.21	1.40	1.33
1	A	325	SER	CA-C	5.21	1.59	1.52
1	A	381	GLY	N-CA	5.16	1.51	1.44
1	A	329	ARG	CA-C	5.01	1.59	1.52

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	ARG	CA-C-N	29.73	165.48	120.89
1	A	127	ARG	C-N-CA	29.73	165.48	120.89
1	C	817	PRO	O-C-N	20.57	130.82	121.15
1	A	368	LEU	CA-CB-CG	18.18	179.92	116.30
1	A	368	LEU	CA-C-N	17.77	150.14	122.24
1	A	368	LEU	C-N-CA	17.77	150.14	122.24
1	A	368	LEU	CD1-CG-CD2	-16.77	73.90	110.80
1	D	74	VAL	N-CA-C	16.25	131.60	108.36
1	D	72	VAL	CA-C-N	15.15	151.11	121.41
1	D	72	VAL	C-N-CA	15.15	151.11	121.41
1	A	212	VAL	CA-C-N	-14.97	99.08	122.59
1	A	212	VAL	C-N-CA	-14.97	99.08	122.59
1	A	329	ARG	CA-CB-CG	13.61	141.31	114.10
1	D	57	VAL	N-CA-C	13.25	136.89	109.34
1	D	74	VAL	CB-CA-C	-12.82	93.41	110.84
1	A	369	LYS	CB-CA-C	-12.75	87.60	109.02
1	A	326	LEU	N-CA-C	12.37	128.59	113.12
1	D	56	VAL	CA-C-N	12.22	143.97	121.97
1	D	56	VAL	C-N-CA	12.22	143.97	121.97
1	A	327	MET	CA-C-N	12.11	147.65	122.58
1	A	327	MET	C-N-CA	12.11	147.65	122.58
1	A	328	THR	CA-C-N	11.95	144.36	121.54
1	A	328	THR	C-N-CA	11.95	144.36	121.54
1	A	127	ARG	CA-C-O	-11.53	106.45	119.14
1	A	329	ARG	CB-CA-C	-10.16	90.21	110.42
1	D	56	VAL	CA-C-O	-10.06	108.21	120.78
1	A	369	LYS	N-CA-C	10.00	127.21	114.31
1	A	328	THR	CA-CB-CG2	9.83	127.22	110.50
1	A	213	TYR	N-CA-C	9.66	124.50	109.52
1	A	820	THR	CA-C-N	-9.51	115.75	122.59
1	A	820	THR	C-N-CA	-9.51	115.75	122.59
1	A	393	GLU	CA-C-N	-9.33	108.34	121.77
1	A	393	GLU	C-N-CA	-9.33	108.34	121.77
1	D	57	VAL	CB-CA-C	-9.25	96.12	111.29
1	A	369	LYS	CA-CB-CG	9.19	132.48	114.10
1	D	58	LYS	CA-CB-CG	9.17	132.44	114.10
1	D	71	LEU	CA-CB-CG	9.04	147.93	116.30
1	B	981	ASN	CA-C-N	9.00	132.75	122.85
1	B	981	ASN	C-N-CA	9.00	132.75	122.85
1	A	344	ILE	CA-C-N	8.94	136.23	121.39
1	A	344	ILE	C-N-CA	8.94	136.23	121.39
1	A	206	VAL	N-CA-C	8.91	121.16	108.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	VAL	O-C-N	-8.81	113.31	123.00
1	A	346	ASN	N-CA-C	8.79	129.53	110.80
1	A	692	TYR	CA-CB-CG	8.72	129.60	113.90
1	A	692	TYR	CB-CA-C	-8.65	101.51	110.33
1	D	73	GLY	N-CA-C	8.46	133.23	113.18
1	A	203	ASN	CA-C-N	8.31	146.94	127.00
1	A	203	ASN	C-N-CA	8.31	146.94	127.00
1	A	323	ILE	CB-CA-C	8.31	124.91	111.29
1	A	331	LYS	CB-CG-CD	8.25	130.27	111.30
1	D	58	LYS	N-CA-C	8.21	122.14	110.40
1	D	1017	LYS	CA-CB-CG	-8.16	97.77	114.10
1	A	328	THR	N-CA-CB	-8.13	96.68	110.51
1	A	368	LEU	CB-CA-C	8.11	122.82	110.08
1	D	57	VAL	O-C-N	-8.10	112.44	122.57
1	D	72	VAL	CA-C-O	-8.10	110.66	120.78
1	A	328	THR	CB-CA-C	8.07	123.21	109.65
1	A	692	TYR	CB-CG-CD2	-8.02	108.77	120.80
1	A	370	GLU	CA-C-N	7.99	135.07	123.17
1	A	370	GLU	C-N-CA	7.99	135.07	123.17
1	A	329	ARG	CB-CG-CD	7.99	129.67	111.30
1	A	128	GLU	CB-CA-C	-7.59	99.31	111.39
1	A	369	LYS	CA-C-O	-7.59	110.34	118.77
1	A	834	ILE	CA-C-N	7.56	135.98	121.54
1	A	834	ILE	C-N-CA	7.56	135.98	121.54
1	A	364	TYR	CA-CB-CG	7.50	127.41	113.90
1	A	692	TYR	CD1-CG-CD2	7.39	129.19	118.10
1	A	203	ASN	C-N-CD	-7.38	104.35	120.60
1	D	72	VAL	N-CA-C	7.35	124.63	109.34
1	A	212	VAL	CG1-CB-CG2	-7.25	94.84	110.80
1	D	74	VAL	CA-C-N	7.23	135.35	121.54
1	D	74	VAL	C-N-CA	7.23	135.35	121.54
1	B	1017	LYS	CA-CB-CG	-7.07	99.96	114.10
1	A	345	ALA	N-CA-C	7.06	120.93	110.48
1	D	73	GLY	CA-C-O	-7.00	108.40	120.57
1	D	55	LEU	CA-CB-CG	6.94	140.59	116.30
1	A	328	THR	N-CA-C	6.94	122.17	113.43
1	A	329	ARG	N-CA-C	6.89	125.48	110.80
1	D	107	ILE	CA-C-N	-6.71	109.40	122.70
1	D	107	ILE	C-N-CA	-6.71	109.40	122.70
1	A	135	HIS	CA-C-N	6.69	132.06	120.68
1	A	135	HIS	C-N-CA	6.69	132.06	120.68
1	A	324	LEU	CD1-CG-CD2	-6.61	96.26	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	ARG	CB-CG-CD	6.60	126.47	111.30
1	A	327	MET	CB-CG-SD	-6.59	92.94	112.70
1	A	324	LEU	N-CA-CB	6.55	119.95	110.65
1	A	118	GLU	CB-CA-C	6.53	123.42	110.42
1	A	205	LEU	CB-CA-C	6.52	122.58	109.68
1	B	834	ILE	CA-C-N	6.46	133.87	121.54
1	B	834	ILE	C-N-CA	6.46	133.87	121.54
1	B	982	ASN	N-CA-C	-6.42	97.84	108.75
1	C	834	ILE	CA-C-N	6.42	133.79	121.54
1	C	834	ILE	C-N-CA	6.42	133.79	121.54
1	A	380	GLY	CA-C-N	6.40	131.91	121.87
1	A	380	GLY	C-N-CA	6.40	131.91	121.87
1	D	834	ILE	CA-C-N	6.38	133.72	121.54
1	D	834	ILE	C-N-CA	6.38	133.72	121.54
1	D	57	VAL	CA-C-O	-6.31	112.89	120.78
1	A	367	PRO	N-CA-C	6.31	125.46	112.47
1	A	205	LEU	CA-CB-CG	6.24	138.14	116.30
1	A	775	LYS	CD-CE-NZ	-6.17	92.15	111.90
1	A	324	LEU	CB-CG-CD2	6.14	129.12	110.70
1	C	817	PRO	CA-C-O	-6.12	115.89	120.73
1	A	330	GLU	N-CA-C	6.10	118.47	109.69
1	D	71	LEU	N-CA-C	6.10	117.56	107.20
1	D	57	VAL	CA-CB-CG1	6.09	120.75	110.40
1	A	212	VAL	CA-C-O	-6.05	113.22	120.78
1	A	328	THR	O-C-N	-5.96	114.11	122.10
1	A	368	LEU	N-CA-CB	-5.94	100.01	110.34
1	A	181	LEU	CA-CB-CG	5.91	137.00	116.30
1	D	73	GLY	CA-C-N	5.85	130.30	122.93
1	D	73	GLY	C-N-CA	5.85	130.30	122.93
1	A	329	ARG	CG-CD-NE	-5.85	99.13	112.00
1	D	72	VAL	CA-CB-CG1	5.84	120.32	110.40
1	A	207	VAL	CA-C-N	5.81	132.64	121.54
1	A	207	VAL	C-N-CA	5.81	132.64	121.54
1	A	327	MET	N-CA-C	5.80	123.17	110.80
1	A	775	LYS	CB-CG-CD	-5.80	97.96	111.30
1	A	833	LEU	CA-C-N	-5.78	111.57	121.97
1	A	833	LEU	C-N-CA	-5.78	111.57	121.97
1	A	206	VAL	CG1-CB-CG2	-5.75	98.14	110.80
1	A	368	LEU	CB-CG-CD2	5.74	127.90	110.70
1	A	371	HIS	N-CA-CB	-5.72	102.90	111.25
1	A	207	VAL	N-CA-C	5.70	116.69	108.48
1	D	1017	LYS	CB-CG-CD	5.67	124.34	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	ARG	CB-CA-C	5.67	119.95	110.43
1	A	845	CYS	N-CA-C	5.67	118.10	111.02
1	A	322	THR	CA-C-N	-5.66	111.78	121.97
1	A	322	THR	C-N-CA	-5.66	111.78	121.97
1	A	128	GLU	N-CA-C	5.60	119.72	111.04
1	A	363	ASP	CA-C-N	5.59	131.41	122.86
1	A	363	ASP	C-N-CA	5.59	131.41	122.86
1	A	692	TYR	N-CA-CB	5.59	119.12	110.12
1	A	207	VAL	CG1-CB-CG2	5.57	123.06	110.80
1	D	259	LYS	CB-CG-CD	5.52	123.99	111.30
1	A	328	THR	CA-C-O	-5.49	113.11	119.64
1	A	118	GLU	CA-C-N	5.48	132.00	121.54
1	A	118	GLU	C-N-CA	5.48	132.00	121.54
1	A	835	ARG	N-CA-C	-5.45	99.20	110.80
1	A	128	GLU	N-CA-CB	5.42	117.80	110.10
1	A	378	ARG	N-CA-CB	-5.40	103.35	111.56
1	A	343	SER	CA-C-N	5.38	131.66	121.97
1	A	343	SER	C-N-CA	5.38	131.66	121.97
1	D	74	VAL	N-CA-CB	5.36	117.42	110.99
1	C	833	LEU	CA-C-N	-5.34	112.36	121.97
1	C	833	LEU	C-N-CA	-5.34	112.36	121.97
1	A	368	LEU	CB-CG-CD1	5.26	126.49	110.70
1	B	833	LEU	CA-C-N	-5.21	112.59	121.97
1	B	833	LEU	C-N-CA	-5.21	112.59	121.97
1	A	119	PHE	N-CA-CB	5.21	119.29	110.49
1	D	55	LEU	CB-CG-CD2	-5.16	95.23	110.70
1	D	71	LEU	CB-CG-CD2	5.11	126.03	110.70
1	A	721	GLY	CA-C-O	-5.10	118.49	122.52
1	A	167	LYS	CA-C-N	-5.01	114.18	121.99
1	A	167	LYS	C-N-CA	-5.01	114.18	121.99

There are no chirality outliers.

All (61) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1020	ASN	Peptide
1	A	109	PRO	Peptide
1	A	118	GLU	Peptide,Mainchain
1	A	119	PHE	Peptide
1	A	120	TYR	Mainchain
1	A	121	VAL	Peptide
1	A	122	CYS	Peptide

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Mol	Chain	Res	Type	Group
1	A	129	GLY	Peptide
1	A	222	ASP	Peptide
1	A	223	ALA	Peptide
1	A	23	SER	Peptide
1	A	24	ALA	Peptide
1	A	247	TYR	Peptide
1	A	3	ALA	Peptide
1	A	323	ILE	Peptide
1	A	328	THR	Peptide
1	A	329	ARG	Peptide
1	A	330	GLU	Peptide
1	A	344	ILE	Peptide
1	A	345	ALA	Peptide
1	A	347	PHE	Peptide
1	A	348	THR	Peptide
1	A	361	ILE	Peptide
1	A	362	ARG	Peptide
1	A	363	ASP	Peptide
1	A	364	TYR	Peptide
1	A	397	THR	Peptide
1	A	420	GLY	Peptide
1	A	529	MET	Peptide
1	A	531	TYR	Peptide
1	A	565	GLU	Peptide
1	A	622	GLY	Peptide
1	A	690	ASP	Peptide
1	A	768	ALA	Peptide
1	A	770	GLU	Peptide
1	A	779	LEU	Peptide
1	A	780	LYS	Peptide
1	A	784	VAL	Peptide
1	A	820	THR	Peptide
1	A	952	SER	Peptide
1	B	1020	ASN	Peptide
1	B	622	GLY	Peptide
1	B	769	SER	Peptide
1	B	952	SER	Peptide
1	B	985	MET	Peptide
1	C	1020	ASN	Peptide
1	C	622	GLY	Peptide
1	D	1044	THR	Peptide
1	D	110	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	D	264	LEU	Peptide
1	D	56	VAL	Peptide
1	D	57	VAL	Peptide
1	D	622	GLY	Peptide
1	D	72	VAL	Peptide
1	D	73	GLY	Peptide
1	D	74	VAL	Peptide
1	D	76	LEU	Peptide
1	D	78	LEU	Peptide
1	D	834	ILE	Peptide
1	D	952	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7906	0	7953	364	0
1	B	7906	0	7956	225	0
1	C	7906	0	7956	159	0
1	D	7906	0	7956	216	0
2	A	48	0	32	19	0
2	B	48	0	32	40	0
All	All	31720	0	31885	925	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (925) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLU:N	1:A:128:GLU:CA	1.72	1.50
1:D:73:GLY:CA	1:D:73:GLY:N	1.72	1.49
1:A:692:TYR:CG	1:A:692:TYR:CD2	2.12	1.35
1:A:692:TYR:CG	1:A:692:TYR:CD1	2.13	1.35
1:A:127:ARG:C	1:A:128:GLU:N	1.84	1.34
1:A:1018:LYS:NZ	2:A:1201:COA:O1A	1.61	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1018:LYS:CE	2:A:1201:COA:O1A	1.86	1.23
2:B:1201:COA:C1B	2:B:1201:COA:O4B	1.64	1.20
1:A:692:TYR:CZ	1:A:692:TYR:CE2	2.29	1.20
1:A:692:TYR:CZ	1:A:692:TYR:CE1	2.34	1.15
1:B:505:GLN:NE2	2:B:1201:COA:H143	1.63	1.13
1:A:969:LEU:HD22	2:A:1201:COA:C4A	1.81	1.10
1:B:572:PHE:HB3	2:B:1201:COA:H133	1.30	1.06
1:D:1018:LYS:HD2	2:B:1201:COA:O1A	1.59	1.03
1:B:505:GLN:HE21	2:B:1201:COA:H143	1.18	1.02
1:B:505:GLN:NE2	2:B:1201:COA:CEP	2.22	1.01
1:A:969:LEU:HD22	2:A:1201:COA:C5A	1.91	1.01
1:A:350:VAL:O	1:A:354:PHE:HB2	1.62	1.00
1:A:120:TYR:HB3	1:A:135:HIS:O	1.63	0.98
1:A:579:TYR:O	1:A:583:MET:HB2	1.64	0.98
1:A:969:LEU:HB3	2:A:1201:COA:C6A	1.95	0.96
1:A:1018:LYS:CD	2:A:1201:COA:O1A	2.18	0.92
1:A:324:LEU:HD12	1:A:364:TYR:H	1.36	0.91
1:B:572:PHE:CB	2:B:1201:COA:H133	2.03	0.89
1:D:1021:LEU:HD21	2:B:1201:COA:C4A	2.06	0.86
1:A:776:ASN:O	1:A:780:LYS:HB2	1.75	0.86
1:B:9:GLN:O	1:B:13:GLU:HB2	1.76	0.85
1:D:776:ASN:O	1:D:780:LYS:HB2	1.76	0.84
1:D:1021:LEU:HD21	2:B:1201:COA:C5A	2.07	0.84
1:D:40:TRP:O	1:D:44:LEU:HB2	1.76	0.84
1:D:1017:LYS:HB3	2:B:1201:COA:H4B	1.60	0.83
1:A:128:GLU:N	1:A:692:TYR:CE1	2.46	0.83
1:B:772:ALA:O	1:B:776:ASN:HB2	1.78	0.83
1:D:34:VAL:O	1:D:105:PHE:HB2	1.79	0.83
1:A:772:ALA:O	1:A:776:ASN:HB2	1.79	0.83
1:A:351:ALA:O	1:A:355:LYS:HB2	1.80	0.82
1:B:505:GLN:HE21	2:B:1201:COA:CEP	1.87	0.81
1:A:128:GLU:N	1:A:692:TYR:CD1	2.49	0.81
1:B:572:PHE:HB3	2:B:1201:COA:CDP	2.11	0.80
1:A:1018:LYS:HD2	2:A:1201:COA:O1A	1.80	0.80
1:C:93:ALA:O	1:C:99:THR:HA	1.82	0.80
1:D:536:ASP:HA	1:D:552:VAL:O	1.81	0.80
1:A:329:ARG:H	1:A:368:LEU:N	1.80	0.79
1:B:670:LEU:O	1:B:674:ILE:HB	1.82	0.78
1:B:3:ALA:HA	1:B:221:VAL:O	1.84	0.77
1:D:199:TYR:O	1:D:219:ALA:HA	1.84	0.77
1:A:603:GLU:HA	1:A:606:THR:HG22	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1021:LEU:CD2	2:B:1201:COA:C4A	2.63	0.77
1:A:119:PHE:H	1:A:205:LEU:HG	1.50	0.76
1:A:181:LEU:O	1:A:184:PHE:HB3	1.85	0.76
1:A:122:CYS:SG	1:A:123:ILE:N	2.58	0.76
1:A:970:ILE:H	2:A:1201:COA:C2A	1.99	0.76
1:B:572:PHE:CD1	2:B:1201:COA:H133	2.21	0.76
1:D:1067:MET:HG2	1:B:1063:LEU:HD21	1.69	0.75
1:D:58:LYS:HB3	1:D:72:VAL:HA	1.69	0.75
1:B:8:GLU:O	1:B:12:LYS:HB2	1.86	0.74
1:A:58:LYS:O	1:A:105:PHE:HA	1.89	0.72
1:B:793:LEU:O	1:B:797:ILE:HB	1.89	0.72
1:A:328:THR:O	1:A:370:GLU:N	2.23	0.72
1:D:872:VAL:HG23	1:B:1067:MET:HE1	1.72	0.72
1:A:724:GLU:HB2	1:A:775:LYS:HD3	1.72	0.72
1:C:206:VAL:O	1:C:213:TYR:HB2	1.90	0.72
1:A:970:ILE:H	2:A:1201:COA:H2A	1.55	0.72
1:A:328:THR:C	1:A:369:LYS:H	1.97	0.72
1:B:572:PHE:CD1	2:B:1201:COA:CDP	2.73	0.71
1:D:58:LYS:HG2	1:D:73:GLY:H	1.54	0.71
1:A:328:THR:H	1:A:368:LEU:HB3	1.55	0.71
1:D:9:GLN:O	1:D:13:GLU:HB2	1.91	0.71
1:A:578:ALA:O	1:A:582:THR:HB	1.90	0.71
1:B:797:ILE:O	1:B:801:TYR:HB2	1.91	0.70
1:C:856:GLY:HA3	1:B:1099:MET:H	1.56	0.70
1:C:344:ILE:HB	1:C:668:ASN:HB3	1.74	0.70
1:A:969:LEU:HB3	2:A:1201:COA:N1A	2.05	0.70
1:A:128:GLU:N	1:A:692:TYR:CZ	2.59	0.70
1:A:770:GLU:HB3	1:A:775:LYS:HD2	1.73	0.70
1:A:324:LEU:HD13	1:A:328:THR:HG21	1.73	0.70
1:A:344:ILE:O	1:A:381:GLY:N	2.19	0.70
1:A:608:LYS:O	1:A:612:LYS:HB2	1.91	0.70
1:A:355:LYS:HA	1:A:358:VAL:HG12	1.74	0.69
1:D:58:LYS:HG3	1:D:106:LEU:HB3	1.75	0.69
1:D:628:GLY:H	1:D:636:ILE:HB	1.56	0.69
1:B:897:THR:HG23	1:B:1064:GLY:HA3	1.73	0.69
1:A:118:GLU:N	1:A:206:VAL:O	2.24	0.69
1:C:897:THR:HG23	1:C:1064:GLY:HA3	1.74	0.69
1:A:414:ILE:HA	1:A:417:MET:HG2	1.74	0.69
1:B:867:MET:HB2	1:B:871:GLY:HA3	1.75	0.69
1:B:911:ILE:O	1:B:915:ARG:HB2	1.93	0.69
1:A:580:ASP:O	1:A:584:GLU:HB2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:908:HIS:HE1	1:D:908:HIS:HE1	1.41	0.68
1:A:128:GLU:N	1:A:128:GLU:HA	2.01	0.68
1:A:128:GLU:N	1:A:692:TYR:CG	2.61	0.68
1:C:340:ILE:HB	1:C:377:VAL:HG12	1.76	0.68
1:A:274:ARG:HA	1:A:336:LYS:HG2	1.76	0.68
1:B:79:ASP:HA	1:B:82:LYS:HG2	1.75	0.68
1:B:350:VAL:O	1:B:354:PHE:HB2	1.92	0.68
1:D:896:VAL:HG21	1:D:990:LEU:HD11	1.76	0.68
1:C:792:GLU:HG2	1:C:795:GLU:HB2	1.75	0.67
1:A:40:TRP:O	1:A:44:LEU:HB2	1.93	0.67
1:D:256:LEU:HA	1:D:259:LYS:HB2	1.77	0.67
1:A:713:ILE:O	1:A:740:ILE:HA	1.94	0.67
1:A:316:THR:O	1:A:320:ALA:HB2	1.94	0.67
1:A:279:VAL:HG13	1:A:341:GLY:H	1.59	0.67
1:C:847:GLU:OE2	1:B:1088:TRP:NE1	2.28	0.67
1:D:73:GLY:HA3	1:D:107:ILE:HA	1.77	0.67
1:D:201:GLU:O	1:D:217:LEU:HA	1.95	0.67
1:C:628:GLY:H	1:C:636:ILE:HB	1.59	0.67
1:A:976:ARG:HG3	1:A:977:VAL:HG23	1.77	0.67
1:D:181:LEU:O	1:D:184:PHE:HB3	1.95	0.67
1:B:572:PHE:CG	2:B:1201:COA:H133	2.30	0.67
1:D:1014:THR:HG22	2:B:1201:COA:H2A	1.75	0.66
1:A:128:GLU:N	1:A:692:TYR:CD2	2.64	0.66
1:D:32:ALA:O	1:D:106:LEU:HA	1.96	0.66
1:B:505:GLN:HE22	2:B:1201:COA:CEP	2.09	0.66
1:C:747:THR:HA	1:C:772:ALA:HB3	1.78	0.66
1:A:328:THR:N	1:A:369:LYS:H	1.94	0.66
1:B:620:ILE:HB	1:B:694:GLY:HA3	1.78	0.66
1:B:118:GLU:HB2	1:B:204:PRO:HB2	1.77	0.65
1:B:340:ILE:HB	1:B:377:VAL:HG22	1.78	0.65
1:A:908:HIS:HE1	1:B:908:HIS:HE1	1.43	0.65
1:A:289:SER:HA	1:A:292:ILE:HD12	1.78	0.65
1:A:715:VAL:O	1:A:742:CYS:HA	1.96	0.64
1:B:61:GLN:HE21	1:B:104:ASN:H	1.45	0.64
1:A:705:GLN:OE1	1:A:735:ARG:NH1	2.30	0.64
1:A:328:THR:HB	1:A:368:LEU:HB2	1.79	0.64
1:A:357:ILE:HA	1:A:360:ALA:HB3	1.78	0.64
1:B:739:PRO:HG2	1:B:804:LEU:HD11	1.77	0.64
1:B:34:VAL:O	1:B:105:PHE:HB2	1.97	0.64
1:A:644:ASP:O	1:A:648:ALA:HB3	1.97	0.64
1:D:620:ILE:HB	1:D:694:GLY:HA3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:ASN:O	1:A:676:ARG:HB2	1.98	0.64
1:D:129:GLY:HA2	1:D:156:VAL:HG13	1.80	0.64
1:A:92:GLU:HA	1:A:100:GLY:O	1.97	0.64
1:A:39:ASP:HB3	1:A:41:ALA:H	1.61	0.64
1:A:123:ILE:HG12	1:A:132:VAL:HG23	1.77	0.64
1:C:350:VAL:O	1:C:354:PHE:HB2	1.96	0.64
1:C:793:LEU:O	1:C:797:ILE:HB	1.98	0.64
1:B:505:GLN:CG	2:B:1201:COA:H132	2.27	0.64
1:A:670:LEU:O	1:A:674:ILE:HB	1.97	0.63
1:B:340:ILE:O	1:B:377:VAL:HA	1.99	0.63
1:A:44:LEU:HA	1:A:50:LEU:HD12	1.80	0.63
1:A:969:LEU:HD22	2:A:1201:COA:N9A	2.14	0.63
1:D:578:ALA:HB3	1:D:601:ILE:HD11	1.81	0.63
1:A:612:LYS:HG2	1:A:616:LYS:HG3	1.80	0.63
1:A:328:THR:CA	1:A:369:LYS:H	2.12	0.63
1:D:776:ASN:O	1:D:780:LYS:CB	2.47	0.63
1:A:723:GLU:H	1:A:775:LYS:HZ3	1.47	0.63
1:A:956:PRO:HA	1:A:959:PHE:HB3	1.81	0.63
1:A:327:MET:H	1:A:368:LEU:HD13	1.63	0.63
1:A:286:VAL:HG11	1:A:745:ILE:HG23	1.79	0.63
1:A:58:LYS:HB3	1:A:66:ARG:HD3	1.79	0.62
1:A:328:THR:H	1:A:368:LEU:CB	2.11	0.62
1:A:392:GLY:O	1:A:396:LYS:HB2	1.99	0.62
1:D:27:ASN:HA	1:D:30:LYS:HD2	1.81	0.62
1:B:802:GLU:O	1:B:806:ALA:HB2	1.99	0.62
1:B:92:GLU:OE1	1:B:99:THR:OG1	2.17	0.62
1:C:61:GLN:HE21	1:C:104:ASN:H	1.47	0.62
1:B:505:GLN:NE2	2:B:1201:COA:CDP	2.63	0.62
1:A:177:LYS:HE2	1:A:207:VAL:HG22	1.82	0.62
1:A:728:CYS:HA	1:A:731:ILE:HB	1.81	0.62
1:C:165:ILE:HG23	1:C:169:LEU:HD23	1.82	0.62
1:B:199:TYR:O	1:B:219:ALA:HA	1.98	0.62
1:A:346:ASN:HA	1:A:381:GLY:HA3	1.80	0.62
1:B:166:LYS:HA	1:B:170:LEU:HB2	1.81	0.62
1:A:93:ALA:O	1:A:99:THR:HA	1.98	0.61
1:D:1021:LEU:HD21	2:B:1201:COA:C8A	2.30	0.61
1:B:358:VAL:HG23	1:B:394:VAL:HG21	1.82	0.61
1:B:42:ARG:HA	1:B:45:GLN:HE21	1.65	0.61
1:B:505:GLN:HB3	1:B:508:ALA:HB3	1.82	0.61
1:A:640:GLY:O	1:A:645:ASN:ND2	2.33	0.61
1:B:355:LYS:HA	1:B:358:VAL:HG12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:986:ARG:HA	1:B:989:ILE:HG22	1.83	0.61
1:D:249:GLU:HB3	1:D:322:THR:HG23	1.82	0.61
1:B:497:THR:O	1:B:521:ARG:NH2	2.33	0.61
1:C:498:LYS:HD2	1:C:527:ALA:HB2	1.83	0.61
1:D:603:GLU:HA	1:D:606:THR:HG22	1.83	0.61
1:A:612:LYS:O	1:A:616:LYS:HB2	2.00	0.61
1:C:249:GLU:HG3	1:C:329:ARG:HH22	1.65	0.61
1:A:362:ARG:HG2	1:A:394:VAL:HG12	1.81	0.61
1:B:4:LYS:HG2	1:B:238:PHE:HB3	1.82	0.61
1:B:164:ASP:O	1:B:168:HIS:HB3	2.01	0.61
1:A:329:ARG:HG2	1:A:367:PRO:C	2.26	0.60
1:D:79:ASP:HA	1:D:82:LYS:HB3	1.83	0.60
1:B:797:ILE:O	1:B:801:TYR:CB	2.49	0.60
1:B:861:GLU:HA	1:B:864:LYS:HG2	1.82	0.60
1:D:497:THR:O	1:D:521:ARG:NH2	2.33	0.60
1:A:582:THR:HG22	1:A:586:MET:HE2	1.81	0.60
1:D:57:VAL:HG23	1:D:72:VAL:H	1.65	0.60
1:A:350:VAL:HG12	1:A:387:GLY:HA3	1.81	0.60
1:A:696:THR:OG1	1:A:697:PHE:N	2.35	0.60
1:D:1018:LYS:CD	2:B:1201:COA:O1A	2.44	0.60
1:C:625:THR:HG22	1:C:627:GLY:H	1.66	0.60
1:C:1051:TYR:OH	1:A:1078:ARG:NH1	2.35	0.60
1:A:118:GLU:HG3	1:A:205:LEU:HA	1.83	0.60
1:A:410:HIS:NE2	1:A:790:PHE:O	2.34	0.60
1:B:139:GLY:H	1:B:204:PRO:HB3	1.67	0.60
1:B:839:SER:OG	1:B:840:PHE:N	2.35	0.60
1:A:128:GLU:N	1:A:692:TYR:CE2	2.69	0.60
1:C:407:THR:OG1	1:C:676:ARG:NH2	2.35	0.60
1:D:847:GLU:OE2	1:A:1088:TRP:NE1	2.33	0.60
1:C:911:ILE:O	1:C:915:ARG:HB2	2.00	0.60
1:D:1088:TRP:NE1	1:A:847:GLU:OE2	2.35	0.60
1:A:817:PRO:HB2	1:B:389:ARG:HD3	1.84	0.59
1:A:991:LYS:HD2	1:A:1008:LEU:HD21	1.84	0.59
1:B:505:GLN:NE2	2:B:1201:COA:H132	2.17	0.59
1:C:60:ASP:HB2	1:C:106:LEU:HB2	1.84	0.59
1:D:1078:ARG:NH1	1:B:1051:TYR:OH	2.36	0.59
1:A:111:VAL:HG13	1:A:113:HIS:HD1	1.66	0.59
1:A:386:GLU:OE2	1:A:389:ARG:NH1	2.36	0.59
1:D:925:THR:HG21	1:B:929:LEU:HG	1.84	0.59
1:A:1018:LYS:HE3	2:A:1201:COA:O1A	1.95	0.59
1:D:582:THR:HG22	1:D:586:MET:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:850:GLN:HE22	1:B:982:ASN:HD21	1.50	0.59
1:B:697:PHE:O	1:B:701:VAL:N	2.34	0.59
1:B:204:PRO:HD2	1:B:215:LEU:HD22	1.85	0.58
1:B:274:ARG:HG3	1:B:275:ILE:HG13	1.85	0.58
1:C:208:THR:OG1	1:C:210:ASP:OD1	2.21	0.58
1:D:1040:CYS:SG	1:D:1041:GLY:N	2.73	0.58
1:D:1021:LEU:HD21	2:B:1201:COA:N9A	2.18	0.58
1:D:9:GLN:NE2	1:D:60:ASP:OD2	2.36	0.58
1:D:270:ASN:ND2	1:D:299:ASN:O	2.36	0.58
1:D:653:ARG:NH2	1:D:679:ASP:O	2.36	0.58
1:A:1044:THR:OG1	1:A:1045:ARG:N	2.37	0.58
1:C:929:LEU:HD13	1:A:925:THR:HG21	1.85	0.57
1:A:521:ARG:NH1	1:A:633:CYS:O	2.37	0.57
1:B:779:LEU:HB3	1:B:784:VAL:HB	1.85	0.57
1:C:64:LYS:HE3	1:C:95:VAL:HB	1.86	0.57
1:A:111:VAL:O	1:A:113:HIS:ND1	2.37	0.57
1:A:316:THR:O	1:A:320:ALA:CB	2.52	0.57
1:B:896:VAL:HG21	1:B:990:LEU:HD11	1.86	0.57
1:B:505:GLN:HE21	2:B:1201:COA:H132	1.69	0.57
1:B:653:ARG:NH2	1:B:679:ASP:O	2.37	0.57
1:D:58:LYS:H	1:D:73:GLY:HA2	1.70	0.57
1:D:140:VAL:HG22	1:D:204:PRO:HD3	1.87	0.57
1:D:867:MET:HB2	1:D:871:GLY:HA3	1.87	0.57
1:A:387:GLY:HA2	1:A:390:VAL:HG12	1.85	0.57
1:A:358:VAL:HG21	1:A:390:VAL:HG22	1.87	0.57
1:A:720:GLY:N	1:A:770:GLU:HG3	2.19	0.57
1:C:118:GLU:HB2	1:C:204:PRO:HB2	1.86	0.57
1:C:270:ASN:ND2	1:C:299:ASN:O	2.38	0.57
1:C:509:VAL:HG13	1:C:526:VAL:HG21	1.86	0.57
1:D:164:ASP:O	1:D:168:HIS:HB3	2.05	0.57
1:D:698:MET:HE3	1:D:726:LYS:HB2	1.87	0.57
1:B:674:ILE:HA	1:B:678:THR:HB	1.86	0.57
1:A:361:ILE:O	1:A:363:ASP:N	2.35	0.57
1:B:844:ILE:HD11	1:B:876:LEU:HD13	1.87	0.57
1:C:867:MET:HB3	1:C:871:GLY:HA3	1.86	0.57
1:A:412:THR:OG1	1:A:791:ASP:OD1	2.19	0.57
1:C:36:PRO:HG3	1:C:89:LEU:HD11	1.87	0.56
1:D:244:ARG:NH2	1:D:268:LEU:O	2.38	0.56
1:B:938:ALA:O	1:B:942:ALA:HB3	2.05	0.56
1:D:974:GLY:HA2	1:D:1021:LEU:HA	1.87	0.56
1:C:647:LEU:HD11	1:C:818:PRO:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:612:LYS:HE2	1:D:616:LYS:HE3	1.88	0.56
1:A:283:GLY:HA2	1:A:666:MET:HE2	1.86	0.56
1:B:499:ALA:HB2	1:B:568:VAL:HG13	1.88	0.56
1:B:505:GLN:NE2	2:B:1201:COA:H141	2.18	0.56
1:C:1035:ASP:O	1:C:1039:ASN:CB	2.53	0.56
1:A:531:TYR:HD2	1:A:534:THR:HG22	1.71	0.56
1:A:340:ILE:HB	1:A:377:VAL:HA	1.88	0.56
1:A:607:ARG:HG3	1:A:692:TYR:HE2	1.71	0.56
1:C:776:ASN:O	1:C:780:LYS:HB2	2.05	0.56
1:C:836:LYS:NZ	1:B:1090:ASP:OD1	2.33	0.56
1:B:129:GLY:HA2	1:B:156:VAL:HG13	1.87	0.56
1:A:82:LYS:HD3	1:A:85:LEU:HD12	1.86	0.56
1:A:275:ILE:HD11	1:A:419:LEU:HD21	1.87	0.56
1:A:521:ARG:HH12	1:A:634:PHE:HD1	1.54	0.56
1:A:723:GLU:H	1:A:775:LYS:NZ	2.04	0.56
1:A:787:PRO:HB3	1:A:796:ILE:HG21	1.88	0.56
1:A:924:LEU:HD13	1:A:1070:ILE:HG13	1.88	0.56
1:D:515:PHE:HZ	1:D:631:PRO:HA	1.70	0.56
1:C:199:TYR:HB3	1:C:220:LYS:HB2	1.88	0.56
1:A:118:GLU:CA	1:A:206:VAL:H	2.18	0.56
1:B:201:GLU:HB3	1:B:218:ALA:HB3	1.88	0.56
1:C:991:LYS:HE3	1:C:995:ARG:HH11	1.71	0.55
1:A:326:LEU:H	1:A:368:LEU:HD23	1.70	0.55
1:A:339:ILE:HG23	1:A:414:ILE:HD11	1.88	0.55
1:D:394:VAL:HA	1:D:397:THR:HG22	1.88	0.55
1:A:128:GLU:HA	1:A:692:TYR:CD2	2.41	0.55
1:A:193:GLU:OE2	1:A:607:ARG:NH2	2.38	0.55
1:A:369:LYS:O	1:A:371:HIS:N	2.39	0.55
1:A:530:VAL:HG12	1:A:556:MET:HG3	1.87	0.55
1:B:509:VAL:HG13	1:B:526:VAL:HG21	1.87	0.55
1:B:668:ASN:HA	1:B:671:ASN:HD22	1.72	0.55
1:C:879:GLN:OE1	1:A:1078:ARG:NH2	2.40	0.55
1:D:344:ILE:HD12	1:D:668:ASN:HB3	1.88	0.55
1:A:641:GLY:HA3	1:A:645:ASN:HD22	1.72	0.55
1:D:12:LYS:HA	1:D:15:LEU:HB3	1.89	0.55
1:D:708:PRO:O	1:D:711:LYS:NZ	2.31	0.55
1:A:327:MET:N	1:A:368:LEU:HB3	2.22	0.55
1:A:328:THR:N	1:A:369:LYS:N	2.53	0.55
1:A:571:ASN:HD22	1:A:596:ILE:HG23	1.71	0.55
1:A:650:LYS:O	1:A:653:ARG:NH1	2.39	0.55
1:A:792:GLU:O	1:A:796:ILE:N	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:970:ILE:N	2:A:1201:COA:C2A	2.69	0.55
1:D:9:GLN:HG3	1:D:106:LEU:HD12	1.88	0.55
1:D:1044:THR:OG1	1:D:1045:ARG:N	2.38	0.55
1:A:645:ASN:O	1:A:649:SER:OG	2.22	0.55
1:A:130:ASP:OD2	1:A:607:ARG:NH2	2.39	0.55
1:A:277:THR:HG22	1:A:339:ILE:HG13	1.88	0.55
1:C:123:ILE:HG12	1:C:132:VAL:HG22	1.89	0.55
1:A:1064:GLY:HA2	1:A:1067:MET:HE3	1.88	0.55
1:B:410:HIS:NE2	1:B:790:PHE:O	2.40	0.54
1:C:622:GLY:O	1:C:625:THR:OG1	2.18	0.54
1:D:63:ILE:HA	1:D:95:VAL:HG21	1.88	0.54
1:D:956:PRO:HB2	1:D:1013:ILE:HD12	1.88	0.54
1:D:1021:LEU:HD21	2:B:1201:COA:N7A	2.22	0.54
1:A:256:LEU:HD21	1:A:264:LEU:HD12	1.89	0.54
1:A:563:HIS:ND1	1:A:565:GLU:OE2	2.37	0.54
1:C:701:VAL:O	1:C:705:GLN:HB2	2.07	0.54
1:D:12:LYS:HG2	1:D:15:LEU:HD23	1.89	0.54
1:A:16:TYR:HB3	1:A:29:PHE:H	1.72	0.54
1:A:742:CYS:HB2	1:A:786:VAL:HG23	1.89	0.54
1:A:139:GLY:H	1:A:204:PRO:HB3	1.71	0.54
1:C:991:LYS:O	1:C:995:ARG:N	2.39	0.54
1:D:730:GLY:HA2	1:D:735:ARG:H	1.73	0.54
1:A:351:ALA:O	1:A:355:LYS:CB	2.54	0.54
1:A:414:ILE:HG22	1:A:417:MET:HE3	1.89	0.54
1:A:692:TYR:CD2	1:A:692:TYR:CE2	2.96	0.54
1:B:163:GLU:HA	1:B:166:LYS:HG2	1.89	0.54
1:A:329:ARG:N	1:A:369:LYS:N	2.56	0.54
1:C:695:SER:HG	1:C:700:HIS:HE2	1.54	0.54
1:A:59:PRO:HG2	1:A:63:ILE:HB	1.88	0.54
1:C:635:LYS:NZ	1:C:639:THR:O	2.40	0.54
1:D:9:GLN:HG2	1:D:33:ARG:HB2	1.88	0.54
1:B:290:ASP:OD1	1:B:747:THR:N	2.40	0.54
1:B:628:GLY:H	1:B:636:ILE:HB	1.73	0.54
1:A:702:LEU:HD12	1:A:735:ARG:HH21	1.73	0.53
1:A:911:ILE:O	1:A:915:ARG:HB2	2.07	0.53
1:B:603:GLU:HA	1:B:606:THR:HG22	1.89	0.53
1:A:328:THR:HG22	1:A:368:LEU:H	1.72	0.53
1:D:27:ASN:ND2	1:D:109:PRO:O	2.42	0.53
1:A:322:THR:O	1:A:325:SER:N	2.36	0.53
1:B:1044:THR:OG1	1:B:1045:ARG:N	2.37	0.53
1:D:44:LEU:HA	1:D:50:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:TYR:HD1	1:A:415:VAL:HG22	1.74	0.53
1:A:635:LYS:NZ	1:A:637:GLY:O	2.35	0.53
1:A:530:VAL:HG11	1:A:560:MET:HE2	1.91	0.53
1:A:661:SER:HA	1:A:716:LEU:HB2	1.91	0.53
1:A:718:GLU:HG3	1:A:719:ILE:H	1.73	0.53
1:B:505:GLN:HE21	2:B:1201:COA:CDP	2.21	0.53
1:C:708:PRO:O	1:C:711:LYS:NZ	2.38	0.53
1:A:505:GLN:O	1:A:509:VAL:N	2.35	0.53
1:C:79:ASP:HA	1:C:82:LYS:HG2	1.91	0.53
1:A:56:VAL:HB	1:A:110:PHE:HB2	1.91	0.53
1:A:200:LEU:HA	1:A:218:ALA:O	2.08	0.53
1:A:513:LEU:HD22	1:A:524:PRO:HB3	1.91	0.53
1:B:199:TYR:HB3	1:B:220:LYS:HB2	1.90	0.53
1:C:268:LEU:HD23	1:C:303:ASN:HB3	1.89	0.53
1:A:1057:LEU:HD13	1:A:1060:ILE:HD12	1.91	0.53
1:D:350:VAL:O	1:D:354:PHE:HB2	2.09	0.53
1:D:492:LEU:HG	1:D:703:ARG:HD2	1.91	0.53
1:C:1088:TRP:HA	1:C:1091:ILE:HD12	1.91	0.52
1:B:1010:VAL:O	1:B:1014:THR:OG1	2.23	0.52
1:B:407:THR:OG1	1:B:676:ARG:NH2	2.42	0.52
1:B:708:PRO:O	1:B:711:LYS:NZ	2.38	0.52
1:A:534:THR:OG1	1:A:535:GLY:N	2.39	0.52
1:A:731:ILE:HG12	1:A:784:VAL:HB	1.90	0.52
1:D:33:ARG:HA	1:D:105:PHE:O	2.10	0.52
1:D:35:THR:H	1:D:38:THR:HG22	1.74	0.52
1:D:58:LYS:HE3	1:D:106:LEU:HD22	1.91	0.52
1:A:57:VAL:HG22	1:A:105:PHE:HD2	1.74	0.52
1:A:292:ILE:HD13	1:A:301:LEU:HD13	1.90	0.52
1:A:342:GLY:O	1:A:378:ARG:NH1	2.42	0.52
1:D:42:ARG:O	1:D:45:GLN:NE2	2.39	0.52
1:A:181:LEU:HD23	1:A:212:VAL:HG12	1.91	0.52
1:A:262:ALA:HA	1:A:309:GLY:HA3	1.91	0.52
1:A:969:LEU:HD22	2:A:1201:COA:C8A	2.40	0.52
1:D:824:ASP:HB3	1:D:827:TRP:HB3	1.91	0.52
1:B:27:ASN:HA	1:B:30:LYS:HD2	1.92	0.52
1:D:95:VAL:HG12	1:D:242:PHE:HD2	1.75	0.52
1:D:727:ILE:HA	1:D:736:LEU:HD12	1.90	0.52
1:D:1078:ARG:NH2	1:B:879:GLN:OE1	2.43	0.52
1:C:58:LYS:O	1:C:106:LEU:HB3	2.09	0.52
1:D:673:ILE:O	1:D:677:THR:OG1	2.25	0.52
1:A:488:LYS:NZ	1:A:616:LYS:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:987:VAL:HG13	1:B:1028:LEU:HD13	1.91	0.52
1:A:191:PHE:CD2	1:A:200:LEU:HD21	2.45	0.52
1:B:57:VAL:HG22	1:B:107:ILE:HG12	1.92	0.52
1:B:77:THR:O	1:B:81:VAL:N	2.41	0.52
1:C:58:LYS:HB2	1:C:66:ARG:HD2	1.90	0.51
1:D:921:VAL:O	1:D:925:THR:OG1	2.22	0.51
1:A:557:ALA:O	1:A:561:ARG:HB2	2.11	0.51
1:A:631:PRO:HB2	1:A:651:LEU:HD22	1.92	0.51
1:A:860:THR:O	1:A:864:LYS:CB	2.57	0.51
1:B:725:TYR:O	1:B:729:ARG:HB2	2.10	0.51
1:C:924:LEU:HD22	1:C:1070:ILE:HD11	1.92	0.51
1:A:120:TYR:HA	1:A:205:LEU:HB3	1.91	0.51
1:A:350:VAL:O	1:A:354:PHE:CB	2.46	0.51
1:A:731:ILE:HG22	1:A:782:ALA:HB3	1.92	0.51
1:B:956:PRO:HB3	1:B:1010:VAL:HG22	1.91	0.51
1:C:653:ARG:NH2	1:C:679:ASP:O	2.43	0.51
1:B:163:GLU:O	1:B:167:LYS:HB3	2.10	0.51
1:C:278:MET:HG3	1:C:319:TYR:HE2	1.75	0.51
1:D:223:ALA:HA	1:D:233:TRP:HH2	1.74	0.51
1:D:327:MET:HE1	1:D:338:LEU:HB2	1.93	0.51
1:A:276:TRP:HA	1:A:302:ALA:HB3	1.92	0.51
1:A:775:LYS:HG2	1:A:778:ALA:HB3	1.93	0.51
1:B:725:TYR:OH	1:B:769:SER:O	2.22	0.51
1:B:873:LEU:O	1:B:877:TRP:HB2	2.10	0.51
1:C:650:LYS:O	1:C:653:ARG:NH1	2.43	0.51
1:A:94:THR:HA	1:A:98:ALA:O	2.11	0.51
1:B:9:GLN:O	1:B:13:GLU:CB	2.55	0.51
1:D:714:VAL:HA	1:D:741:VAL:O	2.11	0.51
1:B:383:ASN:HD21	1:B:831:LEU:HB3	1.75	0.51
1:D:1014:THR:HG22	2:B:1201:COA:C2A	2.41	0.51
1:B:32:ALA:HB3	1:B:107:ILE:HB	1.93	0.51
1:B:974:GLY:HA2	1:B:1021:LEU:HA	1.91	0.51
1:A:139:GLY:N	1:A:204:PRO:HB3	2.26	0.51
1:B:12:LYS:HA	1:B:15:LEU:HB3	1.92	0.51
1:B:568:VAL:HG23	1:B:593:THR:HG23	1.92	0.51
1:B:582:THR:HG22	1:B:586:MET:HE2	1.91	0.51
1:C:902:PRO:HG3	1:A:842:THR:HG21	1.92	0.51
1:A:285:SER:O	1:A:289:SER:OG	2.24	0.51
1:C:1023:LEU:HD11	1:C:1028:LEU:HD12	1.93	0.51
1:D:61:GLN:HE22	1:D:102:LEU:HA	1.76	0.51
1:B:152:LEU:HB2	1:B:169:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:ILE:HD13	1:C:301:LEU:HD13	1.93	0.50
1:C:850:GLN:HE22	1:A:982:ASN:HD21	1.58	0.50
1:A:118:GLU:C	1:A:206:VAL:H	2.19	0.50
1:A:135:HIS:CE1	1:A:137:GLU:HB3	2.46	0.50
1:A:292:ILE:HG21	1:A:301:LEU:HD13	1.93	0.50
1:A:396:LYS:NZ	1:A:402:ILE:H	2.08	0.50
1:B:175:GLU:HA	1:B:178:LYS:HD3	1.93	0.50
1:B:521:ARG:HH12	1:B:634:PHE:HD1	1.59	0.50
1:C:536:ASP:HA	1:C:552:VAL:O	2.11	0.50
1:A:57:VAL:HG23	1:A:107:ILE:HB	1.92	0.50
1:A:264:LEU:HD22	1:A:307:TYR:HB2	1.92	0.50
1:A:538:LYS:HA	1:A:551:PRO:HA	1.92	0.50
1:C:797:ILE:O	1:C:801:TYR:HB2	2.10	0.50
1:D:175:GLU:HA	1:D:178:LYS:HD3	1.93	0.50
1:D:513:LEU:HD22	1:D:524:PRO:HB3	1.93	0.50
1:D:521:ARG:NH1	1:D:633:CYS:O	2.44	0.50
1:D:1035:ASP:O	1:D:1039:ASN:CB	2.59	0.50
1:C:1044:THR:OG1	1:C:1045:ARG:N	2.41	0.50
1:A:288:TYR:CE1	1:A:414:ILE:HG12	2.47	0.50
1:A:500:ILE:HD12	1:A:569:LEU:HB2	1.94	0.50
1:A:1035:ASP:O	1:A:1039:ASN:CB	2.59	0.50
1:B:135:HIS:CE1	1:B:137:GLU:HB2	2.46	0.50
1:B:924:LEU:HD13	1:B:1070:ILE:HG13	1.93	0.50
1:B:1057:LEU:HD13	1:B:1060:ILE:HD12	1.93	0.50
1:C:129:GLY:HA2	1:C:156:VAL:HG13	1.93	0.50
1:C:1088:TRP:NE1	1:B:847:GLU:OE2	2.30	0.50
1:D:924:LEU:HD22	1:D:1070:ILE:HD11	1.91	0.50
1:B:898:ALA:O	1:B:1065:ARG:NE	2.45	0.50
1:A:119:PHE:HA	1:A:205:LEU:C	2.36	0.50
1:A:860:THR:O	1:A:864:LYS:HB2	2.12	0.50
1:D:244:ARG:NH2	1:D:267:THR:OG1	2.44	0.50
1:A:336:LYS:HB3	1:A:373:VAL:HG13	1.93	0.50
1:A:382:PRO:HG3	1:A:642:MET:N	2.26	0.50
1:A:1075:ASP:OD1	1:A:1078:ARG:NH2	2.45	0.50
1:B:671:ASN:O	1:B:675:SER:HB3	2.12	0.50
1:C:664:GLY:O	1:C:667:SER:OG	2.29	0.50
1:D:340:ILE:O	1:D:377:VAL:HA	2.11	0.50
1:A:488:LYS:HE3	1:A:617:GLY:HA3	1.94	0.50
1:D:55:LEU:HB3	1:D:73:GLY:O	2.12	0.49
1:D:58:LYS:CB	1:D:72:VAL:HA	2.40	0.49
1:D:1021:LEU:CD2	2:B:1201:COA:N9A	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:VAL:HG11	1:A:505:GLN:HE21	1.77	0.49
1:A:834:ILE:HD11	1:B:825:TYR:HA	1.94	0.49
1:B:324:LEU:O	1:B:328:THR:OG1	2.25	0.49
1:B:924:LEU:HD22	1:B:1070:ILE:HD11	1.94	0.49
1:B:984:ASP:HB3	1:B:987:VAL:HB	1.94	0.49
1:D:1033:PHE:HB3	1:D:1057:LEU:HD21	1.93	0.49
1:B:776:ASN:O	1:B:780:LYS:HB2	2.12	0.49
1:D:991:LYS:HD2	1:D:1008:LEU:HD21	1.93	0.49
1:A:277:THR:N	1:A:303:ASN:OD1	2.44	0.49
1:B:802:GLU:O	1:B:806:ALA:CB	2.60	0.49
1:C:338:LEU:HB3	1:C:375:ILE:HG12	1.93	0.49
1:C:657:VAL:HG21	1:C:678:THR:HG21	1.93	0.49
1:A:181:LEU:O	1:A:185:ILE:N	2.40	0.49
1:A:183:SER:O	1:A:186:SER:OG	2.27	0.49
1:A:844:ILE:HD11	1:A:876:LEU:HD13	1.95	0.49
1:C:803:ASP:HA	1:C:806:ALA:HB3	1.92	0.49
1:A:328:THR:HG22	1:A:368:LEU:N	2.26	0.49
1:B:572:PHE:CD1	2:B:1201:COA:H131	2.47	0.49
1:C:1029:ILE:O	1:C:1033:PHE:HB2	2.12	0.49
1:D:498:LYS:HD2	1:D:527:ALA:HB2	1.94	0.49
1:C:843:SER:N	1:A:1075:ASP:OD2	2.46	0.49
1:D:529:MET:HB2	1:D:552:VAL:HG22	1.94	0.49
1:A:492:LEU:HD13	1:A:621:ILE:HD11	1.94	0.49
1:A:924:LEU:HD22	1:A:1070:ILE:HD11	1.94	0.49
1:B:181:LEU:O	1:B:184:PHE:HB3	2.12	0.49
1:A:366:GLY:HA3	1:A:367:PRO:HD3	1.61	0.49
1:A:834:ILE:O	1:B:823:MET:N	2.45	0.49
1:B:391:MET:HA	1:B:394:VAL:HG12	1.95	0.49
1:B:505:GLN:HE22	2:B:1201:COA:H143	1.64	0.49
1:B:659:TYR:HA	1:B:714:VAL:O	2.13	0.49
1:C:838:ALA:H	1:D:540:LYS:HZ3	1.59	0.49
1:C:1004:LEU:N	1:C:1035:ASP:OD2	2.44	0.49
1:D:188:LEU:HA	1:D:191:PHE:HB3	1.95	0.49
1:D:1068:GLY:HA2	1:B:876:LEU:HD12	1.94	0.49
1:A:585:THR:HA	1:A:588:TYR:HD2	1.78	0.48
1:B:701:VAL:O	1:B:705:GLN:HB3	2.13	0.48
1:B:899:ASP:HB2	1:B:1068:GLY:HA3	1.94	0.48
1:D:519:CYS:HB2	1:D:632:GLY:HA2	1.95	0.48
1:A:123:ILE:HG23	1:A:132:VAL:HA	1.95	0.48
1:B:257:ASP:HB2	1:B:264:LEU:HB2	1.95	0.48
1:B:747:THR:OG1	1:B:748:CYS:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:GLY:HA2	1:A:636:ILE:HB	1.95	0.48
1:A:969:LEU:HD13	2:A:1201:COA:N7A	2.28	0.48
1:B:504:MET:HE2	1:B:531:TYR:CZ	2.48	0.48
1:D:355:LYS:HA	1:D:358:VAL:HG12	1.95	0.48
1:D:852:LEU:HD21	1:B:900:HIS:HD2	1.78	0.48
1:A:583:MET:O	1:A:587:ASN:ND2	2.47	0.48
1:B:939:LEU:HD12	1:B:1057:LEU:HD12	1.95	0.48
1:D:792:GLU:HA	1:D:795:GLU:HG3	1.94	0.48
1:D:948:LYS:O	1:D:952:SER:OG	2.31	0.48
1:A:328:THR:N	1:A:368:LEU:HB3	2.27	0.48
1:A:497:THR:O	1:A:521:ARG:NH2	2.47	0.48
1:A:644:ASP:O	1:A:648:ALA:CB	2.61	0.48
1:A:675:SER:HA	1:A:680:GLY:HA2	1.95	0.48
1:B:365:GLN:HA	1:B:400:ILE:HD11	1.93	0.48
1:A:65:ARG:NH1	1:A:141:ASP:OD1	2.46	0.48
1:C:188:LEU:O	1:C:192:TYR:N	2.47	0.48
1:C:327:MET:HE1	1:C:338:LEU:HB2	1.96	0.48
1:C:842:THR:HG21	1:A:902:PRO:HG3	1.94	0.48
1:C:873:LEU:O	1:C:877:TRP:HB2	2.14	0.48
1:D:274:ARG:HG3	1:D:275:ILE:HG13	1.96	0.48
1:A:118:GLU:HA	1:A:213:TYR:CA	2.43	0.48
1:B:21:THR:HG21	1:B:184:PHE:HA	1.96	0.48
1:D:312:SER:H	1:D:315:GLN:HB2	1.79	0.48
1:A:55:LEU:HB3	1:A:107:ILE:HD11	1.96	0.48
1:A:265:LYS:HB2	1:A:306:GLU:O	2.13	0.48
1:A:275:ILE:HG23	1:A:337:ILE:HD12	1.96	0.48
1:A:645:ASN:HA	1:A:676:ARG:HH22	1.79	0.48
1:B:869:ILE:HA	1:B:872:VAL:HG22	1.95	0.48
1:C:588:TYR:HB2	1:C:591:ILE:HD12	1.96	0.47
1:C:40:TRP:O	1:C:44:LEU:HB2	2.14	0.47
1:C:567:ASP:OD1	1:C:567:ASP:N	2.47	0.47
1:D:135:HIS:CD2	1:D:149:ALA:HA	2.50	0.47
1:D:494:SER:N	1:D:497:THR:OG1	2.44	0.47
1:D:505:GLN:HG3	1:D:572:PHE:CG	2.50	0.47
1:A:8:GLU:O	1:A:12:LYS:HB2	2.14	0.47
1:A:355:LYS:O	1:A:359:ARG:HB2	2.13	0.47
1:A:657:VAL:HG22	1:A:712:MET:HG3	1.95	0.47
1:C:4:LYS:NZ	1:C:5:ALA:O	2.46	0.47
1:C:336:LYS:O	1:C:373:VAL:HA	2.15	0.47
1:D:311:PRO:HG2	1:D:316:THR:HB	1.97	0.47
1:B:649:SER:O	1:B:649:SER:OG	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:796:ILE:HA	1:B:799:SER:HB3	1.96	0.47
1:A:127:ARG:O	1:A:692:TYR:CE2	2.67	0.47
1:B:63:ILE:HG21	1:B:71:LEU:HD12	1.94	0.47
1:C:375:ILE:HB	1:C:402:ILE:HG12	1.96	0.47
1:A:275:ILE:HG12	1:A:337:ILE:HD12	1.96	0.47
1:A:969:LEU:HD22	2:A:1201:COA:N7A	2.26	0.47
1:B:188:LEU:HA	1:B:191:PHE:HB3	1.95	0.47
1:D:204:PRO:HD2	1:D:215:LEU:HD22	1.96	0.47
1:C:938:ALA:O	1:C:942:ALA:HB3	2.14	0.47
1:D:229:CYS:O	1:D:233:TRP:N	2.46	0.47
1:D:625:THR:OG1	1:D:686:ALA:O	2.29	0.47
1:D:899:ASP:HB2	1:D:1068:GLY:HA3	1.95	0.47
1:B:85:LEU:HB3	1:B:89:LEU:HB2	1.96	0.47
1:B:572:PHE:O	2:B:1201:COA:CCP	2.63	0.47
1:B:956:PRO:HB2	1:B:1013:ILE:HD12	1.95	0.47
1:D:747:THR:OG1	1:D:748:CYS:N	2.48	0.47
1:A:328:THR:C	1:A:369:LYS:N	2.71	0.47
1:A:358:VAL:HG23	1:A:391:MET:HA	1.96	0.47
1:A:724:GLU:H	1:A:775:LYS:HZ3	1.61	0.47
1:B:256:LEU:HA	1:B:259:LYS:HE2	1.97	0.47
1:C:57:VAL:HG12	1:C:107:ILE:HG12	1.96	0.47
1:C:290:ASP:OD1	1:C:747:THR:N	2.48	0.47
1:D:73:GLY:CA	1:D:73:GLY:H	2.06	0.47
1:D:389:ARG:O	1:D:393:GLU:HB2	2.15	0.47
1:D:493:PHE:HB2	1:D:630:LYS:HD3	1.96	0.47
1:A:21:THR:OG1	1:A:22:THR:N	2.48	0.47
1:C:355:LYS:HA	1:C:358:VAL:HG22	1.97	0.47
1:C:1020:ASN:O	1:C:1022:ILE:N	2.48	0.47
1:A:538:LYS:HD2	1:A:549:LEU:HB3	1.96	0.47
1:C:156:VAL:HG23	1:C:611:LYS:HD2	1.96	0.46
1:D:579:TYR:CG	1:D:605:LEU:HD23	2.50	0.46
1:B:225:ALA:HA	1:B:602:PRO:HG3	1.96	0.46
1:B:731:ILE:HD11	1:B:740:ILE:HG13	1.97	0.46
1:D:1029:ILE:O	1:D:1033:PHE:HB2	2.15	0.46
1:A:127:ARG:C	1:A:692:TYR:CZ	2.93	0.46
1:A:578:ALA:O	1:A:582:THR:CB	2.62	0.46
1:A:911:ILE:HG23	1:A:1076:GLN:HG3	1.96	0.46
1:C:612:LYS:HE2	1:C:616:LYS:HE3	1.97	0.46
1:A:502:TRP:HB3	1:A:571:ASN:HA	1.97	0.46
1:B:597:ILE:HG22	2:B:1201:COA:H61	1.97	0.46
1:C:592:ARG:NH2	1:C:617:GLY:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:LYS:HB2	1:B:373:VAL:HG12	1.96	0.46
1:B:602:PRO:HB2	1:B:605:LEU:HD23	1.97	0.46
1:C:7:SER:HA	1:C:62:LEU:HD21	1.98	0.46
1:C:560:MET:HE3	1:C:591:ILE:HD11	1.98	0.46
1:C:701:VAL:O	1:C:705:GLN:CB	2.63	0.46
1:A:724:GLU:HG2	1:A:779:LEU:HD11	1.98	0.46
1:C:643:LEU:O	1:C:647:LEU:HB2	2.15	0.46
1:D:984:ASP:HB3	1:D:987:VAL:HB	1.97	0.46
1:A:292:ILE:HG22	1:A:297:GLY:HA3	1.97	0.46
1:A:382:PRO:HD3	1:A:641:GLY:HA2	1.98	0.46
1:B:167:LYS:HB3	1:B:167:LYS:HE2	1.66	0.46
1:D:54:ASN:O	1:D:110:PHE:N	2.40	0.46
1:D:99:THR:OG1	1:D:100:GLY:N	2.49	0.46
1:D:146:ASP:O	1:D:151:LYS:NZ	2.48	0.46
1:A:328:THR:HG22	1:A:368:LEU:HB2	1.96	0.46
1:C:775:LYS:O	1:C:779:LEU:HB2	2.15	0.46
1:D:40:TRP:HZ3	1:D:78:LEU:HD13	1.81	0.46
1:D:170:LEU:HD11	1:D:182:ALA:HB2	1.96	0.46
1:A:331:LYS:NZ	1:A:333:PRO:HA	2.31	0.46
1:C:928:LEU:HD22	1:C:1062:VAL:HG13	1.98	0.46
1:D:583:MET:HE2	1:D:609:LEU:HD23	1.98	0.46
1:A:660:VAL:HG22	1:A:685:VAL:HB	1.98	0.46
1:A:703:ARG:NH2	1:A:704:TYR:OH	2.48	0.46
1:B:712:MET:HE3	1:B:741:VAL:HG21	1.97	0.46
1:A:127:ARG:C	1:A:692:TYR:CD2	2.94	0.46
1:A:663:SER:HB3	1:A:666:MET:HG2	1.98	0.46
1:B:3:ALA:HB1	1:B:220:LYS:HB3	1.98	0.46
1:B:1035:ASP:O	1:B:1039:ASN:CB	2.64	0.46
1:D:15:LEU:HD12	1:D:19:ILE:HD13	1.98	0.45
1:D:188:LEU:O	1:D:192:TYR:N	2.49	0.45
1:B:1067:MET:HB3	1:B:1067:MET:HE2	1.69	0.45
1:D:635:LYS:NZ	1:D:639:THR:O	2.43	0.45
1:A:208:THR:HB	1:A:209:LYS:H	1.40	0.45
1:B:316:THR:HG23	1:B:356:GLY:HA3	1.99	0.45
1:B:696:THR:H	1:B:699:ASP:HB2	1.81	0.45
1:C:66:ARG:O	1:C:72:VAL:N	2.48	0.45
1:C:495:ARG:O	1:C:521:ARG:NE	2.49	0.45
1:D:8:GLU:CD	1:D:66:ARG:HH12	2.24	0.45
1:D:108:GLU:HA	1:D:109:PRO:HD3	1.84	0.45
1:D:1017:LYS:HB3	2:B:1201:COA:C4B	2.40	0.45
1:A:328:THR:C	1:A:370:GLU:H	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:LEU:HD22	1:A:1062:VAL:HG13	1.99	0.45
1:B:292:ILE:HG21	1:B:301:LEU:HD13	1.98	0.45
1:B:368:LEU:HD12	1:B:373:VAL:HG11	1.98	0.45
1:B:375:ILE:HB	1:B:402:ILE:HA	1.98	0.45
1:B:594:ILE:HD11	1:B:620:ILE:HG12	1.96	0.45
1:C:391:MET:HA	1:C:394:VAL:HG12	1.98	0.45
1:A:288:TYR:HE1	1:A:414:ILE:H	1.65	0.45
1:A:32:ALA:HB3	1:A:107:ILE:O	2.17	0.45
1:B:288:TYR:OH	1:B:411:MET:O	2.33	0.45
1:B:670:LEU:HB3	1:B:674:ILE:HD12	1.98	0.45
1:C:369:LYS:HE3	1:C:400:ILE:HG13	1.97	0.45
1:C:414:ILE:O	1:C:418:ALA:HB2	2.17	0.45
1:D:670:LEU:HD11	1:D:716:LEU:HD13	1.99	0.45
1:A:117:GLU:O	1:A:213:TYR:HB2	2.16	0.45
1:A:331:LYS:HG2	1:A:371:HIS:HB3	1.98	0.45
1:D:415:VAL:HA	1:D:418:ALA:HB3	1.98	0.45
1:B:255:ASP:O	1:B:259:LYS:HB2	2.17	0.45
1:C:488:LYS:NZ	1:C:618:VAL:O	2.50	0.45
1:D:250:GLU:O	1:D:254:ALA:CB	2.64	0.45
1:D:839:SER:HB3	1:B:915:ARG:HH12	1.82	0.45
1:A:500:ILE:HG12	1:A:566:VAL:HG13	1.98	0.45
1:A:647:LEU:HD13	1:A:818:PRO:HG3	1.98	0.45
1:A:956:PRO:HB3	1:A:1010:VAL:HG22	1.97	0.45
1:B:187:GLY:O	1:B:191:PHE:N	2.46	0.45
1:B:985:MET:HA	1:B:988:GLN:HB2	1.98	0.45
1:B:991:LYS:O	1:B:995:ARG:N	2.49	0.45
1:C:61:GLN:NE2	1:C:104:ASN:H	2.12	0.45
1:A:494:SER:N	1:A:497:THR:OG1	2.50	0.45
1:A:510:GLN:O	1:A:514:ASP:CB	2.65	0.45
1:A:630:LYS:HG2	1:A:633:CYS:HB2	1.99	0.45
1:A:1018:LYS:NZ	2:A:1201:COA:P1A	2.80	0.45
1:B:2:SER:O	1:B:2:SER:OG	2.30	0.45
1:C:320:ALA:HA	1:C:323:ILE:HG22	1.99	0.45
1:C:388:LEU:HD22	1:C:404:VAL:HB	1.99	0.45
1:C:707:THR:O	1:C:738:LYS:NZ	2.50	0.45
1:C:915:ARG:HH12	1:A:839:SER:HB3	1.80	0.45
1:A:58:LYS:HB3	1:A:66:ARG:HH11	1.82	0.45
1:A:323:ILE:HG23	1:A:360:ALA:HB1	1.98	0.45
1:B:561:ARG:HD2	1:B:561:ARG:HA	1.79	0.45
1:C:1054:ILE:HD12	1:A:1077:LYS:HB3	1.99	0.44
1:A:57:VAL:HG22	1:A:105:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LYS:HZ2	1:A:209:LYS:C	2.25	0.44
1:B:918:LYS:HE3	1:B:918:LYS:HB3	1.82	0.44
1:C:359:ARG:HE	1:C:359:ARG:HB3	1.62	0.44
1:D:200:LEU:HA	1:D:218:ALA:O	2.18	0.44
1:A:10:THR:HG22	1:A:236:ILE:HD12	1.98	0.44
1:A:118:GLU:HA	1:A:213:TYR:HB2	1.99	0.44
1:A:177:LYS:NZ	1:A:211:GLY:H	2.15	0.44
1:A:969:LEU:HD13	2:A:1201:COA:C5A	2.47	0.44
1:B:492:LEU:HG	1:B:703:ARG:HD2	1.99	0.44
1:C:561:ARG:CZ	1:C:562:LYS:HZ1	2.30	0.44
1:C:705:GLN:NE2	1:C:737:THR:H	2.15	0.44
1:D:540:LYS:NZ	1:D:547:GLU:OE2	2.38	0.44
1:A:283:GLY:HA3	1:A:666:MET:HB3	1.98	0.44
1:A:775:LYS:HA	1:A:778:ALA:HB3	1.99	0.44
1:A:823:MET:H	1:A:823:MET:HG2	1.62	0.44
1:C:825:TYR:HA	1:D:834:ILE:HD11	1.98	0.44
1:C:841:MET:HE2	1:A:1079:LEU:HB3	2.00	0.44
1:A:736:LEU:HD22	1:A:740:ILE:HD11	1.99	0.44
1:B:572:PHE:CG	2:B:1201:COA:CDP	2.98	0.44
1:B:697:PHE:HB2	1:B:723:GLU:HG3	1.98	0.44
1:A:80:GLY:O	1:A:84:TRP:HB2	2.17	0.44
1:A:120:TYR:CB	1:A:135:HIS:O	2.50	0.44
1:B:505:GLN:HG3	2:B:1201:COA:H132	1.98	0.44
1:D:929:LEU:HD22	1:B:925:THR:HG21	1.98	0.44
1:C:796:ILE:HG12	1:C:800:VAL:HG23	1.99	0.44
1:D:9:GLN:O	1:D:13:GLU:CB	2.63	0.44
1:D:268:LEU:HD23	1:D:303:ASN:HB3	1.99	0.44
1:A:106:LEU:HD23	1:A:108:GLU:HB2	1.99	0.44
1:A:324:LEU:HD22	1:A:368:LEU:CD1	2.48	0.44
1:A:834:ILE:HG23	1:A:835:ARG:H	1.83	0.44
1:B:574:SER:HB3	2:B:1201:COA:O9A	2.17	0.44
1:B:983:PRO:HB2	1:B:988:GLN:HG3	2.00	0.44
1:B:1029:ILE:O	1:B:1033:PHE:HB2	2.16	0.44
1:C:133:LEU:HB3	1:C:151:LYS:HD3	1.99	0.44
1:D:57:VAL:HG22	1:D:74:VAL:HG13	2.00	0.44
1:A:345:ALA:HB3	1:A:384:TYR:HB3	1.99	0.44
1:B:506:THR:O	1:B:510:GLN:HB2	2.18	0.44
1:C:12:LYS:NZ	1:C:31:TYR:HB3	2.33	0.44
1:A:340:ILE:O	1:A:377:VAL:HA	2.17	0.44
1:B:225:ALA:HB2	1:B:602:PRO:HB3	1.99	0.44
1:B:233:TRP:HB3	1:B:236:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:ARG:HB2	1:B:414:ILE:HD13	2.00	0.44
1:D:359:ARG:HE	1:D:359:ARG:HB3	1.53	0.43
1:A:191:PHE:HD2	1:A:200:LEU:HD21	1.82	0.43
1:A:229:CYS:O	1:A:233:TRP:N	2.49	0.43
1:A:376:PHE:HD2	1:A:405:PHE:HE2	1.66	0.43
1:B:122:CYS:HA	1:B:200:LEU:O	2.18	0.43
1:C:646:ILE:HG23	1:C:651:LEU:HB2	2.00	0.43
1:C:920:LEU:HD11	1:C:1070:ILE:HG23	1.99	0.43
1:D:55:LEU:C	1:D:75:ASN:H	2.25	0.43
1:D:863:PHE:CE1	1:B:892:MET:HG3	2.54	0.43
1:D:987:VAL:O	1:D:991:LYS:HB2	2.18	0.43
1:B:823:MET:HE2	1:B:828:ALA:HB2	2.00	0.43
1:B:1040:CYS:SG	1:B:1041:GLY:N	2.91	0.43
1:D:928:LEU:HD21	1:D:1066:SER:HB3	2.00	0.43
1:C:35:THR:HG22	1:C:104:ASN:HD22	1.83	0.43
1:C:992:ASP:HA	1:C:995:ARG:HB2	2.00	0.43
1:D:515:PHE:HA	1:D:518:VAL:HG12	2.01	0.43
1:A:824:ASP:HB2	1:A:827:TRP:H	1.83	0.43
1:B:894:LEU:HA	1:B:897:THR:HG22	1.99	0.43
1:B:1026:ASP:OD1	1:B:1026:ASP:N	2.52	0.43
1:C:35:THR:H	1:C:38:THR:HG22	1.84	0.43
1:C:317:TYR:HA	1:C:360:ALA:HB2	2.00	0.43
1:D:73:GLY:HA3	1:D:108:GLU:H	1.83	0.43
1:D:488:LYS:NZ	1:D:618:VAL:O	2.51	0.43
1:A:571:ASN:HB3	1:A:596:ILE:HA	2.01	0.43
1:A:857:MET:HE3	1:A:857:MET:HB2	1.86	0.43
1:B:63:ILE:HD12	1:B:95:VAL:HG21	2.00	0.43
1:B:711:LYS:HA	1:B:711:LYS:HD3	1.87	0.43
1:D:206:VAL:O	1:D:213:TYR:HB2	2.18	0.43
1:D:324:LEU:O	1:D:328:THR:OG1	2.35	0.43
1:B:157:ASP:HB2	1:B:611:LYS:NZ	2.34	0.43
1:D:668:ASN:HA	1:D:671:ASN:HD22	1.83	0.43
1:D:883:PRO:O	1:D:886:SER:OG	2.29	0.43
1:D:1077:LYS:HB3	1:B:1054:ILE:HD12	2.00	0.43
1:A:369:LYS:CD	1:A:373:VAL:H	2.32	0.43
1:A:1013:ILE:O	1:A:1016:SER:OG	2.36	0.43
1:B:56:VAL:HB	1:B:110:PHE:HB2	2.01	0.43
1:B:1018:LYS:HB2	1:B:1021:LEU:HB2	2.00	0.43
1:C:28:ARG:NH1	1:C:29:PHE:H	2.15	0.43
1:D:58:LYS:N	1:D:73:GLY:N	2.67	0.43
1:D:59:PRO:HD3	1:D:71:LEU:HD12	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:VAL:HG23	1:D:611:LYS:HD2	2.01	0.43
1:D:223:ALA:HA	1:D:233:TRP:CH2	2.53	0.43
1:A:703:ARG:O	1:A:707:THR:OG1	2.36	0.43
1:B:85:LEU:HD22	1:B:89:LEU:HB2	2.01	0.43
1:B:628:GLY:HA3	1:B:685:VAL:HG22	2.01	0.43
1:D:288:TYR:OH	1:D:411:MET:O	2.26	0.43
1:A:128:GLU:HB2	1:A:692:TYR:CD1	2.54	0.43
1:A:328:THR:H	1:A:368:LEU:CA	2.32	0.43
1:A:951:ASP:OD1	1:A:1045:ARG:NH1	2.52	0.43
1:B:188:LEU:O	1:B:192:TYR:N	2.50	0.43
1:B:715:VAL:O	1:B:742:CYS:HA	2.19	0.43
1:C:1075:ASP:OD1	1:C:1078:ARG:NH2	2.52	0.43
1:D:872:VAL:HA	1:D:875:LEU:HB2	2.00	0.43
1:D:963:MET:HG3	1:D:970:ILE:HG12	2.00	0.42
1:A:857:MET:HG2	1:A:862:VAL:HG23	2.01	0.42
1:B:135:HIS:CD2	1:B:149:ALA:HA	2.54	0.42
1:D:410:HIS:HB3	1:D:413:ALA:HB2	2.00	0.42
1:D:581:SER:O	1:D:585:THR:OG1	2.25	0.42
1:A:25:ILE:HG13	1:A:184:PHE:CE1	2.54	0.42
1:A:643:LEU:HD23	1:A:643:LEU:HA	1.86	0.42
1:D:509:VAL:HG23	1:D:526:VAL:HG21	2.00	0.42
1:D:978:LYS:HE3	1:D:984:ASP:HA	2.00	0.42
1:A:523:GLU:HA	1:A:524:PRO:HD3	1.90	0.42
1:A:825:TYR:HA	1:B:834:ILE:HD11	2.00	0.42
1:B:513:LEU:HD12	1:B:513:LEU:HA	1.86	0.42
1:B:1086:HIS:HD2	1:B:1091:ILE:HD11	1.85	0.42
1:D:58:LYS:N	1:D:73:GLY:HA2	2.34	0.42
1:D:123:ILE:HG12	1:D:132:VAL:HG22	2.00	0.42
1:D:278:MET:HE1	1:D:320:ALA:HB2	2.00	0.42
1:D:852:LEU:HD23	1:D:852:LEU:HA	1.91	0.42
1:A:276:TRP:HE1	1:A:336:LYS:HD3	1.83	0.42
1:A:327:MET:C	1:A:369:LYS:HB2	2.45	0.42
1:A:345:ALA:HA	1:A:380:GLY:N	2.34	0.42
1:B:135:HIS:HE1	1:B:137:GLU:HB2	1.84	0.42
1:B:1001:THR:O	1:B:1001:THR:OG1	2.37	0.42
1:C:65:ARG:HD3	1:C:65:ARG:HA	1.66	0.42
1:C:123:ILE:HA	1:C:131:TYR:O	2.20	0.42
1:C:857:MET:HE3	1:C:857:MET:HB2	1.93	0.42
1:D:324:LEU:HD23	1:D:324:LEU:HA	1.78	0.42
1:D:939:LEU:HD11	1:D:1029:ILE:HB	2.02	0.42
1:D:1018:LYS:HG3	2:B:1201:COA:O4B	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ARG:NH1	1:A:690:ASP:HB2	2.35	0.42
1:A:522:ASP:OD1	1:A:522:ASP:N	2.41	0.42
1:A:721:GLY:O	1:A:770:GLU:HG2	2.20	0.42
1:B:320:ALA:HA	1:B:323:ILE:HG22	2.01	0.42
1:C:12:LYS:HZ2	1:C:31:TYR:HB3	1.84	0.42
1:C:280:ALA:HB2	1:C:307:TYR:CZ	2.55	0.42
1:C:840:PHE:O	1:C:842:THR:HG22	2.19	0.42
1:D:14:LEU:HD21	1:D:233:TRP:HD1	1.84	0.42
1:D:847:GLU:HA	1:D:852:LEU:HD23	2.00	0.42
1:D:874:GLY:O	1:D:879:GLN:N	2.53	0.42
1:A:229:CYS:HB3	1:A:233:TRP:HB2	2.02	0.42
1:B:227:TYR:CE2	1:B:576:ARG:HA	2.54	0.42
1:B:344:ILE:HB	1:B:668:ASN:HB3	2.01	0.42
1:C:259:LYS:HE2	1:C:259:LYS:HB2	1.91	0.42
1:C:970:ILE:HB	1:C:973:ILE:HD12	2.02	0.42
1:D:989:ILE:HD11	1:B:860:THR:HG22	2.01	0.42
1:A:951:ASP:CG	1:A:1045:ARG:HH11	2.27	0.42
1:C:7:SER:O	1:C:11:GLY:N	2.52	0.42
1:C:274:ARG:HG2	1:C:300:GLU:HG3	2.02	0.42
1:D:386:GLU:HA	1:D:389:ARG:HB2	2.01	0.42
1:A:102:LEU:HB3	1:A:105:PHE:HE1	1.84	0.42
1:A:122:CYS:HB3	1:A:201:GLU:HA	2.00	0.42
1:A:580:ASP:O	1:A:584:GLU:CB	2.64	0.42
1:B:512:MET:HB2	1:B:512:MET:HE2	1.81	0.42
1:B:803:ASP:HA	1:B:806:ALA:HB3	2.01	0.42
1:C:568:VAL:HG13	1:C:593:THR:HG23	2.01	0.42
1:A:175:GLU:HA	1:A:178:LYS:HG2	2.01	0.42
1:A:354:PHE:HA	1:A:357:ILE:H	1.84	0.42
1:A:604:ALA:HA	1:A:607:ARG:HB2	2.02	0.42
1:B:567:ASP:OD1	1:B:567:ASP:N	2.52	0.42
1:C:10:THR:HG23	1:C:236:ILE:HD12	2.01	0.41
1:C:716:LEU:HB3	1:C:745:ILE:HD11	2.02	0.41
1:C:989:ILE:H	1:C:989:ILE:HG12	1.65	0.41
1:D:538:LYS:HB3	1:D:549:LEU:HB3	2.01	0.41
1:D:873:LEU:HD23	1:D:873:LEU:HA	1.90	0.41
1:A:9:GLN:HE22	1:A:32:ALA:HA	1.84	0.41
1:A:127:ARG:C	1:A:692:TYR:CE1	2.99	0.41
1:A:196:TYR:O	1:A:222:ASP:HB2	2.20	0.41
1:A:329:ARG:N	1:A:366:GLY:O	2.53	0.41
1:A:331:LYS:HD3	1:A:332:HIS:C	2.45	0.41
1:A:789:SER:OG	1:A:790:PHE:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:803:ASP:O	1:C:807:ASN:ND2	2.53	0.41
1:C:869:ILE:HA	1:C:872:VAL:HG22	2.02	0.41
1:D:76:LEU:HB3	1:D:77:THR:O	2.20	0.41
1:D:898:ALA:O	1:D:1065:ARG:NE	2.53	0.41
1:D:991:LYS:O	1:D:995:ARG:N	2.43	0.41
1:A:130:ASP:HB3	1:A:192:TYR:HE2	1.85	0.41
1:A:269:LEU:HD23	1:A:301:LEU:HG	2.02	0.41
1:C:157:ASP:HB2	1:C:611:LYS:NZ	2.35	0.41
1:C:175:GLU:HA	1:C:178:LYS:HD3	2.00	0.41
1:C:325:SER:O	1:C:329:ARG:NE	2.53	0.41
1:C:850:GLN:HE22	1:A:982:ASN:ND2	2.18	0.41
1:C:908:HIS:CE1	1:D:908:HIS:HE1	2.30	0.41
1:D:58:LYS:CA	1:D:72:VAL:HA	2.50	0.41
1:D:911:ILE:O	1:D:915:ARG:HB2	2.20	0.41
1:D:940:ASP:O	1:D:944:LYS:HG2	2.20	0.41
1:A:122:CYS:O	1:A:133:LEU:HB2	2.19	0.41
1:A:270:ASN:O	1:A:302:ALA:HA	2.20	0.41
1:A:1023:LEU:HD23	1:A:1023:LEU:HA	1.86	0.41
1:B:561:ARG:O	1:B:561:ARG:NH1	2.53	0.41
1:A:311:PRO:HG2	1:A:316:THR:HB	2.02	0.41
1:A:330:GLU:HA	1:A:371:HIS:HB2	2.00	0.41
1:A:969:LEU:CD2	2:A:1201:COA:C4A	2.74	0.41
1:D:347:PHE:HE1	1:D:638:ASN:HB2	1.86	0.41
1:A:127:ARG:C	1:A:692:TYR:CE2	2.99	0.41
1:A:887:CYS:SG	1:A:888:GLN:N	2.93	0.41
1:A:987:VAL:HG13	1:A:1028:LEU:HD13	2.02	0.41
1:B:165:ILE:HG22	1:B:170:LEU:HG	2.02	0.41
1:A:162:PRO:HA	1:A:165:ILE:HD12	2.00	0.41
1:A:324:LEU:HD23	1:A:360:ALA:O	2.21	0.41
1:A:929:LEU:HD12	1:A:929:LEU:HA	1.82	0.41
1:C:53:GLN:HE21	1:C:109:PRO:HB3	1.85	0.41
1:D:541:PHE:O	1:D:547:GLU:HA	2.20	0.41
1:D:578:ALA:O	1:D:582:THR:OG1	2.26	0.41
1:D:671:ASN:O	1:D:675:SER:HB3	2.21	0.41
1:A:119:PHE:CD1	1:A:207:VAL:HB	2.56	0.41
1:B:668:ASN:HA	1:B:671:ASN:ND2	2.35	0.41
1:C:414:ILE:HA	1:C:417:MET:HG2	2.02	0.41
1:C:585:THR:HG23	1:C:591:ILE:HD13	2.03	0.41
1:D:60:ASP:OD1	1:D:60:ASP:N	2.33	0.41
1:D:381:GLY:HA3	1:D:382:PRO:HD3	1.89	0.41
1:A:34:VAL:HA	1:A:43:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:VAL:HG22	1:A:713:ILE:HD13	2.03	0.41
1:A:707:THR:HA	1:A:708:PRO:HD3	1.91	0.41
1:B:598:ALA:HB3	1:B:601:ILE:HD11	2.02	0.41
1:B:683:GLU:OE2	1:B:684:GLY:N	2.54	0.41
1:B:986:ARG:CZ	1:B:1025:VAL:HG11	2.51	0.41
1:B:1033:PHE:HB3	1:B:1057:LEU:HD11	2.03	0.41
1:C:62:LEU:HD13	1:C:62:LEU:HA	1.93	0.41
1:C:852:LEU:HD23	1:C:852:LEU:HA	1.78	0.41
1:D:40:TRP:CZ3	1:D:78:LEU:HD13	2.56	0.41
1:D:292:ILE:HD13	1:D:301:LEU:HD13	2.03	0.41
1:D:576:ARG:HH21	1:D:576:ARG:HD2	1.73	0.41
1:D:695:SER:HB3	1:D:699:ASP:HB2	2.02	0.41
1:A:792:GLU:HA	1:A:795:GLU:HG3	2.02	0.41
1:A:831:LEU:HD12	1:A:833:LEU:HD23	2.01	0.41
1:B:362:ARG:HH11	1:B:362:ARG:HD2	1.76	0.41
1:B:410:HIS:HB3	1:B:413:ALA:HB2	2.02	0.41
1:C:278:MET:HE3	1:C:319:TYR:HD2	1.85	0.41
1:C:324:LEU:O	1:C:328:THR:OG1	2.27	0.41
1:C:898:ALA:O	1:C:1065:ARG:NE	2.53	0.41
1:D:657:VAL:HG21	1:D:678:THR:HG21	2.02	0.41
1:D:720:GLY:HA2	1:D:770:GLU:HB2	2.02	0.41
1:A:77:THR:HG22	1:A:78:LEU:H	1.86	0.41
1:A:118:GLU:HB2	1:A:205:LEU:HA	2.03	0.41
1:A:277:THR:OG1	1:A:303:ASN:O	2.38	0.41
1:A:331:LYS:HA	1:A:371:HIS:O	2.21	0.41
1:A:417:MET:HB3	1:A:422:ARG:HG2	2.04	0.41
1:B:792:GLU:HA	1:B:795:GLU:H	1.86	0.41
1:C:375:ILE:O	1:C:402:ILE:HA	2.22	0.40
1:D:201:GLU:HB3	1:D:218:ALA:HB3	2.03	0.40
1:D:391:MET:HA	1:D:394:VAL:HG12	2.03	0.40
1:A:692:TYR:CD2	1:A:692:TYR:CB	2.96	0.40
1:A:908:HIS:CE1	1:B:908:HIS:HE1	2.31	0.40
1:C:1054:ILE:HD13	1:C:1054:ILE:HA	1.89	0.40
1:D:57:VAL:O	1:D:71:LEU:HB3	2.21	0.40
1:A:516:ASP:O	1:A:521:ARG:HB3	2.20	0.40
1:B:790:PHE:CZ	1:B:793:LEU:HD22	2.57	0.40
1:C:33:ARG:HG2	1:C:104:ASN:HD21	1.86	0.40
1:C:40:TRP:NE1	1:C:82:LYS:HE3	2.36	0.40
1:C:792:GLU:O	1:C:796:ILE:N	2.45	0.40
1:A:126:THR:OG1	1:A:127:ARG:N	2.54	0.40
1:A:270:ASN:HA	1:A:271:PRO:HD3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:GLY:HA3	1:B:623:PRO:HD3	1.94	0.40
1:C:489:SER:OG	1:C:490:THR:N	2.54	0.40
1:C:797:ILE:O	1:C:801:TYR:CB	2.69	0.40
1:D:920:LEU:O	1:D:923:SER:OG	2.37	0.40
1:A:53:GLN:HB3	1:A:112:PRO:HD3	2.04	0.40
1:A:724:GLU:N	1:A:775:LYS:HZ3	2.19	0.40
1:D:40:TRP:HH2	1:D:78:LEU:HD22	1.85	0.40
1:D:56:VAL:O	1:D:73:GLY:N	2.53	0.40
1:D:741:VAL:HA	1:D:785:PHE:HB2	2.04	0.40
1:D:857:MET:HG2	1:D:862:VAL:HG23	2.03	0.40
1:A:111:VAL:HG13	1:A:113:HIS:ND1	2.35	0.40
1:A:196:TYR:HE1	1:A:604:ALA:H	1.69	0.40
1:A:382:PRO:HB3	1:A:642:MET:HG3	2.03	0.40
1:A:1020:ASN:O	1:A:1022:ILE:N	2.55	0.40
1:B:505:GLN:HE22	2:B:1201:COA:H141	1.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1015/1101 (92%)	886 (87%)	111 (11%)	18 (2%)	6	33
1	B	1017/1101 (92%)	936 (92%)	78 (8%)	3 (0%)	36	71
1	C	1017/1101 (92%)	942 (93%)	73 (7%)	2 (0%)	43	77
1	D	1017/1101 (92%)	930 (91%)	80 (8%)	7 (1%)	18	55
All	All	4066/4404 (92%)	3694 (91%)	342 (8%)	30 (1%)	20	55

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1021	LEU
1	D	59	PRO
1	A	329	ARG
1	A	344	ILE
1	A	362	ARG
1	A	370	GLU
1	A	1021	LEU
1	C	835	ARG
1	D	73	GLY
1	D	835	ARG
1	D	1021	LEU
1	A	122	CYS
1	A	835	ARG
1	B	835	ARG
1	B	1021	LEU
1	D	76	LEU
1	D	1020	ASN
1	A	4	LYS
1	A	119	PHE
1	A	622	GLY
1	A	347	PHE
1	A	367	PRO
1	A	383	ASN
1	A	532	PRO
1	A	747	THR
1	A	554	LYS
1	B	747	THR
1	D	57	VAL
1	A	109	PRO
1	A	720	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	842/909 (93%)	806 (96%)	36 (4%)	26	48
1	B	842/909 (93%)	838 (100%)	4 (0%)	81	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	842/909 (93%)	837 (99%)	5 (1%)	78	80
1	D	842/909 (93%)	829 (98%)	13 (2%)	57	70
All	All	3368/3636 (93%)	3310 (98%)	58 (2%)	54	67

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	111	VAL
1	C	207	VAL
1	C	226[A]	ASP
1	C	226[B]	ASP
1	C	710	VAL
1	D	54	ASN
1	D	56	VAL
1	D	57	VAL
1	D	71	LEU
1	D	74	VAL
1	D	101	PHE
1	D	165	ILE
1	D	226[A]	ASP
1	D	226[B]	ASP
1	D	264	LEU
1	D	386	GLU
1	D	869	ILE
1	D	1057	LEU
1	A	10	THR
1	A	25	ILE
1	A	111	VAL
1	A	118	GLU
1	A	119	PHE
1	A	126	THR
1	A	135	HIS
1	A	177	LYS
1	A	188	LEU
1	A	207	VAL
1	A	208	THR
1	A	221	VAL
1	A	224	THR
1	A	226[A]	ASP
1	A	226[B]	ASP
1	A	324	LEU

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Mol	Chain	Res	Type
1	A	327	MET
1	A	328	THR
1	A	344	ILE
1	A	346	ASN
1	A	348	THR
1	A	364	TYR
1	A	365	GLN
1	A	368	LEU
1	A	369	LYS
1	A	389	ARG
1	A	394	VAL
1	A	500	ILE
1	A	566	VAL
1	A	567	ASP
1	A	568	VAL
1	A	607	ARG
1	A	678	THR
1	A	692	TYR
1	A	715	VAL
1	A	873	LEU
1	B	226[A]	ASP
1	B	226[B]	ASP
1	B	504	MET
1	B	1054	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	61	GLN
1	C	104	ASN
1	C	203	ASN
1	C	270	ASN
1	C	314	GLN
1	C	332	HIS
1	C	563	HIS
1	C	615	GLN
1	C	705	GLN
1	C	777	GLN
1	C	850	GLN
1	C	908	HIS
1	C	1072	HIS
1	D	61	GLN

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Mol	Chain	Res	Type
1	D	113	HIS
1	D	203	ASN
1	D	270	ASN
1	D	332	HIS
1	D	571	ASN
1	D	615	GLN
1	D	671	ASN
1	D	850	GLN
1	D	908	HIS
1	D	981	ASN
1	D	996	GLN
1	D	1058	ASN
1	D	1098	HIS
1	A	9	GLN
1	A	91	GLN
1	A	104	ASN
1	A	150	GLN
1	A	203	ASN
1	A	299	ASN
1	A	314	GLN
1	A	346	ASN
1	A	371	HIS
1	A	510	GLN
1	A	571	ASN
1	A	587	ASN
1	A	615	GLN
1	A	767	GLN
1	A	900	HIS
1	A	908	HIS
1	A	981	ASN
1	B	45	GLN
1	B	61	GLN
1	B	135	HIS
1	B	403	HIS
1	B	505	GLN
1	B	571	ASN
1	B	587	ASN
1	B	671	ASN
1	B	850	GLN
1	B	900	HIS
1	B	908	HIS
1	B	996	GLN

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Mol	Chain	Res	Type
1	B	1076	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	COA	A	1201	-	47,50,50	3.02	19 (40%)	69,75,75	2.01	14 (20%)
2	COA	B	1201	-	47,50,50	2.98	20 (42%)	69,75,75	2.56	20 (28%)

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	1201	-	-	10/48/64/64	0/3/3/3
2	COA	B	1201	-	-	15/48/64/64	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	COA	O4B-C1B	9.50	1.64	1.42
2	A	1201	COA	O4B-C1B	8.55	1.61	1.42
2	A	1201	COA	C9P-N8P	6.95	1.49	1.33
2	A	1201	COA	C2B-C1B	-6.71	1.32	1.53
2	B	1201	COA	C9P-N8P	6.66	1.49	1.33
2	B	1201	COA	C2B-C1B	-6.24	1.33	1.53
2	A	1201	COA	O4B-C4B	-6.23	1.31	1.45
2	B	1201	COA	O4B-C4B	-5.78	1.32	1.45
2	A	1201	COA	C5P-N4P	5.67	1.46	1.33
2	B	1201	COA	C5P-N4P	5.20	1.45	1.33
2	A	1201	COA	C6A-N6A	5.05	1.47	1.34
2	B	1201	COA	C6A-N6A	4.97	1.46	1.34
2	A	1201	COA	P2A-O3A	4.57	1.64	1.59
2	B	1201	COA	CCP-CBP	4.36	1.59	1.52
2	B	1201	COA	P2A-O3A	4.33	1.64	1.59
2	A	1201	COA	P1A-O3A	4.31	1.64	1.59
2	B	1201	COA	P1A-O3A	3.84	1.63	1.59
2	B	1201	COA	C5A-C4A	-3.78	1.32	1.39
2	A	1201	COA	CCP-CBP	3.62	1.58	1.52
2	A	1201	COA	C5A-C4A	-3.61	1.32	1.39
2	A	1201	COA	P3B-O3B	3.55	1.65	1.59
2	A	1201	COA	C8A-N9A	-2.94	1.32	1.37
2	B	1201	COA	P3B-O3B	2.90	1.64	1.59
2	A	1201	COA	O9P-C9P	-2.88	1.17	1.23
2	A	1201	COA	OAP-CAP	-2.74	1.37	1.42
2	A	1201	COA	C6P-C5P	2.71	1.56	1.51
2	B	1201	COA	O9P-C9P	-2.68	1.18	1.23
2	B	1201	COA	C3B-C4B	2.56	1.59	1.52
2	B	1201	COA	C8A-N9A	-2.50	1.33	1.37
2	B	1201	COA	OAP-CAP	-2.48	1.37	1.42
2	B	1201	COA	C6P-C5P	2.47	1.56	1.51
2	A	1201	COA	C5A-N7A	-2.41	1.34	1.39
2	B	1201	COA	O2B-C2B	2.35	1.48	1.43
2	A	1201	COA	O2B-C2B	2.25	1.48	1.43
2	A	1201	COA	P1A-O5B	2.24	1.68	1.59
2	A	1201	COA	O3B-C3B	-2.14	1.36	1.44
2	B	1201	COA	O3B-C3B	-2.05	1.37	1.44
2	B	1201	COA	C8A-N7A	2.04	1.35	1.31
2	B	1201	COA	O5P-C5P	-2.03	1.19	1.23

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	COA	O4B-C1B-N9A	8.24	123.91	108.09
2	A	1201	COA	N6A-C6A-N1A	-7.31	102.10	118.38
2	B	1201	COA	N3A-C2A-N1A	-7.24	117.62	128.58
2	B	1201	COA	N6A-C6A-N1A	-6.90	103.00	118.38
2	B	1201	COA	C5B-C4B-C3B	-6.47	92.84	114.38
2	A	1201	COA	C5A-C6A-N6A	5.80	137.64	123.29
2	B	1201	COA	C2B-C1B-N9A	-5.34	100.03	113.30
2	B	1201	COA	C5A-C6A-N6A	5.33	136.49	123.29
2	A	1201	COA	N3A-C2A-N1A	-5.18	120.74	128.58
2	B	1201	COA	N9A-C8A-N7A	-5.18	106.59	113.94
2	A	1201	COA	N9A-C8A-N7A	-4.55	107.48	113.94
2	A	1201	COA	C5A-C4A-N3A	-4.51	120.51	126.72
2	B	1201	COA	C5A-C4A-N3A	-3.92	121.32	126.72
2	B	1201	COA	C2A-N3A-C4A	3.81	121.14	111.83
2	B	1201	COA	C4A-N9A-C8A	3.40	109.31	105.74
2	B	1201	COA	C6P-C7P-N8P	-3.28	105.02	112.00
2	B	1201	COA	O5B-C5B-C4B	3.18	119.82	108.99
2	A	1201	COA	C2A-N3A-C4A	3.18	119.59	111.83
2	B	1201	COA	C5A-N7A-C8A	3.14	108.38	103.45
2	A	1201	COA	C5A-N7A-C8A	2.97	108.12	103.45
2	A	1201	COA	CAP-C9P-N8P	2.76	121.72	116.48
2	A	1201	COA	C4A-N9A-C8A	2.73	108.60	105.74
2	B	1201	COA	C3B-C2B-C1B	2.72	105.88	99.89
2	B	1201	COA	C2P-C3P-N4P	-2.68	106.23	112.31
2	A	1201	COA	C5B-C4B-C3B	-2.64	105.60	114.38
2	A	1201	COA	N3A-C4A-N9A	2.56	131.52	127.17
2	A	1201	COA	C4A-C5A-N7A	-2.41	107.83	110.58
2	B	1201	COA	C4A-C5A-N7A	-2.39	107.85	110.58
2	A	1201	COA	CDP-CBP-CCP	-2.15	104.67	108.22
2	B	1201	COA	N3A-C4A-N9A	2.14	130.81	127.17
2	B	1201	COA	C6P-C5P-N4P	2.11	120.19	116.34
2	B	1201	COA	C4B-O4B-C1B	-2.03	104.98	109.47
2	B	1201	COA	C7P-C6P-C5P	-2.03	109.01	112.39
2	A	1201	COA	C6P-C5P-N4P	2.01	120.01	116.34

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	COA	CCP-O6A-P2A-O3A
2	A	1201	COA	CDP-CBP-CCP-O6A
2	A	1201	COA	CEP-CBP-CCP-O6A
2	A	1201	COA	CAP-CBP-CCP-O6A

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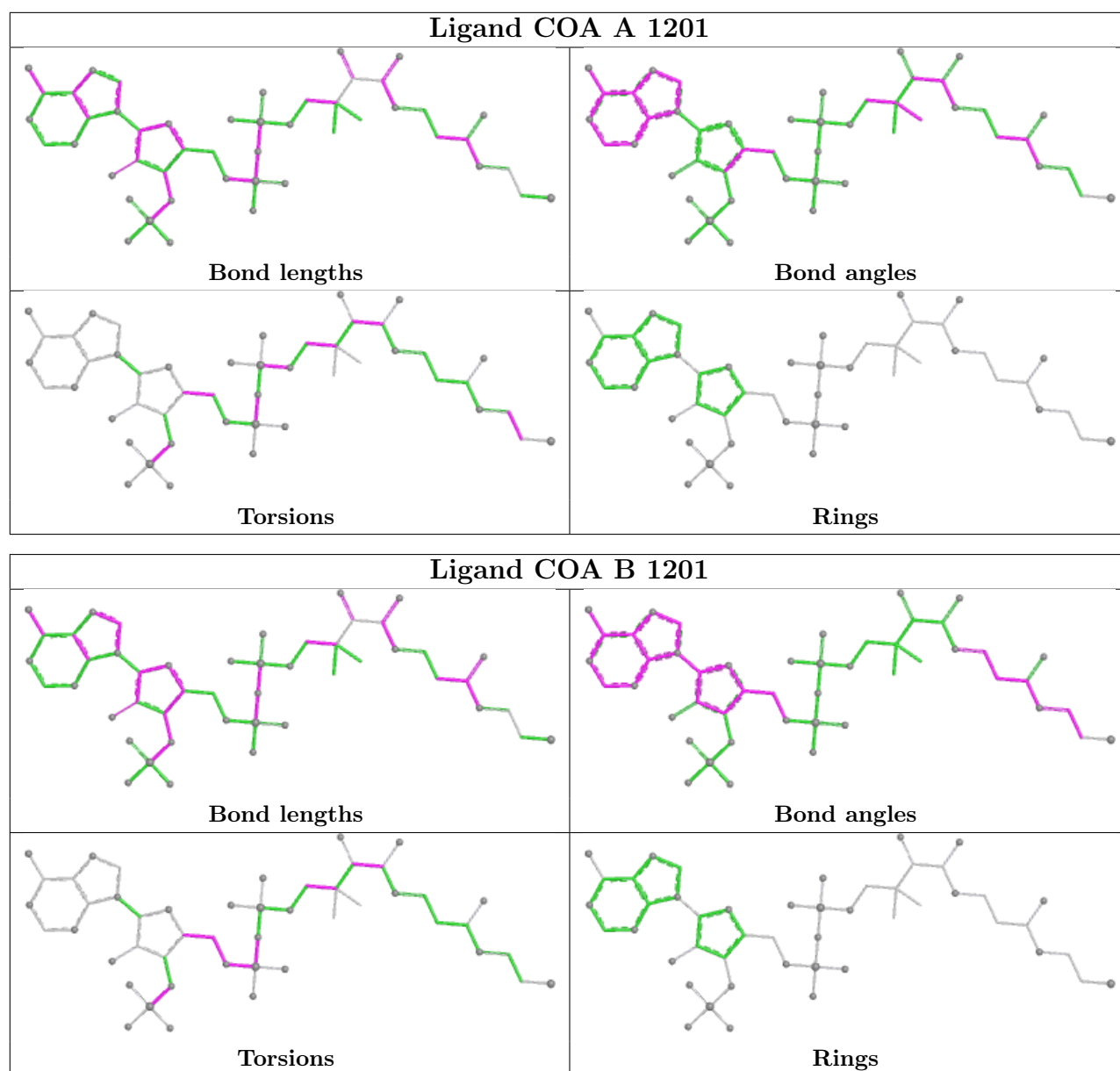
Mol	Chain	Res	Type	Atoms
2	A	1201	COA	N8P-C9P-CAP-OAP
2	B	1201	COA	C5B-O5B-P1A-O1A
2	B	1201	COA	C5B-O5B-P1A-O2A
2	B	1201	COA	C5B-O5B-P1A-O3A
2	B	1201	COA	CDP-CBP-CCP-O6A
2	B	1201	COA	CEP-CBP-CCP-O6A
2	B	1201	COA	CAP-CBP-CCP-O6A
2	B	1201	COA	N8P-C9P-CAP-OAP
2	B	1201	COA	O9P-C9P-CAP-OAP
2	B	1201	COA	C3B-C4B-C5B-O5B
2	A	1201	COA	P2A-O3A-P1A-O5B
2	B	1201	COA	P2A-O3A-P1A-O5B
2	A	1201	COA	O9P-C9P-CAP-OAP
2	B	1201	COA	C4B-C5B-O5B-P1A
2	A	1201	COA	C3B-O3B-P3B-O7A
2	B	1201	COA	C3B-O3B-P3B-O7A
2	A	1201	COA	O4B-C4B-C5B-O5B
2	B	1201	COA	P2A-O3A-P1A-O1A
2	B	1201	COA	O9P-C9P-CAP-CBP
2	A	1201	COA	S1P-C2P-C3P-N4P
2	B	1201	COA	P2A-O3A-P1A-O2A

There are no ring outliers.

2 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	COA	19	0
2	B	1201	COA	40	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	819:PRO	C	820:THR	N	4.94
1	A	127:ARG	C	128:GLU	N	1.84
1	D	73:GLY	C	74:VAL	N	1.62

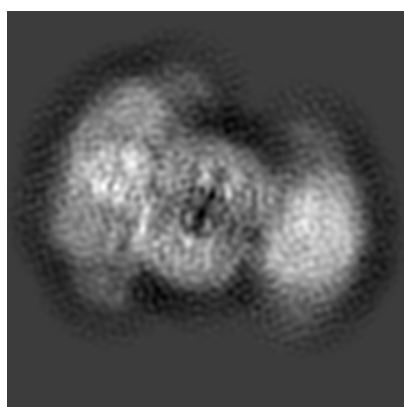
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20784. These allow visual inspection of the internal detail of the map and identification of artifacts.

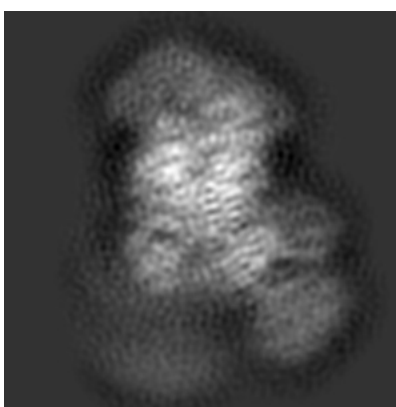
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

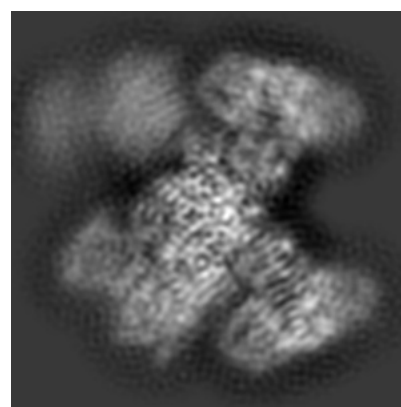
6.1.1 Primary map



X



Y

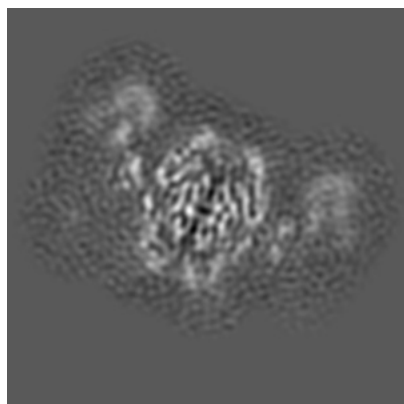


Z

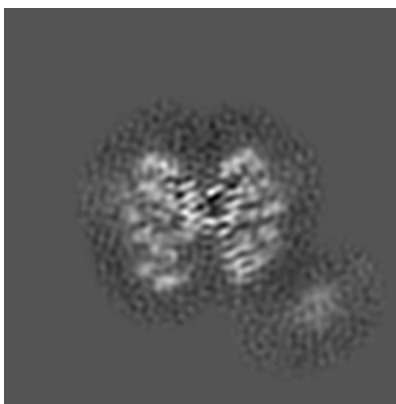
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

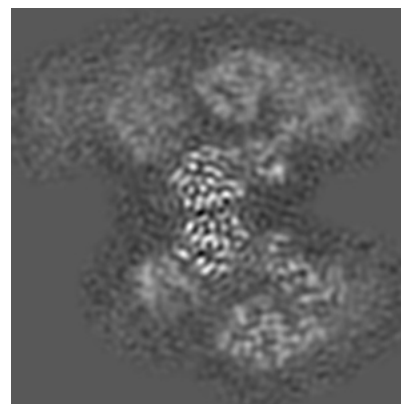
6.2.1 Primary map



X Index: 110



Y Index: 110

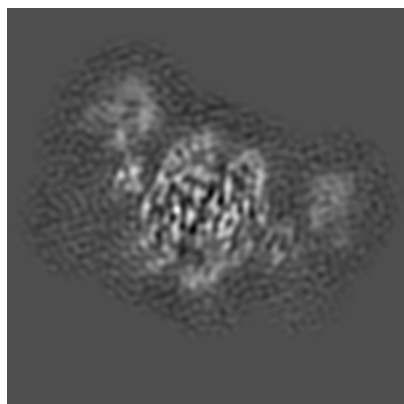


Z Index: 110

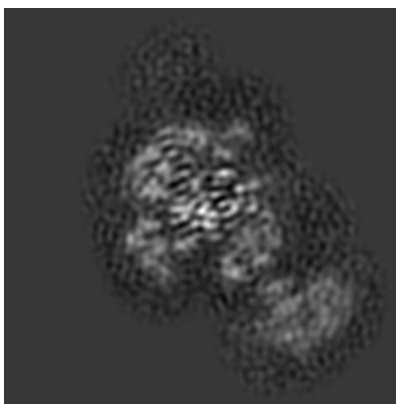
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

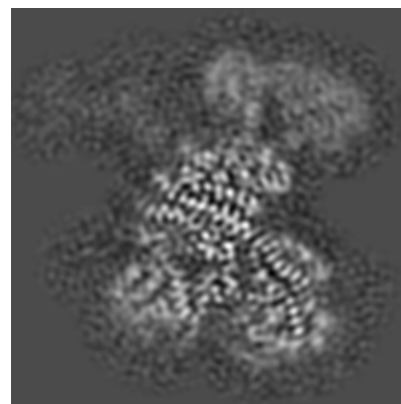
6.3.1 Primary map



X Index: 108



Y Index: 93

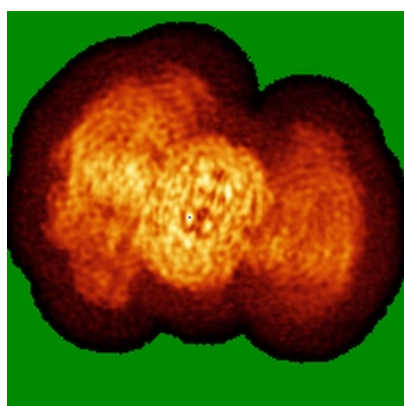


Z Index: 124

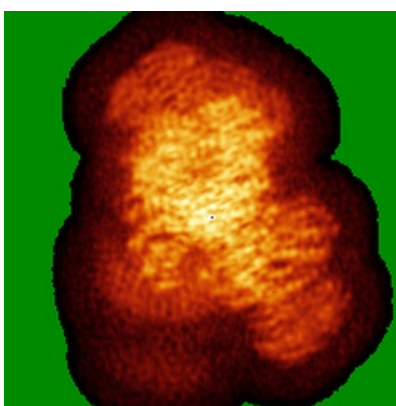
The images above show the largest variance slices of the map in three orthogonal directions.

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

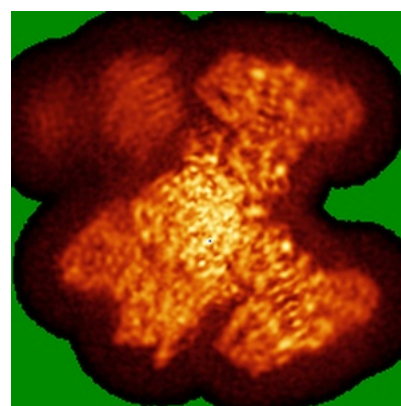
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

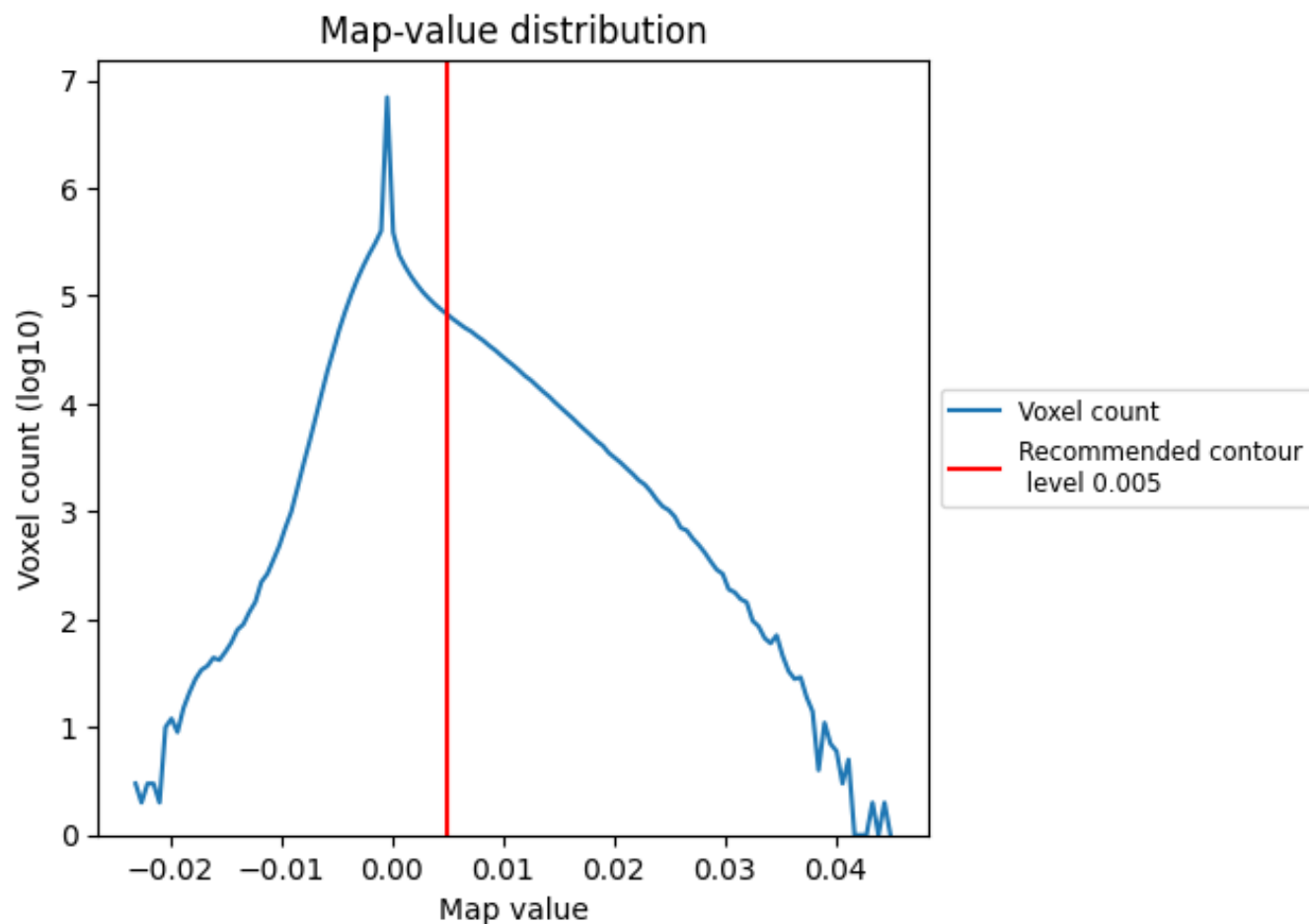
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

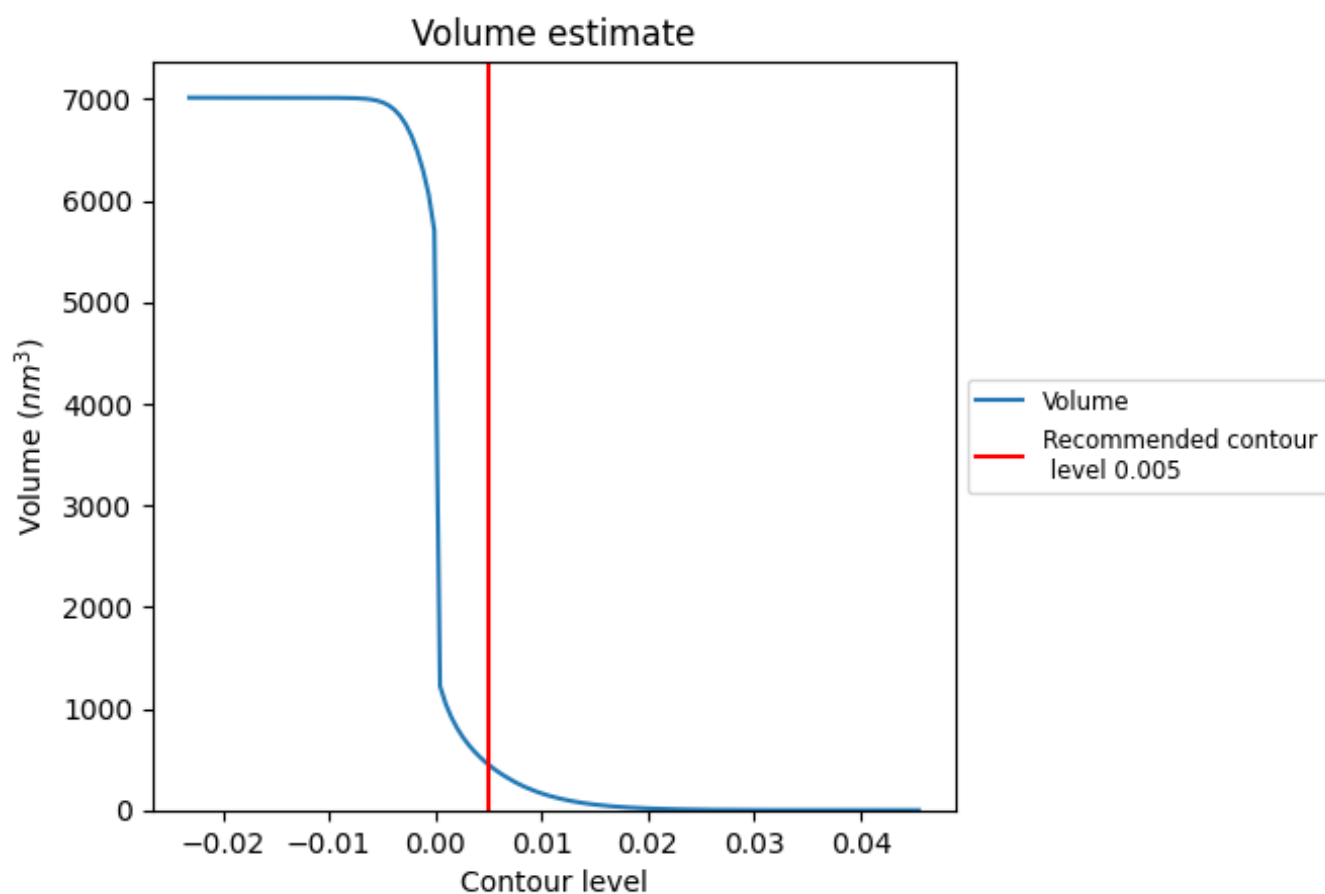
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

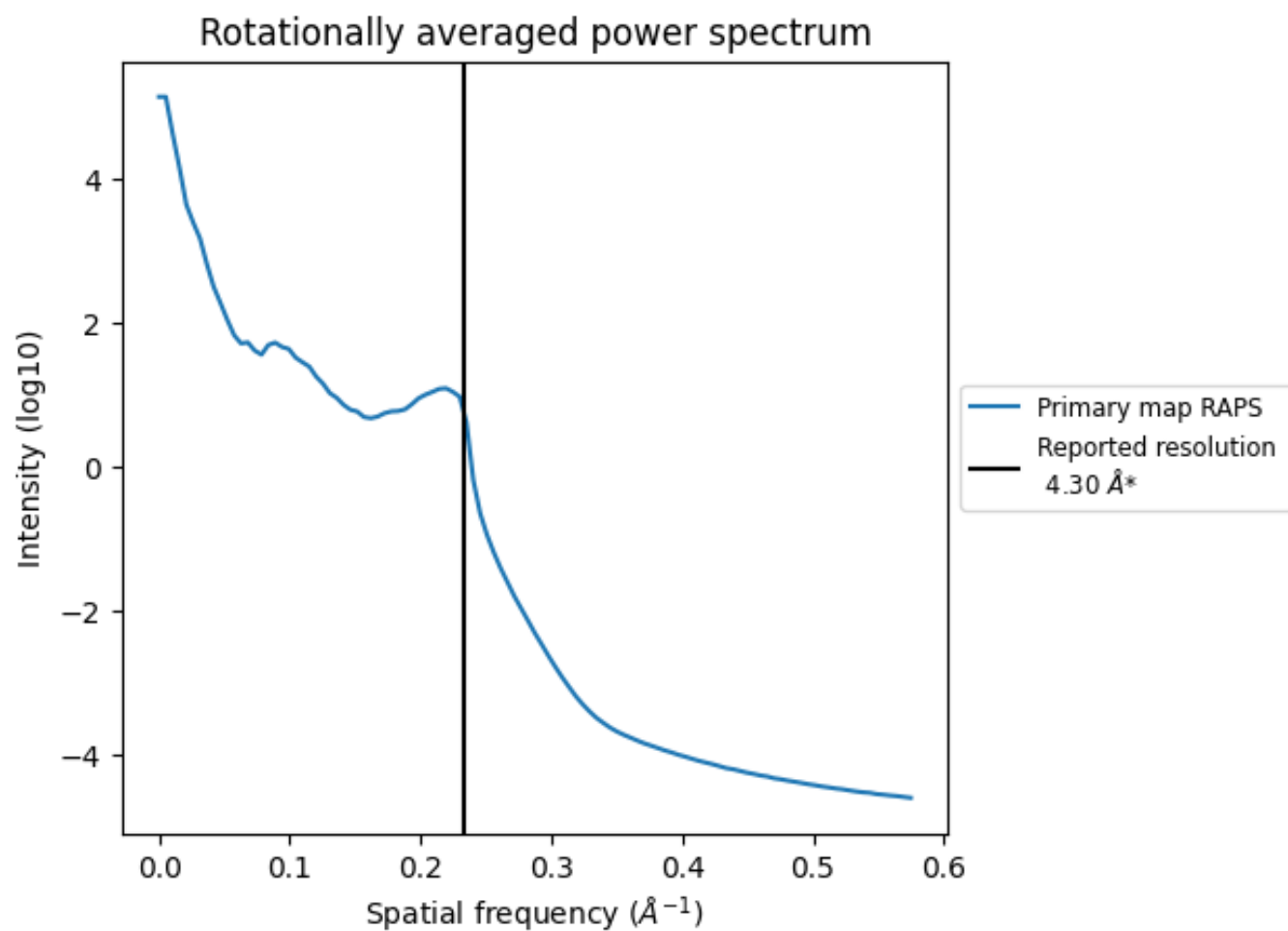
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 448 nm³; this corresponds to an approximate mass of 405 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

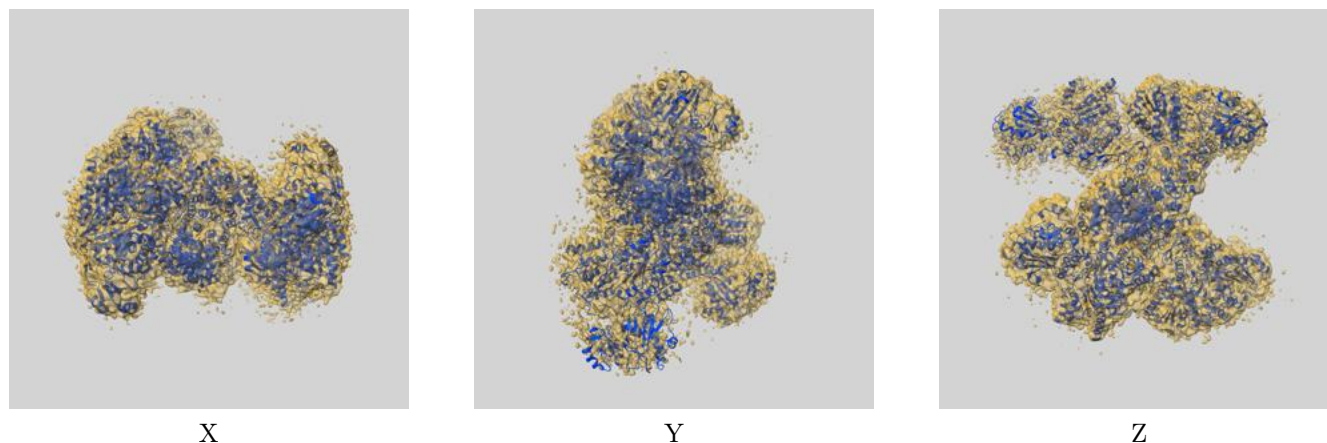
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

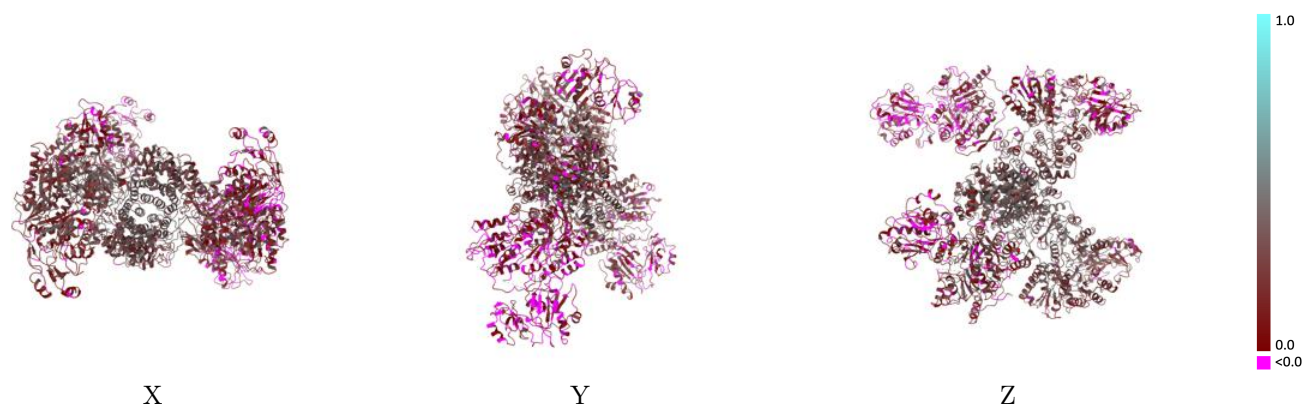
This section contains information regarding the fit between EMDB map EMD-20784 and PDB model 6UIA. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



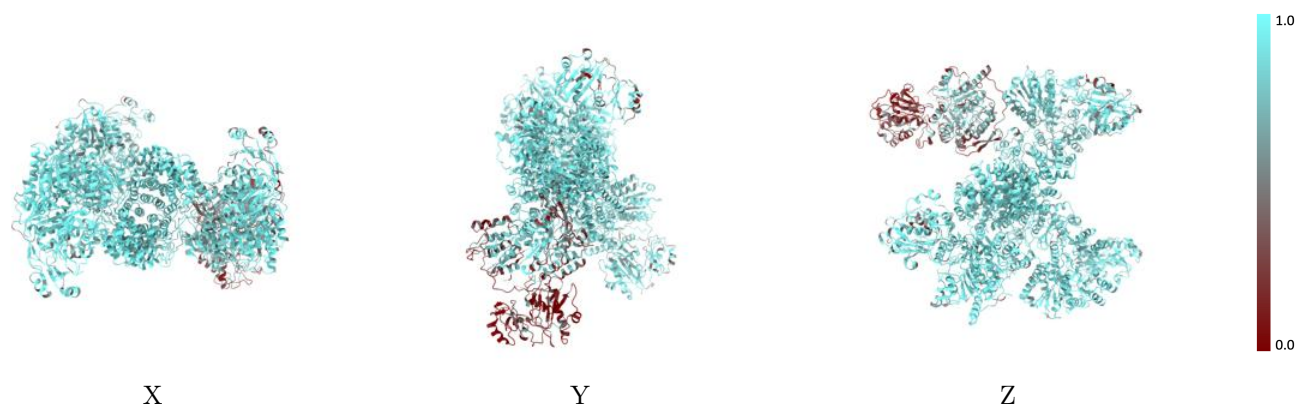
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



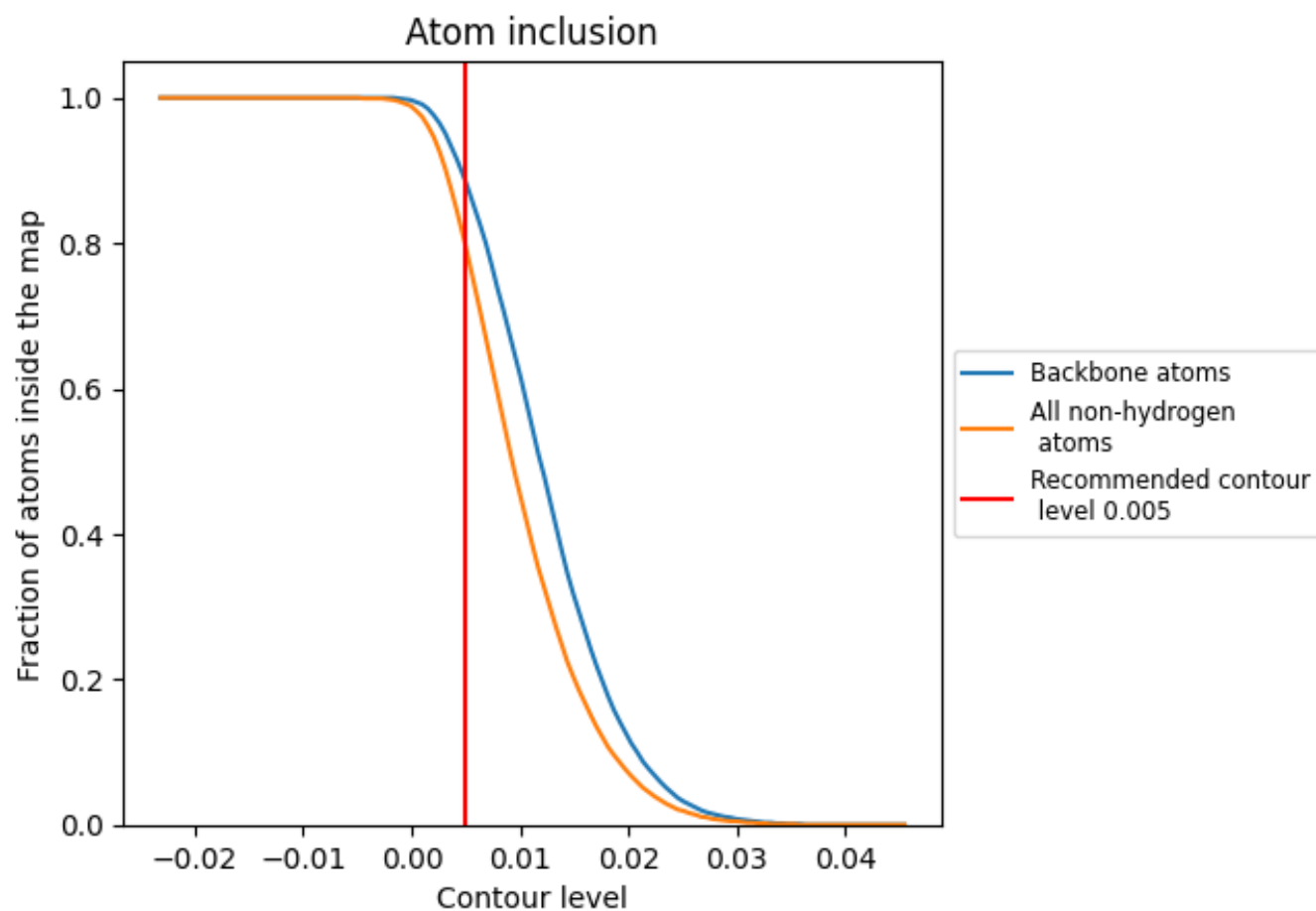
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7950	0.2140
A	0.5660	0.1360
B	0.8460	0.2200
C	0.8960	0.2770
D	0.8710	0.2210

