



Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 10:55 AM EST

PDB ID : 6UIA
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.

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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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

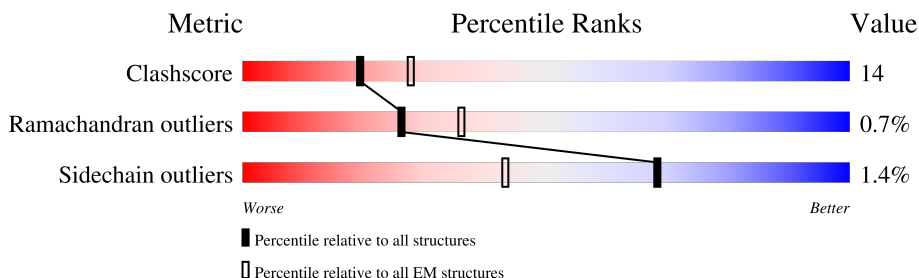
1 Overall quality at a glance

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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](#)

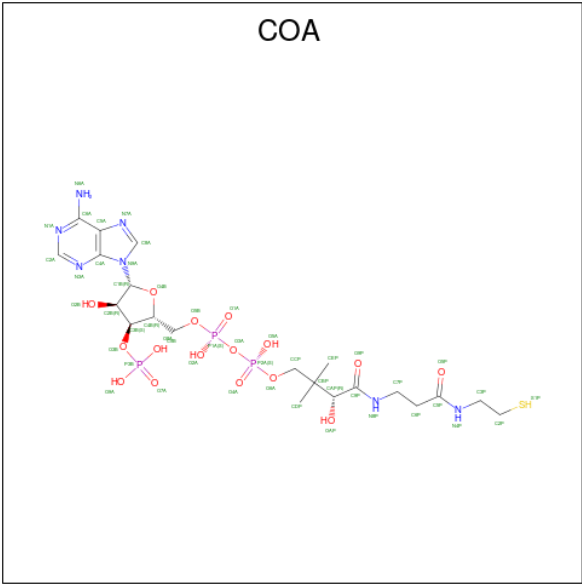
There are 2 unique types of molecules in this entry. The entry contains 31720 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

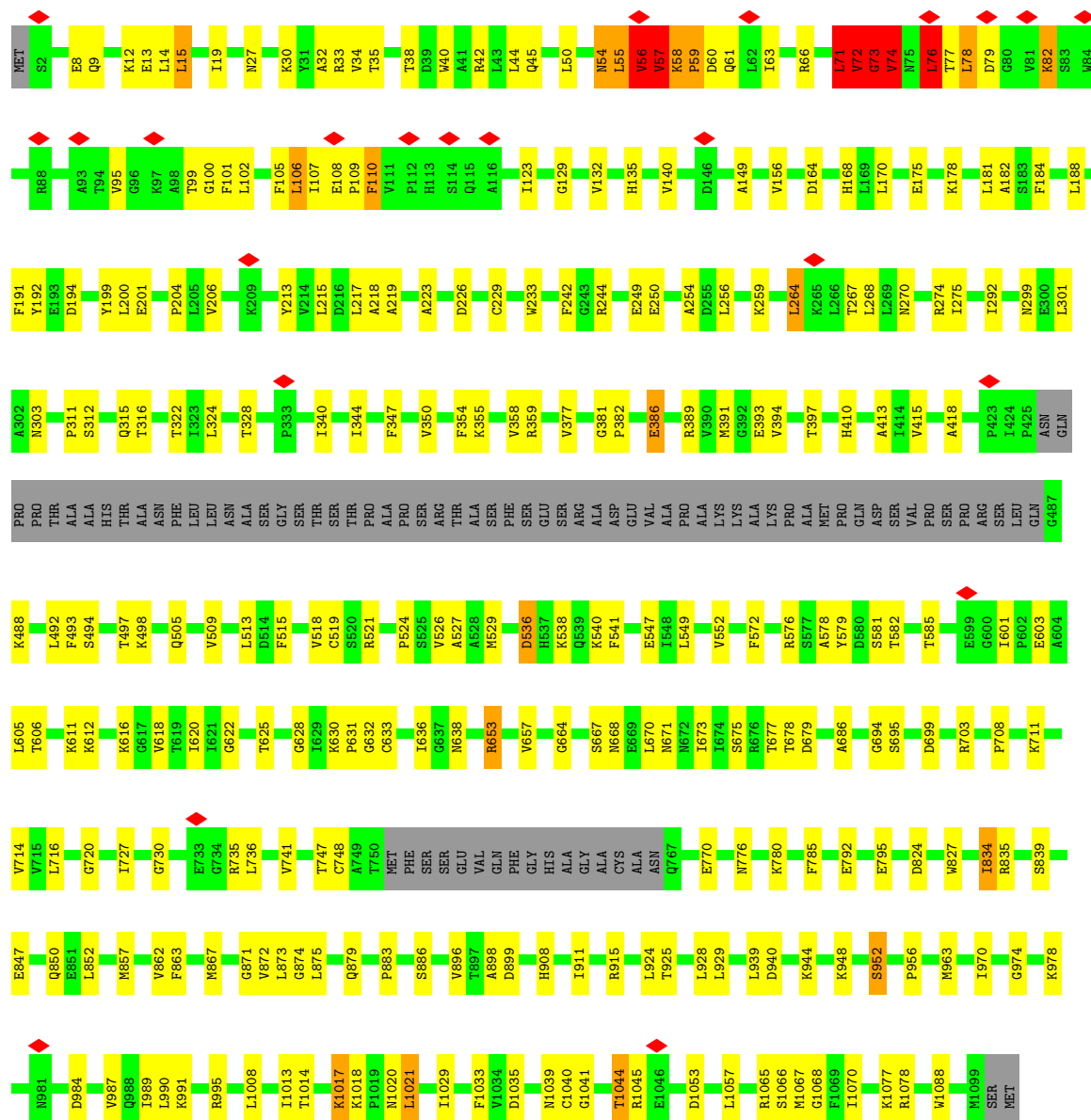
- Molecule 1 is a protein called ATP-citrate synthase.

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

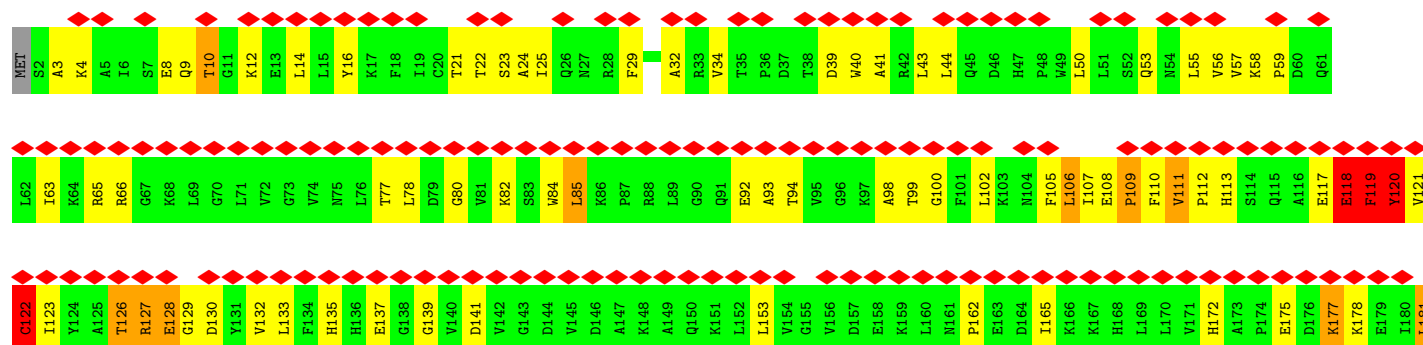
- Molecule 2 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S) (labeled as "Ligand of Interest" by depositor).

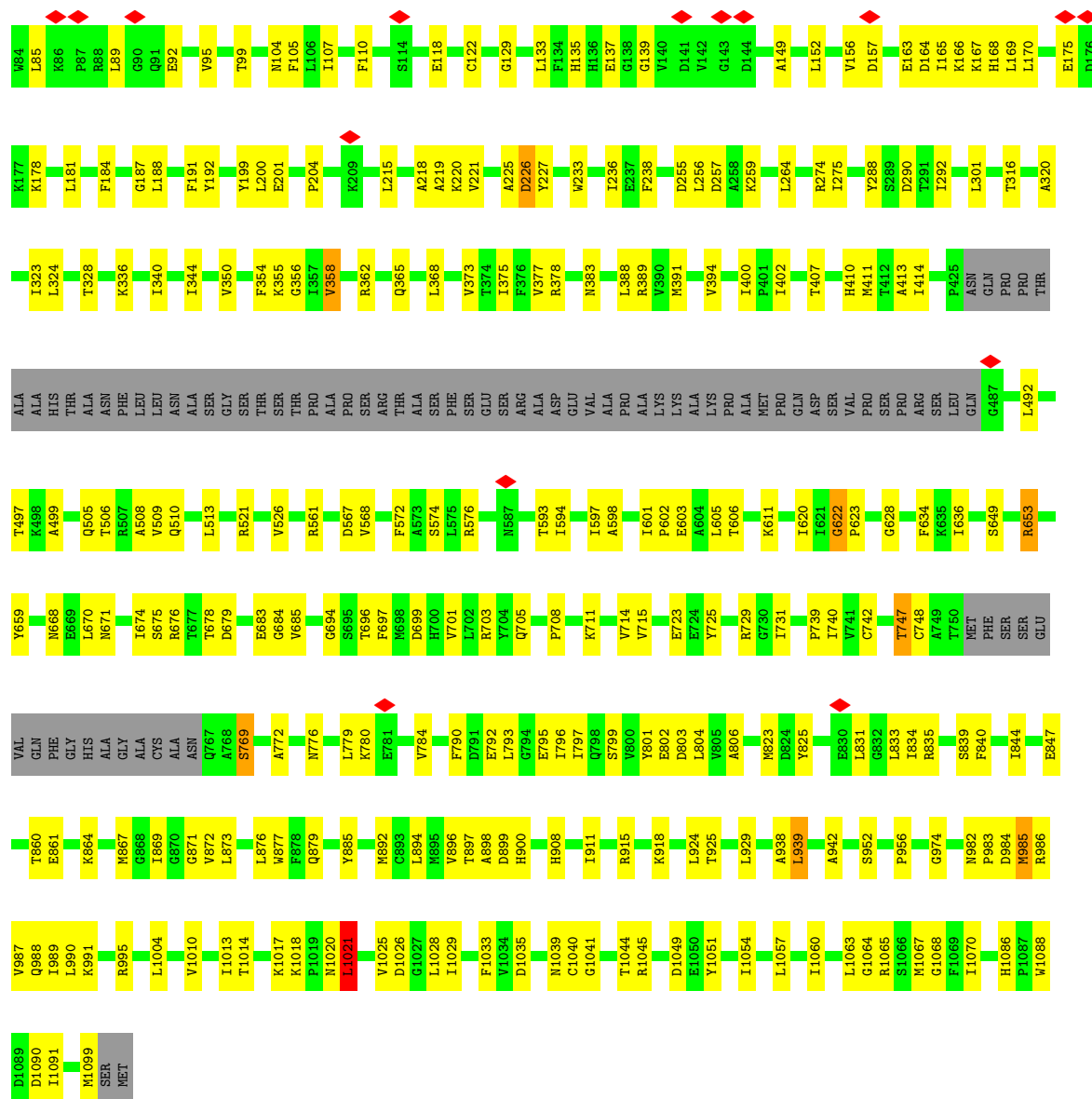


Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
2	A	1	Total 48	21	7	16	3	1	0
2	B	1	Total 48	21	7	16	3	1	0



• 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

5.1 Standard geometry

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	2.48	24/8082 (0.3%)	1.17	72/10939 (0.7%)
1	B	0.41	0/8083	0.73	10/10942 (0.1%)
1	C	0.41	1/8083 (0.0%)	0.67	3/10942 (0.0%)
1	D	0.57	10/8083 (0.1%)	0.85	34/10942 (0.3%)
All	All	1.30	35/32331 (0.1%)	0.88	119/43765 (0.3%)

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 (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	692	TYR	CD1-CE1	133.21	3.39	1.39
1	A	692	TYR	CD2-CE2	104.62	2.96	1.39
1	A	692	TYR	CE1-CZ	74.04	2.34	1.38
1	A	692	TYR	CE2-CZ	69.92	2.29	1.38
1	A	692	TYR	CG-CD1	57.15	2.13	1.39
1	A	692	TYR	CG-CD2	56.23	2.12	1.39
1	A	127	ARG	C-N	22.08	1.84	1.34
1	D	73	GLY	N-CA	17.56	1.72	1.46
1	D	72	VAL	C-N	14.46	1.59	1.33
1	A	128	GLU	N-CA	13.24	1.72	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	73	GLY	C-N	12.46	1.62	1.34
1	D	56	VAL	C-N	10.74	1.58	1.34
1	D	73	GLY	CA-C	10.16	1.68	1.51
1	D	57	VAL	N-CA	8.99	1.64	1.46
1	A	328	THR	C-N	8.89	1.54	1.34
1	A	329	ARG	N-CA	8.23	1.62	1.46
1	A	368	LEU	C-N	8.04	1.52	1.34
1	D	72	VAL	CB-CG1	7.69	1.69	1.52
1	A	328	THR	CA-C	7.56	1.72	1.52
1	A	327	MET	CA-C	7.37	1.72	1.52
1	D	57	VAL	CA-C	7.22	1.71	1.52
1	A	368	LEU	CA-C	6.32	1.69	1.52
1	A	212	VAL	CB-CG1	-6.27	1.39	1.52
1	A	326	LEU	CA-C	6.19	1.69	1.52
1	A	326	LEU	N-CA	6.10	1.58	1.46
1	A	120	TYR	CB-CG	6.10	1.60	1.51
1	C	817	PRO	CA-C	6.02	1.64	1.52
1	D	74	VAL	N-CA	5.76	1.57	1.46
1	A	172	HIS	C-N	5.58	1.46	1.34
1	A	119	PHE	N-CA	5.51	1.57	1.46
1	A	368	LEU	CA-CB	5.47	1.66	1.53
1	D	57	VAL	C-N	5.43	1.46	1.34
1	A	118	GLU	CA-C	5.23	1.66	1.52
1	A	206	VAL	N-CA	5.08	1.56	1.46
1	A	380	GLY	C-N	5.02	1.42	1.33

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	LEU	CA-CB-CG	28.09	179.92	115.30
1	A	692	TYR	CB-CG-CD2	-20.39	108.77	121.00
1	A	127	ARG	C-N-CA	17.51	165.48	121.70
1	D	71	LEU	CA-CB-CG	14.19	147.93	115.30
1	D	72	VAL	C-N-CA	13.72	151.11	122.30
1	A	329	ARG	CA-CB-CG	12.69	141.31	113.40
1	A	368	LEU	CD1-CG-CD2	-12.20	73.90	110.50
1	A	369	LYS	CB-CA-C	-11.40	87.60	110.40
1	A	368	LEU	C-N-CA	11.38	150.14	121.70
1	D	55	LEU	CA-CB-CG	11.00	140.59	115.30
1	A	324	LEU	CB-CG-CD2	10.66	129.12	111.00
1	A	328	THR	CA-CB-CG2	10.58	127.22	112.40
1	A	327	MET	C-N-CA	10.38	147.65	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	692	TYR	CD1-CG-CD2	10.27	129.19	117.90
1	A	329	ARG	CB-CA-C	-10.10	90.21	110.40
1	A	212	VAL	CG1-CB-CG2	-10.04	94.84	110.90
1	A	368	LEU	CB-CG-CD2	9.94	127.90	111.00
1	A	205	LEU	CA-CB-CG	9.93	138.14	115.30
1	D	57	VAL	N-CA-C	9.59	136.89	111.00
1	D	74	VAL	CB-CA-C	-9.47	93.41	111.40
1	A	181	LEU	CA-CB-CG	9.43	137.00	115.30
1	D	55	LEU	CB-CG-CD2	-9.27	95.23	111.00
1	A	692	TYR	CG-CD1-CE1	-9.23	113.92	121.30
1	A	368	LEU	CB-CG-CD1	9.11	126.49	111.00
1	A	328	THR	C-N-CA	9.06	144.36	121.70
1	A	212	VAL	C-N-CA	-9.05	99.08	121.70
1	A	692	TYR	CD1-CE1-CZ	-8.95	111.75	119.80
1	D	56	VAL	C-N-CA	8.91	143.97	121.70
1	D	264	LEU	CB-CG-CD1	-8.87	95.92	111.00
1	D	71	LEU	CB-CG-CD2	8.84	126.03	111.00
1	A	369	LYS	CA-CB-CG	8.67	132.48	113.40
1	D	58	LYS	CA-CB-CG	8.66	132.44	113.40
1	A	692	TYR	CA-CB-CG	8.53	129.60	113.40
1	A	775	LYS	CD-CE-NZ	-8.50	92.15	111.70
1	D	73	GLY	N-CA-C	8.05	133.23	113.10
1	D	57	VAL	CB-CA-C	-8.04	96.12	111.40
1	A	324	LEU	CB-CG-CD1	8.01	124.61	111.00
1	A	206	VAL	CG1-CB-CG2	-7.97	98.14	110.90
1	D	76	LEU	CA-CB-CG	7.75	133.12	115.30
1	D	73	GLY	CA-C-N	7.68	134.11	117.20
1	D	74	VAL	N-CA-C	7.63	131.60	111.00
1	A	207	VAL	CG1-CB-CG2	7.60	123.06	110.90
1	A	203	ASN	C-N-CD	-7.38	104.35	120.60
1	A	364	TYR	CA-CB-CG	7.37	127.41	113.40
1	D	57	VAL	CA-C-N	7.35	133.37	117.20
1	A	331	LYS	CB-CG-CD	7.18	130.27	111.60
1	A	328	THR	N-CA-CB	-7.17	96.68	110.30
1	D	1017	LYS	CA-CB-CG	-7.10	97.77	113.40
1	A	329	ARG	CB-CG-CD	6.95	129.67	111.60
1	A	346	ASN	N-CA-C	6.86	129.53	111.00
1	D	72	VAL	CA-C-N	6.80	129.79	116.20
1	D	73	GLY	CA-C-O	-6.78	108.40	120.60
1	D	15	LEU	CA-CB-CG	6.69	130.70	115.30
1	D	74	VAL	CG1-CB-CG2	6.66	121.55	110.90
1	A	323	ILE	CB-CA-C	6.66	124.91	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	LEU	CA-CB-CG	6.65	130.60	115.30
1	A	368	LEU	CB-CA-C	6.64	122.82	110.20
1	D	57	VAL	CA-CB-CG1	6.57	120.75	110.90
1	A	205	LEU	CB-CA-C	6.52	122.58	110.20
1	A	326	LEU	N-CA-C	6.51	128.59	111.00
1	A	118	GLU	CB-CA-C	6.51	123.42	110.40
1	A	127	ARG	CA-C-O	-6.50	106.45	120.10
1	A	328	THR	CA-C-N	6.50	131.49	117.20
1	A	327	MET	CB-CG-SD	-6.49	92.94	112.40
1	A	357	ILE	CG1-CB-CG2	-6.43	97.25	111.40
1	D	57	VAL	O-C-N	-6.41	112.44	122.70
1	B	833	LEU	CA-CB-CG	6.35	129.90	115.30
1	B	358	VAL	CG1-CB-CG2	-6.34	100.75	110.90
1	D	72	VAL	CA-CB-CG1	6.28	120.32	110.90
1	A	177	LYS	CD-CE-NZ	6.27	126.12	111.70
1	D	72	VAL	CG1-CB-CG2	6.22	120.86	110.90
1	A	269	LEU	CA-CB-CG	6.21	129.59	115.30
1	A	127	ARG	CA-C-N	6.11	130.63	117.20
1	B	1017	LYS	CA-CB-CG	-6.11	99.96	113.40
1	B	133	LEU	CA-CB-CG	6.09	129.32	115.30
1	A	326	LEU	CA-C-N	6.04	130.48	117.20
1	A	329	ARG	CG-CD-NE	-6.03	99.13	111.80
1	A	350	VAL	CG1-CB-CG2	-6.03	101.25	110.90
1	A	702	LEU	CA-CB-CG	6.01	129.12	115.30
1	A	369	LYS	N-CA-C	6.00	127.21	111.00
1	A	369	LYS	CA-C-N	5.94	130.26	117.20
1	A	203	ASN	C-N-CA	5.94	146.94	122.00
1	A	327	MET	CA-CB-CG	5.92	123.37	113.30
1	B	939	LEU	CB-CG-CD1	-5.91	100.96	111.00
1	A	206	VAL	O-C-N	-5.87	113.31	122.70
1	A	344	ILE	C-N-CA	5.81	136.23	121.70
1	C	833	LEU	CA-CB-CG	5.79	128.62	115.30
1	A	362	ARG	CB-CG-CD	5.72	126.47	111.60
1	A	834	ILE	C-N-CA	5.71	135.98	121.70
1	B	1049	ASP	CB-CG-OD1	5.68	123.41	118.30
1	B	1004	LEU	CA-CB-CG	5.67	128.33	115.30
1	D	56	VAL	CA-C-O	-5.66	108.21	120.10
1	A	85	LEU	CA-CB-CG	5.61	128.19	115.30
1	B	15	LEU	CA-CB-CG	5.59	128.15	115.30
1	B	388	LEU	CA-CB-CG	5.57	128.12	115.30
1	C	1053	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	128	GLU	CB-CA-C	-5.54	99.31	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	106	LEU	CA-CB-CG	5.54	128.04	115.30
1	D	74	VAL	C-N-CA	5.46	135.35	121.70
1	A	366	GLY	C-N-CD	-5.43	108.66	120.60
1	D	55	LEU	CB-CG-CD1	5.37	120.13	111.00
1	D	194	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	328	THR	O-C-N	-5.37	114.11	122.70
1	A	329	ARG	N-CA-C	5.36	125.48	111.00
1	A	370	GLU	C-N-CA	5.35	135.07	121.70
1	A	393	GLU	C-N-CA	-5.35	108.34	121.70
1	A	775	LYS	CB-CG-CD	-5.25	97.96	111.60
1	A	643	LEU	CB-CG-CD1	-5.24	102.09	111.00
1	A	368	LEU	N-CA-CB	-5.20	100.01	110.40
1	D	264	LEU	CA-CB-CG	5.16	127.16	115.30
1	A	367	PRO	N-CA-C	5.14	125.46	112.10
1	C	817	PRO	O-C-N	5.12	130.82	121.10
1	B	1021	LEU	CA-CB-CG	-5.06	103.66	115.30
1	D	72	VAL	N-CA-C	5.05	124.63	111.00
1	A	153	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	106	LEU	CA-CB-CG	5.04	126.89	115.30
1	D	536	ASP	CB-CG-OD1	5.03	122.82	118.30
1	A	120	TYR	CB-CG-CD1	5.02	124.01	121.00
1	D	1053	ASP	CB-CG-OD1	5.02	122.81	118.30

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	Mainchain,Peptide
1	A	119	PHE	Peptide
1	A	120	TYR	Mainchain
1	A	121	VAL	Peptide
1	A	122	CYS	Peptide
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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	355	0
1	B	7906	0	7956	219	0
1	C	7906	0	7956	157	0
1	D	7906	0	7956	205	0
2	A	48	0	32	19	0
2	B	48	0	32	40	0
All	All	31720	0	31885	896	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 14.

All (896) 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:1018:LYS:NZ	2:A:1201:COA:O1A	1.61	1.33
1:A:127:ARG:C	1:A:128:GLU:N	1.84	1.29
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:328:THR:C	1:A:369:LYS:H	1.97	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:177:LYS:HZ1	1:A:211:GLY:H	1.46	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:1040:CYS:SG	1:D:1041:GLY:N	2.73	0.59
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:D:612:LYS:HE2	1:D:616:LYS:HE3	1.88	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:B:1044:THR:OG1	1:B:1045:ARG:N	2.37	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:A:329:ARG:HG2	1:A:367:PRO:C	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:1044:THR:OG1	1:D:1045:ARG:N	2.38	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:B:885:TYR:HH	1:B:1040:CYS:HG	1.55	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:1044:THR:OG1	1:C:1045:ARG:N	2.41	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:A:534:THR:OG1	1:A:535:GLY:N	2.39	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:D:44:LEU:HA	1:D:50:LEU:HD12	1.90	0.53
1:A:288:TYR:HD1	1:A:415:VAL:HG22	1.74	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:708:PRO:O	1:C:711:LYS:NZ	2.38	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:D:948:LYS:O	1:D:952:SER:OG	2.31	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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:118:GLU:C	1:A:206:VAL:H	2.19	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: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:C:838:ALA:H	1:D:540:LYS:HZ3	1.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:LEU:O	1:D:192:TYR:N	2.49	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: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:119:PHE:HA	1:A:205:LEU:C	2.36	0.45
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:C:841:MET:HE2	1:A:1079:LEU:HB3	1.99	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:C:561:ARG:HB2	1:C:562:LYS:HZ2	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:747:THR:OG1	1:A:748:CYS:N	2.46	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:705:GLN:NE2	1:C:737:THR:H	2.15	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: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:A:635:LYS:NZ	1:A:637:GLY:O	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:D:872:VAL:HG23	1:B:1067:MET:HE3	2.01	0.43
1:A:571:ASN:HB3	1:A:596:ILE:HA	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:581:SER:O	1:C:585:THR:OG1	2.23	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
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: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:A:177:LYS:HZ2	1:A:209:LYS:C	2.21	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:A:887:CYS:SG	1:A:888:GLN:N	2.93	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: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: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:C:65:ARG:HD3	1:C:65:ARG:HA	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ILE:HA	1:C:131:TYR:O	2.20	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
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: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:C:577:SER:HB3	1:A:964:LYS:HZ1	1.85	0.42
1:C:836:LYS:NZ	1:B:1090:ASP:OD1	2.33	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: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:127:ARG:C	1:A:692:TYR:CZ	2.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:789:SER:OG	1:A:790:PHE:N	2.52	0.41
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:VAL:HA	1:A:43:LEU:HD22	2.03	0.41
1:A:127:ARG:C	1:A:692:TYR:CD2	2.94	0.41
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:664:GLY:O	1:D:667:SER:OG	2.30	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: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:8:GLU:CD	1:D:66:ARG:HH12	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:53:GLN:HB3	1:A:112:PRO:HD3	2.04	0.40
1:A:328:THR:C	1:A:369:LYS:N	2.71	0.40
1:A:652:TYR:OH	1:A:816:VAL:O	2.29	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%)	8	42
1	B	1017/1101 (92%)	936 (92%)	78 (8%)	3 (0%)	41	76
1	C	1017/1101 (92%)	942 (93%)	73 (7%)	2 (0%)	47	81
1	D	1017/1101 (92%)	930 (91%)	80 (8%)	7 (1%)	22	62
All	All	4066/4404 (92%)	3694 (91%)	342 (8%)	30 (1%)	26	62

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	842/909 (93%)	813 (97%)	29 (3%)	37	61
1	B	842/909 (93%)	838 (100%)	4 (0%)	88	93
1	C	842/909 (93%)	834 (99%)	8 (1%)	76	86
1	D	842/909 (93%)	832 (99%)	10 (1%)	71	84
All	All	3368/3636 (93%)	3317 (98%)	51 (2%)	68	80

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	64	LYS
1	C	68	LYS
1	C	209	LYS
1	C	226[A]	ASP
1	C	226[B]	ASP
1	C	653	ARG
1	C	710	VAL
1	C	944	LYS
1	D	54	ASN
1	D	57	VAL
1	D	71	LEU
1	D	74	VAL
1	D	82	LYS
1	D	101	PHE
1	D	226[A]	ASP
1	D	226[B]	ASP
1	D	386	GLU
1	D	653	ARG
1	A	10	THR
1	A	111	VAL
1	A	118	GLU
1	A	119	PHE
1	A	126	THR
1	A	207	VAL
1	A	224	THR
1	A	226[A]	ASP
1	A	226[B]	ASP
1	A	324	LEU
1	A	327	MET
1	A	344	ILE

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Mol	Chain	Res	Type
1	A	346	ASN
1	A	347	PHE
1	A	348	THR
1	A	364	TYR
1	A	365	GLN
1	A	368	LEU
1	A	369	LYS
1	A	378	ARG
1	A	389	ARG
1	A	394	VAL
1	A	500	ILE
1	A	505	GLN
1	A	507	ARG
1	A	567	ASP
1	A	568	VAL
1	A	653	ARG
1	A	692	TYR
1	B	64	LYS
1	B	226[A]	ASP
1	B	226[B]	ASP
1	B	653	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	61	GLN
1	C	104	ASN
1	C	270	ASN
1	C	314	GLN
1	C	332	HIS
1	C	505	GLN
1	C	705	GLN
1	C	807	ASN
1	C	850	GLN
1	C	908	HIS
1	C	1072	HIS
1	C	1076	GLN
1	D	61	GLN
1	D	332	HIS
1	D	671	ASN
1	D	850	GLN
1	D	908	HIS

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Mol	Chain	Res	Type
1	D	961	ASN
1	D	982	ASN
1	D	996	GLN
1	D	1024	ASN
1	A	150	GLN
1	A	299	ASN
1	A	371	HIS
1	A	510	GLN
1	A	571	ASN
1	A	587	ASN
1	A	908	HIS
1	A	961	ASN
1	A	1076	GLN
1	B	45	GLN
1	B	61	GLN
1	B	505	GLN
1	B	587	ASN
1	B	671	ASN
1	B	850	GLN
1	B	900	HIS
1	B	908	HIS
1	B	982	ASN
1	B	1024	ASN

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 monosaccharides 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	B	1201	-	41,50,50	4.01	14 (34%)	52,75,75	2.64	12 (23%)
2	COA	A	1201	-	41,50,50	3.98	15 (36%)	52,75,75	2.41	8 (15%)

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	B	1201	-	-	15/44/64/64	0/3/3/3
2	COA	A	1201	-	-	12/44/64/64	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	COA	O4B-C1B	16.40	1.64	1.41
2	A	1201	COA	O4B-C1B	14.81	1.61	1.41
2	A	1201	COA	C2B-C1B	-14.08	1.32	1.53
2	B	1201	COA	C2B-C1B	-13.10	1.33	1.53
2	A	1201	COA	C9P-N8P	7.46	1.49	1.33
2	B	1201	COA	C9P-N8P	7.15	1.49	1.33
2	A	1201	COA	O4B-C4B	-6.20	1.31	1.45
2	A	1201	COA	C5P-N4P	5.92	1.46	1.33
2	B	1201	COA	O4B-C4B	-5.75	1.32	1.45
2	B	1201	COA	C5P-N4P	5.42	1.45	1.33
2	A	1201	COA	C6A-N6A	3.57	1.47	1.34
2	B	1201	COA	C6A-N6A	3.52	1.46	1.34
2	A	1201	COA	P3B-O3B	3.41	1.65	1.59
2	B	1201	COA	C5A-C4A	-3.25	1.32	1.40
2	A	1201	COA	C5A-C4A	-3.13	1.32	1.40
2	A	1201	COA	C6P-C5P	2.84	1.56	1.51
2	B	1201	COA	P3B-O3B	2.81	1.64	1.59
2	A	1201	COA	O9P-C9P	-2.78	1.17	1.23
2	A	1201	COA	OAP-CAP	-2.63	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	COA	C6P-C5P	2.60	1.56	1.51
2	B	1201	COA	O9P-C9P	-2.59	1.18	1.23
2	B	1201	COA	C3B-C4B	2.48	1.59	1.52
2	B	1201	COA	O2B-C2B	2.46	1.48	1.43
2	B	1201	COA	C2A-N3A	2.43	1.36	1.32
2	B	1201	COA	OAP-CAP	-2.38	1.37	1.42
2	A	1201	COA	O2B-C2B	2.36	1.48	1.43
2	A	1201	COA	C2A-N3A	2.27	1.35	1.32
2	A	1201	COA	P1A-O5B	2.19	1.68	1.59
2	A	1201	COA	O3B-C3B	-2.01	1.36	1.44

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	COA	C5A-C6A-N6A	11.38	137.64	120.35
2	B	1201	COA	C5A-C6A-N6A	10.62	136.49	120.35
2	A	1201	COA	N6A-C6A-N1A	-7.94	102.10	118.57
2	B	1201	COA	N6A-C6A-N1A	-7.50	103.00	118.57
2	B	1201	COA	N3A-C2A-N1A	-7.08	117.62	128.68
2	B	1201	COA	C5B-C4B-C3B	-6.51	92.84	114.40
2	A	1201	COA	N3A-C2A-N1A	-5.08	120.74	128.68
2	A	1201	COA	P2A-O3A-P1A	-4.11	118.72	132.83
2	B	1201	COA	P2A-O3A-P1A	-3.46	120.95	132.83
2	B	1201	COA	C6P-C7P-N8P	-3.41	105.02	111.90
2	B	1201	COA	O5B-C5B-C4B	3.15	119.82	108.99
2	B	1201	COA	C3B-C2B-C1B	2.70	105.88	99.89
2	B	1201	COA	C2P-C3P-N4P	-2.66	106.23	112.31
2	A	1201	COA	C5B-C4B-C3B	-2.65	105.60	114.40
2	B	1201	COA	C1B-N9A-C4A	-2.61	122.06	126.64
2	A	1201	COA	CAP-C9P-N8P	2.58	121.72	116.58
2	B	1201	COA	C6P-C5P-N4P	2.24	120.19	116.42
2	A	1201	COA	CDP-CBP-CCP	-2.18	104.67	108.23
2	A	1201	COA	C6P-C5P-N4P	2.13	120.01	116.42
2	B	1201	COA	C7P-C6P-C5P	-2.01	109.01	112.36

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	COA	C3B-O3B-P3B-O7A
2	A	1201	COA	CCP-O6A-P2A-O3A
2	A	1201	COA	CAP-CBP-CCP-O6A

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Mol	Chain	Res	Type	Atoms
2	A	1201	COA	O9P-C9P-CAP-OAP
2	A	1201	COA	N8P-C9P-CAP-OAP
2	A	1201	COA	S1P-C2P-C3P-N4P
2	B	1201	COA	C5B-O5B-P1A-O1A
2	B	1201	COA	C5B-O5B-P1A-O2A
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	A	1201	COA	CDP-CBP-CCP-O6A
2	A	1201	COA	CEP-CBP-CCP-O6A
2	B	1201	COA	O9P-C9P-CAP-OAP
2	B	1201	COA	C4B-C5B-O5B-P1A
2	A	1201	COA	P2A-O3A-P1A-O5B
2	B	1201	COA	P2A-O3A-P1A-O5B
2	B	1201	COA	C3B-C4B-C5B-O5B
2	A	1201	COA	C5B-O5B-P1A-O3A
2	B	1201	COA	C3B-O3B-P3B-O7A
2	A	1201	COA	O4B-C4B-C5B-O5B
2	B	1201	COA	C3B-O3B-P3B-O8A
2	B	1201	COA	C5B-O5B-P1A-O3A
2	B	1201	COA	P2A-O3A-P1A-O1A
2	A	1201	COA	C5B-O5B-P1A-O2A
2	B	1201	COA	O9P-C9P-CAP-CBP

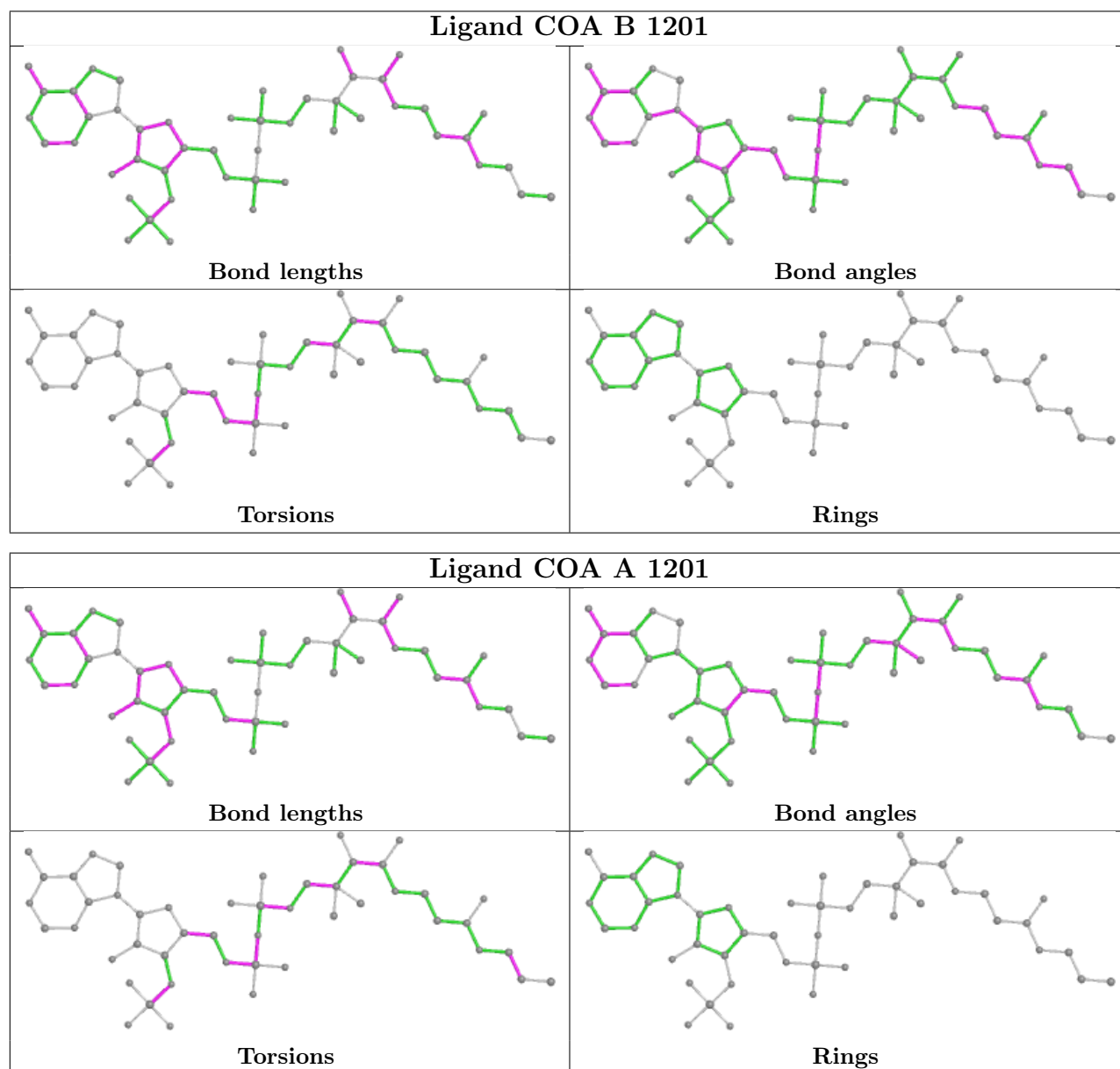
There are no ring outliers.

2 monomers are involved in 59 short contacts:

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:
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Mol	Chain	Number of breaks
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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

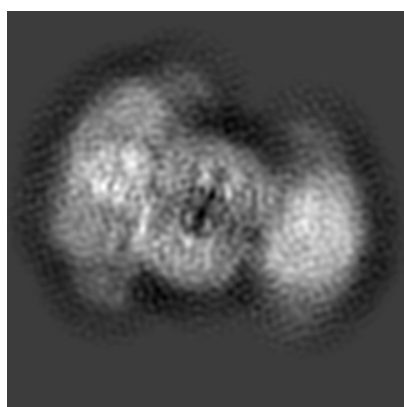
6 Map visualisation [i](#)

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.

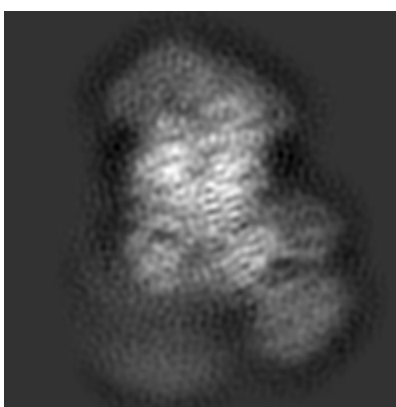
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

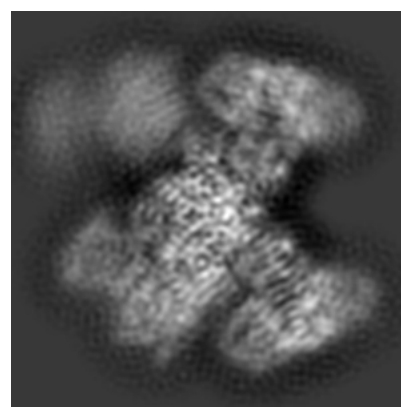
6.1.1 Primary map



X



Y

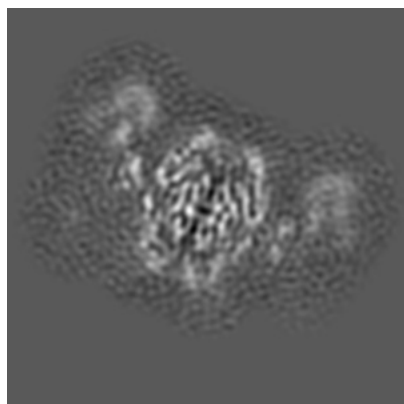


Z

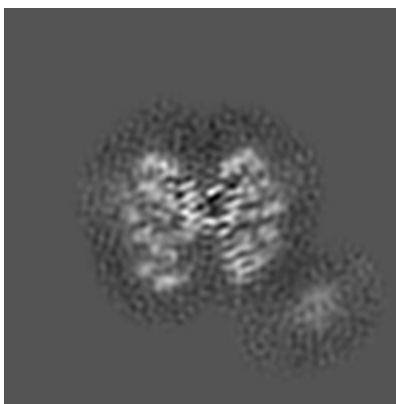
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

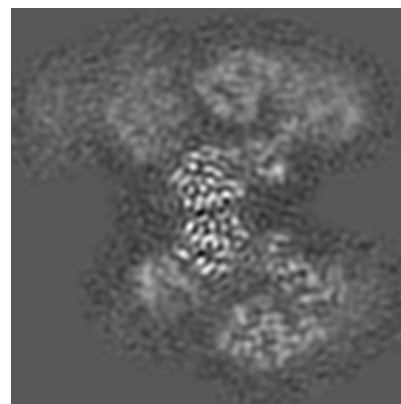
6.2.1 Primary map



X Index: 110



Y Index: 110

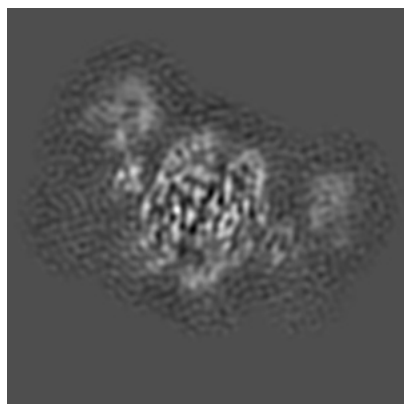


Z Index: 110

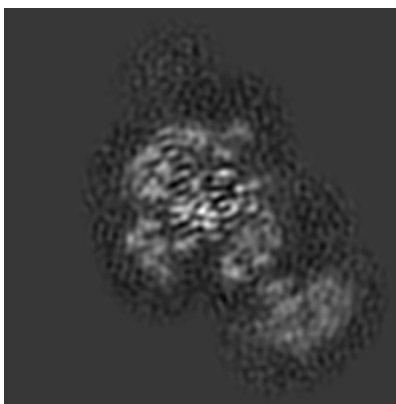
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

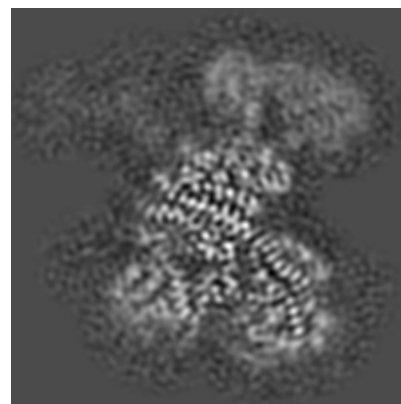
6.3.1 Primary map



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 surface views [i](#)

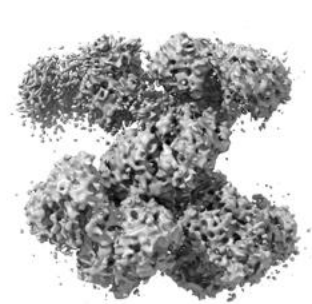
6.4.1 Primary map



X



Y



Z

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.

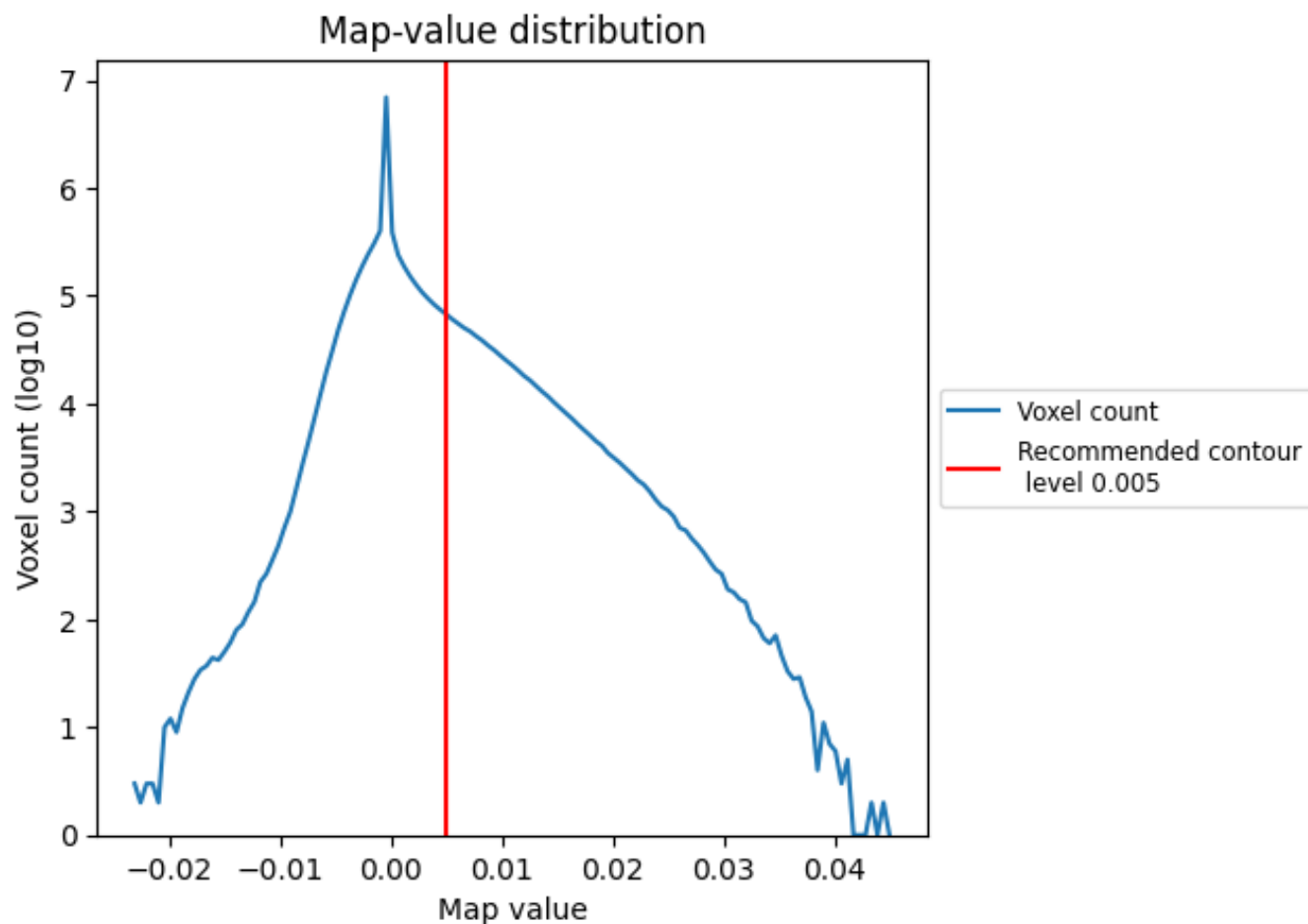
6.5 Mask visualisation

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

7 Map analysis [i](#)

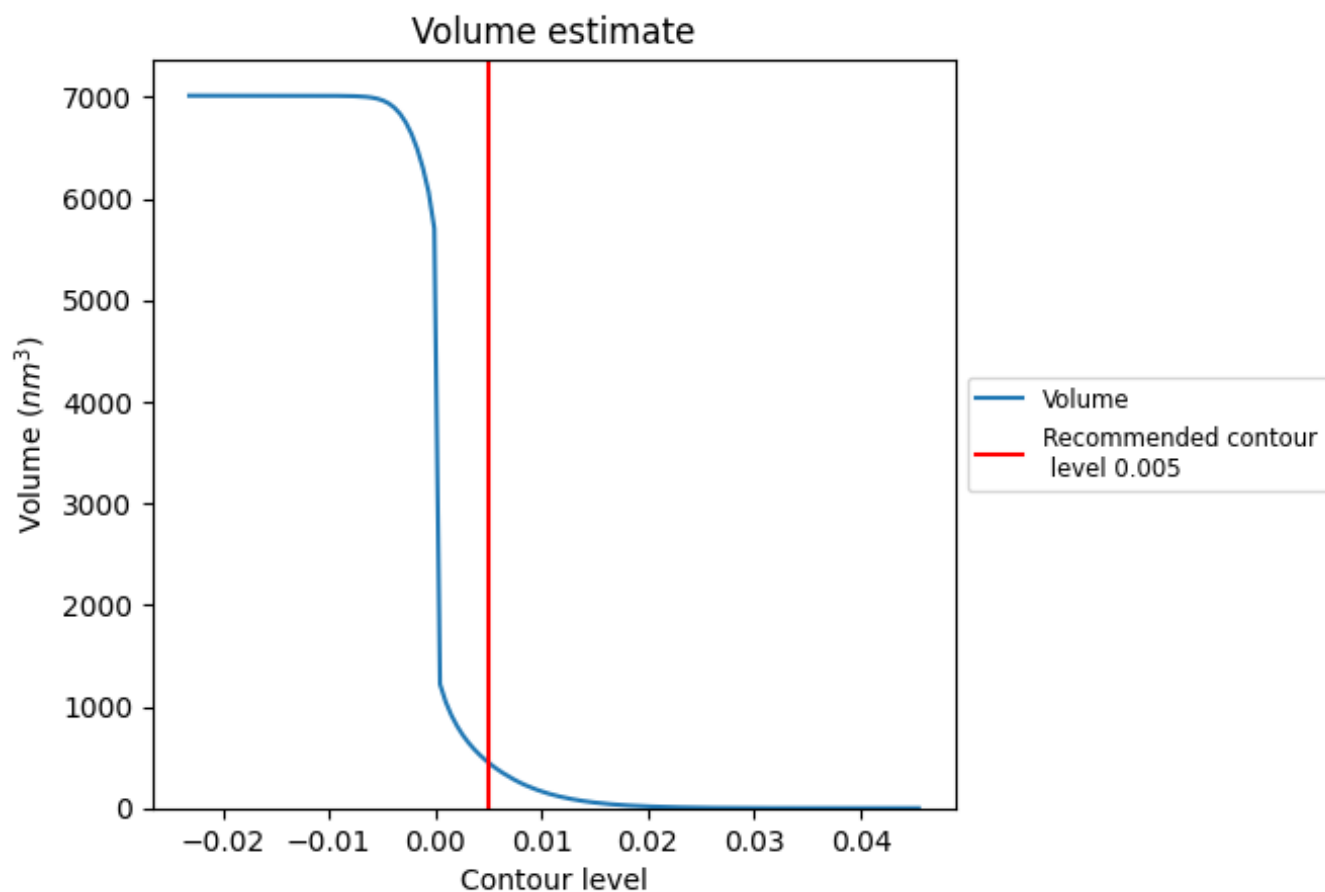
This section contains the results of statistical analysis of the map.

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.

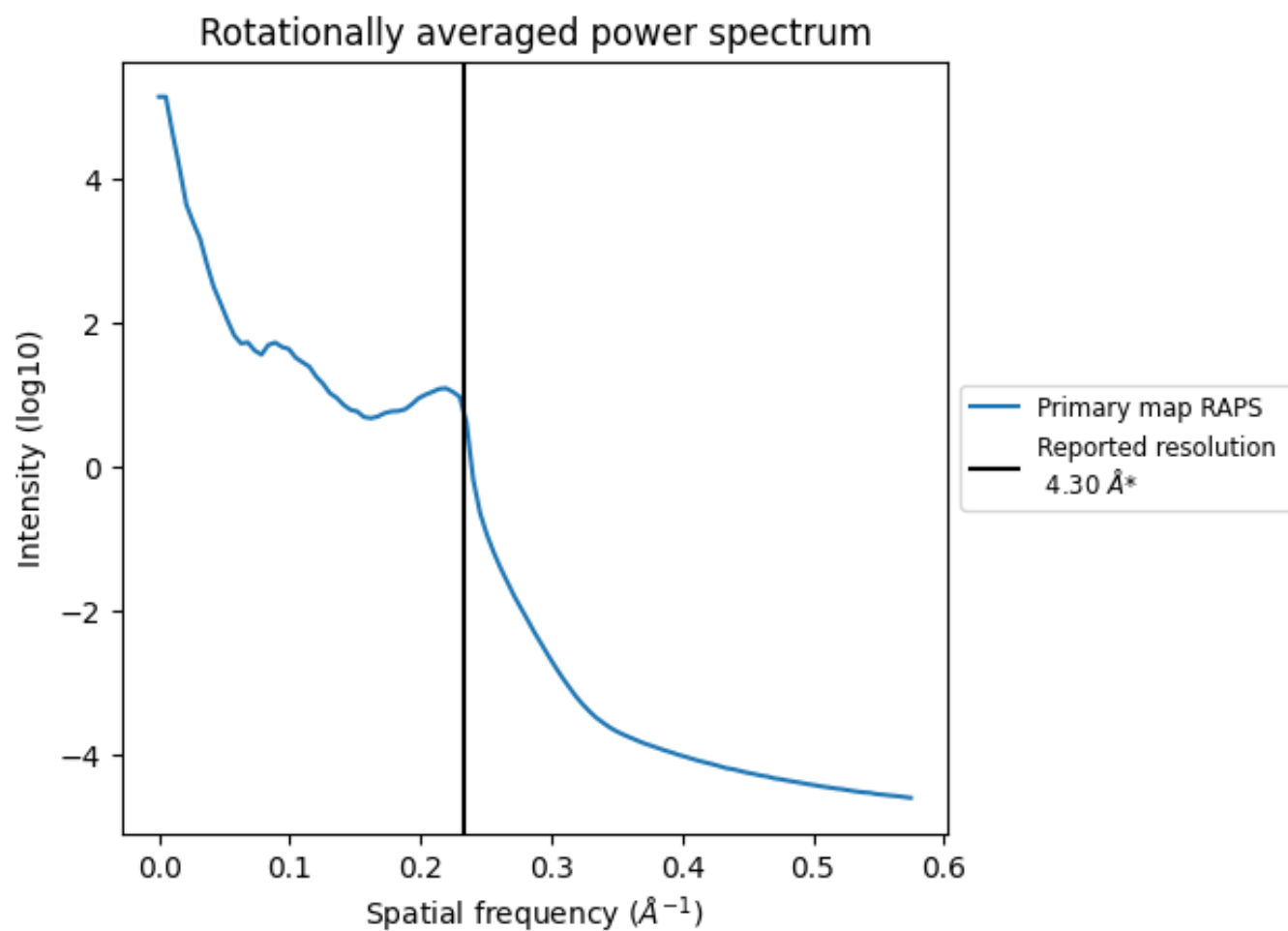
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 448 nm^3 ; 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

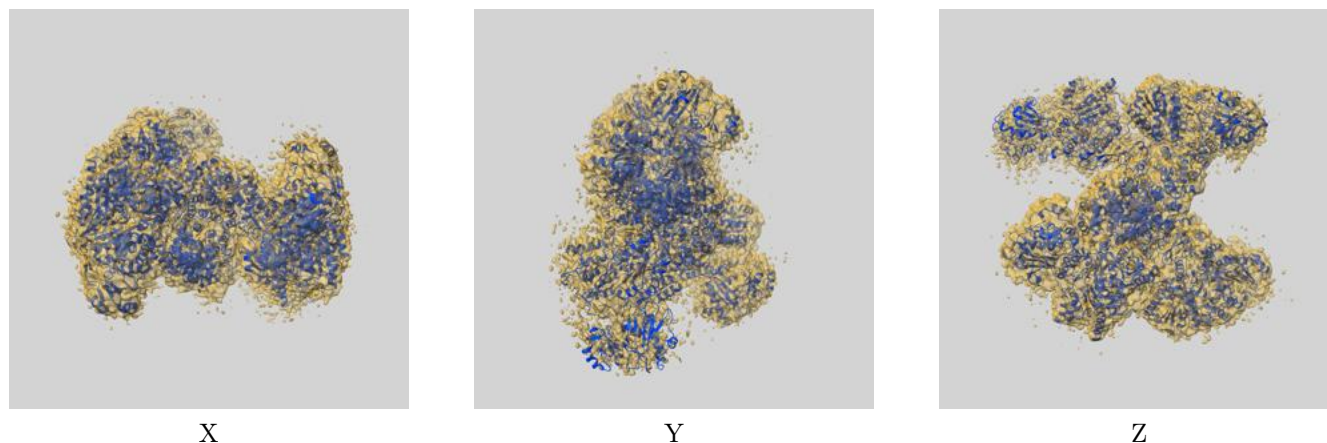
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

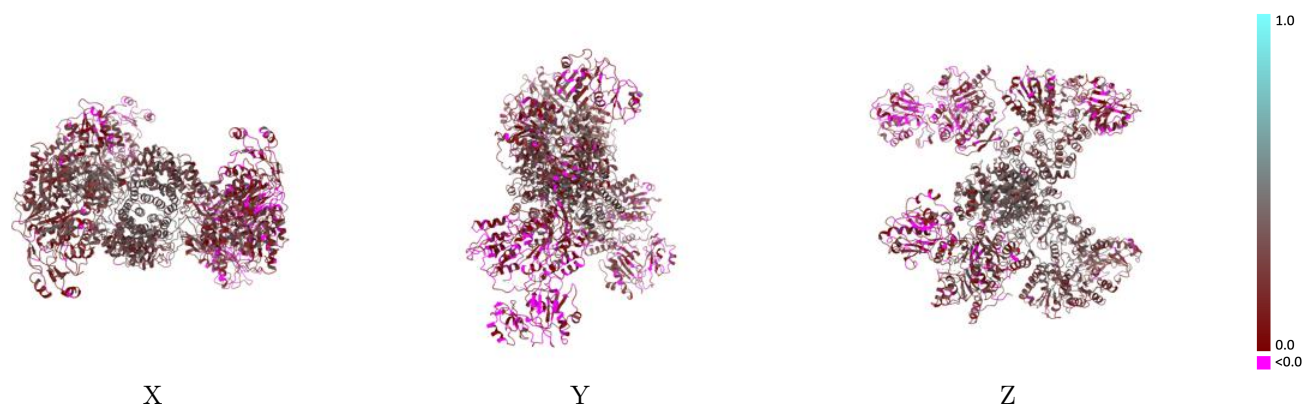
This section contains information regarding the fit between EMDB map EMD-20784 and PDB model 6UIA. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



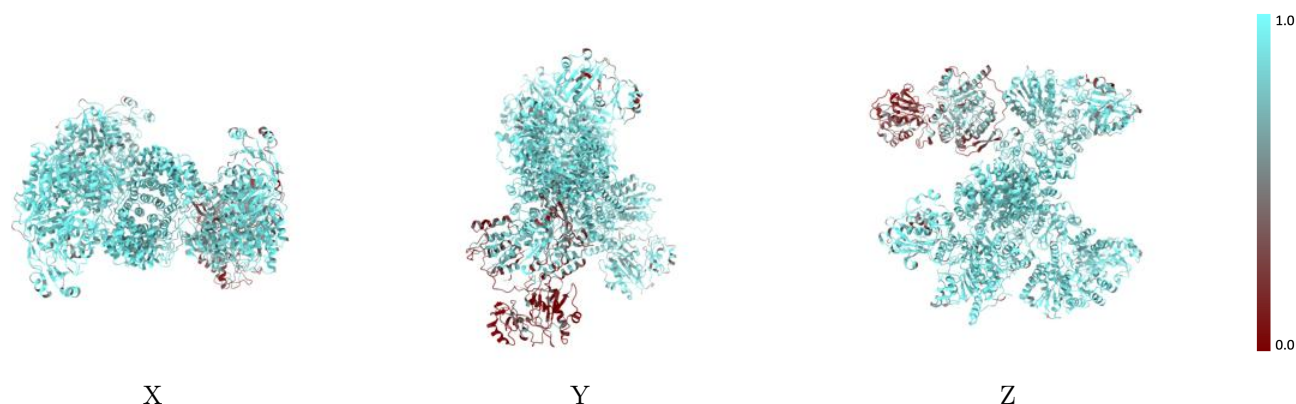
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



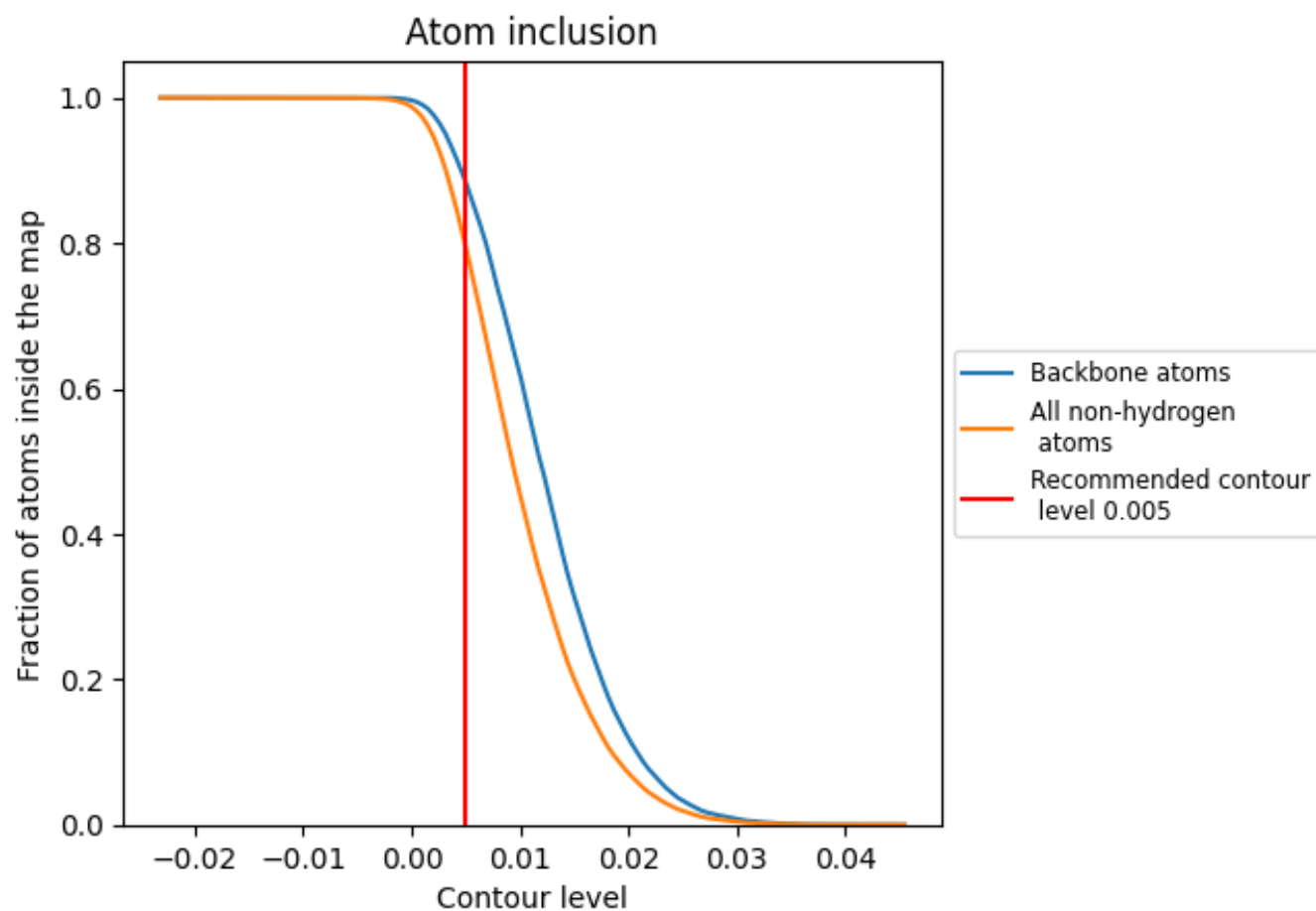
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 79% 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	<div></div> 0.7947	<div></div> 0.2140
A	<div></div> 0.5664	<div></div> 0.1360
B	<div></div> 0.8461	<div></div> 0.2200
C	<div></div> 0.8960	<div></div> 0.2770
D	<div></div> 0.8713	<div></div> 0.2210

