



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:57 PM UTC

PDB ID : 7LO5 / pdb_00007lo5
EMDB ID : EMD-23461
Title : cryoEM structure DrdV-DNA complex
Authors : Shen, B.W.; Stoddard, B.L.
Deposited on : 2021-02-09
Resolution : 2.86 Å(reported)

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:

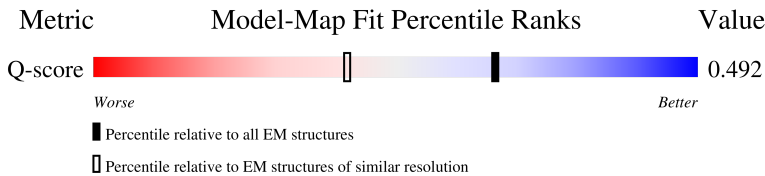
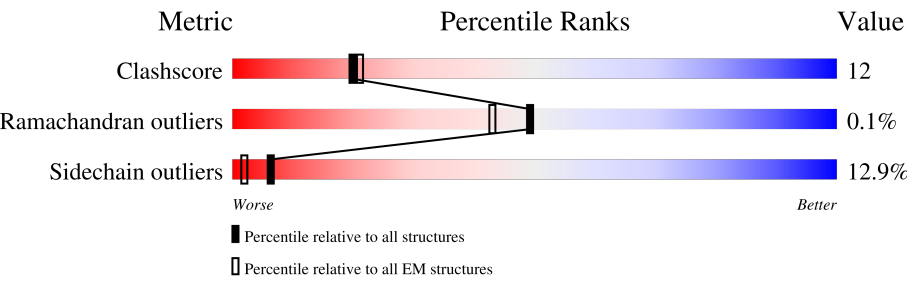
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.86 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	12017 (2.36 - 3.36)

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	1029	73%24%..
1	B	1029	76%21%..
1	C	1029	72%24%..
1	D	1029	31% 61%33%..

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Mol	Chain	Length	Quality of chain
2	E	29	76% 21%
2	G	29	59% 34%
2	I	29	31% 83% 14%
2	K	29	28% 72% 14% 14%
3	F	29	76% 17% 7%
3	H	29	83% 10% 7%
3	J	29	24% 66% 28% 7%
3	L	29	34% 76% 10% 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 37449 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 Site-specific DNA-methyltransferase (adenine-specific).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1016	Total	C	N	O	S	0	0
			8249	5243	1445	1542	19		
1	B	1013	Total	C	N	O	S	0	0
			8230	5232	1441	1538	19		
1	C	1014	Total	C	N	O	S	0	0
			8234	5232	1442	1540	20		
1	D	1012	Total	C	N	O	S	0	0
			8221	5227	1441	1533	20		

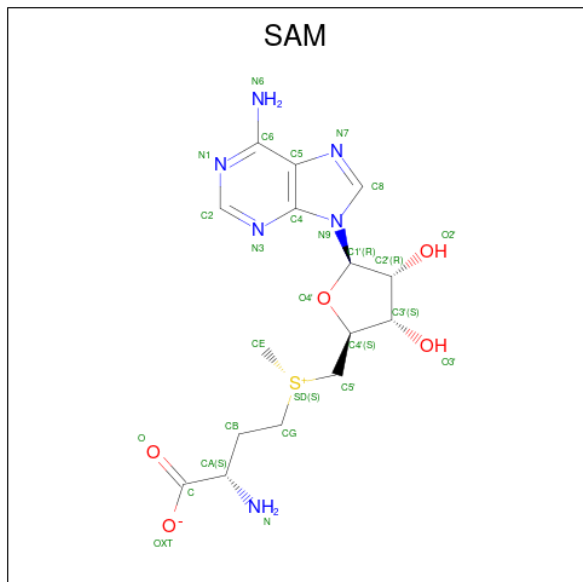
- Molecule 2 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	28	Total	C	N	O	P	0	0
			561	265	107	161	28		
2	G	28	Total	C	N	O	P	0	0
			561	265	107	161	28		
2	I	28	Total	C	N	O	P	0	0
			561	265	107	161	28		
2	K	25	Total	C	N	O	P	0	0
			504	238	98	143	25		

- Molecule 3 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	27	Total	C	N	O	P	0	0
			565	266	103	169	27		
3	H	27	Total	C	N	O	P	0	0
			565	266	103	169	27		
3	J	27	Total	C	N	O	P	0	0
			565	266	103	169	27		
3	L	25	Total	C	N	O	P	0	0
			521	246	93	157	25		

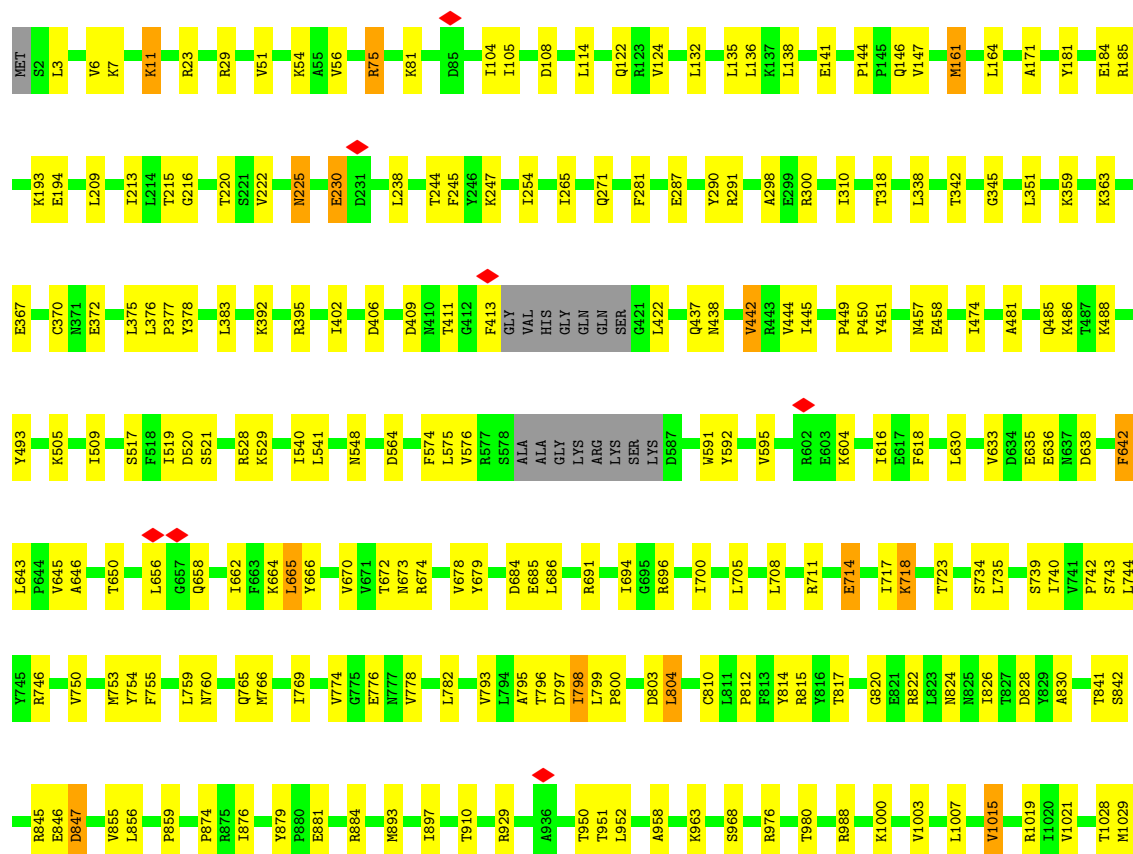
- Molecule 4 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	S	0
			27	15	6	5	1	
4	B	1	Total	C	N	O	S	0
			27	15	6	5	1	
4	C	1	Total	C	N	O	S	0
			27	15	6	5	1	
4	D	1	Total	C	N	O	S	0
			27	15	6	5	1	

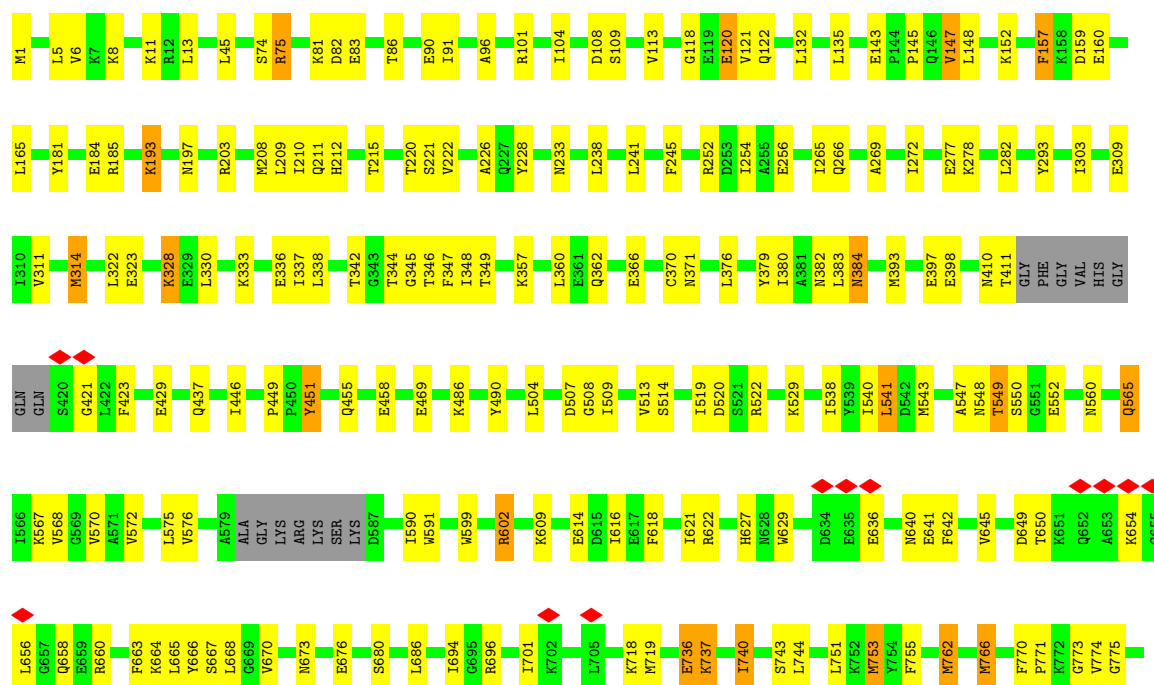
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

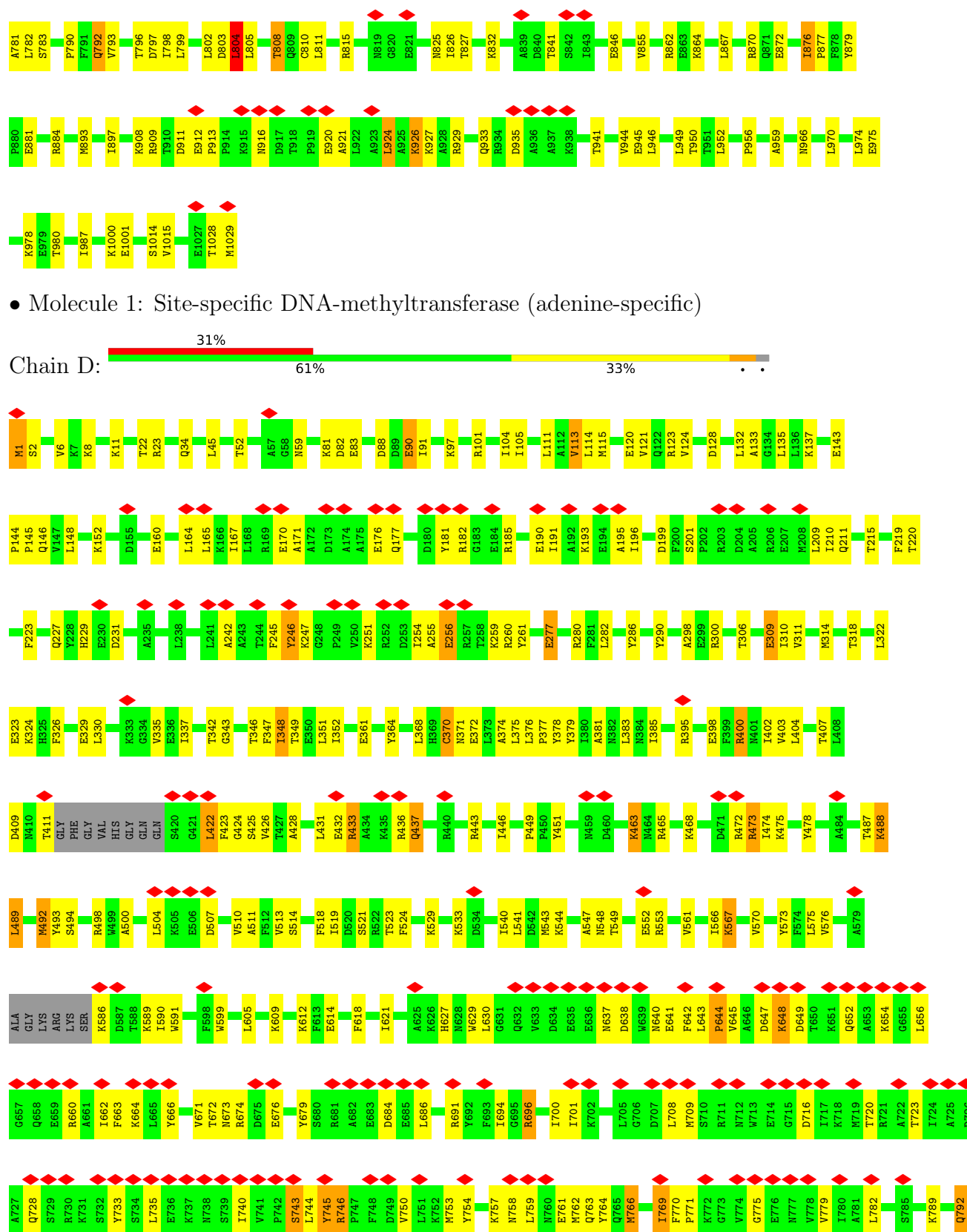
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	B	1	Total	Ca	0
			1	1	
5	C	1	Total	Ca	0
			1	1	
5	D	1	Total	Ca	0
			1	1	

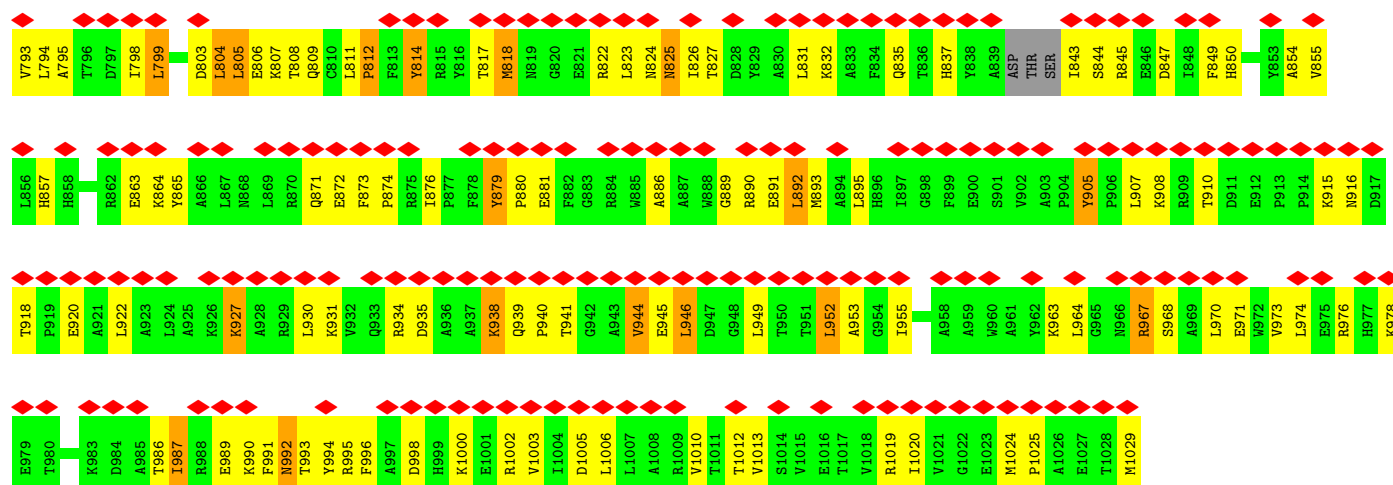


- Molecule 1: Site-specific DNA-methyltransferase (adenine-specific)

Chain C: 72% 24% ..

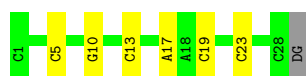






• Molecule 2: DNA (28-MER)

Chain E: 76% 21% .



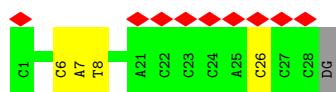
• Molecule 2: DNA (28-MER)

Chain G: 59% 34% . .



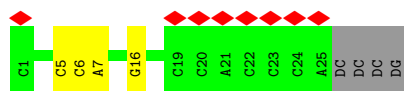
• Molecule 2: DNA (28-MER)

Chain I: 31% 83% 14% .



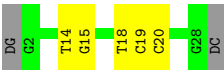
• Molecule 2: DNA (28-MER)

Chain K: 28% 72% 14% 14%

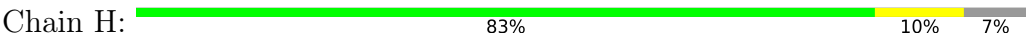


• Molecule 3: DNA (27-MER)

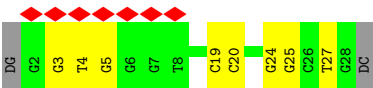
Chain F: 76% 17% 7%



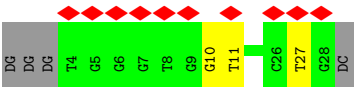
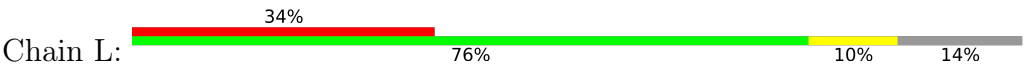
- Molecule 3: DNA (27-MER)



- Molecule 3: DNA (27-MER)



- Molecule 3: DNA (27-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	94920	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.020	Depositor
Minimum map value	-0.381	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.18	Depositor
Map size ($\text{\AA}$)	526.08, 526.08, 526.08	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0275, 1.0275, 1.0275	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: CA, SAM

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	0.86	3/8430 (0.0%)	1.24	13/11391 (0.1%)
1	B	0.88	3/8411 (0.0%)	1.23	11/11367 (0.1%)
1	C	0.88	4/8414 (0.0%)	1.25	9/11371 (0.1%)
1	D	0.89	2/8400 (0.0%)	1.23	18/11348 (0.2%)
2	E	0.41	0/628	0.74	3/962 (0.3%)
2	G	0.51	0/628	0.80	3/962 (0.3%)
2	I	0.39	0/628	0.70	0/962
2	K	0.46	0/565	0.73	1/866 (0.1%)
3	F	0.44	0/633	0.71	1/979 (0.1%)
3	H	0.42	0/633	0.74	0/979
3	J	0.44	0/633	0.81	3/979 (0.3%)
3	L	0.45	0/583	0.74	1/901 (0.1%)
All	All	0.83	12/38586 (0.0%)	1.18	63/53067 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	987	ILE	C-N	7.97	1.44	1.33
1	A	2	SER	C-N	6.70	1.42	1.33
1	A	449	PRO	C-O	-6.31	1.19	1.25
1	C	74	SER	C-N	-6.10	1.24	1.33
1	B	442	VAL	C-N	6.07	1.41	1.33
1	B	449	PRO	C-O	-5.98	1.19	1.24
1	C	449	PRO	C-O	-5.63	1.20	1.24
1	D	449	PRO	C-O	-5.22	1.20	1.24
1	B	485	GLN	C-N	5.19	1.41	1.33
1	D	876	ILE	N-CA	5.12	1.50	1.46
1	A	363	LYS	C-N	-5.06	1.27	1.33
1	C	75	ARG	C-N	5.02	1.40	1.33

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	548	ASN	N-CA-C	-8.32	104.16	112.97
1	C	522	ARG	N-CA-C	-8.03	104.09	114.04
2	G	23	DC	C2'-C3'-O3'	-7.87	99.69	111.50
1	C	548	ASN	N-CA-C	-7.62	104.89	112.97
1	B	638	ASP	N-CA-C	-7.37	104.25	112.57
1	B	804	LEU	N-CA-C	-7.12	103.45	111.07
1	C	987	ILE	O-C-N	6.83	128.87	121.83
1	D	812	PRO	N-CA-C	6.82	120.77	111.22
1	C	804	LEU	N-CA-C	-6.70	103.67	110.97
2	E	17	DA	C2'-C3'-O3'	6.57	121.36	111.50
1	D	548	ASN	N-CA-C	-6.56	106.02	112.97
1	D	745	TYR	N-CA-C	-6.40	106.06	114.31
1	D	764	TYR	CB-CA-C	-6.36	107.43	116.34
1	A	804	LEU	N-CA-C	-6.28	104.35	111.07
1	A	929	ARG	N-CA-C	-6.27	105.65	113.55
2	G	2	DA	C2'-C3'-O3'	-6.09	102.37	111.50
1	C	913	PRO	CA-C-O	-6.02	115.97	120.73
1	B	798	ILE	CB-CA-C	5.90	120.12	110.69
3	J	3	DG	C2'-C3'-O3'	5.89	120.33	111.50
3	F	20	DC	C2'-C3'-O3'	-5.80	102.81	111.50
1	B	442	VAL	O-C-N	5.79	129.23	122.81
2	G	13	DC	C2'-C3'-O3'	-5.78	102.83	111.50
1	A	626	LYS	N-CA-C	-5.75	106.12	113.02
1	B	184	GLU	O-C-N	5.71	128.17	122.12
1	B	108	ASP	N-CA-C	-5.69	102.34	110.59
1	D	409	ASP	CA-CB-CG	5.67	118.27	112.60
1	D	91	ILE	N-CA-C	-5.65	105.00	110.42
3	L	27	DT	C2'-C3'-O3'	5.65	119.97	111.50
1	A	422	LEU	N-CA-C	-5.64	106.19	112.57
1	C	108	ASP	N-CA-C	-5.61	102.16	110.46
1	D	97	LYS	N-CA-C	-5.60	106.50	113.38
1	D	799	LEU	N-CA-C	5.60	117.66	109.71
1	A	876	ILE	N-CA-C	5.57	114.01	107.77
1	D	306	THR	CA-C-O	-5.57	115.67	119.29
1	A	217	ASP	N-CA-C	-5.55	106.55	113.55
1	D	879	TYR	CB-CA-C	5.55	116.34	110.17
1	B	847	ASP	N-CA-C	-5.53	105.83	113.18
1	A	548	ASN	N-CA-C	-5.52	106.59	113.15
1	B	876	ILE	N-CA-C	5.50	114.54	108.05
1	D	426	VAL	N-CA-C	-5.49	105.15	110.42
1	D	488	LYS	N-CA-C	-5.46	106.39	112.57
1	C	565	GLN	N-CA-C	-5.43	107.30	114.31
2	E	19	DC	C4'-C3'-O3'	5.43	118.15	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	490	TYR	N-CA-C	-5.41	106.46	112.57
1	A	728	GLN	N-CA-C	-5.37	106.57	113.23
1	D	193	LYS	N-CA-C	-5.37	106.69	113.18
2	K	16	DG	C2'-C3'-O3'	-5.34	103.49	111.50
1	D	489	LEU	N-CA-C	-5.32	106.82	113.15
1	B	411	THR	N-CA-C	-5.32	106.38	112.92
1	A	24	ASN	CB-CA-C	5.29	118.70	109.65
1	D	745	TYR	CB-CA-C	5.23	117.81	109.02
1	D	220	THR	N-CA-C	-5.14	107.66	114.04
2	E	13	DC	C2'-C3'-O3'	-5.14	103.79	111.50
3	J	27	DT	C2'-C3'-O3'	5.13	119.20	111.50
1	A	121	VAL	N-CA-C	-5.13	107.75	111.90
1	D	874	PRO	CB-CA-C	-5.12	103.11	111.56
1	A	788	ALA	N-CA-C	-5.11	107.12	113.55
1	B	739	SER	N-CA-C	-5.05	108.14	114.56
1	A	881	GLU	CA-C-O	-5.05	115.70	120.90
3	J	20	DC	C2'-C3'-O3'	-5.04	103.94	111.50
1	C	91	ILE	CA-C-O	-5.04	115.83	121.17
1	A	488	LYS	N-CA-C	-5.02	105.63	112.26
1	D	905	TYR	CA-C-O	-5.01	115.04	119.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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	8249	0	8137	176	0
1	B	8230	0	8118	188	0
1	C	8234	0	8128	254	0
1	D	8221	0	8124	262	0
2	E	561	0	310	3	0
2	G	561	0	310	14	0
2	I	561	0	310	4	0
2	K	504	0	277	2	0
3	F	565	0	306	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	565	0	306	5	0
3	J	565	0	306	6	0
3	L	521	0	284	1	0
4	A	27	0	22	1	0
4	B	27	0	22	0	0
4	C	27	0	22	0	0
4	D	27	0	22	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	37449	0	35004	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 12.

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:C:209:LEU:HD21	1:C:245:PHE:CZ	1.32	1.58
1:B:782:LEU:CD2	1:B:793:VAL:HG12	1.35	1.54
1:D:754:TYR:CD2	1:D:759:LEU:HD12	1.49	1.45
1:C:770:PHE:CB	1:C:799:LEU:HD21	1.51	1.38
1:C:645:VAL:HG11	1:C:811:LEU:CD2	1.50	1.38
1:C:770:PHE:CD2	1:C:799:LEU:HD23	1.69	1.28
1:B:645:VAL:HG11	1:B:666:TYR:CD2	1.67	1.28
1:A:645:VAL:HG11	1:A:666:TYR:CD2	1.68	1.28
1:A:645:VAL:CG1	1:A:666:TYR:HD2	1.50	1.23
1:C:209:LEU:CD2	1:C:245:PHE:CZ	2.23	1.22
1:C:222:VAL:CG2	1:C:265:ILE:HG22	1.71	1.20
1:D:247:LYS:HA	1:D:251:LYS:CE	1.72	1.19
1:B:782:LEU:CD2	1:B:793:VAL:CG1	2.21	1.18
1:C:314:MET:HE1	1:C:513:VAL:CG2	1.72	1.18
1:D:519:ILE:CG2	1:D:630:LEU:HD12	1.73	1.17
1:C:770:PHE:HB2	1:C:799:LEU:CD2	1.74	1.17
1:C:538:ILE:HG12	1:C:575:LEU:CD2	1.74	1.17
1:A:225:ASN:HD22	1:A:383:LEU:HD11	1.02	1.16
1:B:766:MET:HE2	1:B:799:LEU:CD1	1.74	1.16
1:C:222:VAL:HG22	1:C:265:ILE:HG22	1.22	1.16
1:D:247:LYS:HA	1:D:251:LYS:CD	1.74	1.16
1:A:696:ARG:NH2	1:A:700:ILE:HG13	1.62	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:ILE:CG2	1:D:385:ILE:HD11	1.78	1.14
1:D:247:LYS:CA	1:D:251:LYS:HE3	1.80	1.12
1:D:247:LYS:HA	1:D:251:LYS:HE3	1.24	1.12
1:A:922:LEU:HD11	1:A:926:LYS:HE3	1.31	1.12
1:C:924:LEU:HD13	1:C:927:LYS:HD2	1.17	1.12
1:C:645:VAL:HG11	1:C:811:LEU:HD22	1.15	1.11
1:B:778:VAL:HG11	1:B:893:MET:HE3	1.12	1.11
1:C:893:MET:HG2	1:C:897:ILE:HD12	1.33	1.11
1:D:891:GLU:CD	1:D:1020:ILE:HD11	1.74	1.11
1:C:935:ASP:CG	1:C:941:THR:HG21	1.75	1.10
1:B:670:VAL:HG21	1:B:799:LEU:HD21	1.35	1.09
1:D:519:ILE:HG22	1:D:630:LEU:HD12	1.27	1.09
1:D:255:ALA:O	1:D:259:LYS:HG3	1.53	1.08
2:G:18:DA:H2''	2:G:19:DC:H5'	1.16	1.08
1:B:766:MET:HE2	1:B:799:LEU:HD12	1.18	1.08
1:C:793:VAL:HG12	1:C:862:ARG:NH2	1.69	1.08
1:C:645:VAL:HG11	1:C:811:LEU:HD21	1.30	1.07
1:B:782:LEU:HD22	1:B:793:VAL:HG12	1.30	1.07
1:C:645:VAL:CG1	1:C:811:LEU:HD22	1.83	1.07
1:C:773:GLY:HA2	1:C:799:LEU:HD11	1.31	1.07
1:A:330:LEU:CD2	1:A:337:ILE:HD11	1.85	1.07
1:C:538:ILE:HG23	1:C:575:LEU:CD2	1.85	1.07
1:D:519:ILE:CG2	1:D:630:LEU:CD1	2.33	1.07
1:A:922:LEU:CD1	1:A:926:LYS:HE3	1.83	1.06
1:A:153:ALA:HB1	1:A:265:ILE:HD13	1.37	1.06
1:A:696:ARG:HH22	1:A:700:ILE:HG13	1.14	1.06
1:A:330:LEU:HD22	1:A:337:ILE:HD11	1.38	1.05
1:C:538:ILE:HG12	1:C:575:LEU:HD22	1.09	1.05
1:D:891:GLU:CG	1:D:1020:ILE:HD11	1.86	1.05
1:D:403:VAL:HG12	1:D:433:ARG:CG	1.86	1.04
1:D:403:VAL:HG12	1:D:433:ARG:HG3	1.08	1.04
1:B:782:LEU:HD23	1:B:793:VAL:HG12	1.10	1.04
1:B:766:MET:CE	1:B:799:LEU:CD1	2.37	1.03
1:D:754:TYR:CE2	1:D:759:LEU:HD12	1.94	1.03
1:C:645:VAL:CG1	1:C:811:LEU:CD2	2.36	1.02
1:C:212:HIS:HB2	1:C:238:LEU:HD21	1.42	1.02
1:D:403:VAL:CG1	1:D:433:ARG:HG3	1.89	1.01
1:B:778:VAL:HG11	1:B:893:MET:CE	1.89	1.01
1:C:519:ILE:HD11	1:C:540:ILE:HG21	1.39	1.01
1:D:886:ALA:O	1:D:890:ARG:HG3	1.59	1.01
1:A:645:VAL:HG11	1:A:666:TYR:HD2	0.85	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1003:VAL:O	1:B:1007:LEU:HD13	1.60	1.00
1:D:891:GLU:HG3	1:D:1020:ILE:HD11	1.40	1.00
1:C:209:LEU:HD21	1:C:245:PHE:CE2	1.97	0.98
1:D:754:TYR:CD2	1:D:759:LEU:CD1	2.46	0.98
1:B:442:VAL:HG11	1:B:445:ILE:HD11	1.40	0.98
1:D:209:LEU:HD21	1:D:245:PHE:CE2	1.99	0.98
1:B:766:MET:CE	1:B:799:LEU:HD12	1.94	0.97
1:D:348:ILE:HG23	1:D:385:ILE:HD11	1.45	0.97
1:B:645:VAL:HG11	1:B:666:TYR:HD2	1.23	0.97
1:B:519:ILE:HG22	1:B:630:LEU:HD12	1.46	0.96
1:D:247:LYS:CA	1:D:251:LYS:HG3	1.96	0.96
1:C:222:VAL:HG21	1:C:265:ILE:CG2	1.96	0.96
1:D:891:GLU:HG3	1:D:1020:ILE:CD1	1.96	0.96
1:C:770:PHE:CB	1:C:799:LEU:CD2	2.36	0.95
1:D:766:MET:CE	1:D:799:LEU:HD22	1.97	0.95
1:A:645:VAL:CG1	1:A:666:TYR:CD2	2.36	0.95
1:C:212:HIS:HB2	1:C:238:LEU:CD2	1.96	0.95
1:B:645:VAL:CG1	1:B:666:TYR:CD2	2.48	0.94
1:B:670:VAL:CG2	1:B:799:LEU:HD21	1.97	0.94
1:D:375:LEU:HD11	1:D:379:TYR:CZ	2.00	0.94
1:C:222:VAL:CG2	1:C:265:ILE:CG2	2.44	0.94
1:C:209:LEU:CD2	1:C:245:PHE:HZ	1.69	0.94
1:C:770:PHE:CD2	1:C:799:LEU:CD2	2.50	0.94
1:D:347:PHE:O	1:D:351:LEU:HG	1.67	0.93
1:D:209:LEU:HD21	1:D:245:PHE:HE2	1.29	0.93
1:C:770:PHE:HD2	1:C:799:LEU:HD23	1.32	0.93
1:D:245:PHE:CD1	1:D:246:TYR:N	2.37	0.93
1:B:171:ALA:HB2	1:B:254:ILE:CD1	1.99	0.92
1:C:538:ILE:CG1	1:C:575:LEU:HD22	1.99	0.92
1:C:924:LEU:HD13	1:C:927:LYS:CD	1.99	0.92
1:D:247:LYS:N	1:D:251:LYS:HG3	1.84	0.92
1:D:754:TYR:HD2	1:D:759:LEU:CD1	1.83	0.92
1:B:519:ILE:CG2	1:B:630:LEU:HD12	1.99	0.92
2:G:18:DA:C2'	2:G:19:DC:H5'	1.97	0.91
1:C:935:ASP:CG	1:C:941:THR:CG2	2.42	0.91
1:A:946:LEU:HD11	1:A:952:LEU:HD13	1.52	0.91
1:C:538:ILE:HG23	1:C:575:LEU:HD23	1.52	0.91
1:B:442:VAL:HG11	1:B:445:ILE:CD1	1.98	0.91
1:C:181:TYR:CE1	1:C:245:PHE:CE2	2.59	0.91
1:A:225:ASN:ND2	1:A:383:LEU:HD11	1.85	0.91
1:C:228:TYR:HE1	1:C:382:ASN:ND2	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:ILE:HG21	1:D:385:ILE:HD11	1.50	0.90
1:A:225:ASN:HD22	1:A:383:LEU:CD1	1.82	0.90
1:C:209:LEU:HD21	1:C:245:PHE:HZ	1.08	0.90
1:C:538:ILE:HG23	1:C:575:LEU:HD21	1.51	0.90
1:B:782:LEU:HD23	1:B:793:VAL:CG1	1.97	0.89
1:B:803:ASP:OD2	3:H:19:DC:C5	2.26	0.89
1:A:800:PRO:HG2	1:A:810:CYS:SG	2.12	0.89
1:D:891:GLU:CG	1:D:1020:ILE:CD1	2.51	0.89
1:C:803:ASP:OD2	3:J:19:DC:C5	2.25	0.89
1:D:891:GLU:CD	1:D:1020:ILE:CD1	2.45	0.89
1:D:519:ILE:HG21	1:D:630:LEU:CD1	2.01	0.89
1:D:529:LYS:HD2	1:D:627:HIS:NE2	1.88	0.89
1:D:905:TYR:HB2	1:D:1012:THR:HG23	1.54	0.88
1:A:922:LEU:CG	1:A:926:LYS:HE3	2.03	0.88
1:C:1:MET:HE2	1:C:609:LYS:HD3	1.53	0.88
1:A:338:LEU:HD11	1:A:437:GLN:NE2	1.89	0.88
1:C:666:TYR:HB3	1:C:811:LEU:CD2	2.04	0.88
1:C:770:PHE:HB2	1:C:799:LEU:HD21	0.90	0.88
1:B:800:PRO:HG3	1:B:810:CYS:SG	2.13	0.87
1:C:773:GLY:HA2	1:C:799:LEU:CD1	2.04	0.87
2:G:18:DA:H2''	2:G:19:DC:C5'	2.04	0.87
1:B:519:ILE:CG2	1:B:630:LEU:CD1	2.53	0.86
1:D:891:GLU:OE2	1:D:1020:ILE:CD1	2.24	0.85
1:C:538:ILE:CG2	1:C:575:LEU:CD2	2.54	0.85
1:A:336:GLU:OE1	1:A:441:PRO:HD2	1.77	0.85
1:B:265:ILE:CD1	1:B:281:PHE:CE1	2.59	0.85
1:C:916:ASN:OD1	1:C:921:ALA:CB	2.24	0.85
1:D:242:ALA:HA	1:D:245:PHE:CE2	2.12	0.85
1:C:314:MET:HE1	1:C:513:VAL:HG21	1.58	0.85
1:C:974:LEU:O	1:C:978:LYS:HG3	1.77	0.85
1:C:924:LEU:CD1	1:C:927:LYS:HD2	2.05	0.84
1:C:793:VAL:HG12	1:C:862:ARG:HH21	1.40	0.84
1:C:181:TYR:HE1	1:C:245:PHE:CE2	1.96	0.84
1:C:538:ILE:CG1	1:C:575:LEU:CD2	2.55	0.84
1:B:171:ALA:CB	1:B:254:ILE:CD1	2.55	0.83
1:D:543:MET:HB3	1:D:561:VAL:HG21	1.58	0.83
1:C:212:HIS:CD2	1:C:238:LEU:HD23	2.13	0.83
1:A:922:LEU:HD11	1:A:926:LYS:CE	2.07	0.83
1:B:171:ALA:HB2	1:B:254:ILE:HD13	1.60	0.83
1:C:272:ILE:O	1:C:278:LYS:CE	2.25	0.83
1:A:743:SER:HA	1:A:798:ILE:HG22	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:ALA:HA	1:D:245:PHE:CZ	2.14	0.82
1:D:519:ILE:HG21	1:D:630:LEU:HD11	1.60	0.82
1:C:924:LEU:HD11	1:C:927:LYS:HZ2	1.45	0.82
1:D:247:LYS:HA	1:D:251:LYS:CG	2.10	0.82
1:A:315:ILE:HG12	1:A:351:LEU:HD21	1.62	0.82
1:C:203:ARG:HH12	1:C:293:TYR:HE1	1.26	0.81
1:D:543:MET:CB	1:D:561:VAL:HG21	2.11	0.81
1:B:778:VAL:CG1	1:B:893:MET:HE3	2.05	0.81
1:C:893:MET:HG2	1:C:897:ILE:CD1	2.10	0.81
1:D:740:ILE:HG12	1:D:754:TYR:HA	1.63	0.81
1:D:209:LEU:CD2	1:D:245:PHE:CE2	2.64	0.81
1:C:209:LEU:CG	1:C:245:PHE:HZ	1.94	0.81
1:B:797:ASP:OD2	1:B:897:ILE:HG23	1.81	0.80
1:A:338:LEU:CD1	1:A:437:GLN:NE2	2.44	0.80
1:A:318:THR:O	1:A:322:LEU:HG	1.82	0.80
1:D:372:GLU:OE2	1:D:377:PRO:CB	2.30	0.80
1:C:338:LEU:HD11	1:C:437:GLN:NE2	1.97	0.79
1:C:519:ILE:HD11	1:C:540:ILE:CG2	2.12	0.79
1:B:122:GLN:HB3	1:B:135:LEU:HD13	1.64	0.79
1:C:272:ILE:O	1:C:278:LYS:HE3	1.82	0.79
1:C:538:ILE:CG2	1:C:575:LEU:HD21	2.12	0.79
1:C:946:LEU:HD11	1:C:952:LEU:HD13	1.65	0.79
1:B:519:ILE:HG21	1:B:630:LEU:CD1	2.13	0.79
1:C:666:TYR:HB3	1:C:811:LEU:HD23	1.65	0.78
1:B:754:TYR:CE2	1:B:759:LEU:HD12	2.19	0.78
1:B:800:PRO:CG	1:B:810:CYS:SG	2.71	0.78
1:C:770:PHE:CG	1:C:799:LEU:CD2	2.65	0.78
1:A:153:ALA:CB	1:A:265:ILE:HD13	2.13	0.78
1:B:1003:VAL:HG12	1:B:1007:LEU:HD11	1.65	0.78
1:B:1003:VAL:HG12	1:B:1007:LEU:CD1	2.14	0.78
1:C:222:VAL:HG21	1:C:265:ILE:HG21	1.65	0.77
1:D:342:THR:OG1	1:D:370:CYS:HB2	1.84	0.77
1:A:330:LEU:HD22	1:A:337:ILE:CD1	2.13	0.77
1:B:171:ALA:CB	1:B:254:ILE:HD11	2.13	0.77
1:C:222:VAL:HG13	1:C:269:ALA:CB	2.14	0.77
1:C:649:ASP:O	1:C:664:LYS:HE3	1.85	0.77
1:B:1003:VAL:O	1:B:1007:LEU:CD1	2.32	0.77
1:D:245:PHE:CE1	1:D:246:TYR:HB2	2.20	0.77
1:D:211:GLN:O	1:D:215:THR:HG22	1.85	0.77
1:C:893:MET:CG	1:C:897:ILE:HD12	2.13	0.77
1:B:754:TYR:HE2	1:B:759:LEU:HD12	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:LEU:HD11	1:C:245:PHE:CZ	2.20	0.77
1:C:744:LEU:N	1:C:798:ILE:CD1	2.48	0.77
1:A:315:ILE:HG12	1:A:351:LEU:CD2	2.16	0.77
1:B:519:ILE:HG22	1:B:630:LEU:CD1	2.13	0.76
1:D:247:LYS:CB	1:D:251:LYS:HE3	2.16	0.76
1:D:246:TYR:O	1:D:251:LYS:CE	2.32	0.76
1:C:774:VAL:HG12	1:C:774:VAL:O	1.85	0.76
1:A:338:LEU:HD11	1:A:437:GLN:HE22	1.50	0.76
1:B:265:ILE:HD11	1:B:281:PHE:CD1	2.20	0.76
1:C:797:ASP:OD2	1:C:897:ILE:CG2	2.34	0.76
1:C:181:TYR:CD1	1:C:245:PHE:CD2	2.74	0.76
1:D:227:GLN:HG2	1:D:231:ASP:OD2	1.85	0.76
1:A:822:ARG:O	1:A:822:ARG:HG3	1.84	0.75
1:C:770:PHE:CG	1:C:799:LEU:HD23	2.22	0.75
1:D:398:GLU:CD	1:D:400:ARG:HH21	1.95	0.75
1:D:691:ARG:HA	1:D:735:LEU:HD21	1.68	0.75
1:B:171:ALA:HB2	1:B:254:ILE:HD11	1.68	0.75
1:C:744:LEU:N	1:C:798:ILE:HD12	2.02	0.75
2:G:18:DA:H61	3:H:11:DT:H3	1.32	0.74
1:B:519:ILE:HG21	1:B:630:LEU:HD11	1.69	0.74
1:A:719:MET:SD	1:A:723:THR:HG21	2.28	0.74
1:C:181:TYR:HE1	1:C:245:PHE:HE2	1.35	0.74
1:C:228:TYR:HE1	1:C:382:ASN:HD22	1.35	0.74
1:A:916:ASN:ND2	1:C:96:ALA:O	2.21	0.73
1:C:547:ALA:HB3	1:C:567:LYS:HB2	1.69	0.73
1:C:893:MET:CG	1:C:897:ILE:CD1	2.66	0.73
1:B:122:GLN:NE2	1:B:138:LEU:HD12	2.04	0.73
1:D:247:LYS:HA	1:D:251:LYS:HD2	1.70	0.73
1:C:309:GLU:HG2	1:C:609:LYS:HD2	1.70	0.72
1:D:247:LYS:CA	1:D:251:LYS:CG	2.67	0.72
1:D:754:TYR:HD2	1:D:759:LEU:HD12	0.96	0.72
1:D:504:LEU:HD21	1:D:510:VAL:HG23	1.71	0.72
1:A:211:GLN:O	1:A:215:THR:HG22	1.89	0.72
1:B:893:MET:O	1:B:897:ILE:HG12	1.88	0.72
1:B:171:ALA:CB	1:B:254:ILE:HD13	2.18	0.72
1:D:543:MET:HB3	1:D:561:VAL:CG2	2.20	0.72
1:C:228:TYR:CE1	1:C:382:ASN:ND2	2.57	0.72
1:C:209:LEU:CD1	1:C:245:PHE:HZ	2.02	0.72
1:C:314:MET:HE1	1:C:513:VAL:HG23	1.68	0.72
1:B:782:LEU:HD22	1:B:793:VAL:CG1	2.03	0.72
1:C:935:ASP:OD2	1:C:941:THR:HG21	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:THR:OG1	1:B:370:CYS:HB2	1.89	0.72
1:D:348:ILE:HG12	1:D:385:ILE:HD13	1.69	0.72
1:D:432:GLU:O	1:D:436:ARG:HG3	1.90	0.72
1:C:209:LEU:HD11	1:C:245:PHE:HZ	1.55	0.71
1:C:771:PRO:HD2	1:C:775:GLY:HA3	1.72	0.71
1:B:75:ARG:HD3	1:B:144:PRO:HG3	1.72	0.71
1:C:916:ASN:OD1	1:C:921:ALA:HB2	1.89	0.71
1:D:443:ARG:HH21	1:D:507:ASP:CG	1.98	0.71
1:D:500:ALA:O	1:D:504:LEU:HD13	1.89	0.71
1:D:504:LEU:HD11	1:D:510:VAL:HG22	1.71	0.71
1:D:674:ARG:HH12	1:D:723:THR:HG21	1.55	0.71
1:B:696:ARG:HH11	1:B:714:GLU:CG	2.04	0.71
1:C:793:VAL:HG12	1:C:862:ARG:HH22	1.54	0.71
1:A:726:ASP:HB2	1:A:731:LYS:HE3	1.71	0.71
1:D:309:GLU:HG3	1:D:605:LEU:HD22	1.73	0.70
1:C:347:PHE:CD1	1:C:446:ILE:HG12	2.26	0.70
1:D:891:GLU:OE2	1:D:1020:ILE:HD13	1.89	0.70
1:B:122:GLN:NE2	1:B:138:LEU:CD1	2.55	0.70
1:B:674:ARG:HH22	1:B:723:THR:HG23	1.55	0.70
1:D:754:TYR:CE2	1:D:759:LEU:CD1	2.70	0.70
1:A:153:ALA:O	1:A:265:ILE:HD11	1.91	0.70
1:D:246:TYR:O	1:D:251:LYS:HE3	1.90	0.70
1:A:342:THR:CG2	1:A:345:GLY:HA2	2.22	0.70
1:C:924:LEU:HD22	1:C:927:LYS:HE3	1.74	0.70
1:B:442:VAL:CG1	1:B:445:ILE:HD11	2.18	0.69
1:D:114:LEU:HB2	1:D:135:LEU:HD11	1.73	0.69
1:A:656:LEU:HD23	1:A:659:GLU:CD	2.16	0.69
1:C:645:VAL:CG1	1:C:811:LEU:HD21	2.13	0.69
1:B:457:ASN:OD1	1:B:718:LYS:NZ	2.24	0.69
1:D:352:ILE:HD11	1:D:385:ILE:HG23	1.74	0.69
1:D:246:TYR:O	1:D:251:LYS:HE2	1.93	0.69
1:C:272:ILE:O	1:C:278:LYS:NZ	2.26	0.69
1:B:879:TYR:HA	1:B:1029:MET:SD	2.33	0.69
1:C:519:ILE:CD1	1:C:540:ILE:HG21	2.19	0.69
1:B:645:VAL:CG1	1:B:666:TYR:HD2	1.99	0.68
1:C:666:TYR:CB	1:C:811:LEU:HD23	2.22	0.68
1:C:924:LEU:CD1	1:C:927:LYS:HZ2	2.06	0.68
1:B:265:ILE:CD1	1:B:281:PHE:CD1	2.75	0.68
1:B:132:LEU:O	1:B:136:LEU:HD13	1.93	0.68
1:D:590:ILE:HG22	1:D:621:ILE:CG1	2.23	0.68
1:A:586:LYS:NZ	1:A:589:LYS:HE3	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:872:GLU:HG2	1:D:873:PHE:H	1.58	0.68
1:D:987:ILE:HA	1:D:991:PHE:HB2	1.74	0.68
1:B:124:VAL:HG22	1:B:135:LEU:HD22	1.76	0.68
1:B:670:VAL:HG21	1:B:799:LEU:CD2	2.19	0.68
1:B:265:ILE:HD13	1:B:281:PHE:CZ	2.29	0.68
1:B:75:ARG:HD3	1:B:144:PRO:CG	2.24	0.68
1:A:336:GLU:CD	1:A:441:PRO:HD2	2.18	0.68
1:D:766:MET:CE	1:D:799:LEU:CD2	2.72	0.68
1:A:132:LEU:O	1:A:136:LEU:HD13	1.94	0.67
1:C:686:LEU:HD23	1:C:740:ILE:HG23	1.75	0.67
1:D:872:GLU:HG2	1:D:873:PHE:N	2.10	0.67
1:C:766:MET:HG3	1:C:799:LEU:HD22	1.74	0.67
1:D:318:THR:O	1:D:322:LEU:HG	1.94	0.67
1:A:342:THR:HG23	1:A:345:GLY:HA2	1.77	0.67
1:C:770:PHE:HB3	1:C:799:LEU:HD21	1.66	0.67
1:A:719:MET:SD	1:A:723:THR:CG2	2.82	0.67
1:A:338:LEU:CD2	1:A:437:GLN:HE21	2.08	0.66
1:C:338:LEU:CD1	1:C:437:GLN:NE2	2.57	0.66
1:A:791:PHE:CE2	1:A:793:VAL:HG13	2.31	0.66
1:A:880:PRO:HD3	1:A:1029:MET:HE3	1.78	0.66
1:B:342:THR:CG2	1:B:345:GLY:HA2	2.26	0.66
1:B:766:MET:HE3	1:B:799:LEU:CD1	2.22	0.66
1:C:504:LEU:HD11	1:C:508:GLY:HA3	1.77	0.66
1:A:363:LYS:HD2	1:A:367:GLU:OE1	1.96	0.66
1:A:817:THR:OG1	1:A:820:GLY:HA3	1.96	0.66
1:D:398:GLU:OE2	1:D:400:ARG:NH2	2.28	0.66
1:A:331:ALA:HB1	1:A:359:LYS:HD2	1.78	0.66
1:B:318:THR:HG23	1:B:509:ILE:HG21	1.77	0.66
1:B:674:ARG:HH22	1:B:723:THR:CG2	2.07	0.66
1:A:684:ASP:OD1	1:A:685:GLU:N	2.30	0.65
1:A:922:LEU:HG	1:A:926:LYS:HE3	1.75	0.65
1:C:157:PHE:HB2	1:C:265:ILE:HD11	1.77	0.65
1:C:272:ILE:C	1:C:278:LYS:HE3	2.22	0.65
1:A:946:LEU:CD1	1:A:952:LEU:HD13	2.27	0.65
1:A:743:SER:HA	1:A:798:ILE:CG2	2.26	0.65
1:C:338:LEU:CD1	1:C:437:GLN:HE21	2.09	0.65
1:A:916:ASN:CG	1:A:918:THR:HG23	2.22	0.64
1:C:803:ASP:OD2	3:J:19:DC:C6	2.49	0.64
1:B:442:VAL:CG1	1:B:445:ILE:CD1	2.75	0.64
1:B:696:ARG:HH11	1:B:714:GLU:HG2	1.61	0.64
1:D:209:LEU:CD2	1:D:245:PHE:CZ	2.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:MET:CE	1:A:723:THR:HG22	2.27	0.64
1:B:766:MET:HE2	1:B:799:LEU:HD11	1.75	0.64
1:C:209:LEU:CD2	1:C:245:PHE:CE2	2.71	0.64
1:C:916:ASN:OD1	1:C:921:ALA:HB3	1.97	0.64
1:B:265:ILE:HD13	1:B:281:PHE:CE1	2.33	0.64
1:D:621:ILE:HD12	1:D:629:TRP:HB3	1.79	0.64
1:C:541:LEU:HD21	1:C:616:ILE:HD13	1.79	0.64
1:C:744:LEU:HB2	1:C:798:ILE:HD11	1.79	0.64
1:B:342:THR:HG23	1:B:345:GLY:HA2	1.80	0.63
1:C:668:LEU:HD22	1:C:802:LEU:CD1	2.28	0.63
1:B:338:LEU:HD11	1:B:437:GLN:NE2	2.14	0.63
1:B:338:LEU:CD1	1:B:437:GLN:NE2	2.61	0.63
1:B:910:THR:OG1	1:B:951:THR:CG2	2.47	0.63
1:C:314:MET:CE	1:C:513:VAL:CG2	2.64	0.63
1:B:742:PRO:O	1:B:798:ILE:HG23	1.99	0.62
1:B:287:GLU:OE2	1:B:291:ARG:NH1	2.32	0.62
1:D:590:ILE:HG22	1:D:621:ILE:HG12	1.81	0.62
1:B:910:THR:OG1	1:B:951:THR:HG23	1.98	0.62
1:C:455:GLN:NE2	1:C:458:GLU:OE1	2.33	0.62
1:D:735:LEU:N	1:D:735:LEU:HD12	2.15	0.62
1:B:700:ILE:HD12	1:B:717:ILE:HD11	1.80	0.62
1:A:742:PRO:O	1:A:798:ILE:HG23	2.00	0.62
1:B:114:LEU:HB2	1:B:135:LEU:HD11	1.81	0.62
1:B:803:ASP:OD2	3:H:19:DC:C6	2.52	0.62
1:A:922:LEU:HD21	1:A:926:LYS:NZ	2.14	0.62
1:D:223:PHE:CE1	1:D:282:LEU:HD21	2.35	0.62
1:D:547:ALA:HB3	1:D:567:LYS:HG2	1.81	0.61
1:A:406:ASP:HB3	1:A:409:ASP:HB2	1.82	0.61
1:A:645:VAL:HG12	1:A:666:TYR:CD2	2.29	0.61
1:B:541:LEU:HD21	1:B:616:ILE:HD13	1.81	0.61
1:C:344:THR:OG1	1:C:346:THR:HG23	2.00	0.61
1:D:372:GLU:OE2	1:D:377:PRO:HB3	1.98	0.61
1:D:375:LEU:HD11	1:D:379:TYR:OH	2.00	0.61
1:D:487:THR:HA	1:D:523:THR:OG1	2.00	0.61
1:D:794:LEU:HD12	1:D:964:LEU:HD11	1.81	0.61
1:A:586:LYS:HZ3	1:A:589:LYS:HE3	1.63	0.61
1:B:171:ALA:HB1	1:B:254:ILE:CD1	2.31	0.61
1:C:649:ASP:OD1	1:C:664:LYS:CD	2.49	0.61
1:D:766:MET:HE1	1:D:799:LEU:CD2	2.31	0.61
1:B:444:VAL:HG22	1:B:509:ILE:HG22	1.82	0.61
1:C:744:LEU:HD23	1:C:804:LEU:HD11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ALA:C	1:A:265:ILE:HD11	2.26	0.61
1:B:338:LEU:CD1	1:B:437:GLN:HE21	2.14	0.61
1:D:181:TYR:CD1	1:D:245:PHE:CD2	2.89	0.60
1:D:750:VAL:HG13	1:D:798:ILE:HD12	1.82	0.60
1:A:916:ASN:OD1	1:A:918:THR:N	2.29	0.60
1:D:375:LEU:HD11	1:D:379:TYR:CE2	2.35	0.60
1:D:519:ILE:CG2	1:D:630:LEU:HD11	2.20	0.60
1:D:744:LEU:HD23	1:D:804:LEU:HD11	1.83	0.60
1:B:636:GLU:O	1:B:636:GLU:HG2	2.01	0.60
1:C:314:MET:HE1	1:C:513:VAL:HG22	1.75	0.60
1:C:797:ASP:OD2	1:C:897:ILE:HG23	2.01	0.60
1:D:645:VAL:HG11	1:D:666:TYR:HB3	1.82	0.60
1:D:750:VAL:HG13	1:D:798:ILE:CD1	2.30	0.60
1:B:765:GLN:NE2	2:G:5:DC:H5'	2.16	0.60
1:B:782:LEU:HD21	1:B:793:VAL:CG1	2.29	0.60
1:B:700:ILE:CD1	1:B:717:ILE:HD11	2.30	0.60
1:D:361:GLU:OE1	1:D:395:ARG:NH1	2.35	0.60
1:A:408:LEU:O	1:A:411:THR:HG23	2.03	0.59
1:D:372:GLU:OE2	1:D:377:PRO:HB2	2.02	0.59
1:D:766:MET:HE1	1:D:799:LEU:HD22	1.83	0.59
1:D:352:ILE:CD1	1:D:385:ILE:HG23	2.32	0.59
1:C:529:LYS:HD2	1:C:627:HIS:CE1	2.37	0.59
1:D:403:VAL:CG1	1:D:433:ARG:CG	2.63	0.59
1:D:402:ILE:O	1:D:402:ILE:HG23	2.03	0.59
1:C:649:ASP:CG	1:C:664:LYS:HD2	2.28	0.59
1:D:348:ILE:HG12	1:D:385:ILE:CD1	2.32	0.59
1:B:817:THR:OG1	1:B:820:GLY:HA3	2.02	0.59
1:A:672:THR:HG22	1:A:674:ARG:HG3	1.84	0.59
1:A:338:LEU:CD1	1:A:437:GLN:HE21	2.16	0.58
1:B:450:PRO:HA	2:G:11:DA:H62	1.67	0.58
1:C:520:ASP:OD1	1:C:520:ASP:O	2.22	0.58
1:A:737:LYS:NZ	1:A:740:ILE:HD12	2.18	0.58
1:B:6:VAL:HG13	1:B:132:LEU:HD23	1.85	0.58
1:A:352:ILE:HG23	1:A:360:LEU:HD21	1.86	0.58
1:C:209:LEU:CD1	1:C:245:PHE:CZ	2.84	0.58
1:B:800:PRO:HG2	1:B:810:CYS:SG	2.42	0.58
1:C:181:TYR:CD1	1:C:245:PHE:HD2	2.19	0.58
1:A:153:ALA:HB1	1:A:265:ILE:CD1	2.24	0.58
1:A:642:PHE:HZ	1:A:830:ALA:HA	1.69	0.58
1:B:893:MET:HG2	1:B:897:ILE:HG13	1.85	0.58
1:D:766:MET:HE2	1:D:799:LEU:HD22	1.80	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:591:TRP:HB3	1:C:618:PHE:HB3	1.86	0.57
1:C:744:LEU:H	1:C:798:ILE:CD1	2.18	0.57
1:D:375:LEU:HG	1:D:379:TYR:CE2	2.39	0.57
1:D:133:ALA:O	1:D:137:LYS:HG3	2.05	0.57
1:D:529:LYS:HD2	1:D:627:HIS:CD2	2.40	0.57
1:A:696:ARG:NH2	1:A:700:ILE:CG1	2.54	0.57
1:C:212:HIS:CB	1:C:238:LEU:CD2	2.79	0.57
1:C:222:VAL:HG13	1:C:269:ALA:HB2	1.87	0.57
1:C:803:ASP:OD2	3:J:19:DC:H5	1.84	0.57
1:A:22:THR:HG23	1:A:27:SER:OG	2.05	0.57
1:D:209:LEU:HD21	1:D:245:PHE:CZ	2.40	0.57
1:A:290:TYR:HB3	1:A:298:ALA:HB2	1.86	0.57
1:A:337:ILE:HG12	1:A:444:VAL:HB	1.87	0.57
1:C:641:GLU:HB3	1:C:877:PRO:HA	1.85	0.57
1:A:347:PHE:O	1:A:351:LEU:HG	2.04	0.57
1:A:916:ASN:ND2	1:A:918:THR:HG23	2.20	0.57
1:B:265:ILE:HD11	1:B:281:PHE:CG	2.40	0.57
1:C:211:GLN:O	1:C:215:THR:HG22	2.05	0.56
1:C:212:HIS:CG	1:C:238:LEU:HD23	2.39	0.56
1:A:696:ARG:HH22	1:A:700:ILE:CG1	2.03	0.56
1:B:674:ARG:NH2	1:B:723:THR:CG2	2.68	0.56
1:C:670:VAL:HG21	1:C:755:PHE:HE1	1.70	0.56
1:C:233:ASN:HB3	1:C:429:GLU:OE1	2.05	0.56
1:D:403:VAL:HG12	1:D:433:ARG:CD	2.35	0.56
1:A:696:ARG:NH2	1:A:699:GLU:OE1	2.38	0.56
1:C:946:LEU:CD1	1:C:952:LEU:HD13	2.35	0.56
1:D:521:SER:OG	1:D:524:PHE:HB2	2.05	0.56
1:A:791:PHE:CE2	1:A:793:VAL:CG1	2.88	0.56
1:D:674:ARG:NH1	1:D:723:THR:HG21	2.21	0.56
1:B:696:ARG:NH1	1:B:714:GLU:HG2	2.20	0.56
1:D:892:LEU:HD13	1:D:1020:ILE:HD12	1.88	0.56
1:B:290:TYR:HB3	1:B:298:ALA:HB2	1.88	0.56
1:C:212:HIS:HB2	1:C:238:LEU:HD23	1.86	0.56
1:C:933:GLN:NE2	1:C:945:GLU:HG2	2.21	0.56
1:B:244:THR:O	1:B:247:LYS:NZ	2.39	0.56
1:D:847:ASP:HA	1:D:850:HIS:HD2	1.71	0.56
1:B:743:SER:HA	1:B:798:ILE:HG22	1.87	0.55
1:A:946:LEU:HD12	1:A:950:THR:HG22	1.87	0.55
1:A:645:VAL:HG22	1:A:663:PHE:HB2	1.88	0.55
1:B:338:LEU:HD13	1:B:437:GLN:HE21	1.71	0.55
1:D:663:PHE:HB3	1:D:825:ASN:HD21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LYS:HG2	1:A:288:ASN:OD1	2.06	0.55
1:C:181:TYR:CE1	1:C:245:PHE:CD2	2.94	0.55
1:C:666:TYR:CB	1:C:811:LEU:CD2	2.81	0.55
1:B:746:ARG:HG3	1:B:976:ARG:HD3	1.89	0.55
1:C:893:MET:CG	1:C:897:ILE:HD11	2.37	0.55
1:A:719:MET:HE1	1:A:723:THR:HG22	1.87	0.55
1:B:517:SER:OG	2:G:10:DG:OP1	2.20	0.55
1:C:538:ILE:CG2	1:C:575:LEU:HD23	2.26	0.55
1:C:649:ASP:OD1	1:C:664:LYS:HE3	2.07	0.55
1:C:770:PHE:HD2	1:C:799:LEU:CD2	2.07	0.55
1:D:758:ASN:OD1	1:D:759:LEU:HG	2.06	0.55
1:C:347:PHE:CE1	1:C:446:ILE:HG12	2.42	0.54
1:D:735:LEU:N	1:D:735:LEU:CD1	2.71	0.54
1:B:744:LEU:CD2	1:B:796:THR:HG22	2.38	0.54
1:B:782:LEU:HD21	1:B:856:LEU:HD13	1.89	0.54
1:C:645:VAL:HG12	1:C:663:PHE:HB2	1.89	0.54
1:B:684:ASP:OD1	1:B:685:GLU:N	2.41	0.54
1:D:743:SER:HB2	1:D:799:LEU:HB2	1.89	0.54
1:D:181:TYR:HD1	1:D:245:PHE:CD2	2.25	0.54
1:D:348:ILE:HA	1:D:351:LEU:HD12	1.90	0.54
1:B:859:PRO:HD3	1:B:1021:VAL:HG13	1.89	0.54
1:C:773:GLY:CA	1:C:799:LEU:HD11	2.22	0.54
1:C:790:PRO:CD	1:C:966:ASN:OD1	2.56	0.54
1:D:973:VAL:HG21	1:D:1010:VAL:HG21	1.89	0.54
1:C:774:VAL:O	1:C:774:VAL:CG1	2.54	0.54
1:D:708:LEU:HD21	1:D:728:GLN:HA	1.89	0.54
1:A:893:MET:CG	1:A:897:ILE:HD12	2.37	0.54
1:B:696:ARG:NH2	1:B:700:ILE:HG13	2.23	0.54
1:B:744:LEU:HD23	1:B:796:THR:HG22	1.90	0.54
2:G:18:DA:N6	3:H:11:DT:H3	2.05	0.54
1:D:905:TYR:HB2	1:D:1012:THR:CG2	2.33	0.54
1:D:996:PHE:HE1	1:D:1003:VAL:HG21	1.73	0.54
1:C:935:ASP:CB	1:C:941:THR:CG2	2.86	0.53
1:B:406:ASP:HB3	1:B:409:ASP:HB2	1.90	0.53
1:C:181:TYR:HD1	1:C:245:PHE:HD2	1.56	0.53
1:D:746:ARG:HG3	1:D:976:ARG:HD3	1.90	0.53
1:A:591:TRP:HB3	1:A:618:PHE:HB3	1.91	0.53
1:A:413:PHE:HZ	1:A:499:TRP:HE1	1.55	0.53
1:C:122:GLN:HB3	1:C:135:LEU:HD12	1.90	0.53
1:D:371:ASN:HD21	1:D:437:GLN:HE22	1.57	0.53
1:D:771:PRO:HD2	1:D:775:GLY:HA3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:872:GLU:CG	1:D:873:PHE:H	2.22	0.53
1:B:287:GLU:O	1:B:291:ARG:HG3	2.09	0.53
1:B:413:PHE:HA	1:B:438:ASN:HB3	1.90	0.53
1:D:854:ALA:HA	1:D:857:HIS:HB2	1.91	0.53
1:A:321:LEU:HD21	1:A:613:PHE:CE2	2.44	0.52
1:D:769:ILE:HG23	1:D:812:PRO:HB3	1.91	0.52
1:A:259:LYS:NZ	1:A:266:GLN:HE22	2.07	0.52
1:D:181:TYR:HD1	1:D:245:PHE:HD2	1.58	0.52
1:D:256:GLU:HA	1:D:259:LYS:HE3	1.90	0.52
1:D:348:ILE:HD11	1:D:368:LEU:HB3	1.91	0.52
1:D:209:LEU:HD23	1:D:245:PHE:CZ	2.44	0.52
1:A:336:GLU:OE1	1:A:441:PRO:CD	2.54	0.52
1:A:668:LEU:HD22	1:A:802:LEU:CD1	2.40	0.52
1:C:797:ASP:OD2	1:C:897:ILE:HG21	2.08	0.52
1:C:743:SER:C	1:C:798:ILE:HD12	2.34	0.52
1:D:223:PHE:CZ	1:D:282:LEU:HG	2.44	0.52
1:D:378:TYR:CE1	1:D:402:ILE:HG12	2.45	0.52
1:D:590:ILE:CG2	1:D:621:ILE:CG1	2.87	0.52
1:A:330:LEU:CD2	1:A:337:ILE:CD1	2.73	0.52
1:B:678:VAL:HG13	1:B:754:TYR:HB3	1.92	0.52
3:F:18:DT:H2''	3:F:19:DC:C6	2.44	0.52
1:C:935:ASP:OD1	1:C:941:THR:HG21	2.06	0.51
1:C:222:VAL:HG13	1:C:269:ALA:HB1	1.90	0.51
1:C:658:GLN:O	1:C:660:ARG:HG3	2.11	0.51
1:A:753:MET:SD	1:A:799:LEU:HD22	2.50	0.51
1:A:828:ASP:OD2	1:A:832:LYS:HE3	2.11	0.51
1:D:314:MET:SD	1:D:513:VAL:HG23	2.50	0.51
1:D:543:MET:CB	1:D:561:VAL:CG2	2.85	0.51
1:B:520:ASP:O	1:B:520:ASP:OD1	2.29	0.51
1:C:649:ASP:CG	1:C:664:LYS:CD	2.83	0.51
1:C:766:MET:HE1	1:C:810:CYS:SG	2.51	0.51
1:D:290:TYR:HB3	1:D:298:ALA:HB2	1.92	0.51
1:A:719:MET:SD	1:A:723:THR:HG22	2.50	0.51
1:D:247:LYS:HB2	1:D:251:LYS:HE3	1.91	0.51
1:D:446:ILE:HG22	1:D:511:ALA:HB3	1.92	0.51
1:D:744:LEU:HD13	1:D:798:ILE:HD11	1.93	0.51
1:B:486:LYS:HB3	2:G:8:DT:H5'	1.91	0.51
1:D:375:LEU:CD1	1:D:379:TYR:CE2	2.94	0.51
1:C:349:THR:HG21	1:C:384:ASN:HD22	1.76	0.51
1:A:916:ASN:ND2	1:A:918:THR:CG2	2.74	0.51
1:B:766:MET:CE	1:B:799:LEU:HD11	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:645:VAL:HG22	1:D:663:PHE:HB2	1.92	0.51
1:D:348:ILE:HG23	1:D:385:ILE:CD1	2.28	0.51
1:A:479:VAL:HG13	1:A:487:THR:HG21	1.93	0.50
1:B:124:VAL:HG22	1:B:135:LEU:CD2	2.41	0.50
1:D:770:PHE:HB2	1:D:799:LEU:HD21	1.92	0.50
1:A:83:GLU:HA	1:A:108:ASP:OD1	2.10	0.50
1:B:146:GLN:CD	1:B:271:GLN:O	2.53	0.50
1:C:762:MET:HG2	2:I:6:DC:H5	1.77	0.50
1:A:929:ARG:O	1:A:931:LYS:HG3	2.10	0.50
1:C:6:VAL:HG13	1:C:132:LEU:HD23	1.93	0.50
1:C:924:LEU:HD13	1:C:927:LYS:CE	2.41	0.50
1:B:114:LEU:CB	1:B:135:LEU:HD11	2.41	0.50
1:C:314:MET:CE	1:C:513:VAL:HG23	2.37	0.50
1:D:849:PHE:CD2	1:D:893:MET:HE1	2.47	0.50
1:B:696:ARG:HH11	1:B:714:GLU:CD	2.19	0.50
1:C:959:ALA:HA	1:C:1014:SER:HB2	1.94	0.50
1:D:591:TRP:HB3	1:D:618:PHE:HB3	1.92	0.50
1:D:905:TYR:CB	1:D:1012:THR:HG23	2.34	0.50
1:D:963:LYS:HA	1:D:968:SER:HA	1.92	0.50
1:A:215:THR:HG21	1:A:379:TYR:HD2	1.77	0.50
1:C:113:VAL:HG13	1:C:120:GLU:HG3	1.93	0.50
1:C:215:THR:HG21	1:C:379:TYR:HD2	1.77	0.50
1:C:790:PRO:HD3	1:C:966:ASN:OD1	2.12	0.50
1:D:637:ASN:HB3	1:D:865:TYR:HE1	1.77	0.50
1:A:881:GLU:OE1	1:A:884:ARG:NE	2.36	0.50
1:B:650:THR:HG23	1:B:665:LEU:HA	1.94	0.50
1:B:766:MET:HE3	1:B:799:LEU:HD13	1.93	0.50
1:C:220:THR:HG22	1:C:226:ALA:HA	1.94	0.50
1:D:792:GLN:HB2	1:D:805:LEU:HG	1.93	0.50
1:D:277:GLU:O	1:D:280:ARG:HG2	2.12	0.49
1:B:519:ILE:CG2	1:B:630:LEU:HD11	2.31	0.49
1:A:153:ALA:C	1:A:265:ILE:CD1	2.85	0.49
1:B:645:VAL:HG12	1:B:646:ALA:N	2.26	0.49
1:B:122:GLN:HE22	1:B:138:LEU:CD1	2.24	0.49
1:D:855:VAL:HG13	1:D:879:TYR:HE2	1.76	0.49
1:A:662:ILE:HA	1:A:830:ALA:HB2	1.95	0.49
1:A:680:SER:HB2	1:A:689:LYS:NZ	2.27	0.49
1:C:538:ILE:CB	1:C:575:LEU:CD2	2.91	0.49
1:D:967:ARG:HB3	1:D:971:GLU:HB3	1.94	0.49
1:D:757:LYS:HA	1:D:763:GLN:NE2	2.27	0.49
1:C:744:LEU:HD22	1:C:796:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:893:MET:HG2	1:A:897:ILE:HD12	1.93	0.49
1:C:520:ASP:O	1:C:520:ASP:CG	2.55	0.49
1:C:667:SER:OG	1:C:810:CYS:SG	2.67	0.49
1:D:905:TYR:HD2	1:D:1012:THR:HG22	1.78	0.49
1:A:22:THR:CG2	1:A:27:SER:OG	2.61	0.49
1:B:122:GLN:HE21	1:B:138:LEU:CD1	2.25	0.49
1:C:513:VAL:HG22	1:C:572:VAL:HG22	1.94	0.49
1:B:54:LYS:HB2	1:B:54:LYS:HE2	1.64	0.49
1:B:132:LEU:HG	1:B:136:LEU:HD13	1.94	0.49
1:C:338:LEU:HD11	1:C:437:GLN:HE21	1.70	0.49
1:D:113:VAL:HG12	1:D:123:ARG:HG3	1.95	0.49
1:D:364:TYR:HE1	1:D:385:ILE:HG22	1.78	0.49
1:A:22:THR:OG1	1:A:24:ASN:ND2	2.46	0.48
1:A:726:ASP:CB	1:A:731:LYS:HE3	2.38	0.48
1:D:504:LEU:HD21	1:D:510:VAL:CG2	2.41	0.48
1:B:338:LEU:HD13	1:B:437:GLN:NE2	2.27	0.48
1:C:538:ILE:HG12	1:C:575:LEU:HD23	1.81	0.48
1:D:81:LYS:HD2	1:D:90:GLU:HB3	1.95	0.48
1:D:746:ARG:HH21	1:D:803:ASP:HB3	1.77	0.48
1:B:376:LEU:HB3	1:B:377:PRO:HD3	1.95	0.48
1:B:963:LYS:HA	1:B:968:SER:HA	1.95	0.48
1:C:621:ILE:HD13	1:C:629:TRP:HB3	1.94	0.48
1:D:59:ASN:OD1	3:H:7:DG:OP1	2.31	0.48
1:D:720:THR:O	1:D:723:THR:OG1	2.31	0.48
1:A:753:MET:SD	1:A:799:LEU:CD2	3.01	0.48
1:A:779:VAL:CG2	1:A:796:THR:OG1	2.61	0.48
1:C:797:ASP:CG	1:C:897:ILE:HG23	2.38	0.48
1:D:514:SER:HB2	1:D:573:TYR:HE2	1.78	0.48
1:D:849:PHE:HD2	1:D:893:MET:HE1	1.79	0.48
1:D:855:VAL:HG13	1:D:879:TYR:CE2	2.47	0.48
1:B:75:ARG:HD3	1:B:144:PRO:HG2	1.96	0.48
1:C:645:VAL:HG13	1:C:811:LEU:CD1	2.44	0.48
1:C:744:LEU:CB	1:C:798:ILE:HD11	2.42	0.48
1:D:223:PHE:HZ	1:D:282:LEU:HG	1.78	0.48
1:D:256:GLU:HA	1:D:259:LYS:CD	2.43	0.48
1:B:679:TYR:CZ	1:B:753:MET:SD	3.07	0.48
1:D:52:THR:OG1	2:G:25:DA:OP1	2.29	0.48
1:B:642:PHE:HZ	1:B:830:ALA:HA	1.79	0.48
1:B:645:VAL:CG1	1:B:666:TYR:CE2	2.96	0.48
1:D:872:GLU:CG	1:D:873:PHE:N	2.76	0.48
1:A:769:ILE:HG23	1:A:812:PRO:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:VAL:HG11	1:B:445:ILE:HD13	1.87	0.48
1:A:521:SER:H	1:A:528:ARG:HH21	1.62	0.48
1:C:338:LEU:HD13	1:C:437:GLN:HE21	1.79	0.48
1:C:753:MET:HE3	1:C:753:MET:HB3	1.65	0.48
2:E:10:DG:H1	3:F:19:DC:H42	1.61	0.48
1:C:338:LEU:HD11	1:C:437:GLN:HE22	1.73	0.47
1:D:247:LYS:N	1:D:251:LYS:CG	2.69	0.47
1:A:586:LYS:NZ	1:A:589:LYS:CE	2.77	0.47
1:A:621:ILE:HD13	1:A:629:TRP:HB3	1.96	0.47
1:C:649:ASP:O	1:C:664:LYS:CE	2.61	0.47
1:D:211:GLN:HG2	1:D:376:LEU:HB2	1.97	0.47
1:D:245:PHE:CD1	1:D:246:TYR:HB2	2.48	0.47
1:D:375:LEU:CG	1:D:379:TYR:CE2	2.97	0.47
1:C:719:MET:HE3	1:C:719:MET:HB3	1.81	0.47
1:D:590:ILE:CG2	1:D:621:ILE:HD11	2.43	0.47
1:A:667:SER:HB2	1:A:765:GLN:HB2	1.97	0.47
1:C:314:MET:SD	1:C:513:VAL:HG23	2.54	0.47
1:C:956:PRO:HG2	1:C:1015:VAL:HG21	1.96	0.47
1:D:938:LYS:HB3	1:D:938:LYS:HE3	1.44	0.47
1:C:101:ARG:HD3	1:C:118:GLY:HA2	1.96	0.47
1:A:348:ILE:HG13	1:A:370:CYS:SG	2.54	0.47
1:A:656:LEU:HA	1:A:659:GLU:HG3	1.95	0.47
1:A:668:LEU:HD22	1:A:802:LEU:HD11	1.95	0.47
1:A:828:ASP:OD1	1:A:832:LYS:HG3	2.14	0.47
1:A:859:PRO:HD3	1:A:1021:VAL:HG13	1.95	0.47
1:D:255:ALA:O	1:D:259:LYS:CG	2.43	0.47
1:D:492:MET:HE3	1:D:492:MET:HB3	1.67	0.47
1:D:930:LEU:HB2	1:D:978:LYS:HG3	1.96	0.47
1:A:828:ASP:CG	1:A:832:LYS:HE3	2.39	0.47
1:A:338:LEU:HD13	1:A:437:GLN:NE2	2.28	0.47
1:C:215:THR:HG21	1:C:379:TYR:CD2	2.50	0.47
1:C:342:THR:CG2	1:C:345:GLY:HA2	2.45	0.47
1:C:893:MET:HG3	1:C:897:ILE:HD11	1.96	0.47
1:D:376:LEU:HB3	1:D:377:PRO:HD3	1.97	0.47
1:A:671:VAL:HG12	1:A:762:MET:HB2	1.97	0.47
1:A:683:GLU:HG3	1:A:740:ILE:HD13	1.96	0.47
1:A:849:PHE:CE2	1:A:893:MET:HE1	2.50	0.47
1:C:529:LYS:CD	1:C:627:HIS:CE1	2.97	0.47
1:A:742:PRO:O	1:A:798:ILE:CG2	2.63	0.46
1:B:744:LEU:HD23	1:B:804:LEU:HD11	1.97	0.46
1:C:45:LEU:HD11	1:C:75:ARG:NH2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:LEU:CD1	1:D:379:TYR:CZ	2.88	0.46
1:D:895:LEU:HD11	1:D:1013:VAL:HA	1.97	0.46
1:D:934:ARG:HA	1:D:940:PRO:HA	1.97	0.46
1:D:219:PHE:CE1	1:D:383:LEU:HD22	2.49	0.46
1:B:591:TRP:HB3	1:B:618:PHE:HB3	1.97	0.46
1:D:348:ILE:CG2	1:D:385:ILE:CD1	2.72	0.46
1:D:794:LEU:HD23	1:D:795:ALA:N	2.30	0.46
1:B:122:GLN:HE21	1:B:138:LEU:HD12	1.79	0.46
1:C:143:GLU:HG3	1:C:147:VAL:HG22	1.97	0.46
1:B:879:TYR:OH	1:B:1028:THR:HG23	2.15	0.46
1:C:507:ASP:OD1	1:C:507:ASP:O	2.34	0.46
1:B:146:GLN:NE2	1:B:271:GLN:O	2.49	0.46
1:C:371:ASN:OD1	1:C:437:GLN:NE2	2.46	0.46
1:C:421:GLY:C	1:C:423:PHE:H	2.24	0.46
1:C:855:VAL:HG11	1:C:876:ILE:HG23	1.98	0.46
1:D:944:VAL:HG23	1:D:952:LEU:HB3	1.98	0.46
1:D:989:GLU:HG3	1:D:990:LYS:HG3	1.98	0.46
1:D:246:TYR:C	1:D:251:LYS:HE3	2.40	0.46
1:D:343:GLY:HA3	4:D:1102:SAM:HA	1.96	0.46
1:D:644:PRO:HG2	1:D:873:PHE:HB3	1.98	0.46
1:A:855:VAL:HG13	1:A:879:TYR:HE2	1.81	0.46
1:B:696:ARG:NH1	1:B:714:GLU:OE2	2.48	0.46
1:C:252:ARG:HG2	1:C:256:GLU:OE2	2.16	0.46
1:D:364:TYR:HE1	1:D:385:ILE:CG2	2.28	0.46
1:D:425:SER:HA	1:D:431:LEU:HB2	1.97	0.46
1:A:331:ALA:HB1	1:A:359:LYS:CD	2.46	0.46
1:C:668:LEU:HD22	1:C:802:LEU:HD11	1.97	0.46
1:D:645:VAL:HG21	1:D:811:LEU:HD22	1.98	0.46
1:A:964:LEU:HD12	1:A:964:LEU:HA	1.78	0.46
1:D:171:ALA:HB2	1:D:254:ILE:HD11	1.97	0.46
1:D:6:VAL:HG13	1:D:132:LEU:HD23	1.98	0.45
1:B:753:MET:HE1	1:B:799:LEU:HD23	1.97	0.45
1:B:845:ARG:C	1:B:847:ASP:H	2.24	0.45
1:C:792:GLN:HG3	1:C:805:LEU:HB3	1.97	0.45
1:A:153:ALA:CB	1:A:265:ILE:CD1	2.90	0.45
1:C:348:ILE:HG13	1:C:370:CYS:SG	2.57	0.45
1:A:497:LEU:O	1:A:501:THR:HG23	2.16	0.45
1:B:209:LEU:HD11	1:B:245:PHE:HE1	1.81	0.45
1:D:145:PRO:HA	1:D:148:LEU:HD12	1.98	0.45
1:B:122:GLN:NE2	1:B:138:LEU:HD11	2.28	0.45
1:B:1003:VAL:C	1:B:1007:LEU:HD13	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:THR:HG23	1:C:345:GLY:HA2	1.99	0.45
1:C:744:LEU:N	1:C:798:ILE:HD11	2.27	0.45
1:D:648:LYS:HZ2	1:D:648:LYS:HG3	1.67	0.45
1:B:171:ALA:HB1	1:B:254:ILE:HD11	1.92	0.45
1:C:410:ASN:O	1:C:411:THR:C	2.59	0.45
1:D:330:LEU:CD2	1:D:337:ILE:HD11	2.47	0.45
1:A:451:TYR:CE1	1:A:514:SER:HA	2.51	0.45
1:C:781:ALA:HB1	1:C:808:THR:HG22	1.99	0.45
1:D:753:MET:HE3	1:D:753:MET:HB2	1.78	0.45
1:D:806:GLU:HG3	1:D:807:LYS:HG3	1.98	0.45
1:A:83:GLU:HB3	1:A:109:SER:OG	2.17	0.45
1:A:595:VAL:HG21	1:A:604:LYS:HG2	1.99	0.45
1:B:766:MET:HG3	1:B:799:LEU:HD11	1.99	0.45
1:C:538:ILE:CB	1:C:575:LEU:HD23	2.46	0.45
1:D:590:ILE:HG21	1:D:621:ILE:HD11	1.99	0.45
1:C:451:TYR:CE1	1:C:514:SER:HA	2.52	0.45
1:C:645:VAL:HG13	1:C:811:LEU:HD13	1.98	0.45
1:D:81:LYS:CD	1:D:90:GLU:HB3	2.47	0.45
1:A:878:PHE:O	1:A:1029:MET:HE1	2.17	0.44
1:B:672:THR:HG23	1:B:760:ASN:HA	1.99	0.44
1:D:209:LEU:HD23	1:D:245:PHE:CE2	2.49	0.44
1:A:645:VAL:HG21	1:A:811:LEU:HD22	1.99	0.44
1:A:779:VAL:HG23	1:A:779:VAL:O	2.18	0.44
1:A:893:MET:HG3	1:A:897:ILE:HD12	1.99	0.44
1:A:982:PRO:HD2	1:A:988:ARG:HG3	2.00	0.44
1:C:736:GLU:H	1:C:736:GLU:HG3	1.46	0.44
1:C:744:LEU:CA	1:C:798:ILE:HD11	2.47	0.44
1:A:315:ILE:HG12	1:A:351:LEU:HD23	1.95	0.44
1:D:195:ALA:HB1	1:D:424:GLY:H	1.82	0.44
1:D:347:PHE:O	1:D:351:LEU:CG	2.53	0.44
1:D:637:ASN:HB3	1:D:865:TYR:CE1	2.52	0.44
3:J:4:DT:H6	3:J:4:DT:H2'	1.64	0.44
1:A:338:LEU:HD21	1:A:437:GLN:HE21	1.79	0.44
1:A:361:GLU:HG3	1:A:365:ARG:HD2	2.00	0.44
1:B:238:LEU:CD2	1:B:375:LEU:HD21	2.48	0.44
1:C:773:GLY:CA	1:C:799:LEU:CD1	2.89	0.44
1:C:737:LYS:HA	1:C:737:LYS:HD2	1.61	0.44
1:B:521:SER:H	1:B:528:ARG:HH12	1.64	0.44
1:B:778:VAL:HG22	1:B:797:ASP:OD1	2.18	0.44
1:D:124:VAL:HG22	1:D:135:LEU:HD22	2.00	0.44
3:J:24:DG:H2''	3:J:25:DG:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:GLU:OE1	1:A:440:ARG:HB3	2.17	0.44
1:B:793:VAL:HG11	1:B:856:LEU:HB3	2.00	0.44
1:C:212:HIS:CB	1:C:238:LEU:HD23	2.47	0.44
1:C:360:LEU:HB3	1:C:393:MET:HE2	2.00	0.44
1:C:744:LEU:HD22	1:C:796:THR:CG2	2.48	0.44
1:B:742:PRO:O	1:B:798:ILE:CG2	2.65	0.44
1:B:795:ALA:HB1	1:B:897:ILE:HD11	2.00	0.44
1:D:403:VAL:HG12	1:D:433:ARG:HD2	2.00	0.44
1:A:746:ARG:HG3	1:A:976:ARG:HD3	1.99	0.44
1:C:181:TYR:CD1	1:C:245:PHE:CE2	3.01	0.44
1:D:533:LYS:HB2	1:D:533:LYS:HE2	1.62	0.44
1:C:602:ARG:H	1:C:602:ARG:HG2	1.60	0.43
1:D:256:GLU:HG3	1:D:259:LYS:NZ	2.33	0.43
1:A:338:LEU:HD13	1:A:369:HIS:HB2	1.99	0.43
1:A:481:ALA:HB1	1:A:529:LYS:HD3	2.00	0.43
1:B:181:TYR:CE2	1:B:185:ARG:HD3	2.54	0.43
1:B:225:ASN:HD22	1:B:225:ASN:HA	1.57	0.43
1:D:256:GLU:HA	1:D:259:LYS:CE	2.47	0.43
2:G:18:DA:C2'	2:G:19:DC:O4'	2.66	0.43
1:B:216:GLY:O	1:B:220:THR:HG23	2.18	0.43
1:C:935:ASP:HB2	1:C:941:THR:CG2	2.47	0.43
1:D:518:PHE:CZ	1:D:519:ILE:HD11	2.53	0.43
1:D:590:ILE:CG2	1:D:621:ILE:HG13	2.48	0.43
1:D:850:HIS:O	1:D:889:GLY:HA3	2.18	0.43
1:A:547:ALA:HB3	1:A:567:LYS:HB3	2.00	0.43
1:B:122:GLN:HB3	1:B:135:LEU:CD1	2.42	0.43
1:B:664:LYS:HD3	1:B:815:ARG:CZ	2.48	0.43
1:C:649:ASP:OD1	1:C:664:LYS:CE	2.66	0.43
1:D:1:MET:HB3	1:D:2:SER:H	1.60	0.43
1:D:209:LEU:HD12	1:D:209:LEU:HA	1.76	0.43
1:D:398:GLU:CD	1:D:400:ARG:NH2	2.70	0.43
1:D:696:ARG:HE	1:D:696:ARG:HB3	1.36	0.43
1:A:855:VAL:HG11	1:A:877:PRO:HD2	2.00	0.43
1:C:208:MET:O	1:C:238:LEU:HD21	2.18	0.43
1:C:926:LYS:HE2	1:C:926:LYS:HB2	1.63	0.43
1:D:740:ILE:HG13	1:D:754:TYR:HD1	1.84	0.43
1:A:340:PRO:HB2	1:A:496:PHE:HE2	1.83	0.43
1:C:884:ARG:HD2	1:C:884:ARG:HA	1.57	0.43
1:D:160:GLU:HB3	1:D:261:TYR:HD1	1.83	0.43
1:A:363:LYS:CD	1:A:367:GLU:OE1	2.65	0.43
1:B:161:MET:HB2	1:B:161:MET:HE2	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:LYS:HB3	2:I:8:DT:H5'	2.00	0.43
1:D:428:ALA:O	1:D:432:GLU:HG3	2.18	0.43
1:A:321:LEU:HD21	1:A:613:PHE:HE2	1.84	0.43
1:B:481:ALA:HB1	1:B:529:LYS:HD3	2.01	0.43
1:D:223:PHE:HE1	1:D:282:LEU:HD21	1.83	0.43
1:D:326:PHE:CZ	1:D:576:VAL:CG2	3.02	0.43
1:D:403:VAL:HG11	1:D:433:ARG:C	2.44	0.43
1:D:463:LYS:HB3	1:D:463:LYS:HE3	1.78	0.43
1:D:782:LEU:HD23	1:D:782:LEU:HA	1.84	0.43
1:D:818:MET:HB3	1:D:818:MET:HE3	1.63	0.43
2:I:26:DC:H5'	3:J:5:DG:H21	1.84	0.43
1:C:181:TYR:CE1	1:C:245:PHE:HE2	2.15	0.43
1:D:589:LYS:HD3	1:D:591:TRP:CZ2	2.54	0.43
2:K:5:DC:H2''	2:K:6:DC:H5''	2.01	0.43
1:B:29:ARG:HH22	2:E:23:DC:H5''	1.84	0.43
1:B:958:ALA:HB3	1:B:1015:VAL:HG23	2.01	0.43
1:C:8:LYS:HD2	1:C:8:LYS:HA	1.79	0.42
1:C:184:GLU:HG2	1:C:241:LEU:HA	2.00	0.42
1:D:196:ILE:HD11	1:D:404:LEU:HD23	2.01	0.42
1:D:372:GLU:CG	1:D:377:PRO:HB2	2.48	0.42
1:B:705:LEU:HA	1:B:708:LEU:HD12	2.01	0.42
1:C:486:LYS:HB2	2:I:7:DA:H1'	2.01	0.42
1:D:478:TYR:HB3	1:D:489:LEU:HD22	2.00	0.42
1:D:590:ILE:HD13	1:D:629:TRP:CE2	2.54	0.42
1:D:761:GLU:HG3	1:D:762:MET:HE2	2.01	0.42
1:C:314:MET:HE2	1:C:572:VAL:HG13	2.01	0.42
1:B:265:ILE:HD12	1:B:281:PHE:CE1	2.52	0.42
1:C:328:LYS:HE2	1:C:328:LYS:HB2	1.63	0.42
1:C:543:MET:HE3	1:C:543:MET:HB3	1.90	0.42
1:C:893:MET:HG3	1:C:897:ILE:CD1	2.48	0.42
1:D:991:PHE:HB3	1:D:992:ASN:H	1.65	0.42
1:C:970:LEU:HA	1:C:970:LEU:HD12	1.75	0.42
1:D:672:THR:HG21	1:D:679:TYR:HE1	1.85	0.42
1:A:75:ARG:HG2	1:A:144:PRO:HG3	2.02	0.42
1:A:916:ASN:OD1	1:A:916:ASN:C	2.62	0.42
1:B:238:LEU:CD2	1:B:375:LEU:CD2	2.97	0.42
1:B:238:LEU:HD22	1:B:375:LEU:HD21	2.02	0.42
1:B:595:VAL:HG21	1:B:604:LYS:HG2	2.02	0.42
1:C:547:ALA:C	1:C:549:THR:H	2.27	0.42
1:C:935:ASP:HB2	1:C:941:THR:HG22	2.02	0.42
1:A:343:GLY:HA3	4:A:1101:SAM:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:VAL:HG21	1:A:1013:VAL:HG23	2.01	0.42
1:C:212:HIS:HD2	1:C:238:LEU:HD23	1.73	0.42
1:D:814:TYR:HA	1:D:825:ASN:H	1.84	0.42
1:A:924:LEU:HD23	1:A:927:LYS:NZ	2.35	0.42
1:D:111:LEU:HD21	1:D:123:ARG:HD3	2.01	0.42
1:D:372:GLU:CD	1:D:377:PRO:HB2	2.45	0.42
1:A:728:GLN:HE21	1:A:728:GLN:HB2	1.59	0.42
1:C:221:SER:HB2	1:C:266:GLN:CD	2.45	0.42
1:C:565:GLN:HE21	1:C:565:GLN:HB2	1.53	0.42
1:D:402:ILE:O	1:D:402:ILE:CG2	2.68	0.42
1:D:908:LYS:HB2	1:D:953:ALA:HB3	2.01	0.42
1:A:54:LYS:HD3	1:A:54:LYS:HA	1.78	0.42
1:D:422:LEU:HD23	1:D:422:LEU:HA	1.86	0.42
1:A:614:GLU:OE1	1:D:586:LYS:NZ	2.51	0.41
1:A:737:LYS:HZ2	1:A:740:ILE:HD12	1.84	0.41
1:B:797:ASP:OD2	1:B:897:ILE:CG2	2.62	0.41
1:C:314:MET:HE3	1:C:314:MET:HB2	1.59	0.41
1:D:946:LEU:HD13	1:D:996:PHE:HZ	1.85	0.41
3:L:10:DG:H2''	3:L:11:DT:H5'	2.02	0.41
1:A:656:LEU:CD2	1:A:659:GLU:CD	2.92	0.41
1:C:680:SER:HB3	1:C:686:LEU:HB2	2.01	0.41
1:C:792:GLN:HB2	1:C:805:LEU:HD22	2.02	0.41
2:K:6:DC:H2''	2:K:7:DA:C8	2.55	0.41
1:A:922:LEU:HD21	1:A:926:LYS:HZ1	1.83	0.41
1:C:145:PRO:HA	1:C:148:LEU:HB2	2.02	0.41
1:C:771:PRO:C	1:C:773:GLY:H	2.28	0.41
1:D:254:ILE:HD13	1:D:254:ILE:HA	1.89	0.41
1:D:1006:LEU:HD12	1:D:1006:LEU:HA	1.81	0.41
1:B:378:TYR:CE1	1:B:402:ILE:HG12	2.55	0.41
1:C:815:ARG:HH21	1:C:825:ASN:HA	1.84	0.41
1:A:215:THR:HG21	1:A:379:TYR:CD2	2.56	0.41
1:A:766:MET:C	1:A:768:SER:H	2.28	0.41
1:B:769:ILE:HG23	1:B:812:PRO:HB3	2.03	0.41
1:D:694:ILE:HG23	1:D:733:TYR:HB2	2.03	0.41
1:A:80:SER:HA	1:A:107:GLU:HB3	2.03	0.41
1:A:87:LEU:HD12	1:A:87:LEU:HA	1.88	0.41
1:A:515:ASN:HA	1:A:569:GLY:O	2.20	0.41
1:B:230:GLU:H	1:B:230:GLU:HG3	1.70	0.41
1:B:338:LEU:HD11	1:B:437:GLN:HE22	1.86	0.41
1:B:422:LEU:HD23	1:B:422:LEU:HA	1.88	0.41
1:B:755:PHE:HA	1:B:760:ASN:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:855:VAL:HG13	1:B:879:TYR:HE2	1.85	0.41
1:C:666:TYR:HB3	1:C:811:LEU:HD21	1.94	0.41
1:D:529:LYS:HD2	1:D:627:HIS:CE1	2.51	0.41
1:A:363:LYS:HD2	1:A:363:LYS:HA	1.91	0.41
1:B:656:LEU:HD12	1:B:656:LEU:HA	1.85	0.41
1:D:286:TYR:HE1	1:D:377:PRO:HG3	1.85	0.41
1:A:700:ILE:O	1:A:703:LEU:HB2	2.20	0.41
1:B:645:VAL:CG1	1:B:646:ALA:N	2.84	0.41
1:C:212:HIS:CG	1:C:238:LEU:CD2	3.02	0.41
1:C:879:TYR:HE1	1:C:1029:MET:H	1.69	0.41
1:D:256:GLU:HA	1:D:259:LYS:HD2	2.03	0.41
1:D:342:THR:HG21	1:D:381:ALA:HB1	2.01	0.41
1:D:547:ALA:C	1:D:549:THR:H	2.28	0.41
2:G:1:DC:H2''	2:G:2:DA:C8	2.56	0.41
1:A:87:LEU:HD22	1:A:108:ASP:HB2	2.03	0.41
1:A:161:MET:HE2	1:A:161:MET:HB2	1.82	0.41
1:A:330:LEU:HD23	1:A:337:ILE:HD11	1.91	0.41
1:A:507:ASP:OD1	1:A:507:ASP:O	2.39	0.41
1:A:774:VAL:HG13	1:A:774:VAL:O	2.21	0.41
1:A:968:SER:OG	1:A:971:GLU:HG3	2.21	0.41
1:A:1006:LEU:HD12	1:A:1006:LEU:HA	1.91	0.41
1:B:592:TYR:CE1	1:B:630:LEU:HD11	2.56	0.41
1:B:662:ILE:HA	1:B:830:ALA:HB2	2.03	0.41
1:B:711:ARG:HE	1:B:711:ARG:HB3	1.57	0.41
1:B:951:THR:HG23	1:B:951:THR:O	2.20	0.41
1:C:636:GLU:H	1:C:636:GLU:HG3	1.63	0.41
1:C:924:LEU:HD21	1:C:927:LYS:NZ	2.36	0.41
1:D:374:ALA:HB3	1:D:377:PRO:HG2	2.03	0.41
1:B:814:TYR:CE1	1:B:824:ASN:OD1	2.74	0.41
1:C:165:LEU:HD23	1:C:165:LEU:HA	1.94	0.41
1:C:193:LYS:HA	1:C:197:ASN:O	2.21	0.41
1:C:347:PHE:CD1	1:C:446:ILE:CD1	3.04	0.41
1:D:905:TYR:CD2	1:D:1012:THR:HG22	2.55	0.41
1:A:108:ASP:O	1:A:126:MET:HE2	2.20	0.40
1:B:766:MET:CG	1:B:799:LEU:HD11	2.51	0.40
1:C:924:LEU:HD22	1:C:927:LYS:CE	2.48	0.40
1:D:567:LYS:HB2	1:D:567:LYS:HE2	1.93	0.40
2:G:18:DA:H2'	2:G:19:DC:C6	2.56	0.40
1:A:744:LEU:CD2	1:A:796:THR:HG22	2.50	0.40
1:A:762:MET:HE1	2:E:5:DC:H2'	2.03	0.40
1:C:282:LEU:HD13	1:C:380:ILE:HG23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:781:ALA:HB1	1:C:808:THR:CG2	2.51	0.40
1:D:372:GLU:CD	1:D:377:PRO:CB	2.94	0.40
2:G:18:DA:H2''	2:G:19:DC:O4'	2.20	0.40
1:A:636:GLU:H	1:A:636:GLU:HG3	1.58	0.40
1:C:590:ILE:HD13	1:C:629:TRP:CE2	2.56	0.40
1:B:442:VAL:CG1	1:B:445:ILE:HD13	2.50	0.40
1:D:165:LEU:HD23	1:D:165:LEU:HA	1.86	0.40
1:D:473:ARG:HE	1:D:473:ARG:HB3	1.39	0.40
1:D:927:LYS:HA	1:D:927:LYS:HD3	1.80	0.40
1:B:11:LYS:HB2	1:B:11:LYS:HE2	1.74	0.40
1:B:509:ILE:HD11	1:B:574:PHE:HB3	2.03	0.40
1:D:195:ALA:HA	1:D:423:PHE:HA	2.03	0.40
3:F:14:DT:H2''	3:F:15:DG:C8	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all 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	1010/1029 (98%)	951 (94%)	58 (6%)	1 (0%)	48	68
1	B	1007/1029 (98%)	948 (94%)	58 (6%)	1 (0%)	48	68
1	C	1008/1029 (98%)	939 (93%)	69 (7%)	0	100	100
1	D	1004/1029 (98%)	925 (92%)	75 (8%)	4 (0%)	30	48
All	All	4029/4116 (98%)	3763 (93%)	260 (6%)	6 (0%)	49	68

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	246	TYR
1	D	880	PRO

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Mol	Chain	Res	Type
1	B	874	PRO
1	D	644	PRO
1	D	1025	PRO
1	A	874	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	863/872 (99%)	776 (90%)	87 (10%)	7	15
1	B	861/872 (99%)	786 (91%)	75 (9%)	9	21
1	C	862/872 (99%)	756 (88%)	106 (12%)	4	8
1	D	860/872 (99%)	684 (80%)	176 (20%)	1	1
All	All	3446/3488 (99%)	3002 (87%)	444 (13%)	6	7

All (444) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	17	VAL
1	A	37	SER
1	A	46	ARG
1	A	54	LYS
1	A	56	VAL
1	A	59	ASN
1	A	92	GLN
1	A	94	LYS
1	A	95	LEU
1	A	104	ILE
1	A	105	ILE
1	A	111	LEU
1	A	113	VAL
1	A	146	GLN
1	A	147	VAL
1	A	159	ASP

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Mol	Chain	Res	Type
1	A	161	MET
1	A	184	GLU
1	A	185	ARG
1	A	191	ILE
1	A	193	LYS
1	A	199	ASP
1	A	214	LEU
1	A	220	THR
1	A	238	LEU
1	A	240	GLN
1	A	260	ARG
1	A	272	ILE
1	A	303	ILE
1	A	307	PRO
1	A	311	VAL
1	A	318	THR
1	A	329	GLU
1	A	361	GLU
1	A	366	GLU
1	A	403	VAL
1	A	425	SER
1	A	426	VAL
1	A	436	ARG
1	A	445	ILE
1	A	451	TYR
1	A	458	GLU
1	A	463	LYS
1	A	466	GLU
1	A	472	ARG
1	A	493	TYR
1	A	513	VAL
1	A	519	ILE
1	A	525	ASP
1	A	540	ILE
1	A	560	ASN
1	A	566	ILE
1	A	570	VAL
1	A	576	VAL
1	A	600	ARG
1	A	611	THR
1	A	635	GLU
1	A	642	PHE

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Mol	Chain	Res	Type
1	A	643	LEU
1	A	651	LYS
1	A	665	LEU
1	A	678	VAL
1	A	694	ILE
1	A	701	ILE
1	A	703	LEU
1	A	735	LEU
1	A	737	LYS
1	A	750	VAL
1	A	759	LEU
1	A	768	SER
1	A	782	LEU
1	A	783	SER
1	A	792	GLN
1	A	799	LEU
1	A	821	GLU
1	A	826	ILE
1	A	842	SER
1	A	846	GLU
1	A	863	GLU
1	A	870	ARG
1	A	872	GLU
1	A	890	ARG
1	A	897	ILE
1	A	945	GLU
1	A	988	ARG
1	A	995	ARG
1	B	3	LEU
1	B	7	LYS
1	B	11	LYS
1	B	23	ARG
1	B	51	VAL
1	B	56	VAL
1	B	75	ARG
1	B	81	LYS
1	B	104	ILE
1	B	105	ILE
1	B	141	GLU
1	B	147	VAL
1	B	161	MET
1	B	164	LEU

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Mol	Chain	Res	Type
1	B	193	LYS
1	B	194	GLU
1	B	213	ILE
1	B	215	THR
1	B	222	VAL
1	B	225	ASN
1	B	230	GLU
1	B	300	ARG
1	B	310	ILE
1	B	351	LEU
1	B	359	LYS
1	B	363	LYS
1	B	367	GLU
1	B	372	GLU
1	B	383	LEU
1	B	392	LYS
1	B	395	ARG
1	B	451	TYR
1	B	458	GLU
1	B	474	ILE
1	B	488	LYS
1	B	493	TYR
1	B	505	LYS
1	B	540	ILE
1	B	564	ASP
1	B	575	LEU
1	B	576	VAL
1	B	633	VAL
1	B	635	GLU
1	B	642	PHE
1	B	643	LEU
1	B	658	GLN
1	B	665	LEU
1	B	673	ASN
1	B	686	LEU
1	B	691	ARG
1	B	694	ILE
1	B	714	GLU
1	B	718	LYS
1	B	734	SER
1	B	735	LEU
1	B	740	ILE

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Mol	Chain	Res	Type
1	B	750	VAL
1	B	774	VAL
1	B	776	GLU
1	B	822	ARG
1	B	826	ILE
1	B	828	ASP
1	B	841	THR
1	B	842	SER
1	B	846	GLU
1	B	881	GLU
1	B	884	ARG
1	B	929	ARG
1	B	950	THR
1	B	952	LEU
1	B	980	THR
1	B	988	ARG
1	B	1000	LYS
1	B	1015	VAL
1	B	1019	ARG
1	C	5	LEU
1	C	11	LYS
1	C	13	LEU
1	C	81	LYS
1	C	82	ASP
1	C	83	GLU
1	C	86	THR
1	C	90	GLU
1	C	104	ILE
1	C	109	SER
1	C	120	GLU
1	C	121	VAL
1	C	147	VAL
1	C	152	LYS
1	C	157	PHE
1	C	159	ASP
1	C	160	GLU
1	C	185	ARG
1	C	193	LYS
1	C	210	ILE
1	C	254	ILE
1	C	277	GLU
1	C	303	ILE

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Mol	Chain	Res	Type
1	C	311	VAL
1	C	314	MET
1	C	322	LEU
1	C	323	GLU
1	C	328	LYS
1	C	330	LEU
1	C	333	LYS
1	C	336	GLU
1	C	337	ILE
1	C	357	LYS
1	C	362	GLN
1	C	366	GLU
1	C	376	LEU
1	C	383	LEU
1	C	384	ASN
1	C	397	GLU
1	C	398	GLU
1	C	451	TYR
1	C	469	GLU
1	C	509	ILE
1	C	541	LEU
1	C	549	THR
1	C	550	SER
1	C	552	GLU
1	C	560	ASN
1	C	568	VAL
1	C	570	VAL
1	C	576	VAL
1	C	599	TRP
1	C	602	ARG
1	C	614	GLU
1	C	622	ARG
1	C	640	ASN
1	C	642	PHE
1	C	650	THR
1	C	654	LYS
1	C	656	LEU
1	C	665	LEU
1	C	673	ASN
1	C	676	GLU
1	C	694	ILE
1	C	696	ARG

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Mol	Chain	Res	Type
1	C	701	ILE
1	C	718	LYS
1	C	736	GLU
1	C	737	LYS
1	C	740	ILE
1	C	751	LEU
1	C	753	MET
1	C	762	MET
1	C	766	MET
1	C	782	LEU
1	C	783	SER
1	C	792	GLN
1	C	804	LEU
1	C	808	THR
1	C	826	ILE
1	C	827	THR
1	C	832	LYS
1	C	841	THR
1	C	846	GLU
1	C	864	LYS
1	C	867	LEU
1	C	870	ARG
1	C	872	GLU
1	C	876	ILE
1	C	881	GLU
1	C	908	LYS
1	C	909	ARG
1	C	911	ASP
1	C	912	GLU
1	C	920	GLU
1	C	924	LEU
1	C	926	LYS
1	C	929	ARG
1	C	944	VAL
1	C	949	LEU
1	C	950	THR
1	C	975	GLU
1	C	980	THR
1	C	1000	LYS
1	C	1001	GLU
1	C	1028	THR
1	D	1	MET

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Mol	Chain	Res	Type
1	D	8	LYS
1	D	11	LYS
1	D	22	THR
1	D	23	ARG
1	D	34	GLN
1	D	45	LEU
1	D	82	ASP
1	D	83	GLU
1	D	88	ASP
1	D	90	GLU
1	D	101	ARG
1	D	104	ILE
1	D	105	ILE
1	D	113	VAL
1	D	115	MET
1	D	120	GLU
1	D	121	VAL
1	D	128	ASP
1	D	143	GLU
1	D	144	PRO
1	D	146	GLN
1	D	152	LYS
1	D	164	LEU
1	D	167	ILE
1	D	170	GLU
1	D	176	GLU
1	D	177	GLN
1	D	182	ARG
1	D	185	ARG
1	D	190	GLU
1	D	191	ILE
1	D	199	ASP
1	D	201	SER
1	D	210	ILE
1	D	229	HIS
1	D	256	GLU
1	D	260	ARG
1	D	277	GLU
1	D	300	ARG
1	D	309	GLU
1	D	310	ILE
1	D	311	VAL

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Mol	Chain	Res	Type
1	D	323	GLU
1	D	324	LYS
1	D	329	GLU
1	D	335	VAL
1	D	346	THR
1	D	348	ILE
1	D	349	THR
1	D	370	CYS
1	D	400	ARG
1	D	407	THR
1	D	411	THR
1	D	422	LEU
1	D	433	ARG
1	D	437	GLN
1	D	451	TYR
1	D	463	LYS
1	D	465	ARG
1	D	468	LYS
1	D	472	ARG
1	D	473	ARG
1	D	474	ILE
1	D	475	LYS
1	D	488	LYS
1	D	492	MET
1	D	493	TYR
1	D	494	SER
1	D	498	ARG
1	D	540	ILE
1	D	541	LEU
1	D	544	LYS
1	D	552	GLU
1	D	553	ARG
1	D	566	ILE
1	D	567	LYS
1	D	570	VAL
1	D	575	LEU
1	D	599	TRP
1	D	609	LYS
1	D	612	LYS
1	D	614	GLU
1	D	638	ASP
1	D	640	ASN

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Mol	Chain	Res	Type
1	D	641	GLU
1	D	642	PHE
1	D	643	LEU
1	D	647	ASP
1	D	648	LYS
1	D	649	ASP
1	D	652	GLN
1	D	654	LYS
1	D	656	LEU
1	D	660	ARG
1	D	662	ILE
1	D	664	LYS
1	D	671	VAL
1	D	673	ASN
1	D	676	GLU
1	D	684	ASP
1	D	686	LEU
1	D	696	ARG
1	D	700	ILE
1	D	701	ILE
1	D	709	MET
1	D	716	ASP
1	D	743	SER
1	D	745	TYR
1	D	746	ARG
1	D	766	MET
1	D	769	ILE
1	D	779	VAL
1	D	789	LYS
1	D	792	GLN
1	D	793	VAL
1	D	804	LEU
1	D	805	LEU
1	D	808	THR
1	D	809	GLN
1	D	814	TYR
1	D	817	THR
1	D	818	MET
1	D	822	ARG
1	D	823	LEU
1	D	824	ASN
1	D	825	ASN

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Mol	Chain	Res	Type
1	D	826	ILE
1	D	827	THR
1	D	831	LEU
1	D	832	LYS
1	D	835	GLN
1	D	837	HIS
1	D	843	ILE
1	D	844	SER
1	D	845	ARG
1	D	863	GLU
1	D	864	LYS
1	D	871	GLN
1	D	881	GLU
1	D	892	LEU
1	D	907	LEU
1	D	910	THR
1	D	915	LYS
1	D	916	ASN
1	D	918	THR
1	D	920	GLU
1	D	922	LEU
1	D	927	LYS
1	D	931	LYS
1	D	935	ASP
1	D	938	LYS
1	D	939	GLN
1	D	941	THR
1	D	944	VAL
1	D	945	GLU
1	D	946	LEU
1	D	949	LEU
1	D	952	LEU
1	D	955	ILE
1	D	967	ARG
1	D	970	LEU
1	D	974	LEU
1	D	986	THR
1	D	987	ILE
1	D	992	ASN
1	D	993	THR
1	D	994	TYR
1	D	995	ARG

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Mol	Chain	Res	Type
1	D	998	ASP
1	D	1000	LYS
1	D	1002	ARG
1	D	1005	ASP
1	D	1019	ARG
1	D	1024	MET
1	D	1029	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	33	GLN
1	A	116	GLN
1	A	122	GLN
1	A	187	HIS
1	A	225	ASN
1	A	227	GLN
1	A	233	ASN
1	A	266	GLN
1	A	279	GLN
1	A	384	ASN
1	A	410	ASN
1	A	437	GLN
1	A	448	ASN
1	A	454	ASN
1	A	537	HIS
1	A	546	ASN
1	A	637	ASN
1	A	673	ASN
1	A	728	GLN
1	A	760	ASN
1	A	824	ASN
1	A	896	HIS
1	A	966	ASN
1	A	977	HIS
1	B	10	GLN
1	B	33	GLN
1	B	59	ASN
1	B	116	GLN
1	B	122	GLN
1	B	225	ASN

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Mol	Chain	Res	Type
1	B	227	GLN
1	B	232	ASN
1	B	288	ASN
1	B	325	HIS
1	B	327	GLN
1	B	371	ASN
1	B	384	ASN
1	B	437	GLN
1	B	448	ASN
1	B	565	GLN
1	B	620	HIS
1	B	673	ASN
1	B	760	ASN
1	B	763	GLN
1	B	765	GLN
1	B	857	HIS
1	B	868	ASN
1	B	896	HIS
1	B	933	GLN
1	C	33	GLN
1	C	59	ASN
1	C	73	GLN
1	C	116	GLN
1	C	212	HIS
1	C	225	ASN
1	C	232	ASN
1	C	236	GLN
1	C	327	GLN
1	C	448	ASN
1	C	560	ASN
1	C	565	GLN
1	C	627	HIS
1	C	673	ASN
1	C	728	GLN
1	C	792	GLN
1	C	809	GLN
1	C	824	ASN
1	C	837	HIS
1	C	857	HIS
1	C	868	ASN
1	D	10	GLN
1	D	59	ASN

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Mol	Chain	Res	Type
1	D	60	ASN
1	D	73	GLN
1	D	92	GLN
1	D	122	GLN
1	D	211	GLN
1	D	229	HIS
1	D	237	GLN
1	D	266	GLN
1	D	288	ASN
1	D	294	ASN
1	D	325	HIS
1	D	369	HIS
1	D	371	ASN
1	D	401	ASN
1	D	410	ASN
1	D	438	ASN
1	D	448	ASN
1	D	565	GLN
1	D	628	ASN
1	D	792	GLN
1	D	835	GLN
1	D	857	HIS
1	D	871	GLN
1	D	916	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SAM	D	1102	-	27,29,29	0.51	1 (3%)	34,42,42	0.74	0
4	SAM	B	1101	-	27,29,29	0.59	1 (3%)	34,42,42	0.74	1 (2%)
4	SAM	A	1101	-	27,29,29	0.53	1 (3%)	34,42,42	0.60	0
4	SAM	C	1101	-	27,29,29	0.51	1 (3%)	34,42,42	0.67	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SAM	D	1102	-	-	4/17/33/33	0/3/3/3
4	SAM	B	1101	-	-	6/17/33/33	0/3/3/3
4	SAM	A	1101	-	-	4/17/33/33	0/3/3/3
4	SAM	C	1101	-	-	11/17/33/33	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1101	SAM	OXT-C	-2.62	1.22	1.30
4	A	1101	SAM	OXT-C	-2.25	1.23	1.30
4	D	1102	SAM	OXT-C	-2.10	1.23	1.30
4	C	1101	SAM	OXT-C	-2.09	1.24	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1101	SAM	C2'-C1'-N9	2.04	118.36	113.30

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1101	SAM	O4'-C4'-C5'-SD
4	A	1101	SAM	C3'-C4'-C5'-SD
4	B	1101	SAM	N-CA-CB-CG
4	C	1101	SAM	N-CA-CB-CG
4	C	1101	SAM	C-CA-CB-CG
4	C	1101	SAM	CA-CB-CG-SD
4	C	1101	SAM	O4'-C4'-C5'-SD
4	C	1101	SAM	C3'-C4'-C5'-SD
4	D	1102	SAM	O4'-C4'-C5'-SD
4	D	1102	SAM	C3'-C4'-C5'-SD
4	B	1101	SAM	C-CA-CB-CG
4	C	1101	SAM	OXT-C-CA-CB
4	A	1101	SAM	CA-CB-CG-SD
4	D	1102	SAM	CA-CB-CG-SD
4	B	1101	SAM	O4'-C4'-C5'-SD
4	C	1101	SAM	O-C-CA-CB
4	B	1101	SAM	C3'-C4'-C5'-SD
4	C	1101	SAM	C2'-C1'-N9-C8
4	C	1101	SAM	C2'-C1'-N9-C4
4	D	1102	SAM	O4'-C1'-N9-C8
4	C	1101	SAM	O4'-C1'-N9-C8
4	B	1101	SAM	O4'-C1'-N9-C8
4	B	1101	SAM	CB-CG-SD-C5'
4	C	1101	SAM	CB-CG-SD-C5'
4	A	1101	SAM	O4'-C1'-N9-C8

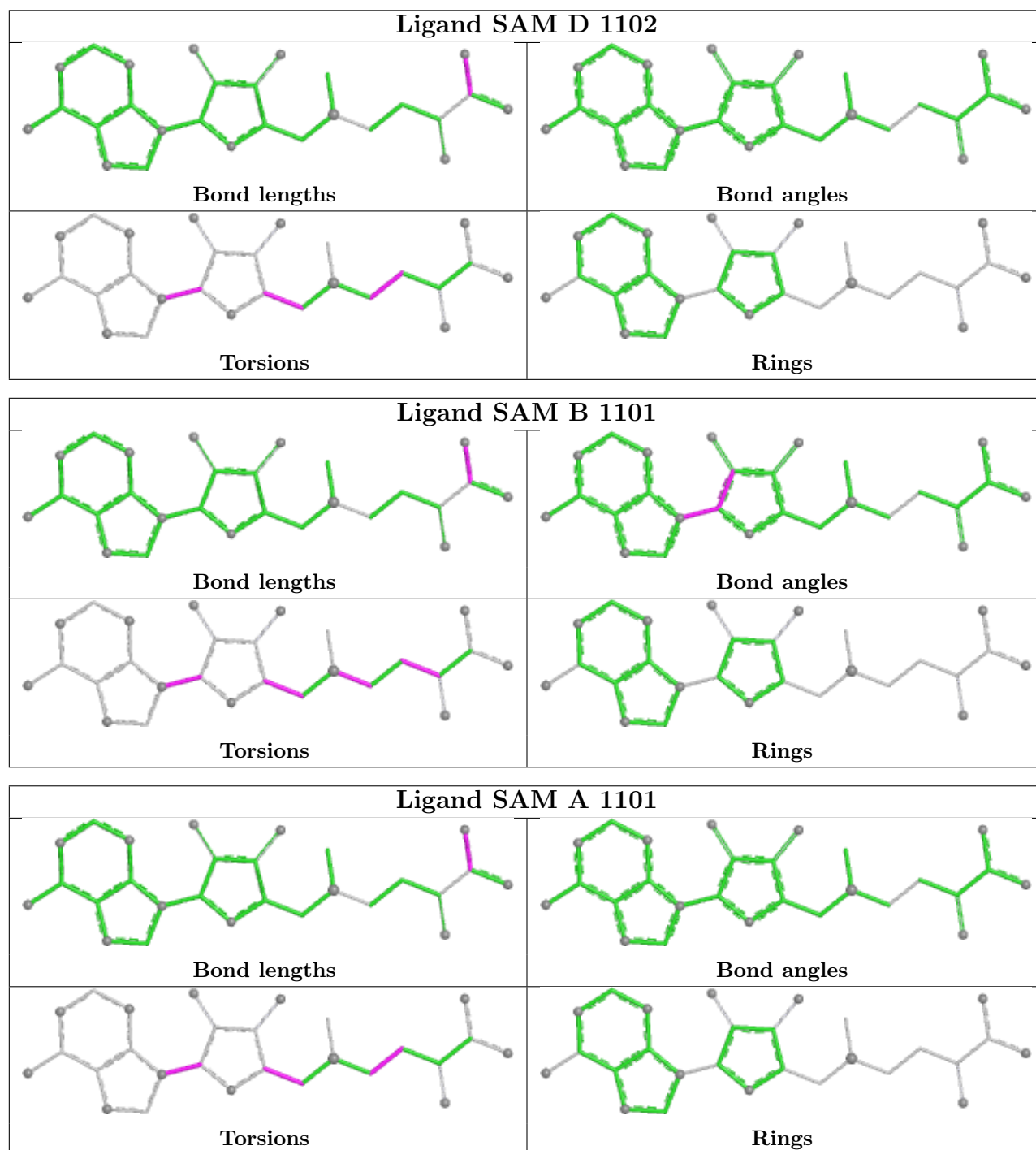
There are no ring outliers.

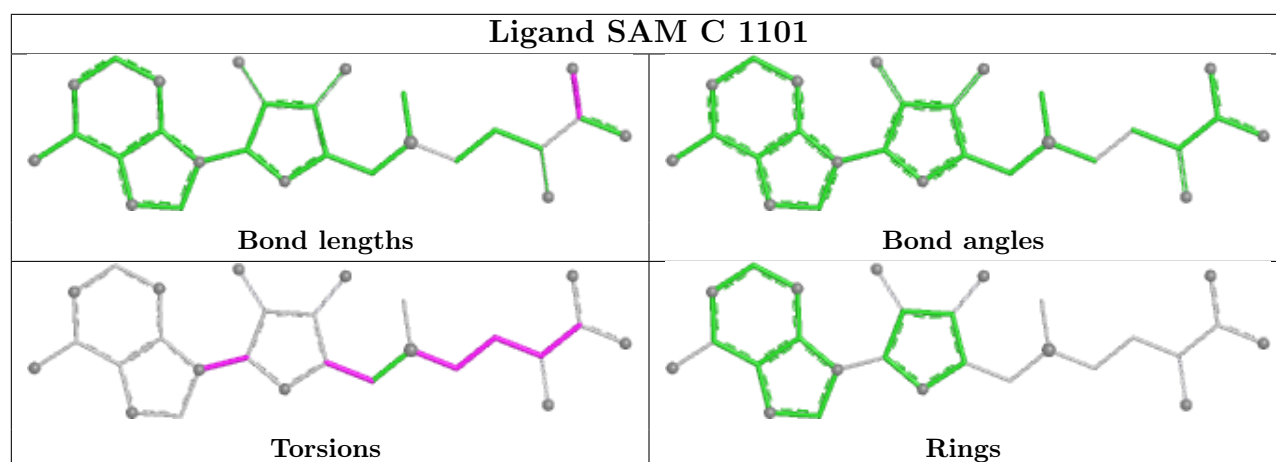
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1102	SAM	1	0
4	A	1101	SAM	1	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](#)

There are no chain breaks in this entry.

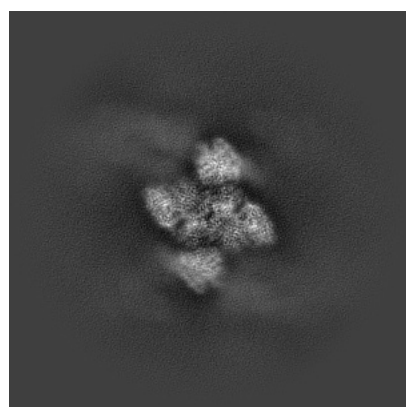
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23461. These allow visual inspection of the internal detail of the map and identification of artifacts.

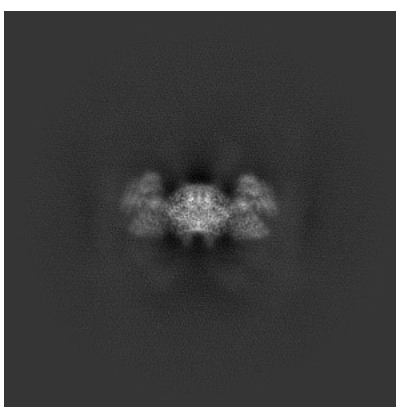
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

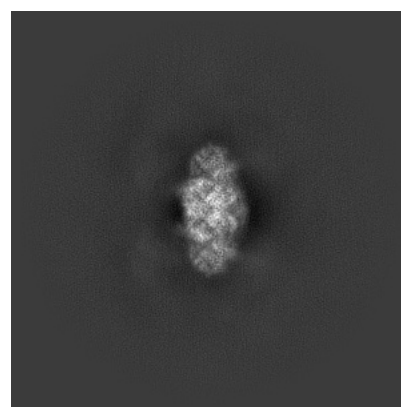
6.1.1 Primary map



X



Y

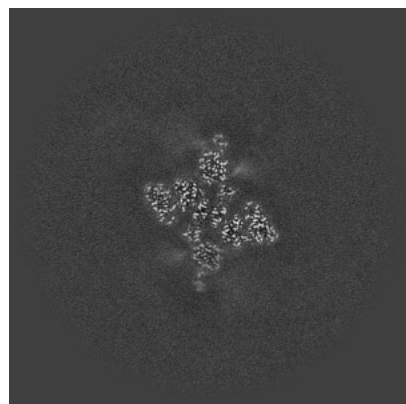


Z

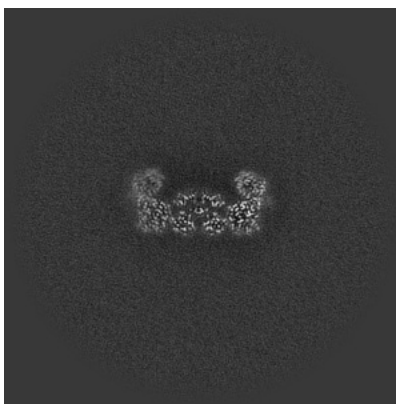
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

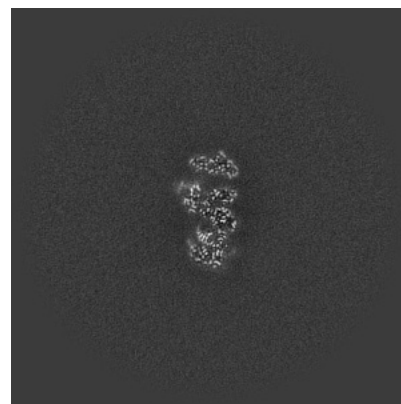
6.2.1 Primary map



X Index: 256



Y Index: 256

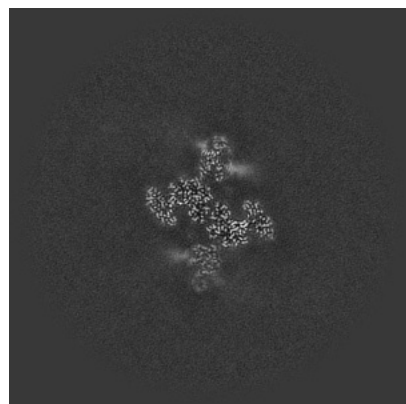


Z Index: 256

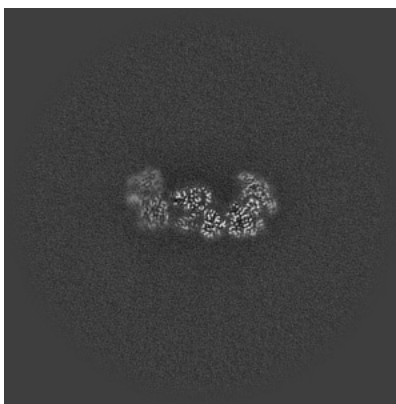
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

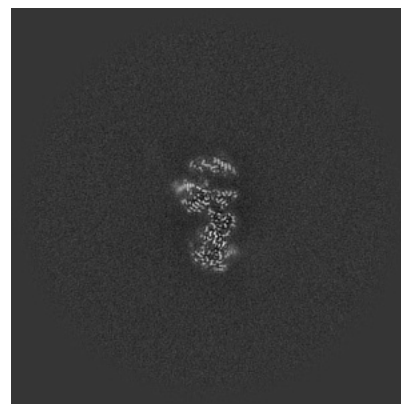
6.3.1 Primary map



X Index: 262



Y Index: 263

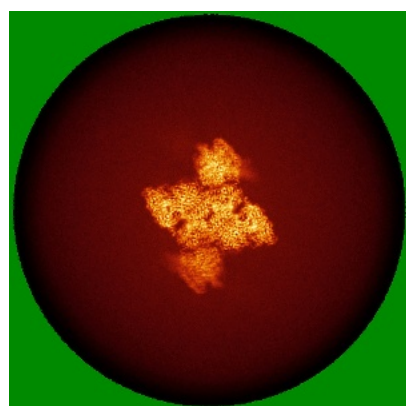


Z Index: 261

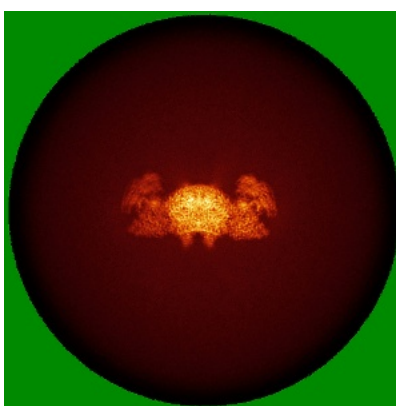
The images above show the largest variance slices of the map in three orthogonal directions.

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

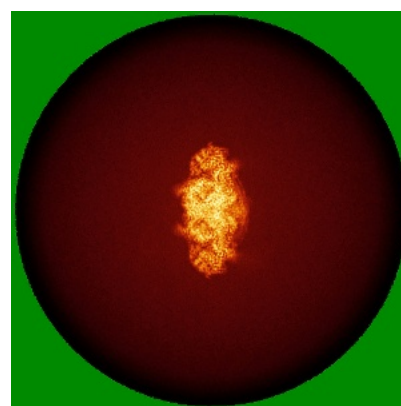
6.4.1 Primary map



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

This section was not generated.

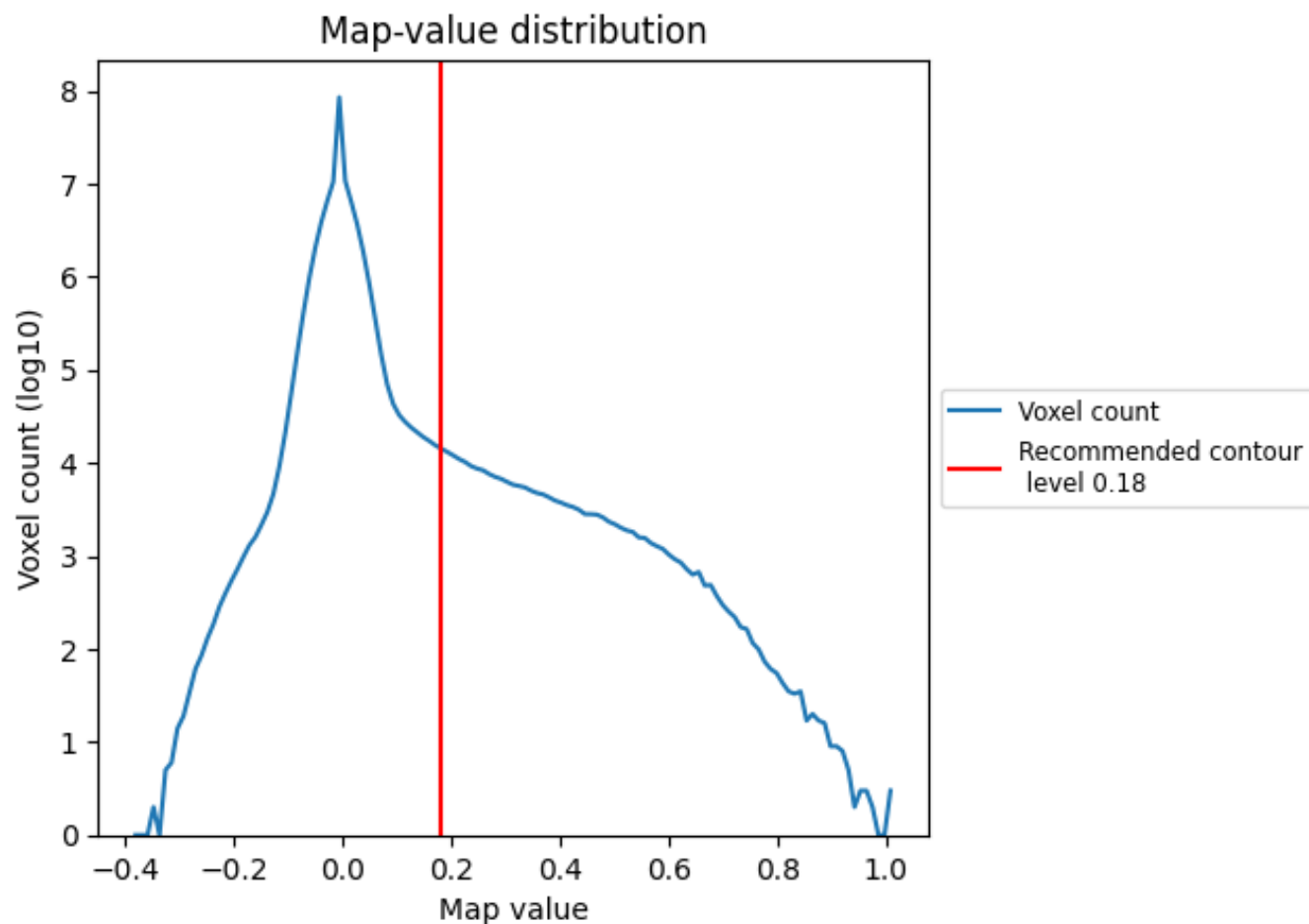
6.6 Mask visualisation

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

7 Map analysis [i](#)

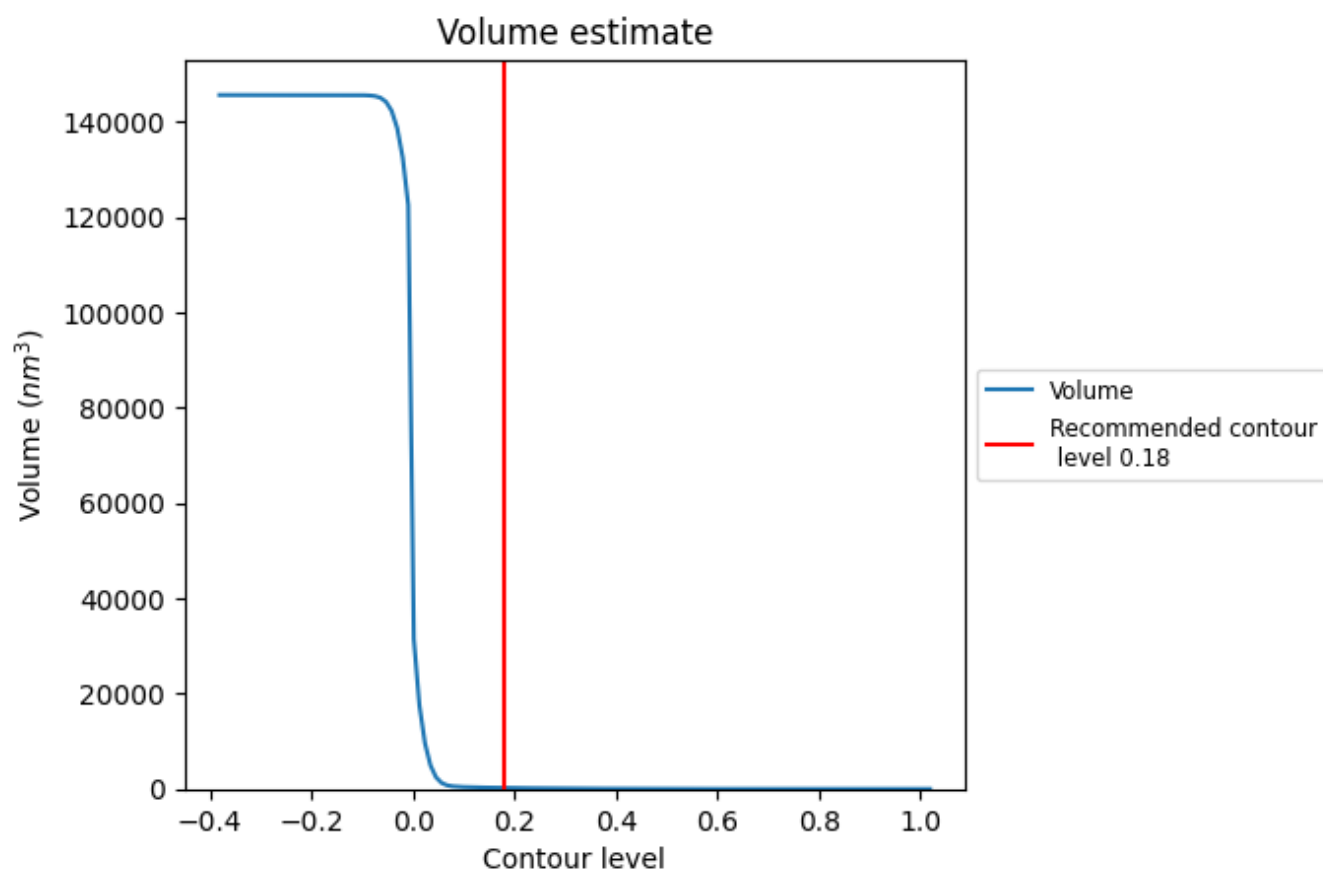
This section contains the results of statistical analysis of the map.

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.

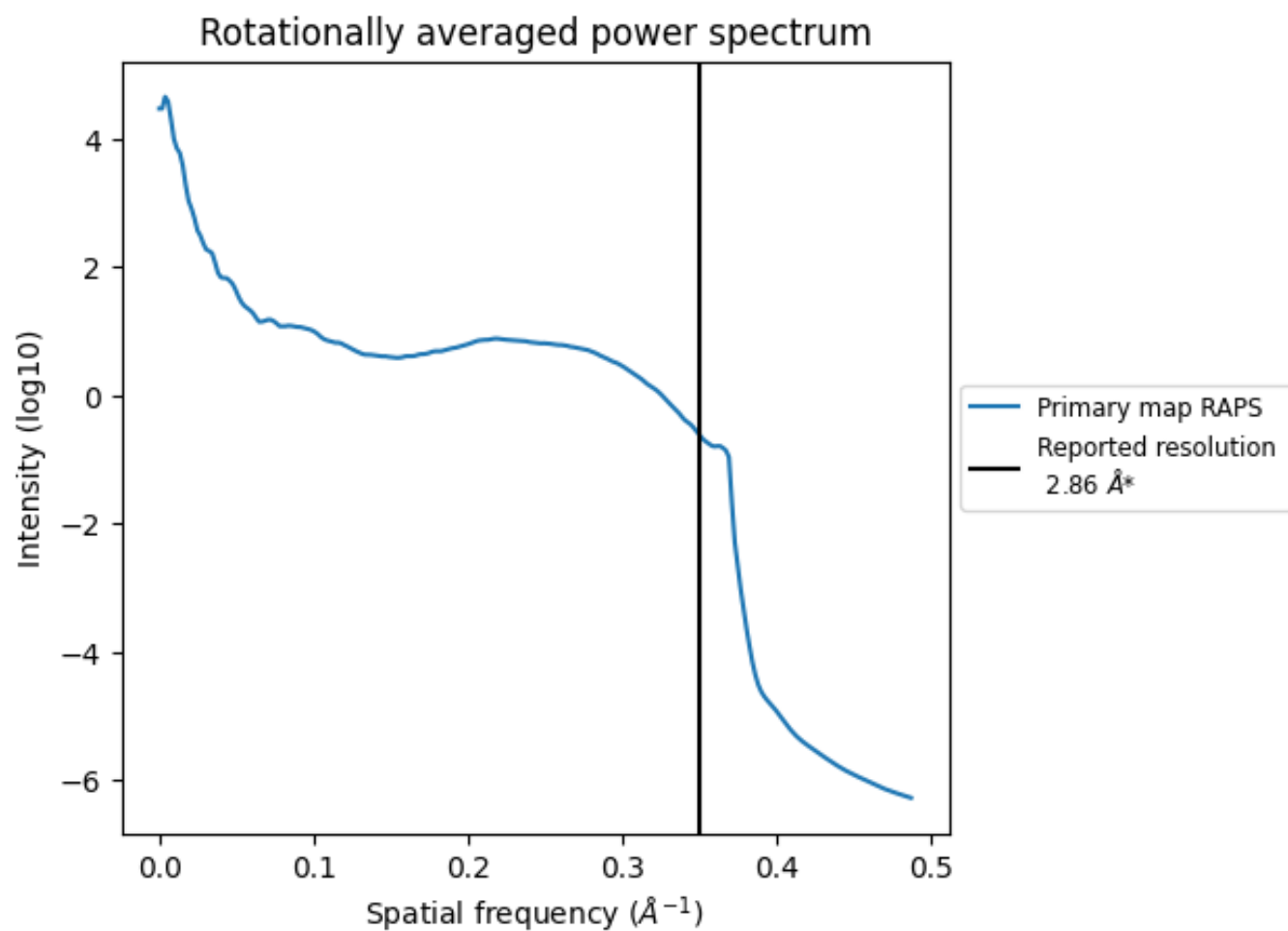
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 224 nm³; this corresponds to an approximate mass of 202 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 0.350 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

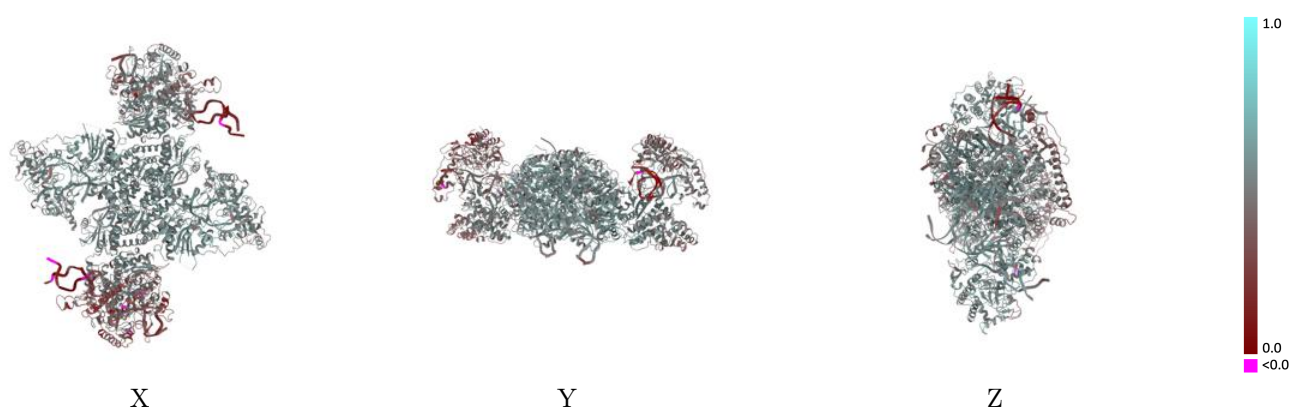
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23461 and PDB model 7LO5. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

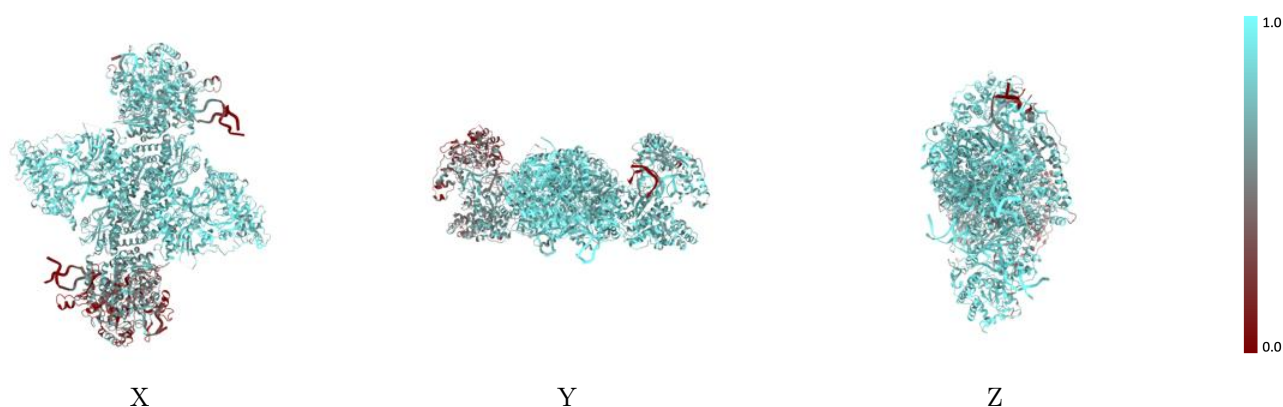
This section was not generated.

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



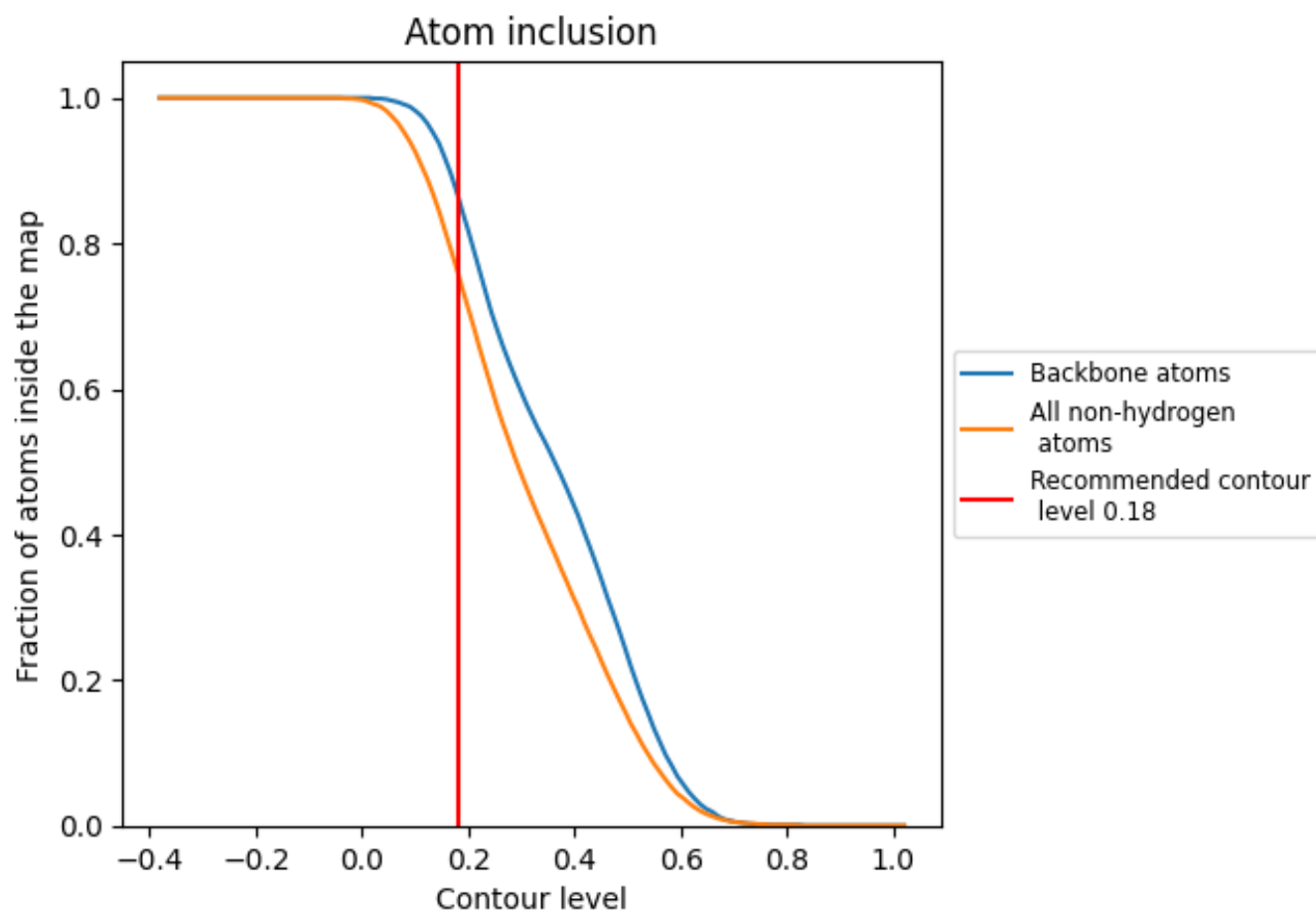
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 76% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7600	0.4920
A	0.8530	0.5430
B	0.8530	0.5430
C	0.7920	0.4940
D	0.5280	0.4200
E	0.9700	0.5450
F	0.9560	0.5420
G	0.9520	0.5410
H	0.9520	0.5530
I	0.6470	0.3530
J	0.6600	0.3540
K	0.5570	0.2910
L	0.5220	0.2670

1.0

0.0

<0.0