



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:48 PM UTC

PDB ID : 6DBQ / pdb_00006dbq
EMDB ID : EMD-7847
Title : Cryo-EM structure of RAG in complex with 12-RSS and 23-RSS substrate DNAs
Authors : Wu, H.; Liao, M.; Ru, H.; Mi, W.
Deposited on : 2018-05-03
Resolution : 4.22 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
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

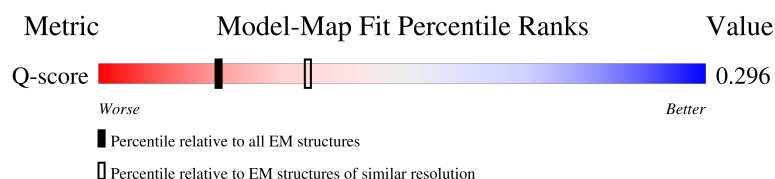
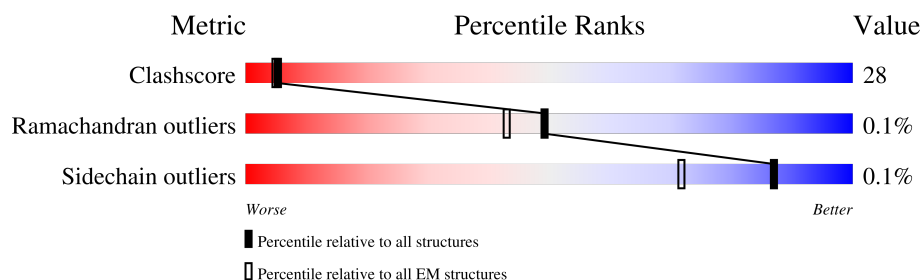
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.22 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.



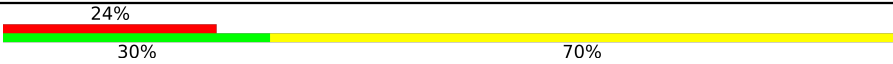
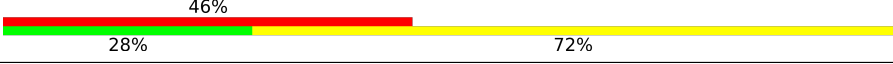
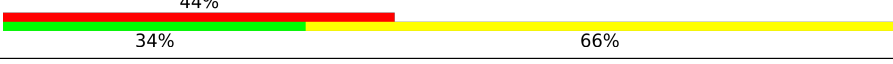
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4772 (3.72 - 4.72)

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	1159	
1	C	1159	
2	B	533	
2	D	533	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	50	
4	F	50	
5	G	61	
6	H	61	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19956 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 Recombination activating gene 1 - MBP chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	621	Total	C	N	O	S	0	0
			4999	3128	899	935	37		
1	C	616	Total	C	N	O	S	0	0
			4972	3113	893	929	37		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-127	MET	-	initiating methionine	UNP P0AEX9
A	-126	GLY	-	expression tag	UNP P0AEX9
A	-125	SER	-	expression tag	UNP P0AEX9
A	-124	SER	-	expression tag	UNP P0AEX9
A	-123	HIS	-	expression tag	UNP P0AEX9
A	-122	HIS	-	expression tag	UNP P0AEX9
A	-121	HIS	-	expression tag	UNP P0AEX9
A	-120	HIS	-	expression tag	UNP P0AEX9
A	-119	HIS	-	expression tag	UNP P0AEX9
A	-118	HIS	-	expression tag	UNP P0AEX9
A	-117	GLY	-	expression tag	UNP P0AEX9
A	-116	THR	-	expression tag	UNP P0AEX9
A	-115	LYS	-	expression tag	UNP P0AEX9
A	-114	THR	-	expression tag	UNP P0AEX9
A	251	GLY	-	linker	UNP P0AEX9
A	252	THR	-	linker	UNP P0AEX9
A	253	ASP	-	linker	UNP P0AEX9
A	254	TYR	-	linker	UNP P0AEX9
A	255	ASP	-	linker	UNP P0AEX9
A	256	ILE	-	linker	UNP P0AEX9
A	257	PRO	-	linker	UNP P0AEX9
A	258	THR	-	linker	UNP P0AEX9
A	259	THR	-	linker	UNP P0AEX9
A	260	LEU	-	linker	UNP P0AEX9
A	261	GLU	-	linker	UNP P0AEX9
A	262	VAL	-	linker	UNP P0AEX9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	263	LEU	-	linker	UNP P0AEX9
A	264	PHE	-	linker	UNP P0AEX9
A	265	GLN	-	linker	UNP P0AEX9
A	266	GLY	-	linker	UNP P0AEX9
A	267	PRO	-	linker	UNP P0AEX9
A	268	LEU	-	linker	UNP P0AEX9
A	269	GLY	-	linker	UNP P0AEX9
A	270	SER	-	linker	UNP P0AEX9
C	-127	MET	-	initiating methionine	UNP P0AEX9
C	-126	GLY	-	expression tag	UNP P0AEX9
C	-125	SER	-	expression tag	UNP P0AEX9
C	-124	SER	-	expression tag	UNP P0AEX9
C	-123	HIS	-	expression tag	UNP P0AEX9
C	-122	HIS	-	expression tag	UNP P0AEX9
C	-121	HIS	-	expression tag	UNP P0AEX9
C	-120	HIS	-	expression tag	UNP P0AEX9
C	-119	HIS	-	expression tag	UNP P0AEX9
C	-118	HIS	-	expression tag	UNP P0AEX9
C	-117	GLY	-	expression tag	UNP P0AEX9
C	-116	THR	-	expression tag	UNP P0AEX9
C	-115	LYS	-	expression tag	UNP P0AEX9
C	-114	THR	-	expression tag	UNP P0AEX9
C	251	GLY	-	linker	UNP P0AEX9
C	252	THR	-	linker	UNP P0AEX9
C	253	ASP	-	linker	UNP P0AEX9
C	254	TYR	-	linker	UNP P0AEX9
C	255	ASP	-	linker	UNP P0AEX9
C	256	ILE	-	linker	UNP P0AEX9
C	257	PRO	-	linker	UNP P0AEX9
C	258	THR	-	linker	UNP P0AEX9
C	259	THR	-	linker	UNP P0AEX9
C	260	LEU	-	linker	UNP P0AEX9
C	261	GLU	-	linker	UNP P0AEX9
C	262	VAL	-	linker	UNP P0AEX9
C	263	LEU	-	linker	UNP P0AEX9
C	264	PHE	-	linker	UNP P0AEX9
C	265	GLN	-	linker	UNP P0AEX9
C	266	GLY	-	linker	UNP P0AEX9
C	267	PRO	-	linker	UNP P0AEX9
C	268	LEU	-	linker	UNP P0AEX9
C	269	GLY	-	linker	UNP P0AEX9
C	270	SER	-	linker	UNP P0AEX9

- Molecule 2 is a protein called Recombination activating gene 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	351	Total	C	N	O	S	0	0
			2714	1716	470	509	19		
2	D	351	Total	C	N	O	S	0	0
			2714	1716	470	509	19		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q1RLW7
B	-1	GLY	-	expression tag	UNP Q1RLW7
B	0	SER	-	expression tag	UNP Q1RLW7
D	-2	GLY	-	expression tag	UNP Q1RLW7
D	-1	GLY	-	expression tag	UNP Q1RLW7
D	0	SER	-	expression tag	UNP Q1RLW7

- Molecule 3 is a DNA chain called Molecule name: Forward strand of 12-RSS substrate DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	50	Total	C	N	O	P	0	0
			1023	486	192	295	50		

- Molecule 4 is a DNA chain called Molecule name: Reverse strand of 12-RSS substrate DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	50	Total	C	N	O	P	0	0
			1027	489	183	305	50		

- Molecule 5 is a DNA chain called Molecule name: Forward strand of 23-RSS substrate DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	61	Total	C	N	O	P	0	0
			1245	593	223	368	61		

- Molecule 6 is a DNA chain called Reverse strand of 23-RSS substrate DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	61	Total	C	N	O	P	0	0
			1256	596	235	364	61		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total 1	Zn 1	0
7	C	1	Total 1	Zn 1	0

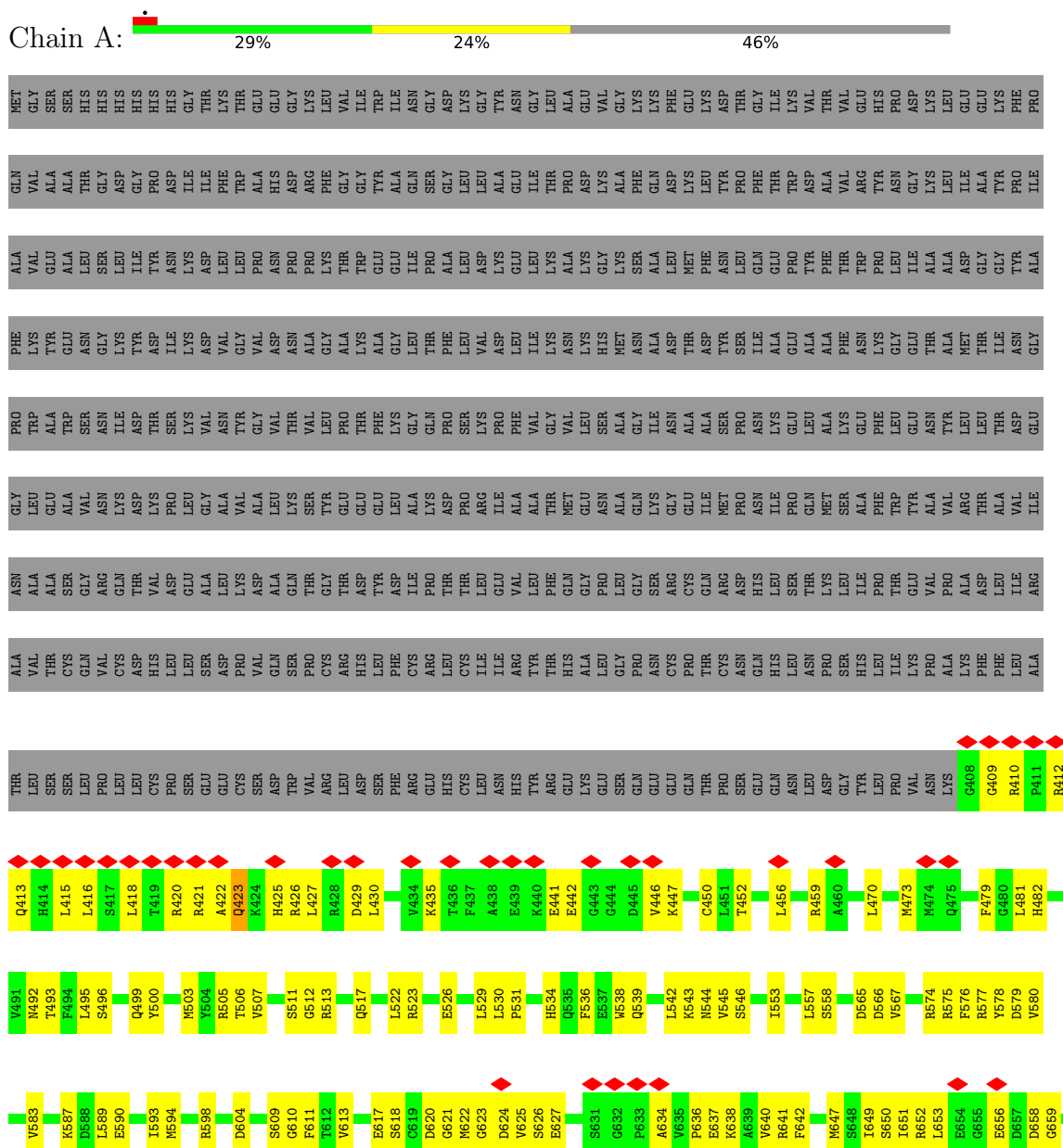
- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
8	A	2	Total 2	Ca 2	0
8	C	2	Total 2	Ca 2	0

3 Residue-property plots

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

- Molecule 1: Recombination activating gene 1 - MBP chimera

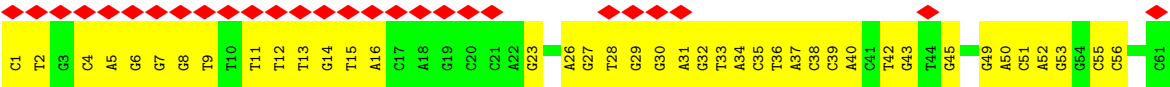




PHE	GLU	GLU	T250	M171	Y90	GLY
	SER	GLU		M172	L91	GLY
LEU	LEU	ASP	L256	M173	I92	GLY
ARG	GLU	GLU	T257		H93	M1
LEU	GLU	GLU		D177	G94	S2
PHE	GLN	ASP	A261	C178	G95	
ASP	LEU	GLU	F350	P179	R96	P5
	SER	SER	Y268	P190	T97	L6
	GLN	GLN	H269		P98	T7
	ASP	THR	E270	L184	N99	A8
	GLY	GLY			N100	V9
	SER	ASP	T273	H195	E101	X10
	THR	THR	F274	T196	L102	C11
	LYS	ILE		L197	S103	
	PHE	LYS	Y277	P198	S104	Q16
	CYS	CYS		E199	S105	
	LEU	CYS	E280	L200	L106	L21
	ASP	LEU	T281	T201	Y107	L22
	HIS	SER	Q282	B202	M108	D23
	GLY	CYS	K283	G203	L109	L24
	GLY	GLN	R284	Q204	S110	
	LEU	VAL				V28
	PRO	GLU	T288	H207	L122	
	LYS	PRO	Y289	V208	R123	K34
	GLN	ASN		A209	C124	G35
	GLU	ILE	L292	L210	E125	W36
	MET	TRP	D293	A211	E126	
	THR	GLU	D294	R212	K127	T43
	PRO	PRO		Q213	G44	G44
	PRO	TRP	W299	D214	G131	I45
	LYS	TYR	E300	C215	D132	
	GLN	SER	S301	V216		V48
	MET	THR	R302	V217	S135	R49
	LEU	GLU		F218	A136	
	PRO	LEU	P305		R137	E54
	VAL	THR	Q306	I223	Y138	L55
	LYS	ARG			G139	K56
	ARG	PRO	T316	S226	H140	L57
	VAL	ALA	W317	D227	T141	R58
	PRO	MET	F318	C228	L142	
	MET	ILE	G319	R229		F62
	LYS	PHE	G320	P230	S147	
	MET	CYS		S231	R148	N65
	THR	SER	G323	R232	G149	S67
	HIS	ARG		L233		
	ARG	GLY	T326	L234	V154	R73
	LYS	GLU		R235	L155	
	ALA	GLY	A330	L236	F156	
	PRO	GLY	I331	H237	G157	A76
	VAL	HIS	P332	V238	G158	I77
	SER	TRP	S333	E239	R159	A78
	LEU	VAL		L240		
	LYS	HIS		L241	M162	A82
	ASP	ASP	W336		P163	Q83
	VAL	VAL	P337	L242	G164	D94
	THR	GLN	T338	G243		G85
	PRO	CYS	P339	S244		K86
	ALA	MET	P340	T245	R167	P87
	LYS	GLU	E341	V246	T168	E88
	THR	LEU			G170	C90
	PRO	PRO	A342			

- Molecule 2: Recombination activating gene 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48002	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.182	Depositor
Minimum map value	-0.085	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	237.69601, 237.69601, 237.69601	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.238, 1.238, 1.238	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, ZN

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	0.23	0/5097	0.65	6/6856 (0.1%)
1	C	0.27	1/5067 (0.0%)	0.80	8/6812 (0.1%)
2	B	0.28	0/2784	0.65	11/3784 (0.3%)
2	D	0.27	1/2784 (0.0%)	0.63	4/3784 (0.1%)
3	E	0.25	0/1148	0.47	0/1768
4	F	0.24	0/1150	0.49	0/1774
5	G	0.25	0/1394	0.44	0/2148
6	H	0.25	0/1410	0.48	0/2175
All	All	0.26	2/20834 (0.0%)	0.64	29/29101 (0.1%)

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	1
1	C	0	1
2	B	0	3
2	D	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	83	GLN	CG-CD	-5.43	1.38	1.52
1	C	817	HIS	CG-CD2	5.03	1.41	1.35

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	432	ASN	CB-CG-ND2	-33.20	66.60	116.40
1	C	432	ASN	CB-CG-OD1	25.20	171.21	120.80
1	A	423	GLN	CG-CD-NE2	-24.84	79.13	116.40
1	A	423	GLN	CG-CD-OE1	18.39	157.58	120.80
1	C	432	ASN	OD1-CG-ND2	-15.82	106.78	122.60
1	C	816	LEU	CA-C-N	-14.84	98.06	122.54
1	C	816	LEU	C-N-CA	-14.84	98.06	122.54
1	A	423	GLN	OE1-CD-NE2	-14.27	108.33	122.60
1	C	817	HIS	CB-CG-CD2	-13.69	113.41	131.20
2	D	83	GLN	CG-CD-NE2	-12.64	97.44	116.40
2	B	344	HIS	N-CA-CB	-11.96	90.27	110.49
2	D	83	GLN	CB-CG-CD	10.18	129.90	112.60
2	D	83	GLN	CA-CB-CG	9.49	133.07	114.10
2	B	344	HIS	CB-CA-C	8.31	126.95	110.42
2	B	10	ASN	CB-CA-C	-8.02	94.46	110.42
2	B	9	VAL	CA-C-N	6.98	134.87	121.54
2	B	9	VAL	C-N-CA	6.98	134.87	121.54
1	C	817	HIS	N-CA-CB	6.71	120.42	110.49
2	B	10	ASN	CB-CG-ND2	-6.38	106.83	116.40
2	B	339	PRO	CA-C-N	6.35	142.25	127.00
2	B	339	PRO	C-N-CA	6.35	142.25	127.00
1	A	423	GLN	CA-CB-CG	6.18	126.46	114.10
2	B	339	PRO	C-N-CD	-6.03	107.34	120.60
1	A	423	GLN	CB-CG-CD	5.76	122.39	112.60
2	B	344	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	A	423	GLN	N-CA-C	-5.27	105.59	112.23
1	C	817	HIS	N-CA-C	-5.25	106.56	113.17
2	D	234	ILE	CA-CB-CG1	-5.08	101.76	110.40
2	B	10	ASN	N-CA-CB	5.07	119.06	110.49

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	423	GLN	Sidechain
2	B	10	ASN	Sidechain,Mainchain
2	B	344	HIS	Sidechain
1	C	817	HIS	Sidechain
2	D	83	GLN	Sidechain

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	4999	0	4954	271	0
1	C	4972	0	4937	253	0
2	B	2714	0	2665	167	0
2	D	2714	0	2665	181	0
3	E	1023	0	561	68	0
4	F	1027	0	566	67	0
5	G	1245	0	687	99	0
6	H	1256	0	685	52	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	2	0	0	0	0
8	C	2	0	0	0	0
All	All	19956	0	17720	1049	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 28.

All (1049) 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)
5:G:12:DT:O4	6:H:50:DA:N6	1.60	1.34
2:D:123:ARG:NH2	2:D:125:GLU:OE2	1.70	1.25
2:D:232:ARG:HH11	2:D:234:ILE:CG1	1.49	1.23
1:C:435:LYS:NZ	1:C:439:GLU:OE2	1.81	1.12
1:A:789:GLU:OE2	1:A:797:ARG:NH1	1.84	1.10
2:D:137:ARG:NH1	2:D:178:CYS:SG	2.25	1.09
2:D:338:THR:HG22	2:D:340:PRO:HA	1.30	1.08
1:A:505:ARG:NH1	1:C:1029:LYS:O	1.89	1.05
1:A:447:LYS:NZ	1:C:463:GLU:OE2	1.88	1.04
1:A:740:LEU:HD11	1:A:770:ARG:HH12	1.24	1.00
2:D:232:ARG:HH11	2:D:234:ILE:HG12	1.27	0.98
2:B:99:ASN:OD1	2:B:101:GLU:OE2	1.81	0.97
1:A:869:MET:HE3	1:A:870:ARG:HG2	1.47	0.96
2:D:232:ARG:HH11	2:D:234:ILE:HG13	1.30	0.96
2:B:97:THR:OG1	2:B:101:GLU:OE2	1.86	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:10:DT:C4	5:G:11:DG:C6	2.57	0.93
1:C:523:ARG:NH1	3:E:24:DC:OP2	2.02	0.92
2:D:232:ARG:NH1	2:D:234:ILE:CG1	2.31	0.92
5:G:32:DC:N4	6:H:30:DG:O6	2.02	0.92
5:G:30:DC:H2"	5:G:31:DT:H71	1.51	0.92
1:A:861:LYS:HZ2	1:A:862:LYS:HZ2	1.08	0.92
2:B:76:ALA:HB3	2:B:93:HIS:O	1.71	0.91
3:E:31:DC:O2	4:F:20:DG:N2	2.05	0.90
2:D:58:ARG:NH1	5:G:7:DG:OP1	2.04	0.90
2:D:232:ARG:NH1	2:D:234:ILE:HG13	1.87	0.90
1:C:598:ARG:NH1	1:C:604:ASP:OD2	2.04	0.90
1:A:546:SER:O	1:A:577:ARG:NH1	2.06	0.89
2:B:97:THR:OG1	2:B:99:ASN:OD1	1.89	0.89
2:B:137:ARG:NH1	2:B:178:CYS:SG	2.46	0.89
1:C:877:ARG:HH12	1:C:916:ARG:NH1	1.73	0.87
2:B:331:ILE:O	2:B:343:TYR:HA	1.76	0.86
1:C:590:GLU:OE2	1:C:714:GLY:N	2.08	0.85
5:G:9:DC:N3	6:H:53:DG:N1	2.24	0.85
2:B:10:ASN:ND2	2:B:10:ASN:C	2.34	0.85
1:A:413:GLN:O	1:A:426:ARG:NH1	2.10	0.85
2:B:10:ASN:HD22	2:B:11:CYS:CB	1.88	0.84
2:B:43:THR:HG22	2:B:45:ILE:H	1.43	0.84
2:D:147:SER:OG	2:D:240:LEU:HD22	1.77	0.84
1:A:617:GLU:OE2	1:A:701:ARG:NH1	2.10	0.83
1:A:624:ASP:HA	1:A:637:GLU:HB3	1.59	0.83
1:C:577:ARG:NH2	1:C:579:ASP:OD2	2.11	0.83
3:E:31:DC:N3	4:F:20:DG:N1	2.27	0.82
1:A:652:ARG:NH1	1:A:656:GLU:O	2.12	0.82
1:C:819:ASP:OD2	1:C:916:ARG:NH2	2.12	0.82
2:D:28:VAL:HG13	2:D:48:VAL:HB	1.61	0.82
1:C:590:GLU:HG2	1:C:713:VAL:HG23	1.62	0.81
1:C:575:ARG:NH1	1:C:576:PHE:O	2.14	0.81
1:C:760:SER:HB3	1:C:954:ILE:HD11	1.61	0.80
1:A:686:ASP:OD1	1:A:688:GLU:N	2.14	0.80
1:A:774:GLU:HG3	1:A:778:ARG:HH12	1.46	0.80
1:A:523:ARG:NH2	5:G:24:DG:OP2	2.14	0.79
1:A:738:GLU:OE2	1:A:775:ASN:ND2	2.16	0.79
1:A:481:LEU:O	1:A:517:GLN:NE2	2.16	0.79
1:C:538:TRP:CZ3	1:C:704:MET:CE	2.65	0.79
1:A:858:GLN:O	1:A:862:LYS:NZ	2.16	0.79
1:C:486:CYS:HG	1:C:500:TYR:HH	1.17	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:GLN:HB3	2:B:223:ILE:HG12	1.64	0.78
5:G:9:DC:O2	6:H:53:DG:N2	2.11	0.78
5:G:12:DT:O2	6:H:50:DA:H2	1.66	0.78
1:C:713:VAL:HG13	1:C:718:ARG:HD2	1.63	0.78
2:D:148:ARG:HH12	2:D:239:GLU:HB3	1.48	0.77
2:D:86:LYS:NZ	2:D:87:PRO:O	2.17	0.77
1:C:709:LEU:HB3	1:C:720:PHE:HB2	1.67	0.77
1:A:598:ARG:NH1	1:A:604:ASP:OD2	2.16	0.77
1:A:861:LYS:HZ2	1:A:862:LYS:NZ	1.83	0.77
2:D:123:ARG:NH2	2:D:125:GLU:CD	2.41	0.76
1:A:861:LYS:NZ	1:A:862:LYS:HZ2	1.84	0.76
2:B:6:LEU:HD11	2:B:347:GLN:HB2	1.66	0.76
1:C:814:ASP:OD2	1:C:817:HIS:N	2.19	0.76
2:D:232:ARG:HE	2:D:234:ILE:HD11	1.50	0.76
3:E:28:DA:H2''	3:E:29:DG:OP2	1.86	0.76
6:H:39:DC:H2'	6:H:40:DA:C8	2.21	0.76
1:C:731:GLU:HG3	1:C:735:ARG:HD2	1.67	0.75
2:D:140:HIS:HD2	2:D:155:LEU:HD11	1.50	0.75
2:B:65:ASN:O	2:B:123:ARG:NH1	2.18	0.75
2:D:148:ARG:O	2:D:150:LYS:NZ	2.19	0.75
1:A:991:ARG:NH1	4:F:34:DG:O3'	2.19	0.74
2:D:258:ILE:HD13	2:D:284:ARG:HD2	1.67	0.74
4:F:36:DA:H2''	4:F:37:DA:OP2	1.85	0.74
1:A:598:ARG:HH12	1:A:604:ASP:CG	1.96	0.74
2:B:104:SER:HB2	2:B:136:ALA:HB2	1.70	0.74
2:B:49:ARG:HH22	2:B:58:ARG:HD2	1.52	0.74
3:E:7:DG:H2''	3:E:8:DC:OP2	1.87	0.74
2:B:10:ASN:HD22	2:B:11:CYS:HB2	1.50	0.73
2:D:58:ARG:HH22	5:G:7:DG:H5''	1.53	0.73
2:D:56:LYS:HZ3	5:G:8:DC:H5''	1.54	0.73
5:G:12:DT:C4	6:H:50:DA:N6	2.54	0.73
2:D:49:ARG:NH1	2:D:58:ARG:HH21	1.87	0.73
2:B:270:GLU:OE2	2:B:270:GLU:N	2.22	0.73
5:G:12:DT:O2	6:H:50:DA:C2	2.41	0.72
2:B:148:ARG:HH12	2:B:239:GLU:HB3	1.53	0.72
2:B:49:ARG:HH22	2:B:58:ARG:HH11	1.35	0.72
2:B:283:LYS:HB2	2:B:317:TRP:HE1	1.54	0.72
1:C:617:GLU:OE2	1:C:729:TYR:OH	2.08	0.72
1:A:486:CYS:SG	1:A:500:TYR:OH	2.48	0.72
1:C:825:GLU:OE2	1:C:950:TYR:OH	2.07	0.71
1:C:1002:LYS:HA	1:C:1005:GLU:HB3	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:836:GLU:HB3	1:C:839:GLN:HB2	1.72	0.71
1:A:741:GLU:N	1:A:741:GLU:OE2	2.22	0.71
1:C:738:GLU:OE2	1:C:775:ASN:ND2	2.24	0.71
1:A:688:GLU:OE2	2:B:73:ARG:NE	2.24	0.71
1:A:735:ARG:NH2	1:A:748:ILE:O	2.23	0.71
1:A:415:LEU:HD21	1:A:427:LEU:HD11	1.73	0.71
1:C:784:LYS:NZ	2:D:126:GLU:OE1	2.23	0.71
4:F:37:DA:OP2	4:F:37:DA:H8	1.74	0.71
1:A:421:ARG:NH2	6:H:14:DG:O6	2.24	0.71
1:A:493:THR:OG1	1:C:499:GLN:OE1	2.09	0.70
1:A:869:MET:HE3	1:A:870:ARG:CG	2.21	0.70
1:A:412:ARG:NH2	6:H:11:DT:OP1	2.24	0.70
1:A:774:GLU:HG3	1:A:778:ARG:NH1	2.07	0.70
5:G:11:DG:H1'	5:G:12:DT:H5'	1.73	0.70
2:B:48:VAL:HG23	2:B:55:LEU:HD11	1.74	0.69
5:G:10:DT:N3	5:G:11:DG:C5	2.60	0.69
2:B:49:ARG:HH12	2:B:58:ARG:NH1	1.90	0.69
1:A:575:ARG:NH1	1:A:576:PHE:O	2.26	0.69
5:G:10:DT:C6	5:G:11:DG:N7	2.60	0.69
4:F:22:DC:H2''	4:F:23:DT:OP2	1.92	0.69
1:A:892:VAL:HG13	1:A:898:ARG:HG2	1.74	0.69
2:B:230:PRO:HB2	2:B:232:ARG:HG2	1.75	0.69
2:B:270:GLU:HB3	2:B:289:TYR:HE1	1.57	0.69
2:D:96:ARG:NH1	2:D:161:TYR:OH	2.25	0.69
5:G:12:DT:O4	6:H:50:DA:C6	2.46	0.69
3:E:18:DA:H2'	3:E:19:DC:C6	2.28	0.69
5:G:30:DC:H2''	5:G:31:DT:C7	2.23	0.69
1:C:641:ARG:NH1	1:C:987:ASN:OD1	2.24	0.68
4:F:12:DT:C6	4:F:13:DT:H72	2.29	0.68
1:C:861:LYS:HE3	1:C:862:LYS:HG3	1.75	0.68
4:F:42:DG:OP2	4:F:42:DG:H2'	1.93	0.68
2:D:338:THR:HG22	2:D:340:PRO:CA	2.18	0.68
1:A:740:LEU:HD11	1:A:770:ARG:NH1	2.04	0.68
5:G:49:DA:H2	6:H:13:DT:H3	1.38	0.68
1:A:749:CYS:SG	1:A:959:HIS:NE2	2.66	0.68
2:B:277:TYR:HA	2:B:284:ARG:H	1.58	0.68
1:C:988:LYS:O	1:C:991:ARG:HB2	1.93	0.68
5:G:31:DT:O2	6:H:32:DG:N2	2.26	0.68
1:C:418:LEU:HD11	1:C:426:ARG:NH1	2.10	0.67
2:D:284:ARG:NE	2:D:286:GLU:OE2	2.28	0.67
5:G:10:DT:C2	5:G:11:DG:C5	2.82	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:538:TRP:CZ3	1:C:704:MET:HE2	2.27	0.67
1:A:872:ASN:ND2	3:E:18:DA:OP1	2.27	0.67
2:D:56:LYS:NZ	5:G:8:DC:H5''	2.09	0.67
1:A:771:SER:N	1:A:774:GLU:OE2	2.27	0.67
1:A:885:VAL:HG21	1:A:905:MET:HG2	1.77	0.67
2:B:28:VAL:HG13	2:B:48:VAL:HG13	1.76	0.67
1:C:538:TRP:CZ3	1:C:704:MET:HE1	2.28	0.67
3:E:41:DA:H8	3:E:41:DA:OP2	1.76	0.67
2:D:232:ARG:NE	2:D:234:ILE:HD11	2.10	0.67
1:C:771:SER:O	1:C:775:ASN:ND2	2.28	0.67
1:A:426:ARG:NH2	1:C:442:GLU:OE1	2.28	0.66
5:G:10:DT:C4	5:G:11:DG:O6	2.48	0.66
2:D:82:ALA:HB2	2:D:88:GLU:HB2	1.77	0.66
1:A:447:LYS:HZ2	1:C:463:GLU:CD	2.00	0.66
1:C:538:TRP:CE3	1:C:704:MET:HE1	2.30	0.66
5:G:10:DT:H2''	5:G:11:DG:H8	1.61	0.66
2:D:210:LEU:HD13	2:D:292:LEU:HD21	1.78	0.66
2:B:62:PHE:HE1	2:B:122:LEU:HB2	1.59	0.65
2:D:168:THR:OG1	2:D:171:ASN:HB2	1.96	0.65
3:E:27:DC:OP2	3:E:27:DC:H2'	1.96	0.65
1:A:566:ASP:OD2	2:B:138:TYR:OH	2.14	0.65
1:A:755:THR:N	1:A:758:GLU:OE2	2.21	0.65
2:D:290:VAL:HG13	2:D:297:VAL:HG23	1.77	0.65
4:F:31:DT:H2''	4:F:32:DG:OP2	1.96	0.65
3:E:21:DG:H2'	3:E:22:DT:H71	1.77	0.65
1:A:506:THR:HG21	1:C:489:ILE:HG12	1.79	0.65
1:A:622:MET:HG2	1:A:625:VAL:HG12	1.77	0.65
1:A:664:GLN:O	1:A:666:GLN:NE2	2.30	0.65
2:B:212:ARG:NH1	2:B:213:GLN:OE1	2.30	0.65
1:C:418:LEU:HB2	1:C:423:GLN:HG3	1.78	0.65
1:C:735:ARG:NH1	1:C:743:SER:HA	2.12	0.65
1:C:903:LYS:HZ3	1:C:907:LEU:HG	1.62	0.65
4:F:36:DA:H8	4:F:36:DA:OP2	1.80	0.65
2:B:10:ASN:C	2:B:10:ASN:HD22	2.02	0.65
1:C:735:ARG:NH1	1:C:742:ALA:HA	2.12	0.65
3:E:18:DA:H2'	3:E:19:DC:H6	1.62	0.65
1:A:618:SER:OG	1:A:728:GLY:O	2.14	0.64
2:D:80:PHE:HD2	2:D:89:CYS:HB2	1.60	0.64
1:A:641:ARG:NH1	1:A:987:ASN:OD1	2.30	0.64
2:D:249:CYS:SG	2:D:250:THR:N	2.70	0.64
5:G:30:DC:C2'	5:G:31:DT:H71	2.24	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:GLU:HB2	1:A:713:VAL:HG23	1.79	0.64
1:A:682:VAL:HG12	1:A:683:ASP:H	1.61	0.64
4:F:32:DG:H2''	4:F:33:DT:OP2	1.97	0.64
1:A:671:GLU:OE1	1:A:671:GLU:N	2.30	0.64
1:A:620:ASP:OD1	1:A:621:GLY:N	2.31	0.64
1:C:832:ASP:HB3	1:C:837:VAL:HG11	1.79	0.64
1:A:482:HIS:HB3	1:A:485:VAL:HG23	1.80	0.63
1:A:553:ILE:HG12	1:A:576:PHE:HE1	1.62	0.63
2:B:10:ASN:ND2	2:B:10:ASN:O	2.30	0.63
5:G:10:DT:C4	5:G:11:DG:C5	2.86	0.63
1:A:623:GLY:HA2	1:A:638:LYS:HD3	1.81	0.63
1:A:817:HIS:C	1:A:819:ASP:H	2.07	0.63
1:A:817:HIS:O	1:A:819:ASP:N	2.32	0.63
2:B:229:ARG:NH2	2:B:280:GLU:OE1	2.27	0.63
1:A:861:LYS:NZ	1:A:862:LYS:NZ	2.44	0.62
2:B:277:TYR:OH	2:B:316:THR:OG1	2.14	0.62
2:B:316:THR:HG23	2:B:332:PRO:HG3	1.80	0.62
1:C:588:ASP:OD2	1:C:1018:SER:OG	2.18	0.62
4:F:7:DG:H2'	4:F:8:DG:H8	1.65	0.62
1:C:609:SER:HB3	1:C:653:LEU:HD11	1.81	0.62
5:G:10:DT:N1	5:G:11:DG:C8	2.68	0.62
2:B:199:GLU:OE2	2:B:199:GLU:N	2.33	0.62
2:D:328:LEU:HD11	2:D:345:PHE:HD2	1.63	0.62
4:F:10:DT:H2'	4:F:11:DT:H71	1.82	0.62
1:A:496:SER:OG	1:A:499:GLN:N	2.29	0.61
1:C:741:GLU:N	1:C:741:GLU:OE1	2.32	0.61
2:D:1:MET:SD	2:D:302:ARG:NH1	2.73	0.61
2:D:49:ARG:NH1	2:D:58:ARG:HD2	2.14	0.61
2:D:123:ARG:HH21	2:D:125:GLU:CD	2.00	0.61
5:G:32:DC:H2''	5:G:33:DC:H5	1.64	0.61
5:G:9:DC:N4	6:H:53:DG:O6	2.26	0.61
2:B:333:SER:OG	2:B:344:HIS:ND1	2.01	0.61
2:D:140:HIS:CD2	2:D:155:LEU:HD11	2.32	0.61
1:A:531:PRO:HG3	1:A:576:PHE:CE2	2.35	0.61
2:B:148:ARG:HH11	2:B:241:LEU:HD13	1.65	0.61
3:E:35:DA:H2	4:F:17:DC:H42	1.49	0.61
1:A:754:SER:HB2	1:A:758:GLU:HB2	1.81	0.61
1:A:818:CYS:SG	1:A:915:TRP:NE1	2.72	0.61
2:B:217:TYR:HB3	2:B:233:LEU:HD21	1.82	0.61
1:C:795:ARG:NH1	2:D:39:ARG:NH1	2.49	0.61
1:C:840:LYS:NZ	1:C:843:PRO:HA	2.16	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:MET:HA	2:B:349:SER:O	2.01	0.61
4:F:28:DC:H2''	4:F:29:DA:C8	2.36	0.61
2:B:49:ARG:HH22	2:B:58:ARG:NH1	1.99	0.61
1:C:871:MET:HG3	1:C:875:TYR:HB3	1.81	0.61
5:G:32:DC:H2''	5:G:33:DC:OP2	2.00	0.61
5:G:36:DT:H3	6:H:26:DA:H61	1.47	0.61
1:A:473:MET:HE1	1:C:470:LEU:HB2	1.83	0.60
1:A:613:VAL:HG23	1:A:649:ILE:HD13	1.82	0.60
6:H:26:DA:H2''	6:H:27:DG:H5'	1.82	0.60
3:E:26:DA:H2''	3:E:27:DC:OP2	2.01	0.60
2:B:7:THR:OG1	2:B:54:GLU:OE1	2.20	0.60
1:C:594:MET:SD	1:C:718:ARG:NH1	2.67	0.60
1:C:870:ARG:HD3	5:G:17:DC:N4	2.17	0.60
1:A:760:SER:OG	1:A:950:TYR:O	2.19	0.60
2:D:38:LYS:NZ	6:H:49:DG:OP1	2.34	0.60
1:A:420:ARG:NE	5:G:43:DC:OP1	2.24	0.60
1:A:740:LEU:CD1	1:A:770:ARG:HH12	2.07	0.60
1:C:566:ASP:CG	2:D:159:ARG:HH12	2.09	0.60
4:F:29:DA:H8	4:F:29:DA:OP2	1.84	0.60
1:C:622:MET:SD	1:C:987:ASN:ND2	2.74	0.60
1:A:505:ARG:HH12	1:C:1029:LYS:C	2.02	0.60
2:B:10:ASN:ND2	2:B:11:CYS:SG	2.75	0.60
1:C:748:ILE:HG21	1:C:756:ARG:HE	1.66	0.60
2:D:28:VAL:CG1	2:D:48:VAL:HB	2.32	0.60
2:D:257:THR:HG23	2:D:284:ARG:HH22	1.66	0.59
1:A:675:ARG:NE	1:A:1017:THR:O	2.36	0.59
1:C:795:ARG:HH12	2:D:39:ARG:NH1	2.00	0.59
2:B:82:ALA:HB2	2:B:88:GLU:HB3	1.84	0.59
2:B:269:HIS:N	2:B:270:GLU:OE2	2.36	0.59
2:D:8:ALA:HA	2:D:55:LEU:HB3	1.84	0.59
2:D:232:ARG:NH1	2:D:234:ILE:HG12	2.10	0.59
3:E:14:DT:H2'	3:E:14:DT:OP2	2.01	0.59
1:A:915:TRP:HB2	1:A:975:ILE:HD12	1.83	0.59
2:B:2:SER:O	2:B:348:VAL:HA	2.02	0.59
1:C:951:ASP:OD1	1:C:951:ASP:N	2.35	0.59
1:C:652:ARG:NH2	1:C:657:ASP:O	2.36	0.59
2:B:62:PHE:CE1	2:B:122:LEU:HB2	2.38	0.59
3:E:6:DG:H8	3:E:6:DG:OP2	1.86	0.59
1:A:753:ASP:OD1	1:A:753:ASP:N	2.36	0.59
1:A:412:ARG:HE	6:H:11:DT:H5''	1.66	0.59
2:B:239:GLU:HB2	2:B:246:VAL:HG13	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:33:GLN:NE2	2:D:37:PRO:HA	2.17	0.59
1:A:771:SER:O	1:A:775:ASN:ND2	2.36	0.58
2:D:134:PRO:HG3	2:D:155:LEU:HD23	1.85	0.58
4:F:21:DT:H2''	4:F:22:DC:OP2	2.02	0.58
1:A:627:GLU:HG3	1:A:994:ARG:NH1	2.18	0.58
2:B:10:ASN:ND2	2:B:11:CYS:CB	2.65	0.58
1:C:814:ASP:OD1	1:C:815:ALA:N	2.36	0.58
2:D:79:HIS:NE2	2:D:88:GLU:OE2	2.37	0.58
3:E:21:DG:H4'	3:E:22:DT:OP1	2.03	0.58
5:G:41:DG:H2''	5:G:42:DG:C8	2.39	0.58
2:B:10:ASN:ND2	2:B:11:CYS:HB2	2.17	0.58
1:A:442:GLU:OE1	1:C:426:ARG:NH2	2.36	0.58
3:E:29:DG:OP2	3:E:29:DG:H2'	2.03	0.58
4:F:45:DC:H2''	4:F:46:DA:OP2	2.03	0.58
1:A:574:ARG:NH2	1:A:1003:THR:O	2.37	0.58
1:A:956:ASN:HD21	1:A:960:LYS:HZ2	1.52	0.58
1:C:840:LYS:HZ2	1:C:843:PRO:HA	1.69	0.58
1:A:420:ARG:NH1	1:C:459:ARG:HD3	2.19	0.57
2:B:274:PHE:CE2	2:B:348:VAL:HG21	2.39	0.57
6:H:28:DT:H2'	6:H:28:DT:OP2	2.04	0.57
2:B:168:THR:HG22	2:B:170:GLN:H	1.69	0.57
2:D:306:GLN:OE1	2:D:306:GLN:N	2.31	0.57
2:D:322:LEU:H	2:D:327:ALA:HA	1.68	0.57
3:E:22:DT:H2''	3:E:23:DG:C8	2.39	0.57
6:H:39:DC:H2'	6:H:40:DA:H8	1.66	0.57
1:A:435:LYS:HD2	1:A:446:VAL:HG21	1.86	0.57
2:D:307:TRP:HB3	2:D:311:ILE:HG23	1.84	0.57
4:F:27:DG:C6	4:F:28:DC:N4	2.73	0.57
2:B:73:ARG:HH12	2:B:96:ARG:NH1	2.03	0.57
5:G:10:DT:C2	5:G:11:DG:C8	2.92	0.57
1:A:986:GLY:O	1:A:989:LEU:HB2	2.04	0.57
2:D:49:ARG:HH12	2:D:58:ARG:HH21	1.51	0.57
2:D:310:GLU:OE1	2:D:346:TYR:OH	2.17	0.57
5:G:10:DT:C1'	5:G:11:DG:C8	2.88	0.57
1:A:903:LYS:HD3	1:A:941:LEU:HD22	1.86	0.57
2:B:148:ARG:NH1	2:B:241:LEU:HD13	2.19	0.57
2:D:6:LEU:HD11	2:D:347:GLN:HB2	1.87	0.57
2:D:152:ALA:HB2	2:D:240:LEU:HD21	1.86	0.57
3:E:37:DC:H1'	4:F:14:DG:H22	1.69	0.57
5:G:35:DC:H2'	5:G:36:DT:O4'	2.05	0.57
2:B:289:TYR:HD2	2:B:300:GLU:HB3	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:23:DT:OP2	4:F:23:DT:H2'	2.05	0.57
2:D:147:SER:OG	2:D:240:LEU:HD13	2.05	0.56
1:A:538:TRP:CH2	1:A:579:ASP:HB2	2.39	0.56
1:A:590:GLU:HB2	1:A:713:VAL:CG2	2.35	0.56
1:C:557:LEU:O	2:D:173:ASN:ND2	2.25	0.56
1:A:763:MET:SD	1:A:943:SER:OG	2.61	0.56
1:A:824:THR:HB	1:A:871:MET:HE3	1.88	0.56
2:B:212:ARG:HG3	2:B:269:HIS:NE2	2.20	0.56
2:D:71:PRO:HG2	2:D:98:PRO:HG3	1.86	0.56
3:E:37:DC:H2''	3:E:38:DA:C8	2.41	0.56
2:B:162:MET:HE1	2:B:171:ASN:HB3	1.88	0.56
1:C:619:CYS:HB2	1:C:642:PHE:CD2	2.41	0.56
1:A:470:LEU:HD13	1:C:470:LEU:HD13	1.86	0.56
1:A:530:LEU:HD22	1:A:531:PRO:HD2	1.86	0.56
2:B:333:SER:CB	2:B:344:HIS:ND1	2.68	0.56
2:B:65:ASN:C	2:B:123:ARG:HH11	2.14	0.56
2:B:235:ARG:HB3	2:B:250:THR:HG23	1.87	0.56
2:B:338:THR:HG22	2:B:340:PRO:HA	1.87	0.56
1:C:558:SER:OG	2:D:172:TRP:N	2.39	0.56
5:G:51:DA:H2''	5:G:52:DA:OP2	2.06	0.56
6:H:34:DA:H2''	6:H:35:DC:OP2	2.06	0.56
2:D:331:ILE:O	2:D:343:TYR:HA	2.06	0.55
5:G:52:DA:OP2	5:G:52:DA:H2'	2.06	0.55
5:G:30:DC:C2'	5:G:31:DT:C7	2.84	0.55
2:B:10:ASN:HD22	2:B:11:CYS:N	2.05	0.55
5:G:16:DA:H2''	5:G:17:DC:H5'	1.88	0.55
1:A:817:HIS:ND1	1:A:957:TYR:OH	2.35	0.55
1:A:988:LYS:HZ2	3:E:20:DA:P	2.29	0.55
1:C:779:TYR:CZ	1:C:804:LYS:HB2	2.42	0.55
2:D:307:TRP:HB2	2:D:312:SER:HB2	1.87	0.55
3:E:20:DA:H2''	3:E:21:DG:C8	2.41	0.55
2:B:212:ARG:HG3	2:B:269:HIS:CE1	2.41	0.55
5:G:32:DC:C2	5:G:33:DC:N4	2.75	0.55
1:A:492:ASN:O	1:A:492:ASN:ND2	2.32	0.55
1:A:536:PHE:HB3	1:A:711:ILE:HD13	1.89	0.55
1:C:536:PHE:CE2	1:C:549:TRP:HB2	2.42	0.55
2:D:148:ARG:N	2:D:149:GLY:HA2	2.22	0.55
1:A:872:ASN:OD1	1:A:875:TYR:N	2.26	0.55
1:C:409:GLY:HA2	4:F:9:DT:H1'	1.87	0.55
1:C:675:ARG:NH2	1:C:1018:SER:HA	2.21	0.55
2:D:39:ARG:NH2	6:H:51:DC:OP2	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:10:DT:N3	5:G:11:DG:C6	2.75	0.55
1:A:912:LYS:HA	1:A:915:TRP:CZ3	2.42	0.55
5:G:44:DT:N3	5:G:45:DG:O6	2.39	0.55
1:A:553:ILE:HG12	1:A:576:PHE:CE1	2.40	0.55
1:A:487:LEU:HD22	1:A:526:GLU:HB2	1.88	0.54
1:C:708:ARG:HG2	1:C:721:ARG:HG2	1.88	0.54
1:C:735:ARG:HG2	1:C:740:LEU:HD12	1.88	0.54
2:D:277:TYR:HA	2:D:283:LYS:HA	1.87	0.54
5:G:10:DT:O4	5:G:11:DG:O6	2.25	0.54
6:H:35:DC:OP2	6:H:35:DC:H2'	2.08	0.54
1:A:731:GLU:N	1:A:731:GLU:OE1	2.40	0.54
1:A:748:ILE:HD13	1:A:756:ARG:HD2	1.89	0.54
2:B:108:MET:HE1	2:B:127:LYS:NZ	2.22	0.54
1:C:735:ARG:HB3	1:C:740:LEU:HB2	1.89	0.54
2:D:1:MET:N	2:D:349:SER:O	2.37	0.54
1:A:883:GLU:OE1	1:A:883:GLU:N	2.33	0.54
1:A:959:HIS:HE2	1:A:964:HIS:HE1	1.56	0.54
1:A:871:MET:SD	1:A:871:MET:N	2.80	0.54
2:D:284:ARG:HB2	2:D:284:ARG:NH1	2.22	0.54
3:E:31:DC:C2	4:F:20:DG:N2	2.72	0.54
4:F:20:DG:H2'	4:F:21:DT:C6	2.42	0.54
1:A:429:ASP:HB2	1:C:437:PHE:HE2	1.73	0.54
1:C:641:ARG:HH11	1:C:987:ASN:CG	2.14	0.54
2:D:229:ARG:HE	2:D:259:THR:HG21	1.72	0.54
5:G:33:DC:H2'	5:G:34:DA:C4	2.42	0.54
2:D:6:LEU:HD22	2:D:53:GLY:HA2	1.88	0.54
2:D:159:ARG:HA	2:D:178:CYS:H	1.73	0.54
1:A:687:HIS:O	1:A:691:THR:OG1	2.22	0.54
1:C:628:LYS:HG2	1:C:994:ARG:NH1	2.23	0.54
5:G:15:DT:H2'	5:G:16:DA:H8	1.73	0.54
1:C:865:LEU:HD21	1:C:878:ARG:HG2	1.89	0.54
1:A:840:LYS:NZ	1:A:847:GLU:OE2	2.32	0.53
1:A:956:ASN:HD21	1:A:960:LYS:NZ	2.05	0.53
2:B:339:PRO:HB2	2:B:341:GLU:H	1.73	0.53
1:C:675:ARG:NH1	1:C:675:ARG:HG3	2.23	0.53
3:E:21:DG:H2''	3:E:22:DT:O5'	2.08	0.53
5:G:10:DT:C2'	5:G:11:DG:C8	2.91	0.53
5:G:32:DC:H1'	5:G:33:DC:C5	2.43	0.53
1:A:452:THR:O	1:A:456:LEU:HG	2.08	0.53
1:A:779:TYR:CZ	1:A:804:LYS:HB2	2.43	0.53
2:B:270:GLU:HB3	2:B:289:TYR:CE1	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:ASP:HB2	1:A:799:LYS:HG2	1.91	0.53
2:D:58:ARG:NH2	5:G:7:DG:H5''	2.21	0.53
4:F:27:DG:H2'	4:F:28:DC:C6	2.43	0.53
6:H:33:DT:OP2	6:H:33:DT:H2'	2.08	0.53
2:D:212:ARG:HG3	2:D:269:HIS:NE2	2.22	0.53
5:G:10:DT:N1	5:G:11:DG:N7	2.56	0.53
6:H:15:DT:H2''	6:H:16:DA:H5''	1.90	0.53
1:C:984:GLU:O	1:C:987:ASN:HB2	2.09	0.53
5:G:31:DT:C2	6:H:32:DG:N2	2.76	0.53
1:C:788:SER:HB2	2:D:65:ASN:HA	1.90	0.53
5:G:28:DT:H2''	5:G:29:DA:N7	2.24	0.53
1:A:534:HIS:CE1	1:A:587:LYS:HD2	2.43	0.53
1:A:922:ARG:HB3	1:A:922:ARG:NH1	2.24	0.53
1:C:534:HIS:CG	1:C:587:LYS:HZ2	2.27	0.53
1:C:885:VAL:HG21	1:C:905:MET:HG2	1.90	0.53
1:C:942:LEU:HD22	1:C:946:PHE:HB2	1.91	0.53
2:D:123:ARG:NH2	2:D:125:GLU:CG	2.71	0.53
4:F:7:DG:H2'	4:F:8:DG:C8	2.43	0.53
1:A:543:LYS:O	1:A:545:VAL:HG23	2.09	0.53
1:C:578:TYR:HB2	1:C:700:GLU:OE2	2.09	0.53
1:C:608:THR:HB	1:C:718:ARG:HG2	1.91	0.53
1:A:539:GLN:NE2	1:A:710:ILE:HG13	2.24	0.53
1:A:730:ASP:N	1:A:730:ASP:OD1	2.41	0.53
1:C:523:ARG:HH22	3:E:23:DG:H2'	1.74	0.53
2:B:49:ARG:NH2	2:B:58:ARG:HD2	2.21	0.52
1:C:410:ARG:HD2	3:E:41:DA:H2	1.74	0.52
2:D:188:GLU:OE2	2:D:189:PHE:HA	2.09	0.52
1:A:578:TYR:HA	1:A:677:LEU:HD21	1.91	0.52
2:D:212:ARG:NH1	2:D:269:HIS:HD2	2.07	0.52
5:G:10:DT:C2	5:G:11:DG:C4	2.98	0.52
1:C:773:ASP:OD1	1:C:773:ASP:N	2.40	0.52
1:A:613:VAL:HG22	1:A:649:ILE:HB	1.91	0.52
2:B:299:MET:SD	2:B:300:GLU:N	2.83	0.52
1:C:641:ARG:HH11	1:C:987:ASN:HA	1.73	0.52
3:E:31:DC:OP2	3:E:31:DC:H6	1.93	0.52
5:G:48:DC:H2''	5:G:49:DA:C8	2.44	0.52
2:D:266:ILE:HD13	2:D:350:PHE:CD2	2.44	0.52
5:G:34:DA:H8	5:G:34:DA:OP2	1.93	0.52
2:B:256:LEU:HD12	2:B:257:THR:H	1.74	0.52
1:C:999:ARG:N	1:C:1000:GLN:HA	2.25	0.52
6:H:12:DT:H2''	6:H:13:DT:H5'	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:ASP:OD1	1:A:567:VAL:N	2.39	0.52
1:C:675:ARG:HG3	1:C:675:ARG:HH11	1.74	0.52
1:C:991:ARG:O	1:C:994:ARG:HB3	2.10	0.52
1:A:696:PRO:HG3	2:B:172:TRP:HB3	1.91	0.52
1:A:828:LYS:HB3	1:A:949:ARG:NH2	2.25	0.52
2:B:277:TYR:OH	2:B:317:TRP:O	2.14	0.52
1:C:563:SER:OG	1:C:566:ASP:OD2	2.26	0.52
2:D:60:ILE:HG22	2:D:61:SER:H	1.75	0.52
2:B:131:GLY:HA3	2:B:132:ASP:C	2.35	0.51
1:C:622:MET:HE3	1:C:991:ARG:HH11	1.75	0.51
2:D:73:ARG:NH2	2:D:100:ASN:OD1	2.43	0.51
2:D:217:TYR:HD2	2:D:233:LEU:HD21	1.75	0.51
1:A:870:ARG:HH22	1:A:872:ASN:HA	1.74	0.51
2:B:148:ARG:N	2:B:149:GLY:HA2	2.25	0.51
1:C:889:CYS:O	1:C:898:ARG:NE	2.43	0.51
2:D:311:ILE:HB	2:D:346:TYR:HE2	1.75	0.51
5:G:27:DG:H2''	5:G:28:DT:OP2	2.10	0.51
5:G:28:DT:OP2	5:G:28:DT:H2'	2.09	0.51
1:A:832:ASP:OD2	1:A:949:ARG:NH1	2.42	0.51
1:A:865:LEU:HD11	1:A:878:ARG:HB3	1.92	0.51
1:A:959:HIS:O	1:A:963:ALA:CB	2.59	0.51
2:D:141:THR:HG21	2:D:209:ALA:HB3	1.91	0.51
3:E:41:DA:C8	3:E:41:DA:H5'	2.45	0.51
1:A:622:MET:HE1	1:A:990:PHE:HB3	1.93	0.51
2:B:21:LEU:HD12	2:B:320:GLY:HA3	1.92	0.51
5:G:52:DA:H2''	5:G:53:DA:C8	2.46	0.51
2:B:108:MET:HE3	2:B:125:GLU:HB2	1.92	0.51
3:E:31:DC:N4	4:F:20:DG:O6	2.43	0.51
1:A:641:ARG:HH11	1:A:987:ASN:HA	1.76	0.51
2:B:249:CYS:SG	2:B:250:THR:N	2.84	0.51
1:C:650:SER:HA	1:C:662:ILE:HG13	1.93	0.51
1:C:709:LEU:O	1:C:719:SER:HA	2.10	0.51
1:A:594:MET:HE1	1:A:718:ARG:NH1	2.26	0.51
1:A:817:HIS:C	1:A:819:ASP:N	2.67	0.51
2:B:289:TYR:HB3	2:B:300:GLU:OE1	2.11	0.51
2:D:145:ILE:HB	2:D:214:ASP:HA	1.92	0.51
2:B:23:ASP:OD1	2:B:24:LEU:N	2.43	0.51
2:B:218:PHE:HB2	2:B:234:ILE:HB	1.91	0.51
1:C:926:ASP:OD1	1:C:926:ASP:N	2.39	0.51
2:D:78:ALA:HB1	2:D:144:VAL:HG23	1.93	0.51
4:F:36:DA:OP2	4:F:36:DA:C8	2.61	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:55:DC:H2''	6:H:56:DC:C6	2.46	0.51
1:A:479:PHE:HA	1:C:513:ARG:NH2	2.26	0.51
1:A:959:HIS:NE2	1:A:964:HIS:HE1	2.09	0.51
2:B:8:ALA:HB2	2:B:55:LEU:HD23	1.92	0.51
3:E:9:DC:H2''	3:E:10:DT:H71	1.92	0.51
2:B:94:GLY:H	2:B:140:HIS:CE1	2.29	0.51
5:G:55:DC:H4'	5:G:56:DC:OP1	2.11	0.51
1:A:908:TYR:O	1:A:911:MET:HG2	2.11	0.50
1:C:737:MET:HE1	1:C:807:MET:SD	2.51	0.50
1:C:975:ILE:C	1:C:977:ALA:H	2.19	0.50
1:A:505:ARG:NH1	1:C:1029:LYS:C	2.65	0.50
1:C:415:LEU:HD21	1:C:427:LEU:HD11	1.92	0.50
2:D:229:ARG:HH22	2:D:280:GLU:HA	1.76	0.50
3:E:17:DC:H2''	3:E:18:DA:C8	2.46	0.50
3:E:20:DA:H2'	3:E:20:DA:OP2	2.11	0.50
2:B:99:ASN:CG	2:B:101:GLU:OE2	2.53	0.50
5:G:13:DC:C5	5:G:14:DT:H73	2.46	0.50
2:B:147:SER:HB3	2:B:240:LEU:H	1.76	0.50
2:B:300:GLU:OE2	2:B:302:ARG:HD3	2.11	0.50
1:C:641:ARG:NH1	1:C:987:ASN:HA	2.26	0.50
2:D:229:ARG:HH12	2:D:280:GLU:HG2	1.75	0.50
4:F:36:DA:OP2	4:F:36:DA:H2'	2.12	0.50
2:B:49:ARG:NH2	2:B:58:ARG:HH11	2.06	0.50
2:B:49:ARG:NH1	2:B:58:ARG:NH1	2.59	0.50
2:D:135:SER:N	2:D:137:ARG:HH21	2.09	0.50
3:E:8:DC:OP2	3:E:8:DC:H2'	2.12	0.50
6:H:32:DG:H2''	6:H:33:DT:OP2	2.11	0.50
1:A:650:SER:OG	1:A:651:ILE:N	2.44	0.50
1:C:534:HIS:CG	1:C:587:LYS:NZ	2.80	0.50
2:D:43:THR:HG23	2:D:62:PHE:CE1	2.47	0.50
2:D:202:ASP:OD2	2:D:223:ILE:HD13	2.10	0.50
1:C:540:PRO:HD2	1:C:707:SER:HA	1.94	0.50
1:A:849:ARG:HH11	1:A:849:ARG:HB2	1.77	0.50
1:A:988:LYS:HZ2	3:E:20:DA:H3'	1.77	0.50
1:C:778:ARG:NH2	1:C:799:LYS:HB2	2.27	0.50
2:D:269:HIS:HB3	2:D:292:LEU:HB2	1.94	0.50
1:C:452:THR:HA	1:C:455:LEU:HD12	1.94	0.50
1:C:752:CYS:SG	1:C:766:HIS:ND1	2.84	0.50
3:E:21:DG:H2'	3:E:22:DT:C6	2.46	0.50
1:A:859:LEU:O	1:A:864:LYS:N	2.44	0.49
2:B:140:HIS:HB3	2:B:158:GLY:HA3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:896:GLU:OE1	1:C:896:GLU:N	2.36	0.49
1:C:992:ARG:HB2	5:G:21:DG:OP1	2.12	0.49
1:C:860:ARG:HG2	1:C:866:LYS:HE3	1.94	0.49
6:H:1:DC:H3'	6:H:2:DT:H71	1.92	0.49
1:A:788:SER:HB2	2:B:65:ASN:HA	1.94	0.49
1:A:1013:HIS:O	1:A:1017:THR:HG22	2.12	0.49
2:D:49:ARG:CZ	2:D:58:ARG:HD2	2.42	0.49
3:E:29:DG:H2''	3:E:30:DA:OP2	2.12	0.49
3:E:44:DC:H4'	3:E:45:DC:OP1	2.11	0.49
1:C:515:ILE:O	1:C:517:GLN:NE2	2.44	0.49
1:C:877:ARG:NH1	1:C:916:ARG:NH1	2.51	0.49
1:C:538:TRP:CZ3	1:C:709:LEU:HB2	2.48	0.49
4:F:41:DA:H2''	4:F:42:DG:OP2	2.12	0.49
1:A:418:LEU:HB3	1:A:422:ALA:HB3	1.95	0.49
2:B:86:LYS:NZ	2:B:123:ARG:HD3	2.28	0.49
2:B:164:PRO:HA	2:B:167:ARG:HB2	1.94	0.49
1:C:790:SER:OG	1:C:791:ALA:N	2.45	0.49
1:A:832:ASP:CG	1:A:949:ARG:HH12	2.21	0.49
1:A:869:MET:HB3	3:E:16:DA:H4'	1.95	0.49
1:A:999:ARG:NH1	1:A:1004:PHE:CG	2.81	0.49
6:H:29:DG:H2''	6:H:30:DG:OP2	2.12	0.49
1:A:493:THR:O	1:C:499:GLN:NE2	2.41	0.49
1:A:877:ARG:HA	1:A:880:MET:HE2	1.94	0.49
1:A:988:LYS:NZ	3:E:20:DA:P	2.85	0.49
1:C:740:LEU:HD21	1:C:770:ARG:HH12	1.78	0.49
2:D:130:VAL:HB	2:D:191:CYS:HA	1.93	0.49
2:D:222:HIS:HB2	2:D:259:THR:HG22	1.94	0.49
6:H:30:DG:H2''	6:H:31:DA:C8	2.48	0.49
4:F:40:DC:H1'	4:F:41:DA:C8	2.48	0.49
1:A:687:HIS:CD2	2:B:36:TRP:HE1	2.31	0.49
5:G:5:DT:H2'	5:G:5:DT:OP2	2.13	0.49
1:A:538:TRP:CD2	1:A:542:LEU:HD21	2.46	0.48
1:A:590:GLU:O	1:A:593:ILE:HG12	2.13	0.48
1:A:926:ASP:OD1	1:A:926:ASP:N	2.39	0.48
1:C:619:CYS:SG	1:C:620:ASP:N	2.85	0.48
2:D:47:GLY:N	2:D:60:ILE:HD11	2.27	0.48
2:D:212:ARG:NH1	2:D:293:ASP:HA	2.27	0.48
2:D:235:ARG:HB3	2:D:250:THR:HG23	1.94	0.48
6:H:35:DC:H2''	6:H:36:DT:C6	2.48	0.48
1:A:737:MET:HG2	1:A:806:PHE:CE1	2.48	0.48
1:C:415:LEU:O	1:C:423:GLN:NE2	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:638:LYS:HD2	1:C:683:ASP:OD2	2.13	0.48
1:C:749:CYS:HB3	1:C:752:CYS:O	2.13	0.48
1:A:429:ASP:HB2	1:C:437:PHE:CE2	2.47	0.48
1:A:911:MET:HB2	1:A:931:TYR:CE2	2.49	0.48
2:B:89:CYS:SG	2:B:110:SER:HB2	2.53	0.48
2:B:226:SER:OG	2:B:228:CYS:SG	2.56	0.48
1:C:431:LYS:NZ	3:E:34:DG:OP1	2.42	0.48
2:D:80:PHE:CE1	2:D:151:THR:HG21	2.49	0.48
2:D:265:PRO:HB3	2:D:271:TYR:CZ	2.49	0.48
4:F:27:DG:H2''	4:F:28:DC:H5'	1.96	0.48
5:G:10:DT:H2''	5:G:11:DG:C8	2.45	0.48
1:C:555:ASP:N	1:C:555:ASP:OD1	2.46	0.48
1:A:420:ARG:HH11	1:C:459:ARG:HD3	1.78	0.48
5:G:9:DC:H2''	5:G:10:DT:OP2	2.12	0.48
1:A:968:ILE:HG23	1:A:971:ARG:HD3	1.96	0.48
4:F:32:DG:OP2	4:F:32:DG:H8	1.94	0.48
5:G:32:DC:C2'	5:G:33:DC:H5	2.27	0.48
1:A:858:GLN:NE2	1:A:890:GLU:OE1	2.47	0.48
3:E:45:DC:H42	4:F:6:DG:H22	1.61	0.48
1:A:410:ARG:HB2	5:G:52:DA:H2	1.78	0.48
1:A:694:LEU:O	1:A:698:VAL:HG23	2.13	0.48
1:A:771:SER:HB3	1:A:774:GLU:OE2	2.14	0.48
1:A:825:GLU:OE2	1:A:950:TYR:OH	2.24	0.48
1:A:893:PRO:C	1:A:898:ARG:HH21	2.22	0.48
1:C:796:ASP:O	1:C:799:LYS:HD2	2.12	0.48
2:B:93:HIS:HA	2:B:94:GLY:HA2	1.62	0.48
1:C:985:SER:HB2	1:C:988:LYS:HZ1	1.78	0.48
4:F:37:DA:OP2	4:F:37:DA:C8	2.62	0.48
5:G:32:DC:C1'	5:G:33:DC:C5	2.97	0.48
1:A:490:ARG:O	1:A:493:THR:HG22	2.14	0.47
1:A:829:ILE:O	1:A:833:GLU:HB2	2.14	0.47
1:A:839:GLN:N	1:A:839:GLN:OE1	2.46	0.47
1:A:849:ARG:HB2	1:A:849:ARG:NH1	2.29	0.47
2:B:16:GLN:HB3	2:B:34:LYS:HB3	1.95	0.47
2:B:229:ARG:O	2:B:257:THR:OG1	2.20	0.47
2:B:316:THR:OG1	2:B:317:TRP:N	2.47	0.47
1:C:889:CYS:HB2	1:C:898:ARG:HG3	1.95	0.47
2:D:113:SER:OG	2:D:114:ARG:N	2.47	0.47
5:G:10:DT:O4	5:G:11:DG:C6	2.67	0.47
1:A:589:LEU:O	1:A:593:ILE:HG23	2.14	0.47
1:A:737:MET:HG2	1:A:806:PHE:HE1	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:PRO:HA	2:B:346:TYR:HD1	1.79	0.47
2:B:87:PRO:HA	2:B:88:GLU:HA	1.50	0.47
1:C:845:ARG:O	1:C:849:ARG:NE	2.35	0.47
5:G:44:DT:H2'	5:G:45:DG:C8	2.49	0.47
1:A:534:HIS:CG	1:A:587:LYS:HD2	2.49	0.47
2:B:214:ASP:OD2	2:B:237:HIS:HE1	1.96	0.47
1:C:993:PHE:HE2	1:C:1013:HIS:HA	1.79	0.47
2:D:158:GLY:N	2:D:204:GLN:O	2.45	0.47
4:F:17:DC:H2''	4:F:18:DC:N1	2.29	0.47
1:A:683:ASP:OD1	1:A:685:SER:N	2.29	0.47
1:A:834:ILE:HD13	1:A:891:LEU:HD12	1.97	0.47
1:C:651:ILE:HB	1:C:662:ILE:HD11	1.94	0.47
2:D:158:GLY:O	2:D:178:CYS:HB3	2.14	0.47
3:E:5:DT:O2	4:F:47:DG:N2	2.48	0.47
1:A:610:GLY:O	1:A:651:ILE:HD12	2.14	0.47
2:B:85:GLY:O	2:B:87:PRO:HD3	2.15	0.47
1:A:626:SER:OG	4:F:34:DG:OP1	2.26	0.47
1:A:700:GLU:OE2	2:B:169:THR:HG21	2.15	0.47
1:A:713:VAL:HG13	1:A:718:ARG:NE	2.30	0.47
2:B:66:SER:HB3	2:B:123:ARG:HB2	1.96	0.47
1:C:489:ILE:O	1:C:493:THR:HG22	2.14	0.47
1:C:538:TRP:CE3	1:C:704:MET:CE	2.96	0.47
1:C:835:GLY:HA3	1:C:851:TRP:CE2	2.49	0.47
2:D:27:ASP:OD1	2:D:28:VAL:N	2.47	0.47
2:D:145:ILE:HD11	2:D:152:ALA:HB3	1.96	0.47
1:A:641:ARG:NH1	1:A:987:ASN:N	2.62	0.47
1:A:738:GLU:HG3	1:A:738:GLU:O	2.14	0.47
1:A:959:HIS:O	1:A:963:ALA:HB3	2.15	0.47
1:A:985:SER:O	1:A:988:LYS:HB3	2.15	0.47
1:A:988:LYS:NZ	3:E:20:DA:H3'	2.30	0.47
1:C:628:LYS:N	1:C:994:ARG:HH12	2.13	0.47
2:D:41:CYS:SG	2:D:43:THR:HB	2.54	0.47
4:F:28:DC:H2'	4:F:28:DC:OP2	2.14	0.47
5:G:32:DC:H2''	5:G:33:DC:C5	2.45	0.47
2:B:333:SER:HG	2:B:344:HIS:CG	2.18	0.47
2:B:339:PRO:HD2	2:B:341:GLU:O	2.14	0.47
1:C:779:TYR:CE2	1:C:804:LYS:HB2	2.49	0.47
4:F:17:DC:H2''	4:F:18:DC:C6	2.50	0.47
1:A:410:ARG:HB2	5:G:52:DA:C2	2.50	0.47
1:C:961:THR:HA	1:C:965:VAL:HG23	1.97	0.47
4:F:33:DT:H1'	4:F:34:DG:H5'	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:ALA:HB3	2:B:91:LEU:HB2	1.97	0.47
1:C:512:GLY:HA2	1:C:513:ARG:HB3	1.97	0.47
1:C:582:LEU:HD23	1:C:582:LEU:HA	1.55	0.47
2:D:268:TYR:O	2:D:269:HIS:ND1	2.46	0.47
2:B:302:ARG:HH11	2:B:351:GLN:HG3	1.79	0.46
1:C:486:CYS:SG	1:C:522:LEU:HD11	2.56	0.46
1:C:708:ARG:HG2	1:C:721:ARG:HH11	1.79	0.46
4:F:15:DT:H2''	4:F:16:DT:C5	2.49	0.46
5:G:22:DT:H2''	5:G:23:DG:H8	1.80	0.46
2:B:93:HIS:HB2	2:B:106:LEU:HA	1.97	0.46
1:C:487:LEU:HB2	1:C:522:LEU:HD13	1.97	0.46
1:C:814:ASP:OD1	1:C:816:LEU:N	2.47	0.46
2:D:80:PHE:CD2	2:D:89:CYS:HB2	2.46	0.46
5:G:22:DT:H2''	5:G:23:DG:C8	2.51	0.46
1:A:908:TYR:HB2	1:A:938:PHE:HE2	1.80	0.46
1:C:543:LYS:O	1:C:545:VAL:HG23	2.15	0.46
2:D:97:THR:HB	2:D:99:ASN:O	2.15	0.46
2:D:233:LEU:HB3	2:D:252:LEU:HD23	1.98	0.46
5:G:56:DC:H2'	5:G:57:DT:H71	1.97	0.46
1:A:565:ASP:OD1	1:A:566:ASP:N	2.48	0.46
1:A:649:ILE:HG23	1:A:663:PHE:HB3	1.97	0.46
1:A:942:LEU:HD21	1:A:950:TYR:CE2	2.50	0.46
1:C:742:ALA:HA	1:C:743:SER:HA	1.52	0.46
2:D:226:SER:OG	2:D:228:CYS:SG	2.60	0.46
3:E:8:DC:H2''	3:E:9:DC:C6	2.50	0.46
3:E:34:DG:N1	4:F:17:DC:C2	2.76	0.46
5:G:10:DT:C2	5:G:11:DG:N7	2.83	0.46
5:G:32:DC:N4	6:H:30:DG:C6	2.72	0.46
1:A:558:SER:OG	2:B:173:ASN:N	2.46	0.46
1:A:485:VAL:HG13	1:A:1024:PHE:HB3	1.98	0.46
1:C:528:GLU:HA	1:C:533:PHE:CD2	2.50	0.46
1:C:576:PHE:CE1	1:C:1010:LEU:HD21	2.51	0.46
2:D:212:ARG:NH1	2:D:269:HIS:CD2	2.83	0.46
1:C:961:THR:HG23	1:C:962:LEU:HG	1.98	0.46
1:C:1019:LYS:O	1:C:1022:GLN:N	2.49	0.46
4:F:18:DC:H2'	4:F:19:DA:C8	2.51	0.46
1:A:409:GLY:HA2	6:H:9:DT:O2	2.15	0.46
1:C:487:LEU:O	1:C:491:VAL:HG13	2.16	0.46
1:C:610:GLY:C	1:C:651:ILE:HD12	2.40	0.46
4:F:26:DA:H2''	4:F:27:DG:C8	2.50	0.46
2:B:306:GLN:OE1	2:B:306:GLN:N	2.40	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:72:LEU:HB3	2:D:95:GLY:HA3	1.97	0.46
2:D:229:ARG:NH2	2:D:280:GLU:OE2	2.49	0.46
1:A:416:LEU:HD21	1:C:448:SER:HB3	1.98	0.46
1:A:422:ALA:HB1	6:H:12:DT:H5"	1.97	0.46
1:A:693:ILE:O	1:A:696:PRO:HD2	2.16	0.46
1:C:725:ARG:HE	1:C:810:GLN:NE2	2.14	0.46
1:C:795:ARG:NH2	2:D:39:ARG:NH1	2.63	0.46
2:D:261:ALA:HB1	2:D:273:ILE:HG23	1.97	0.46
1:A:534:HIS:ND1	1:A:587:LYS:HD2	2.31	0.45
1:A:544:ASN:O	1:A:544:ASN:ND2	2.49	0.45
1:C:914:VAL:HG21	1:C:931:TYR:HD2	1.80	0.45
1:C:1023:LYS:HA	1:C:1023:LYS:HD3	1.77	0.45
2:D:49:ARG:NH1	2:D:58:ARG:HB3	2.31	0.45
2:D:88:GLU:HG3	2:D:89:CYS:N	2.31	0.45
1:A:1021:LEU:HD12	1:A:1021:LEU:H	1.82	0.45
2:B:241:LEU:O	2:B:244:SER:OG	2.26	0.45
1:C:789:GLU:CD	1:C:797:ARG:HE	2.24	0.45
2:D:49:ARG:HH11	2:D:58:ARG:HB3	1.80	0.45
2:B:277:TYR:HD1	2:B:283:LYS:HA	1.80	0.45
2:B:302:ARG:HE	2:B:350:PHE:HE1	1.64	0.45
2:D:96:ARG:HD2	2:D:138:TYR:CD2	2.51	0.45
3:E:15:DT:C2	3:E:16:DA:C6	3.04	0.45
5:G:30:DC:C2	5:G:31:DT:C4	3.04	0.45
1:A:716:LEU:HB2	1:A:718:ARG:HE	1.81	0.45
1:A:919:CYS:HB3	1:A:922:ARG:NH1	2.31	0.45
2:B:10:ASN:HD22	2:B:11:CYS:CA	2.29	0.45
2:B:204:GLN:HB3	2:B:223:ILE:CG1	2.40	0.45
1:C:512:GLY:HA2	1:C:513:ARG:C	2.40	0.45
2:D:333:SER:HB2	2:D:342:ALA:HA	1.99	0.45
1:A:621:GLY:HA2	1:A:640:VAL:HA	1.99	0.45
2:B:49:ARG:HH12	2:B:58:ARG:HH12	1.62	0.45
2:B:318:PHE:CE1	2:B:330:ALA:HB3	2.51	0.45
1:C:482:HIS:HB3	1:C:485:VAL:HG23	1.98	0.45
1:C:795:ARG:HH12	2:D:39:ARG:HH12	1.62	0.45
2:D:87:PRO:HA	2:D:88:GLU:HA	1.71	0.45
4:F:13:DT:C2	4:F:14:DG:C8	3.05	0.45
1:C:651:ILE:HD11	1:C:653:LEU:HB2	1.98	0.45
2:D:242:LEU:HA	2:D:243:GLY:HA2	1.53	0.45
1:A:624:ASP:HA	1:A:637:GLU:CB	2.39	0.45
1:A:863:MET:HA	1:A:863:MET:HE2	1.97	0.45
1:C:465:LYS:HZ2	6:H:23:DG:P	2.39	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:20:DA:H2''	3:E:21:DG:H8	1.82	0.45
4:F:41:DA:H2''	4:F:42:DG:C8	2.51	0.45
5:G:12:DT:H2''	5:G:13:DC:C6	2.52	0.45
5:G:34:DA:H2''	5:G:35:DC:O4'	2.17	0.45
1:C:859:LEU:O	1:C:865:LEU:N	2.41	0.45
2:D:310:GLU:OE2	2:D:344:HIS:ND1	2.50	0.45
4:F:13:DT:C2	4:F:14:DG:N7	2.84	0.45
1:A:459:ARG:HH21	1:C:420:ARG:NH1	2.14	0.45
1:C:669:ASN:O	1:C:982:GLY:HA2	2.17	0.45
1:C:752:CYS:HG	1:C:766:HIS:CG	2.35	0.45
1:A:450:CYS:SG	1:C:454:PHE:HA	2.57	0.45
1:C:733:MET:HE3	1:C:733:MET:HB2	1.90	0.45
1:C:880:MET:HG3	1:C:909:LEU:HD21	1.99	0.45
2:D:86:LYS:HA	2:D:86:LYS:HD2	1.78	0.45
2:D:234:ILE:HA	2:D:234:ILE:HD13	1.63	0.45
2:D:274:PHE:CZ	2:D:348:VAL:HG21	2.52	0.45
2:B:208:VAL:HG21	2:B:261:ALA:HB3	1.98	0.44
1:C:613:VAL:HG12	1:C:615:VAL:HG23	2.00	0.44
1:A:609:SER:HB3	1:A:653:LEU:HD11	1.99	0.44
1:A:692:ALA:HA	2:B:100:ASN:ND2	2.31	0.44
1:A:919:CYS:HB3	1:A:922:ARG:HH12	1.83	0.44
2:B:282:GLN:NE2	2:B:283:LYS:O	2.51	0.44
1:C:688:GLU:OE2	2:D:73:ARG:HD3	2.18	0.44
1:C:816:LEU:HD22	1:C:981:GLU:HB2	1.98	0.44
2:D:16:GLN:HG3	2:D:18:GLY:O	2.18	0.44
2:D:148:ARG:HH12	2:D:239:GLU:CB	2.22	0.44
4:F:9:DT:H2'	4:F:10:DT:C6	2.53	0.44
5:G:33:DC:H2'	5:G:34:DA:C5	2.52	0.44
1:A:536:PHE:HB3	1:A:711:ILE:CD1	2.47	0.44
2:D:1:MET:CA	2:D:349:SER:O	2.65	0.44
5:G:10:DT:C2'	5:G:11:DG:H8	2.26	0.44
6:H:7:DG:O5'	6:H:7:DG:H8	2.00	0.44
1:A:526:GLU:O	1:A:529:LEU:N	2.47	0.44
1:A:529:LEU:HD13	1:A:1021:LEU:HD11	2.00	0.44
1:A:797:ARG:O	1:A:799:LYS:NZ	2.40	0.44
1:C:752:CYS:HB2	1:C:964:HIS:CE1	2.52	0.44
1:C:861:LYS:HE2	1:C:861:LYS:HB3	1.87	0.44
1:C:975:ILE:HG12	1:C:976:GLY:N	2.32	0.44
2:D:39:ARG:HB2	6:H:50:DA:OP1	2.18	0.44
3:E:27:DC:H2''	3:E:28:DA:C8	2.52	0.44
1:A:893:PRO:O	1:A:898:ARG:NH2	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:950:TYR:HB3	1:A:954:ILE:HD11	2.00	0.44
2:D:339:PRO:HB2	2:D:341:GLU:H	1.82	0.44
2:B:135:SER:OG	2:B:137:ARG:NH2	2.50	0.44
2:B:274:PHE:CZ	2:B:348:VAL:CG2	3.01	0.44
2:D:19:PHE:HE2	2:D:21:LEU:HD21	1.83	0.44
3:E:1:DG:H2''	3:E:2:DA:C8	2.53	0.44
4:F:31:DT:OP2	4:F:31:DT:H6	1.99	0.44
2:B:141:THR:OG1	2:B:156:PHE:O	2.29	0.44
1:C:709:LEU:HD12	1:C:710:ILE:H	1.81	0.44
1:C:778:ARG:HH21	1:C:799:LYS:HB2	1.83	0.44
1:C:903:LYS:NZ	1:C:907:LEU:HG	2.32	0.44
1:C:975:ILE:HG12	1:C:976:GLY:H	1.82	0.44
2:D:219:LEU:HD11	2:D:256:LEU:N	2.32	0.44
5:G:24:DG:H1'	5:G:25:DT:H5'	2.00	0.44
1:A:611:PHE:HB3	1:A:649:ILE:HD11	1.99	0.44
1:A:658:ASP:OD1	1:A:659:GLY:N	2.50	0.44
1:A:950:TYR:HB3	1:A:954:ILE:CD1	2.47	0.44
2:B:277:TYR:HA	2:B:284:ARG:N	2.30	0.44
1:C:725:ARG:HE	1:C:810:GLN:HE21	1.65	0.44
1:C:985:SER:O	1:C:987:ASN:N	2.50	0.44
1:C:1011:LYS:NZ	3:E:24:DC:OP1	2.51	0.44
2:D:257:THR:O	2:D:284:ARG:NH1	2.51	0.44
1:C:586:LEU:HD23	1:C:586:LEU:HA	1.75	0.44
1:C:669:ASN:OD1	1:C:979:ALA:HB3	2.17	0.44
2:D:43:THR:HG22	2:D:45:ILE:H	1.82	0.44
5:G:11:DG:C4	5:G:12:DT:C5	3.05	0.44
1:A:578:TYR:OH	1:A:724:PHE:HE2	2.01	0.43
1:A:649:ILE:HG22	1:A:663:PHE:HD2	1.83	0.43
1:C:691:THR:HG22	1:C:806:PHE:CZ	2.53	0.43
3:E:33:DG:H5'	3:E:33:DG:C8	2.52	0.43
2:D:197:LEU:HA	2:D:197:LEU:HD23	1.69	0.43
5:G:30:DC:H2''	5:G:31:DT:OP2	2.17	0.43
1:A:558:SER:OG	1:A:558:SER:O	2.33	0.43
2:B:217:TYR:HE1	2:B:235:ARG:HG3	1.83	0.43
1:C:731:GLU:OE2	1:C:960:LYS:NZ	2.36	0.43
1:C:946:PHE:HA	1:C:948:TYR:CE1	2.53	0.43
6:H:8:DG:H2'	6:H:9:DT:C6	2.53	0.43
1:A:511:SER:O	1:A:513:ARG:N	2.51	0.43
2:B:8:ALA:HA	2:B:55:LEU:HB3	2.00	0.43
2:D:129:LEU:HB3	2:D:192:CYS:SG	2.58	0.43
2:D:285:MET:HE1	2:D:312:SER:HA	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:325:GLY:O	2:D:350:PHE:N	2.46	0.43
3:E:15:DT:H1'	3:E:16:DA:N7	2.33	0.43
5:G:5:DT:OP2	5:G:5:DT:H6	2.02	0.43
1:A:755:THR:HG23	1:A:758:GLU:OE2	2.18	0.43
1:A:778:ARG:HD3	1:A:798:VAL:O	2.18	0.43
2:B:1:MET:C	2:B:305:PRO:HG3	2.43	0.43
2:B:49:ARG:NH2	2:B:58:ARG:NH1	2.66	0.43
2:B:197:LEU:HD23	2:B:197:LEU:HA	1.88	0.43
1:C:522:LEU:HA	1:C:525:ALA:HB3	2.01	0.43
1:C:616:LYS:HB2	1:C:647:MET:HG3	1.99	0.43
1:C:686:ASP:OD1	1:C:686:ASP:N	2.51	0.43
2:D:45:ILE:C	2:D:46:PHE:HD1	2.26	0.43
2:D:96:ARG:HG2	2:D:102:LEU:CD2	2.48	0.43
4:F:27:DG:O5'	4:F:27:DG:H8	2.01	0.43
1:C:859:LEU:HB3	1:C:865:LEU:HB2	2.01	0.43
1:C:860:ARG:HH12	1:C:864:LYS:HE2	1.83	0.43
2:D:228:CYS:SG	2:D:230:PRO:HD3	2.59	0.43
2:D:317:TRP:HB3	2:D:331:ILE:HD13	2.00	0.43
5:G:33:DC:N3	6:H:30:DG:N2	2.66	0.43
1:A:836:GLU:O	1:A:840:LYS:HB3	2.18	0.43
1:A:882:ARG:HA	1:A:885:VAL:HB	2.00	0.43
1:C:972:ASP:OD1	1:C:972:ASP:N	2.52	0.43
2:D:123:ARG:HH22	2:D:125:GLU:CD	2.24	0.43
3:E:26:DA:C2'	3:E:27:DC:OP2	2.66	0.43
5:G:11:DG:C5	5:G:12:DT:C7	3.01	0.43
1:C:621:GLY:HA2	1:C:640:VAL:HG22	2.01	0.43
1:C:716:LEU:HD12	1:C:718:ARG:HH21	1.84	0.43
3:E:5:DT:C2	4:F:47:DG:N2	2.86	0.43
3:E:45:DC:N4	4:F:6:DG:H22	2.17	0.43
1:A:870:ARG:NH2	1:A:872:ASN:HA	2.34	0.43
1:A:974:SER:OG	1:A:975:ILE:N	2.51	0.43
2:B:137:ARG:HB2	2:B:159:ARG:O	2.19	0.43
1:C:735:ARG:HH12	1:C:742:ALA:HA	1.81	0.43
1:C:795:ARG:CZ	2:D:39:ARG:NH1	2.82	0.43
2:D:131:GLY:HA3	2:D:132:ASP:C	2.44	0.43
3:E:16:DA:H5'	3:E:16:DA:C8	2.54	0.43
3:E:40:DA:H2''	3:E:41:DA:OP2	2.19	0.43
4:F:43:DG:H4'	4:F:44:DC:OP1	2.18	0.43
1:A:810:GLN:HG3	1:A:971:ARG:HH11	1.84	0.43
2:B:323:GLY:O	2:B:326:THR:OG1	2.30	0.43
1:C:587:LYS:O	1:C:590:GLU:HB2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:675:ARG:HD3	1:C:1017:THR:HB	1.99	0.43
1:C:811:PRO:HG2	1:C:971:ARG:HH12	1.84	0.43
6:H:4:DC:H2''	6:H:5:DA:C8	2.54	0.43
6:H:29:DG:H1'	6:H:30:DG:H5'	2.00	0.43
1:A:787:PHE:CG	1:A:797:ARG:NH1	2.87	0.42
2:B:22:LEU:HD22	2:B:90:TYR:CD1	2.54	0.42
2:B:109:LEU:HD21	2:B:122:LEU:HD13	2.01	0.42
2:B:167:ARG:NH1	2:B:172:TRP:CE2	2.87	0.42
1:C:545:VAL:HA	2:D:169:THR:HG23	2.01	0.42
1:C:681:PHE:HZ	1:C:994:ARG:HH21	1.67	0.42
1:C:904:LEU:HD12	1:C:904:LEU:O	2.19	0.42
1:A:577:ARG:NH2	1:A:579:ASP:OD2	2.49	0.42
1:A:997:ASN:HD22	1:A:1012:HIS:CE1	2.37	0.42
1:C:667:LYS:HE3	1:C:670:SER:OG	2.18	0.42
3:E:8:DC:H2''	3:E:9:DC:C5	2.54	0.42
6:H:37:DA:H2''	6:H:38:DC:H6	1.84	0.42
1:A:683:ASP:OD1	1:A:684:GLU:N	2.52	0.42
2:B:9:VAL:HG11	2:B:56:LYS:HD2	2.01	0.42
2:B:66:SER:HB3	2:B:123:ARG:HA	2.01	0.42
1:C:729:TYR:HB2	1:C:734:VAL:CG2	2.49	0.42
1:C:813:LEU:HD23	1:C:813:LEU:H	1.84	0.42
2:D:189:PHE:C	2:D:191:CYS:H	2.27	0.42
3:E:31:DC:OP2	3:E:31:DC:C6	2.73	0.42
4:F:46:DA:O5'	4:F:46:DA:C8	2.72	0.42
2:B:83:GLN:N	2:B:87:PRO:HB3	2.34	0.42
2:B:207:HIS:ND1	2:B:207:HIS:O	2.53	0.42
2:B:268:TYR:N	2:B:270:GLU:OE2	2.53	0.42
2:B:341:GLU:OE1	2:B:343:TYR:N	2.51	0.42
1:C:680:MET:HG2	1:C:693:ILE:HG21	2.01	0.42
1:C:810:GLN:OE1	1:C:811:PRO:HD2	2.20	0.42
1:C:828:LYS:HE2	1:C:949:ARG:HH22	1.84	0.42
2:D:22:LEU:HD13	2:D:90:TYR:CG	2.54	0.42
1:A:487:LEU:HA	1:A:522:LEU:HD11	2.01	0.42
2:B:49:ARG:HH12	2:B:58:ARG:HH11	1.67	0.42
2:B:217:TYR:CE1	2:B:235:ARG:HG3	2.53	0.42
2:B:233:LEU:HD23	2:B:234:ILE:N	2.35	0.42
1:C:573:SER:O	1:C:574:ARG:NH1	2.45	0.42
1:C:828:LYS:HE2	1:C:828:LYS:HB3	1.80	0.42
5:G:2:DA:H1'	5:G:3:DT:H5'	2.02	0.42
1:A:610:GLY:O	1:A:652:ARG:N	2.53	0.42
1:A:679:LEU:C	1:A:680:MET:HG3	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:LEU:HD11	2:B:92:ILE:HD11	2.01	0.42
2:B:294:ASP:N	2:B:294:ASP:OD1	2.50	0.42
1:C:818:CYS:SG	1:C:819:ASP:N	2.93	0.42
1:A:640:VAL:HB	1:A:680:MET:HE3	2.01	0.42
1:A:681:PHE:CE1	1:A:1006:LEU:HD21	2.54	0.42
1:A:778:ARG:HB3	1:A:798:VAL:HG22	2.01	0.42
2:B:135:SER:N	2:B:137:ARG:HH21	2.17	0.42
2:B:332:PRO:HA	2:B:342:ALA:O	2.20	0.42
1:C:732:LYS:HE3	1:C:732:LYS:HB2	1.89	0.42
1:C:860:ARG:NH1	1:C:864:LYS:HE2	2.35	0.42
1:C:971:ARG:NH1	1:C:972:ASP:OD2	2.52	0.42
2:D:21:LEU:O	2:D:22:LEU:HD23	2.20	0.42
1:A:594:MET:O	1:A:598:ARG:HG2	2.19	0.42
1:A:634:ALA:C	1:A:636:PRO:HD3	2.45	0.42
1:C:834:ILE:HD13	1:C:834:ILE:HA	1.94	0.42
1:C:956:ASN:O	1:C:959:HIS:HB3	2.19	0.42
5:G:49:DA:N3	6:H:14:DG:N2	2.68	0.42
1:A:421:ARG:HH12	1:A:425:HIS:HD2	1.68	0.42
1:A:771:SER:O	1:A:774:GLU:HG2	2.19	0.42
1:A:821:GLY:O	1:A:825:GLU:HB2	2.20	0.42
2:B:184:LEU:HG	2:B:195:HIS:CD2	2.55	0.42
2:B:201:THR:HB	2:B:232:ARG:HH12	1.85	0.42
1:C:814:ASP:CG	1:C:817:HIS:H	2.22	0.42
1:C:883:GLU:OE1	1:C:883:GLU:N	2.48	0.42
2:D:1:MET:HA	2:D:349:SER:O	2.20	0.42
4:F:35:DT:H2''	4:F:36:DA:C8	2.55	0.42
5:G:17:DC:H6	5:G:17:DC:H2'	1.75	0.42
1:A:487:LEU:HD11	1:A:1015:LEU:HD13	2.02	0.42
1:A:580:VAL:O	1:A:583:VAL:HG22	2.20	0.42
1:A:709:LEU:O	1:A:719:SER:HA	2.20	0.42
2:B:73:ARG:NH1	2:B:96:ARG:NH1	2.66	0.42
1:C:991:ARG:HA	1:C:991:ARG:HD2	1.87	0.42
5:G:54:DC:H2''	5:G:55:DC:C6	2.54	0.42
1:A:892:VAL:CG1	1:A:898:ARG:HG2	2.44	0.41
2:B:21:LEU:O	2:B:22:LEU:HD23	2.20	0.41
1:C:1006:LEU:HD23	1:C:1006:LEU:HA	1.58	0.41
2:D:1:MET:C	2:D:305:PRO:HG3	2.45	0.41
3:E:6:DG:OP2	3:E:6:DG:C8	2.70	0.41
5:G:11:DG:N1	5:G:12:DT:C4	2.88	0.41
6:H:42:DT:H3'	6:H:43:DG:C8	2.55	0.41
1:A:982:GLY:O	1:A:985:SER:HB3	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:ASP:N	2:B:177:ASP:OD1	2.52	0.41
1:C:588:ASP:OD1	1:C:1019:LYS:HB2	2.20	0.41
2:D:93:HIS:HA	2:D:94:GLY:HA2	1.66	0.41
2:D:283:LYS:CD	2:D:317:TRP:HE1	2.33	0.41
2:D:328:LEU:HD11	2:D:345:PHE:CD2	2.51	0.41
3:E:33:DG:H2''	3:E:34:DG:C8	2.55	0.41
1:A:642:PHE:HB3	1:A:678:CYS:HB3	2.01	0.41
2:B:180:PRO:HB3	2:B:203:GLY:N	2.36	0.41
2:D:43:THR:HG22	2:D:45:ILE:N	2.34	0.41
2:D:86:LYS:NZ	2:D:87:PRO:C	2.76	0.41
2:D:315:ARG:HG3	2:D:316:THR:HG23	2.01	0.41
2:D:321:SER:O	2:D:321:SER:OG	2.36	0.41
3:E:18:DA:H2''	3:E:19:DC:O5'	2.20	0.41
1:C:519:LEU:HD23	1:C:519:LEU:HA	1.71	0.41
1:C:705:MET:H	1:C:705:MET:HG2	1.67	0.41
3:E:34:DG:C8	3:E:35:DA:C6	3.08	0.41
5:G:42:DG:O5'	5:G:42:DG:H8	2.03	0.41
6:H:5:DA:H2''	6:H:6:DG:N7	2.35	0.41
1:A:492:ASN:OD1	1:A:1025:MET:HE3	2.21	0.41
1:A:851:TRP:HA	1:A:854:THR:HG22	2.02	0.41
1:A:895:GLU:OE2	1:A:898:ARG:NH2	2.53	0.41
1:A:991:ARG:HH11	4:F:34:DG:C3'	2.32	0.41
2:B:10:ASN:CG	2:B:11:CYS:SG	3.03	0.41
1:C:864:LYS:HD3	1:C:864:LYS:HA	1.95	0.41
2:D:24:LEU:CD2	2:D:29:TYR:CD2	3.03	0.41
2:D:202:ASP:OD2	2:D:223:ILE:HG21	2.21	0.41
2:D:287:CYS:SG	2:D:304:PRO:HA	2.61	0.41
4:F:13:DT:H6	4:F:13:DT:H2'	1.66	0.41
1:A:680:MET:HE3	1:A:680:MET:HB2	1.85	0.41
1:A:822:ASN:OD1	1:A:822:ASN:N	2.52	0.41
2:B:108:MET:HE1	2:B:127:LYS:HZ3	1.83	0.41
2:B:215:CYS:HG	2:B:237:HIS:CE1	2.39	0.41
1:C:895:GLU:OE1	1:C:898:ARG:NH1	2.54	0.41
3:E:29:DG:H1'	3:E:30:DA:C8	2.55	0.41
4:F:47:DG:H2''	4:F:48:DA:OP2	2.20	0.41
6:H:42:DT:H3'	6:H:43:DG:N7	2.35	0.41
2:B:142:LEU:HD12	2:B:154:VAL:O	2.21	0.41
1:C:498:SER:O	1:C:502:LYS:HG3	2.20	0.41
1:C:534:HIS:CE1	1:C:587:LYS:NZ	2.89	0.41
1:C:628:LYS:HB2	4:F:32:DG:H4'	2.01	0.41
1:C:680:MET:HB2	1:C:680:MET:HE3	1.72	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:217:TYR:OH	2:D:235:ARG:NH2	2.52	0.41
4:F:13:DT:H4'	4:F:14:DG:OP1	2.21	0.41
6:H:7:DG:H2'	6:H:8:DG:H8	1.85	0.41
6:H:45:DG:H2'	6:H:45:DG:N3	2.36	0.41
1:A:489:ILE:HD11	1:C:503:MET:HA	2.02	0.41
1:A:740:LEU:HD21	1:A:770:ARG:HH22	1.85	0.41
1:A:880:MET:HE3	1:A:880:MET:HB2	1.93	0.41
1:A:903:LYS:HE2	1:A:907:LEU:HD11	2.02	0.41
1:C:452:THR:O	1:C:456:LEU:HG	2.21	0.41
1:C:738:GLU:HA	1:C:805:PRO:HB3	2.01	0.41
1:C:838:TYR:OH	1:C:897:ARG:HG3	2.21	0.41
1:C:1029:LYS:HE2	1:C:1029:LYS:HB3	1.78	0.41
2:D:286:GLU:HA	2:D:304:PRO:HB3	2.03	0.41
5:G:11:DG:C5	5:G:12:DT:H73	2.55	0.41
1:A:430:LEU:HB2	1:C:437:PHE:CG	2.56	0.41
1:A:820:ILE:O	1:A:824:THR:HG22	2.20	0.41
1:A:860:ARG:HH21	1:A:867:PRO:HD2	1.85	0.41
1:A:968:ILE:O	1:A:971:ARG:HG2	2.20	0.41
1:A:1019:LYS:HB2	1:A:1019:LYS:HE2	1.74	0.41
1:A:1024:PHE:HD1	1:A:1024:PHE:HA	1.73	0.41
2:B:76:ALA:CB	2:B:93:HIS:O	2.57	0.41
2:B:162:MET:HE3	2:B:162:MET:HB2	1.85	0.41
2:B:212:ARG:HG2	2:B:213:GLN:OE1	2.20	0.41
1:C:485:VAL:HG22	1:C:1024:PHE:CG	2.56	0.41
1:C:655:GLY:C	1:C:656:GLU:CD	2.89	0.41
1:C:795:ARG:HH22	2:D:39:ARG:NH1	2.18	0.41
2:D:130:VAL:O	2:D:192:CYS:N	2.37	0.41
2:D:256:LEU:CD2	2:D:288:THR:HG21	2.51	0.41
2:D:290:VAL:CG1	2:D:297:VAL:HG23	2.49	0.41
4:F:14:DG:C5	4:F:15:DT:C4	3.09	0.41
4:F:15:DT:H2''	4:F:16:DT:C4	2.55	0.41
1:A:503:MET:O	1:A:507:VAL:HG12	2.21	0.41
2:B:180:PRO:O	2:B:200:LEU:HD23	2.21	0.41
1:C:481:LEU:HD23	1:C:481:LEU:HA	1.78	0.41
1:C:492:ASN:OD1	1:C:1025:MET:HG2	2.20	0.41
1:C:798:VAL:O	1:C:801:VAL:HG23	2.20	0.41
1:C:840:LYS:HD3	1:C:843:PRO:HB3	2.03	0.41
2:D:259:THR:OG1	2:D:277:TYR:O	2.26	0.41
2:D:275:GLY:HA3	2:D:317:TRP:HH2	1.86	0.41
3:E:33:DG:C2	3:E:34:DG:C6	3.09	0.41
6:H:51:DC:H2''	6:H:52:DA:C8	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:VAL:HG12	1:A:683:ASP:N	2.33	0.40
1:A:897:ARG:HH12	1:A:945:MET:HG3	1.86	0.40
1:A:993:PHE:HE2	1:A:1013:HIS:HA	1.86	0.40
2:B:210:LEU:HD23	2:B:210:LEU:HA	1.88	0.40
1:C:579:ASP:OD1	1:C:579:ASP:N	2.53	0.40
2:D:147:SER:OG	2:D:240:LEU:CD2	2.61	0.40
5:G:11:DG:N2	5:G:12:DT:C2	2.90	0.40
1:A:816:LEU:HD13	1:A:981:GLU:HG2	2.03	0.40
2:B:273:ILE:HB	2:B:288:THR:OG1	2.21	0.40
1:C:665:GLU:HG2	1:C:668:PRO:HB3	2.03	0.40
1:C:778:ARG:NH2	1:C:798:VAL:O	2.49	0.40
2:D:274:PHE:HZ	2:D:348:VAL:HG11	1.86	0.40
4:F:31:DT:OP2	4:F:31:DT:C6	2.74	0.40
1:A:593:ILE:HD11	1:A:713:VAL:HG21	2.03	0.40
1:A:647:MET:HB3	1:A:647:MET:HE3	1.80	0.40
1:A:686:ASP:OD1	1:A:686:ASP:C	2.65	0.40
1:A:862:LYS:HE2	1:A:887:ALA:HB1	2.02	0.40
1:A:894:SER:O	1:A:898:ARG:HG3	2.22	0.40
2:B:48:VAL:HG23	2:B:55:LEU:CD1	2.48	0.40
2:B:101:GLU:C	2:B:102:LEU:HD12	2.46	0.40
2:B:197:LEU:HD12	2:B:249:CYS:HB3	2.03	0.40
2:B:269:HIS:O	2:B:292:LEU:HD23	2.22	0.40
1:C:833:GLU:OE2	1:C:948:TYR:OH	2.35	0.40
1:C:989:LEU:HA	1:C:989:LEU:HD23	1.74	0.40
4:F:27:DG:C2'	4:F:28:DC:H5'	2.51	0.40
5:G:34:DA:OP2	5:G:34:DA:C8	2.73	0.40
1:A:529:LEU:HD23	1:A:529:LEU:HA	1.88	0.40
1:A:778:ARG:HE	1:A:799:LYS:CE	2.34	0.40
1:C:577:ARG:HB3	1:C:579:ASP:OD1	2.22	0.40
1:C:597:LEU:HD21	1:C:603:ASP:O	2.22	0.40
1:C:795:ARG:NH1	2:D:39:ARG:HH11	2.18	0.40
2:D:96:ARG:HG2	2:D:102:LEU:HD22	2.03	0.40
2:D:150:LYS:H	2:D:150:LYS:HG2	1.61	0.40
2:D:233:LEU:O	2:D:234:ILE:HD13	2.21	0.40
2:D:234:ILE:HG23	2:D:234:ILE:HD12	1.49	0.40
2:D:238:VAL:HG12	2:D:247:LEU:HG	2.04	0.40
3:E:19:DC:H2''	3:E:20:DA:C8	2.57	0.40
5:G:4:DC:H2''	5:G:5:DT:OP2	2.21	0.40
5:G:32:DC:N4	6:H:30:DG:H1	2.19	0.40
1:A:441:GLU:OE1	1:C:412:ARG:NH1	2.55	0.40
1:A:495:LEU:HD22	1:A:499:GLN:HB2	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:LEU:HD12	1:A:557:LEU:H	1.87	0.40
2:B:67:SER:OG	2:B:124:CYS:O	2.24	0.40
1:C:474:MET:HE3	1:C:474:MET:HB3	1.85	0.40
2:D:131:GLY:HA2	2:D:132:ASP:HB2	2.03	0.40
2:D:159:ARG:HB3	2:D:176:VAL:O	2.21	0.40
3:E:16:DA:H2''	3:E:17:DC:OP2	2.21	0.40
3:E:35:DA:H2''	3:E:36:DA:OP2	2.22	0.40
4:F:17:DC:H6	4:F:17:DC:H2'	1.59	0.40
4:F:20:DG:C2'	4:F:21:DT:H5'	2.52	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	619/1159 (53%)	558 (90%)	59 (10%)	2 (0%)	36	71
1	C	612/1159 (53%)	551 (90%)	61 (10%)	0	100	100
2	B	349/533 (66%)	306 (88%)	43 (12%)	0	100	100
2	D	349/533 (66%)	312 (89%)	37 (11%)	0	100	100
All	All	1929/3384 (57%)	1727 (90%)	200 (10%)	2 (0%)	49	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	818	CYS
1	A	512	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	547/1000 (55%)	546 (100%)	1 (0%)	87	85
1	C	545/1000 (54%)	544 (100%)	1 (0%)	87	85
2	B	303/465 (65%)	303 (100%)	0	100	100
2	D	303/465 (65%)	303 (100%)	0	100	100
All	All	1698/2930 (58%)	1696 (100%)	2 (0%)	87	88

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	956	ASN
1	C	1029	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	425	HIS
1	A	775	ASN
1	A	910	GLN
1	A	956	ASN
1	A	964	HIS
1	A	997	ASN
2	B	10	ASN
2	B	100	ASN
2	B	146	ASN
2	B	173	ASN
1	C	775	ASN
1	C	842	ASN
2	D	16	GLN
2	D	33	GLN
2	D	146	ASN
2	D	171	ASN
2	D	204	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

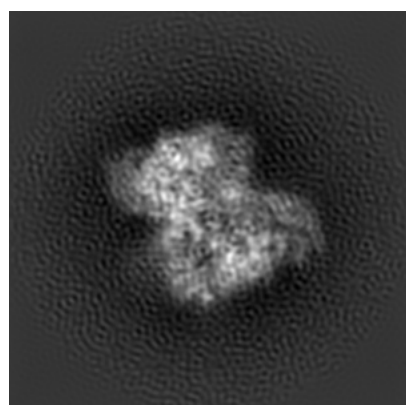
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7847. These allow visual inspection of the internal detail of the map and identification of artifacts.

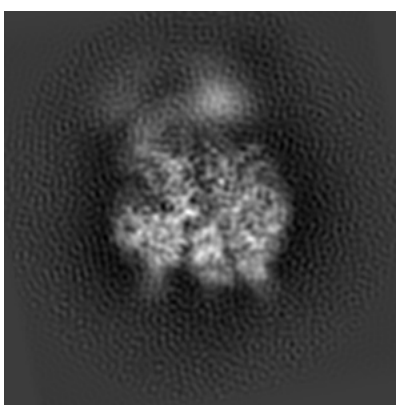
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

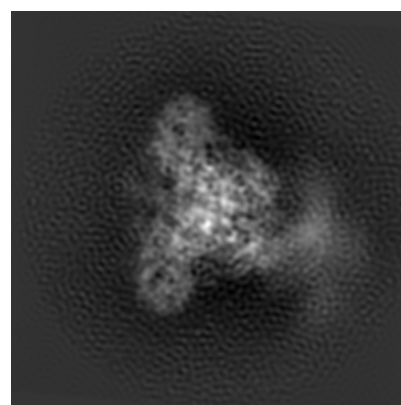
6.1.1 Primary map



X



Y

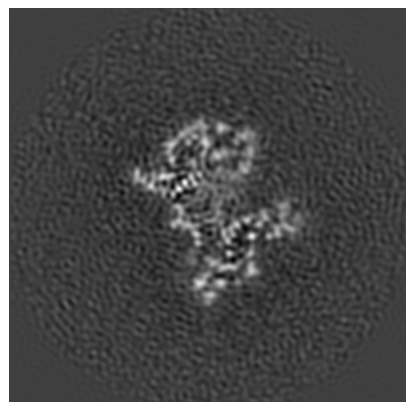


Z

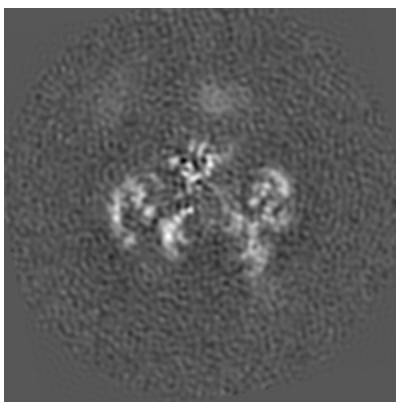
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

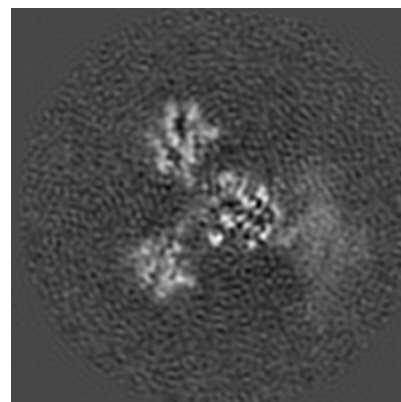
6.2.1 Primary map



X Index: 96



Y Index: 96

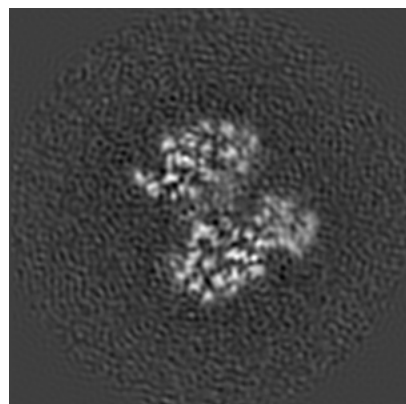


Z Index: 96

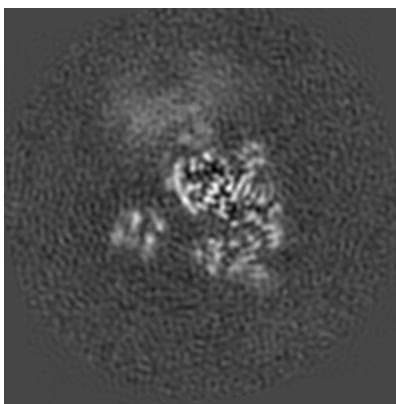
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

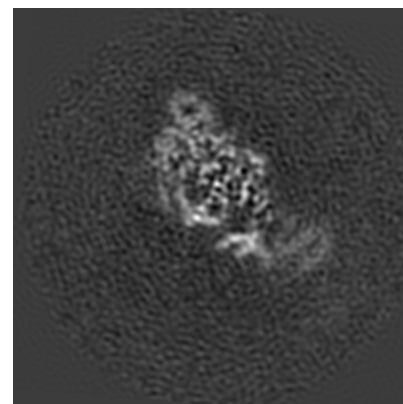
6.3.1 Primary map



X Index: 92



Y Index: 82

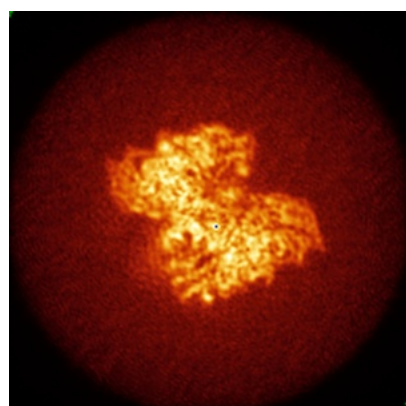


Z Index: 83

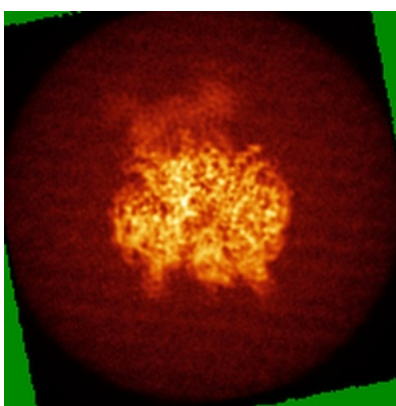
The images above show the largest variance slices of the map in three orthogonal directions.

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

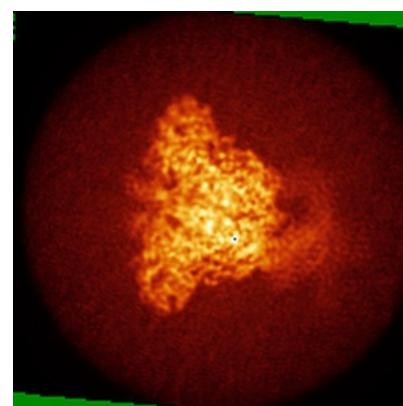
6.4.1 Primary map



X



Y

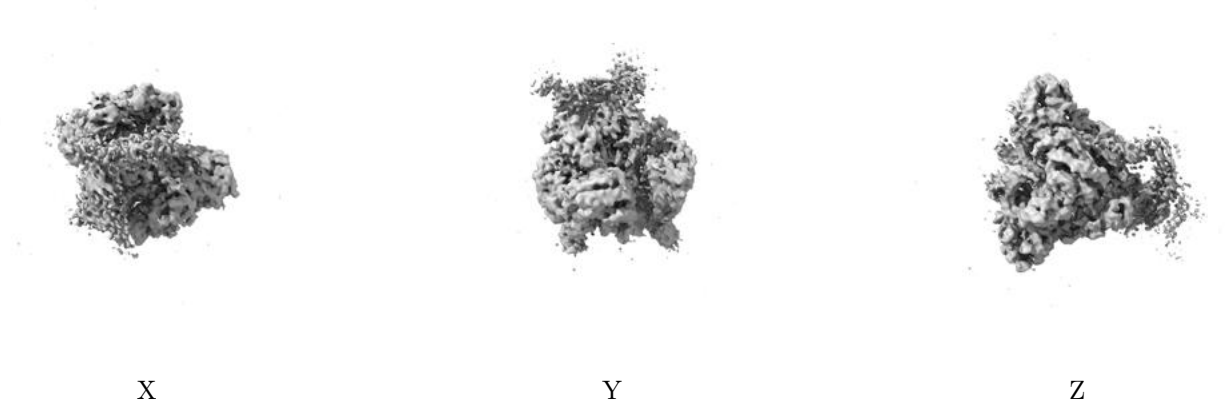


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

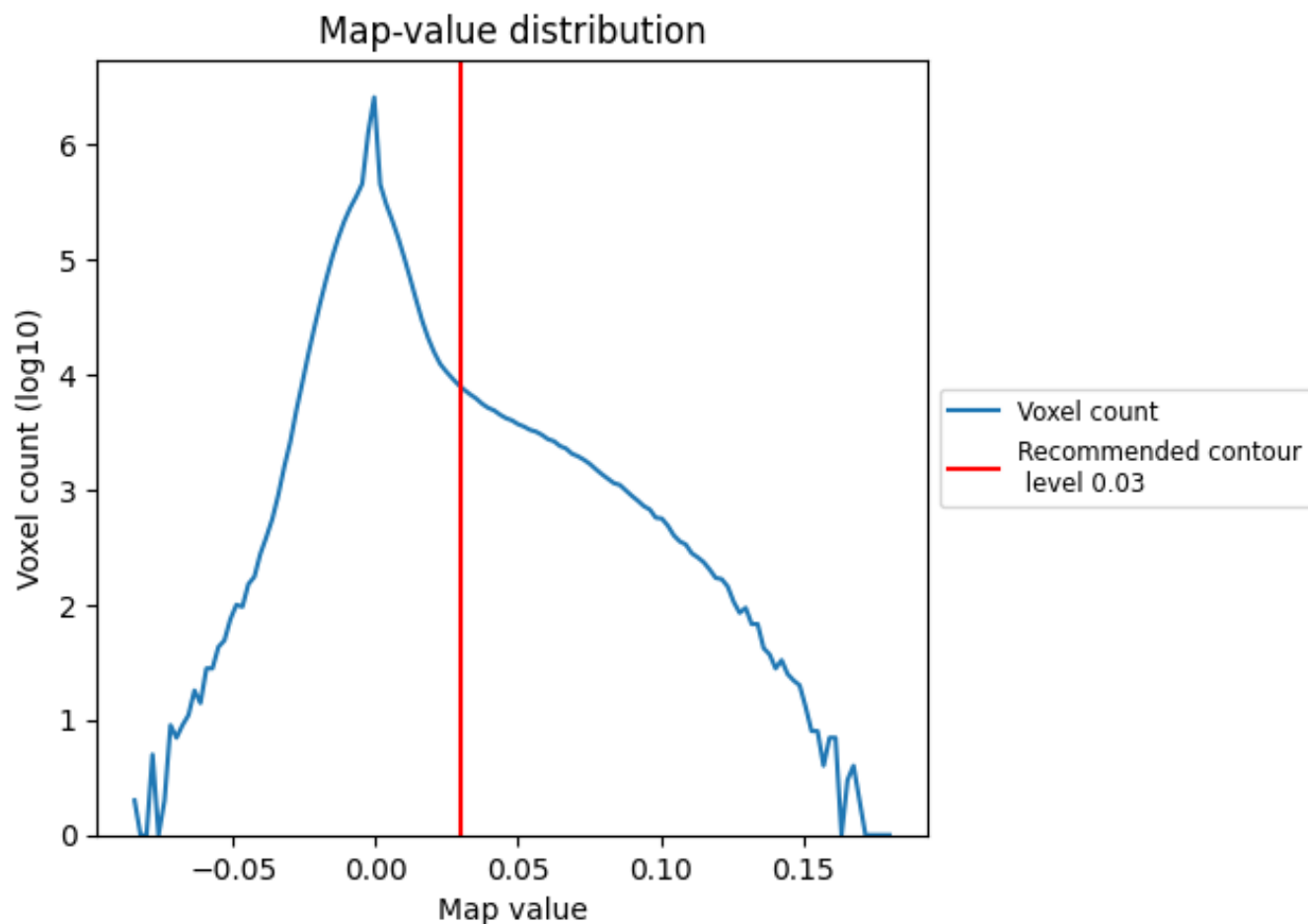
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

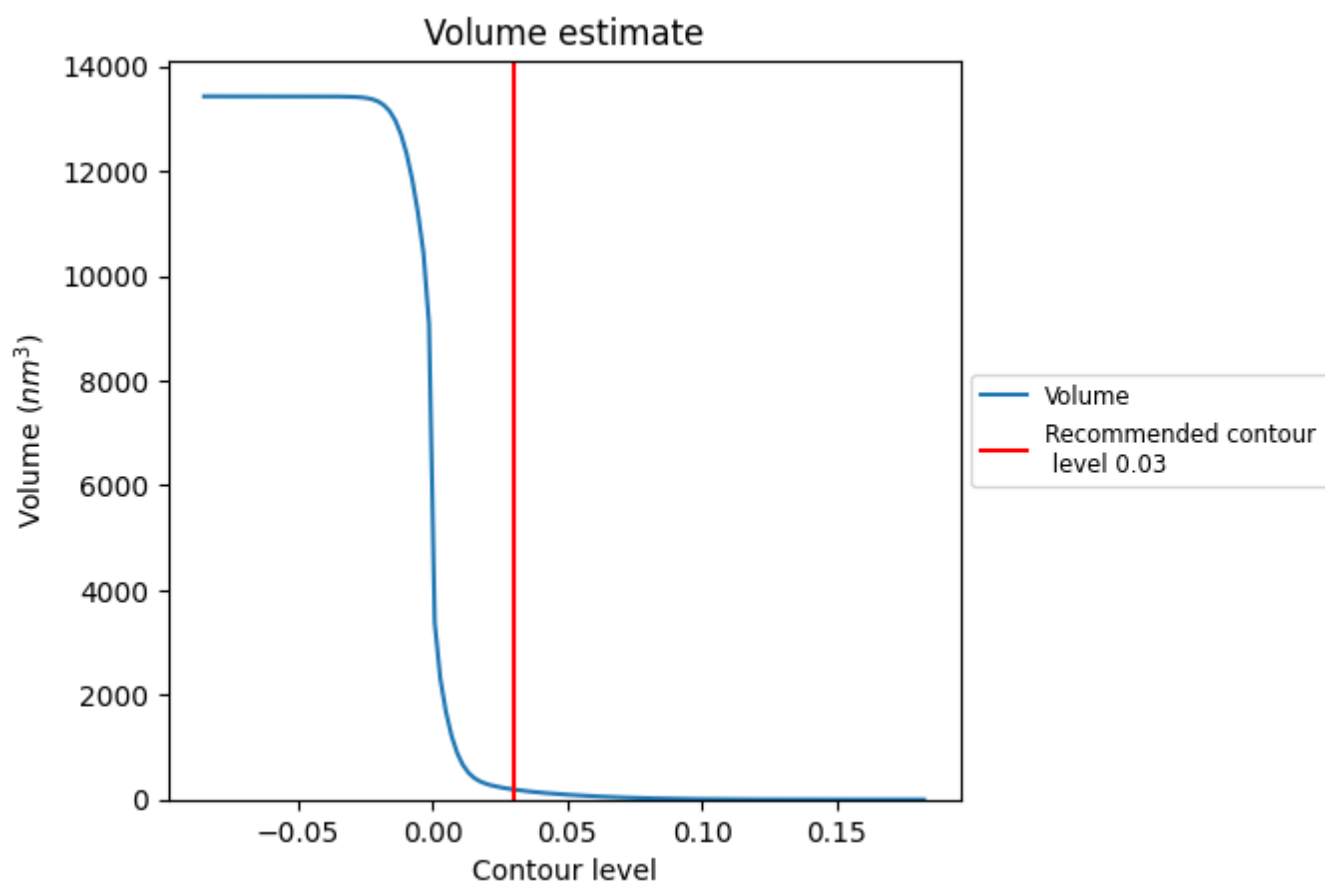
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

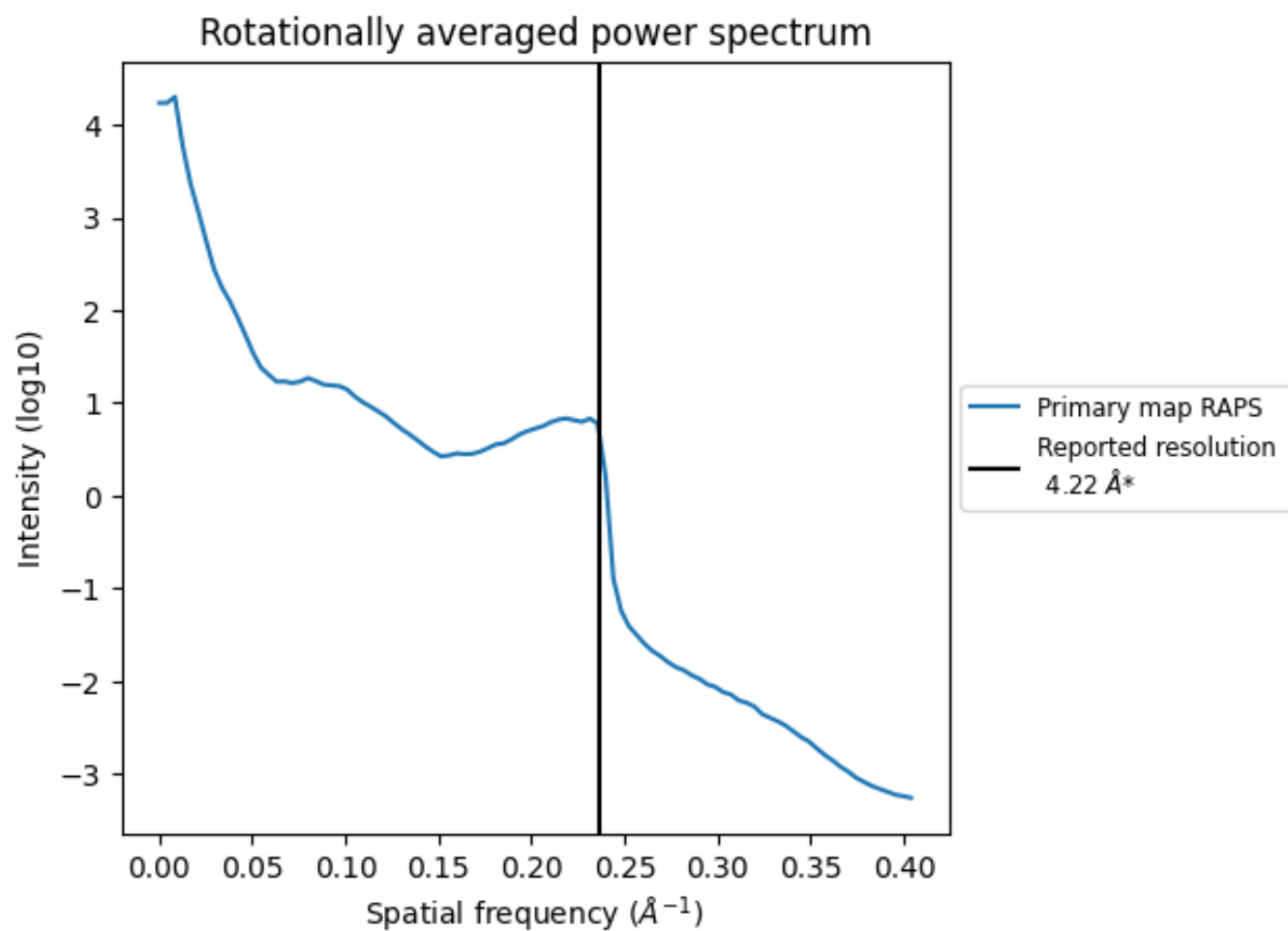
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 193 nm³; this corresponds to an approximate mass of 175 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 0.237 Å⁻¹

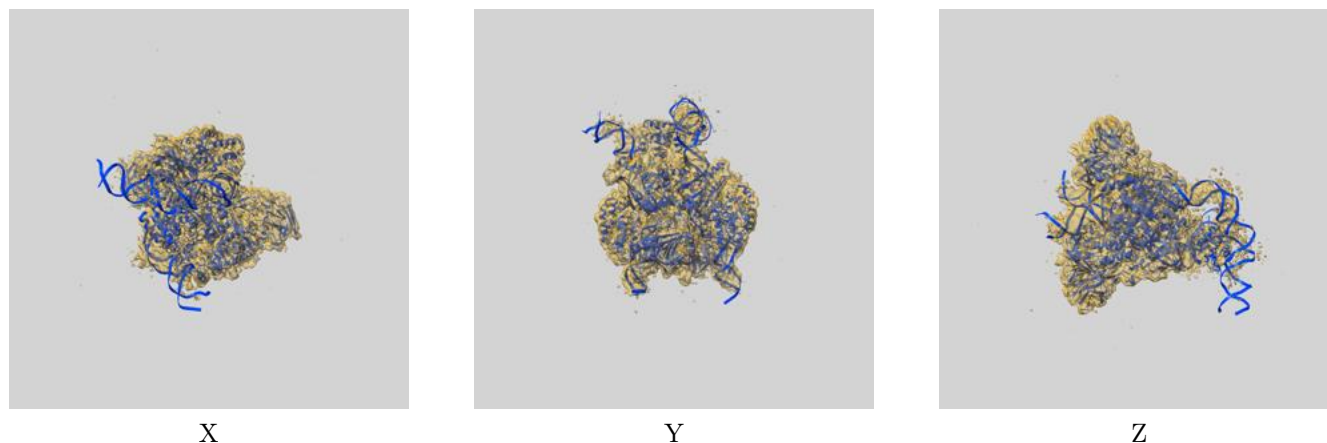
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

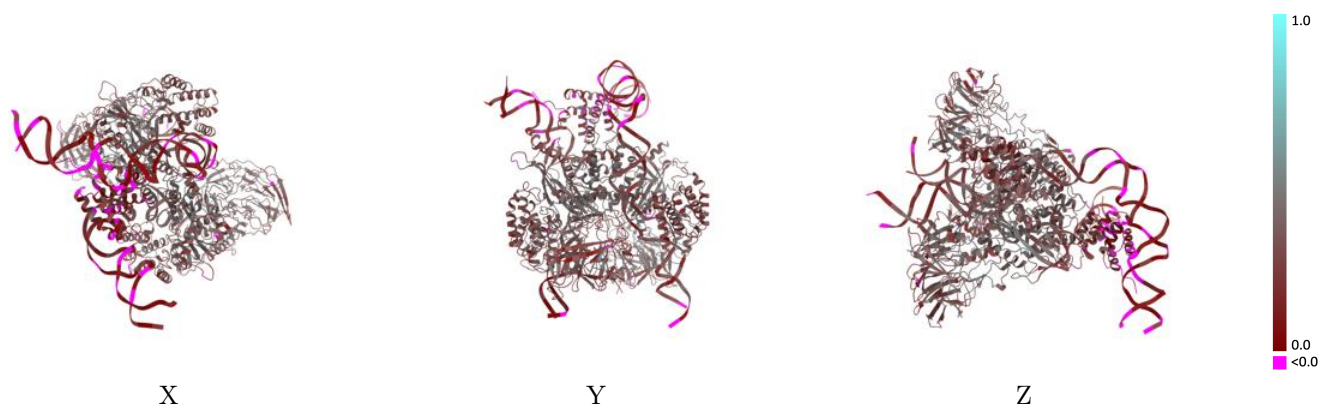
This section contains information regarding the fit between EMDB map EMD-7847 and PDB model 6DBQ. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



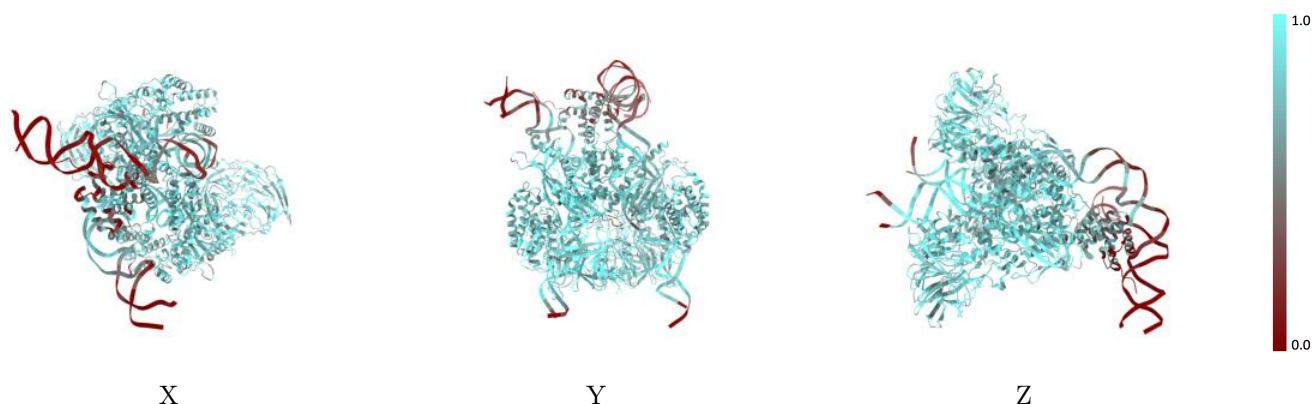
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



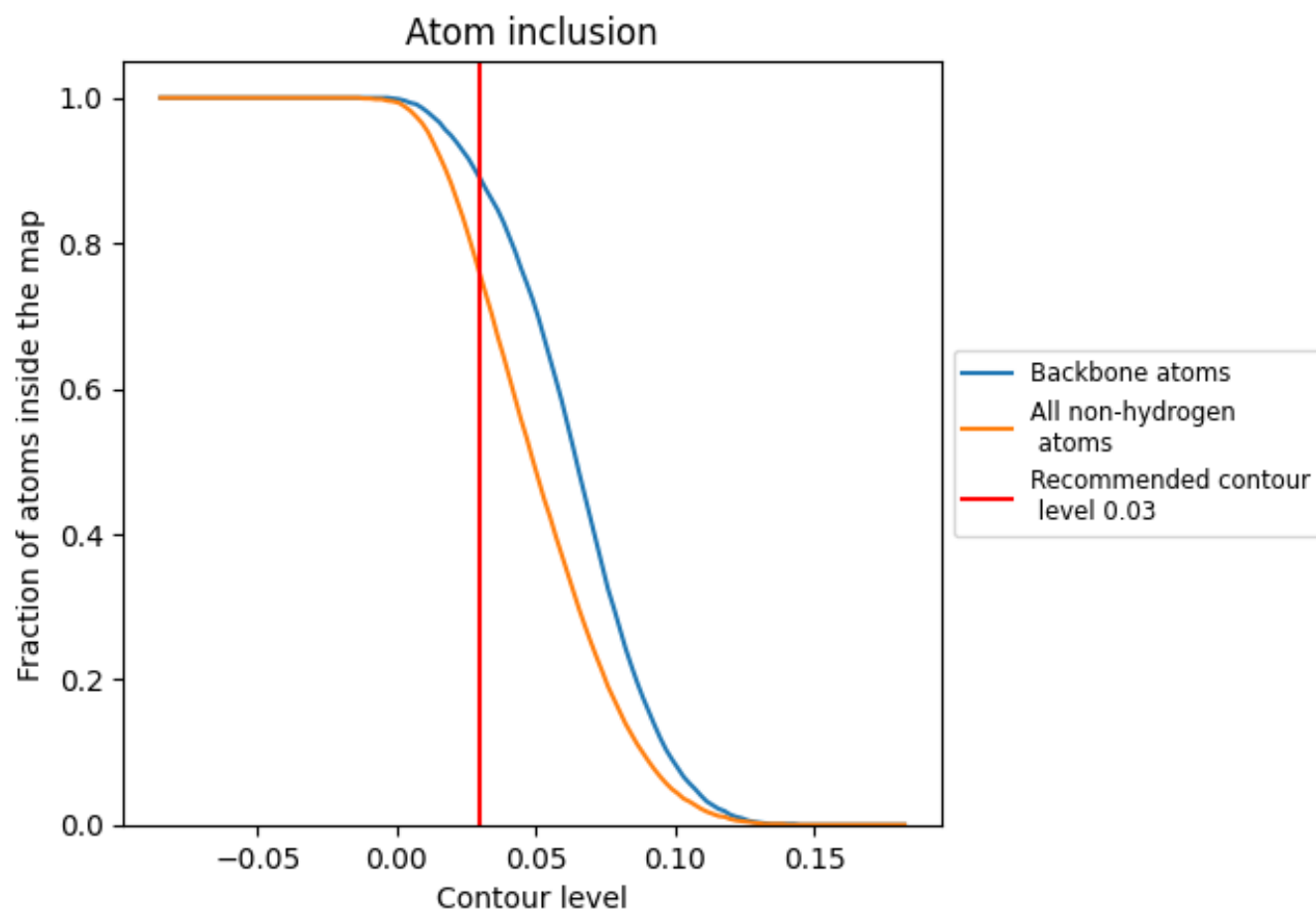
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7580	0.2960
A	0.7870	0.3220
B	0.8450	0.3320
C	0.8000	0.3280
D	0.8280	0.3380
E	0.6870	0.2030
F	0.7400	0.2100
G	0.4890	0.1660
H	0.4850	0.1640

1.0

0.0

<0.0