



## Full wwPDB EM Validation Report ⓘ

Apr 18, 2024 – 03:25 pm BST

PDB ID : 8S55  
EMDB ID : EMD-19726  
Title : RNA polymerase II early elongation complex bound to TFIIE and TFIIF - state a (composite structure)  
Authors : Zhan, Y.; Grabbe, F.; Oberbeckmann, E.; Dienemann, C.; Cramer, P.  
Deposited on : 2024-02-22  
Resolution : 3.40 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

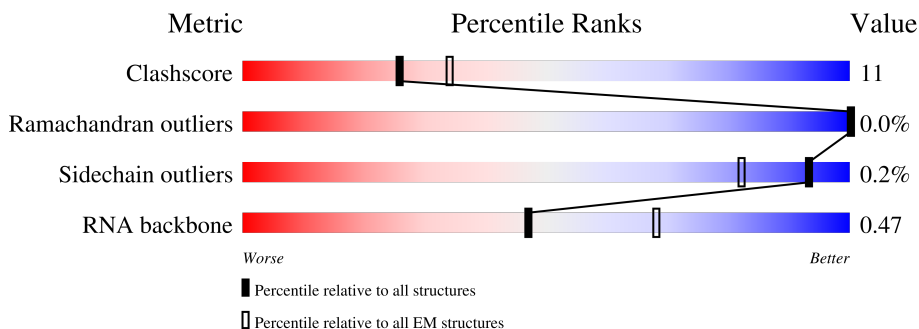
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 Å.

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









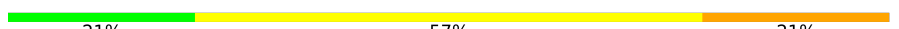

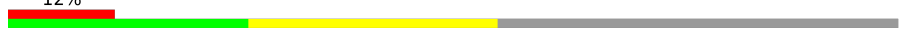



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 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	1984	60% (green), 11% (yellow), 29% (grey)
2	B	1300	73% (green), 14% (yellow), 13% (grey)
3	C	275	79% (green), 15% (yellow), 7% (grey)
4	D	184	35% (green), 35% (yellow), 30% (grey), 1% (red)
5	E	210	87% (green), 12% (yellow)
6	F	127	53% (green), 12% (yellow), 35% (grey), 1% (red)
7	G	172	48% (green), 52% (yellow), 1% (red)

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Mol	Chain	Length	Quality of chain
8	H	150	 85% 13%
9	I	125	 73% 18% 9% 8%
10	J	67	 82% 18%
11	K	117	 79% 18%
12	L	58	 74% 24%
13	N	139	 20% 5% 75%
14	P	14	 21% 57% 21%
15	Q	517	 11% 16% 73%
16	R	249	 12% 27% 28% 45%
17	T	139	 19% 14% 67%
18	W	439	 21% 25% 17% 57%
19	X	291	 33% 37% 22% 41%

## 2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 38148 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 DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1417	11234	7070	2010	2082	72	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1130	9030	5714	1587	1665	64	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	257	2059	1294	351	408	6	0	0

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	128	1050	656	178	212	4	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	209	1720	1089	300	323	8	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	82	657	418	113	121	5	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	171	1351	875	219	249	8	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	148	1186	750	194	237	5	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	114	927	571	166	179	11	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	67	533	345	90	92	6	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	114	916	591	151	172	2	0	0

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	44	372	231	72	63	6	0	0

- Molecule 13 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
13	N	35	712	339	132	207	34	0	0

- Molecule 14 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	14	Total	C	N	O	P	0	0
			296	133	56	93	14		

- Molecule 15 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	138	Total	C	N	O	S	0	0
			1138	719	208	208	3		

- Molecule 16 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	137	Total	C	N	O	S	0	0
			1070	666	193	209	2		

- Molecule 17 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	46	Total	C	N	O	P	0	0
			949	449	175	279	46		

- Molecule 18 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	187	Total	C	N	O	S	0	0
			1535	964	275	285	11		

- Molecule 19 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	171	Total	C	N	O	S	0	0
			1403	895	243	261	4		

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
20	A	2	Total	Zn	0
			2	2	
20	B	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
20	C	1	Total 1	Zn 1	0
20	I	2	Total 2	Zn 2	0
20	J	1	Total 1	Zn 1	0
20	L	1	Total 1	Zn 1	0
20	W	1	Total 1	Zn 1	0

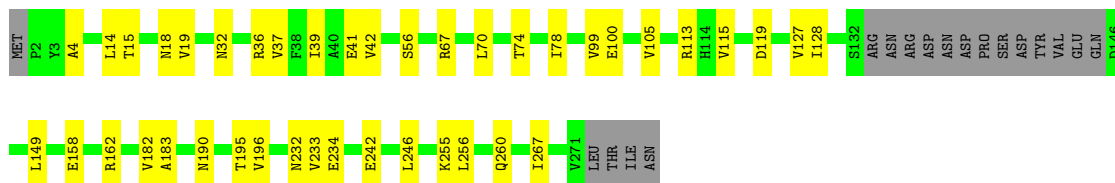
- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
21	P	1	Total 1	Mg 1	0

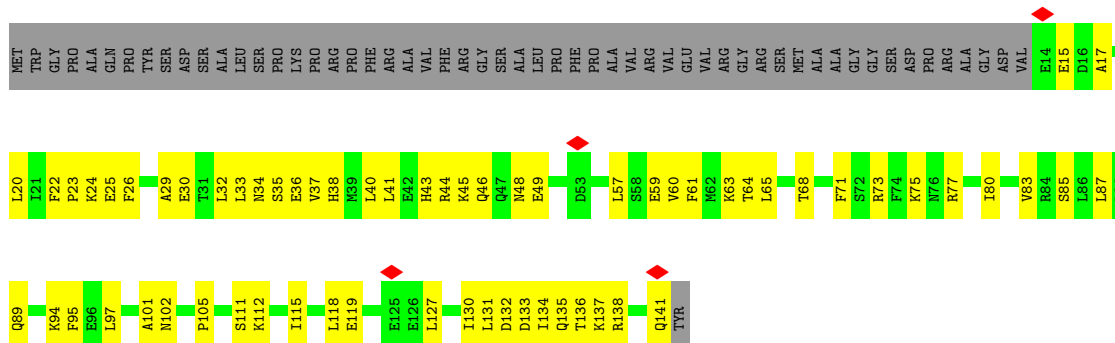
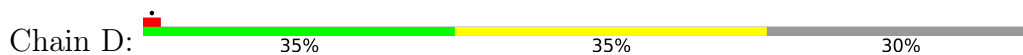




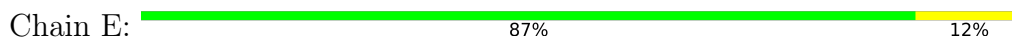




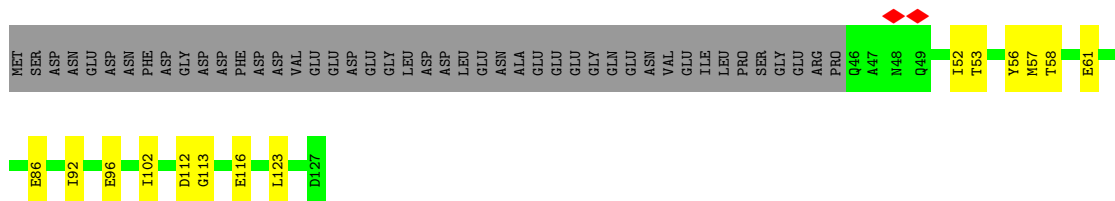
- Molecule 4: RNA polymerase II subunit D



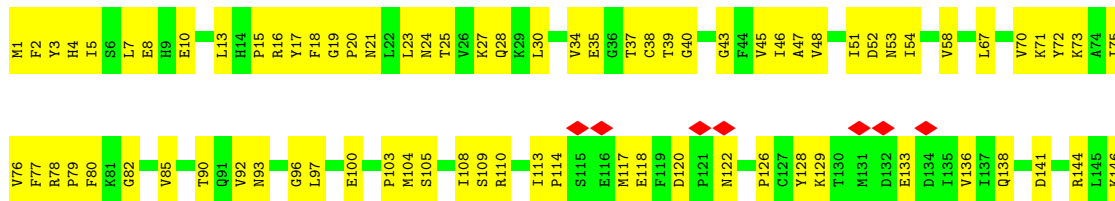
- Molecule 5: DNA-directed RNA polymerase II subunit E



- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



- Molecule 7: DNA-directed RNA polymerase II subunit RPB7









MET	ASP	PRO	PRO	SER	LEU	LEU	ARG	GLU	ARG	GLU	LEU	PHE	LYS	LYS	ARG	ALA	LEU	SER	THR	PRO	VAL	VAL	GLU	LYS	ARG	SER	ALA	SER	SER	GLU	SER	SER	SER	SER	SER	SER	LYS	LYS	LYS	LYS	THR	LYS	THR	LYS	VAL	VAL	GLU	GLU	HIS	GLY	GLY	SER	SER	GLY	SER	SER	GLN	ASN	ASP	HIS	SER	ASN	GLY
SER	PHE	ASN	LEU	LYS	ALA	LEU	SER	GLY	SER	SER	G72	Y73	K74	F75	G76	V77	L78	A79	R80	I81	V82	M83	Y84	M85	R86	T87	R88	H89	Q90	R91	G92	D93	T94	H95	P96	L97	T98	L99	D100	E101	I102	L103	D104	E105	T106	Q107	H108	L109	D110	I111	G112	L113	K114	Q115	K116	Q117	W118	L119	M120				
T121	E122	A123	L124	V125	M126	N127	P128	E131	V132	I133	D134	G135	K136	Y137	K140	P141	K142	Y143	N144	V145	R146	D147	K148	K149	A150	H151	L152	R153	L154	L155	H158	D159	Q160	R161	G162	L163	I166	L167	L168	E169	D170	I171	E172	E173	A174	L175	P176	N177	S178	Q179	K180	K183	A184	L185									
G186	D187	Q188	I189	V192	N193	R194	P195	D196	K197	K198	K199	I200	L201	F202	F203	K206	S207	C208	Q209	F210	S211	V212	D213	E214	E215	K216	L219	S222	V223	T224	V225	D226	S227	M228	E231	E234	E235	T236	L237	K238	R239	Q240	G241	I242	SER	SER	MET	GLN	GLU	SER	GLY	PRO	LYS										
LYS	VAL	ALA	PRO	ILE	GLN	ARG	ARG	LYS	LYS	PRO	ALA	SER	GLN	LYS	ARG	ARG	LYS	HIS	LEU	ALA	GLY	VAL	LEU	LYS	ASP	TYR	SER	ASP	ILE	THR	SER	LYS	S222	V223	T224	V225	D226	S227	M228	E231	E234	E235	T236	L237	K238	R239	Q240	G241	I242	SER	SER	MET	GLN	GLU	SER	GLY	PRO	LYS					

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	47.040	Depositor
Minimum map value	-23.056	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.37	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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: MG, 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	0.29	0/11439	0.58	0/15440
2	B	0.29	0/9210	0.58	0/12431
3	C	0.28	0/2102	0.54	0/2857
4	D	0.24	0/1064	0.43	0/1428
5	E	0.29	0/1751	0.59	0/2366
6	F	0.31	0/667	0.65	0/901
7	G	0.26	0/1382	0.47	0/1874
8	H	0.32	0/1207	0.59	0/1628
9	I	0.29	0/948	0.60	1/1284 (0.1%)
10	J	0.30	0/542	0.59	0/730
11	K	0.29	0/935	0.53	0/1266
12	L	0.30	0/377	0.71	0/500
13	N	0.96	0/797	1.30	0/1225
14	P	0.76	0/330	1.12	0/511
15	Q	0.25	0/1167	0.50	0/1576
16	R	0.25	0/1083	0.51	0/1459
17	T	0.89	0/1064	1.27	0/1642
18	W	0.24	0/1560	0.48	0/2097
19	X	0.23	0/1427	0.42	0/1916
All	All	0.35	0/39052	0.63	1/53131 (0.0%)

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	2
2	B	0	1
All	All	0	3



There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	20	CYS	CA-CB-SG	5.28	123.51	114.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	ARG	Sidechain
1	A	351	ARG	Sidechain
2	B	1085	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11234	0	11366	159	0
2	B	9030	0	9073	150	0
3	C	2059	0	2007	28	0
4	D	1050	0	1033	85	0
5	E	1720	0	1737	26	0
6	F	657	0	684	10	0
7	G	1351	0	1358	96	0
8	H	1186	0	1147	15	0
9	I	927	0	859	17	0
10	J	533	0	553	9	0
11	K	916	0	939	15	0
12	L	372	0	378	1	0
13	N	712	0	395	7	0
14	P	296	0	154	20	0
15	Q	1138	0	1103	128	0
16	R	1070	0	1086	103	0
17	T	949	0	518	27	0
18	W	1535	0	1540	63	0
19	X	1403	0	1428	55	0
20	A	2	0	0	0	0
20	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	C	1	0	0	0	0
20	I	2	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
20	W	1	0	0	0	0
21	P	1	0	0	0	0
All	All	38148	0	37358	853	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 11.

All (853) 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)
2:B:747:LEU:CD2	17:T:49:DG:OP1	1.77	1.32
2:B:747:LEU:HD23	17:T:49:DG:OP1	1.35	1.15
1:A:264:VAL:HG21	14:P:5:C:H4'	1.38	1.05
2:B:747:LEU:HD21	17:T:49:DG:OP1	1.58	1.03
7:G:113:ILE:HG23	7:G:117:MET:HE2	1.40	1.03
7:G:82:GLY:HA2	7:G:146:LYS:HE2	1.42	1.00
7:G:129:LYS:HG2	7:G:136:VAL:HG13	1.44	0.99
8:H:96:VAL:HG12	8:H:116:VAL:HG22	1.45	0.98
5:E:29:THR:CG2	5:E:32:GLU:HG3	1.94	0.98
18:W:184:ILE:HD12	18:W:187:ILE:HD13	1.42	0.97
15:Q:24:LYS:HD3	16:R:99:SER:HB3	1.49	0.94
4:D:60:VAL:HG13	7:G:103:PRO:HB3	1.49	0.93
7:G:52:ASP:HB3	7:G:71:LYS:HG3	1.50	0.93
19:X:99:LEU:HD22	19:X:120:MET:HE3	1.50	0.92
5:E:29:THR:CG2	5:E:32:GLU:CG	2.53	0.85
2:B:841:ARG:HH11	14:P:3:A:C1'	1.91	0.84
1:A:264:VAL:HG21	14:P:5:C:C4'	2.11	0.81
2:B:707:CYS:SG	2:B:726:SER:OG	2.39	0.80
18:W:107:LEU:HD21	18:W:184:ILE:HD11	1.63	0.80
3:C:15:THR:OG1	3:C:18:ASN:OD1	2.00	0.80
1:A:406:VAL:HG21	1:A:419:ILE:HD11	1.63	0.79
15:Q:18:VAL:HG12	16:R:40:VAL:HG11	1.64	0.79
18:W:144:LEU:HD22	18:W:155:THR:H	1.48	0.79
15:Q:110:PHE:HB3	15:Q:146:PHE:HB3	1.65	0.79
1:A:358:ARG:NH2	17:T:46:DG:OP1	2.15	0.78
2:B:783:ALA:HB2	2:B:1041:ILE:HG23	1.65	0.78
5:E:29:THR:HG22	5:E:32:GLU:CD	2.03	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:30:ALA:HB1	16:R:91:GLN:HE21	1.49	0.76
1:A:79:THR:OG1	1:A:80:GLU:OE1	2.04	0.76
1:A:29:ASP:OD2	1:A:33:ARG:NH1	2.19	0.75
14:P:10:C:H2'	14:P:11:G:C8	2.22	0.75
15:Q:15:VAL:O	15:Q:135:PHE:N	2.21	0.73
1:A:1458:ILE:HD11	2:B:1107:LEU:HD12	1.70	0.73
18:W:168:MET:HG2	18:W:169:PRO:HD3	1.69	0.73
1:A:1375:ARG:NE	1:A:1403:ASP:OD1	2.22	0.73
18:W:22:ILE:HD11	18:W:30:HIS:HB3	1.69	0.73
4:D:71:PHE:O	4:D:73:ARG:NH2	2.22	0.72
2:B:952:GLU:O	3:C:36:ARG:NH2	2.23	0.72
3:C:41:GLU:OE2	3:C:255:LYS:NZ	2.18	0.72
5:E:51:GLY:O	5:E:54:ARG:NH1	2.23	0.71
2:B:1040:GLN:NE2	3:C:196:VAL:O	2.23	0.71
2:B:1032:PHE:O	3:C:32:ASN:ND2	2.24	0.71
1:A:998:PRO:O	1:A:1059:ARG:NH2	2.24	0.70
7:G:147:ILE:HG23	7:G:159:ALA:HB1	1.73	0.70
2:B:591:ARG:NH1	2:B:663:GLU:OE2	2.24	0.70
14:P:10:C:H2'	14:P:11:G:H8	1.56	0.70
2:B:1091:ARG:NH2	2:B:1092:ASP:OD1	2.25	0.70
15:Q:166:ARG:HE	15:Q:170:VAL:HG23	1.55	0.70
2:B:146:LYS:O	16:R:152:ASN:ND2	2.23	0.70
3:C:234:GLU:OE1	10:J:42:ARG:NH1	2.25	0.70
17:T:41:DA:H2'	17:T:42:DA:C8	2.27	0.70
2:B:381:GLU:OE1	2:B:381:GLU:N	2.25	0.70
3:C:190:ASN:ND2	3:C:195:THR:O	2.25	0.70
16:R:136:SER:O	16:R:139:VAL:HG12	1.92	0.70
7:G:54:ILE:HD13	7:G:70:VAL:HG13	1.74	0.70
1:A:1206:ARG:NH2	1:A:1263:ASN:O	2.25	0.69
1:A:264:VAL:HG11	14:P:5:C:O2'	1.91	0.69
6:F:53:THR:OG1	6:F:116:GLU:OE1	2.08	0.69
4:D:41:LEU:HD12	4:D:68:THR:HG21	1.74	0.69
1:A:931:ARG:NH2	1:A:936:GLU:OE1	2.25	0.69
1:A:197:GLU:N	1:A:197:GLU:OE1	2.25	0.69
4:D:30:GLU:OE2	7:G:4:HIS:ND1	2.27	0.68
2:B:841:ARG:NH1	14:P:3:A:H1'	2.07	0.68
7:G:40:GLY:HA2	7:G:157:ILE:HD11	1.76	0.68
15:Q:29:MET:HG3	16:R:96:PHE:CD1	2.27	0.68
5:E:29:THR:HG21	5:E:32:GLU:HG3	1.75	0.68
6:F:58:THR:OG1	6:F:61:GLU:OE1	2.08	0.68
5:E:29:THR:HG23	5:E:32:GLU:HG3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ARG:NH2	13:N:65:DC:OP1	2.23	0.67
2:B:1085:ARG:NE	17:T:45:DT:OP1	2.26	0.67
4:D:34:ASN:OD1	4:D:102:ASN:ND2	2.28	0.67
16:R:21:VAL:HG22	16:R:114:ALA:HB3	1.76	0.67
19:X:98:THR:HG22	19:X:136:LYS:HG2	1.77	0.67
9:I:40:ARG:NH2	15:Q:174:PHE:HB3	2.10	0.67
2:B:611:GLU:OE1	2:B:613:ARG:NH2	2.28	0.66
5:E:3:ASP:OD1	5:E:49:SER:OG	2.11	0.66
7:G:39:THR:O	7:G:43:GLY:N	2.27	0.66
19:X:159:ASP:HB2	19:X:203:PHE:HB3	1.76	0.66
4:D:32:LEU:HD12	4:D:36:GLU:HG2	1.77	0.66
7:G:10:GLU:N	7:G:10:GLU:OE1	2.26	0.66
1:A:948:ILE:HD12	1:A:1007:ILE:HG21	1.78	0.66
2:B:31:SER:OG	2:B:766:TYR:OH	2.00	0.66
19:X:235:GLU:HA	19:X:238:LYS:HZ3	1.61	0.65
4:D:64:THR:HG21	7:G:46:ILE:HG12	1.78	0.65
8:H:26:SER:HB2	8:H:45:ILE:HD11	1.78	0.65
1:A:457:ILE:HD11	1:A:515:ILE:HD12	1.77	0.65
4:D:131:LEU:O	4:D:135:GLN:HG2	1.97	0.65
15:Q:100:LEU:HD22	15:Q:110:PHE:HD2	1.62	0.65
4:D:57:LEU:HD13	4:D:61:PHE:CE2	2.31	0.65
2:B:543:GLU:OE1	15:Q:121:ASN:ND2	2.29	0.65
1:A:349:ARG:NH2	1:A:353:ASN:OD1	2.29	0.65
2:B:474:THR:OG1	2:B:732:ALA:O	2.07	0.65
4:D:43:HIS:O	4:D:46:GLN:HG3	1.97	0.65
1:A:876:ASP:O	1:A:890:ARG:NH2	2.29	0.65
15:Q:166:ARG:HH11	15:Q:171:LEU:H	1.45	0.65
18:W:173:ALA:O	18:W:177:LEU:HG	1.96	0.64
15:Q:157:ALA:HA	15:Q:160:ALA:HB3	1.78	0.64
15:Q:29:MET:HG3	16:R:96:PHE:HD1	1.63	0.64
14:P:6:C:H2'	14:P:7:A:C8	2.32	0.64
2:B:206:TYR:OH	2:B:390:ASN:O	2.16	0.64
7:G:165:ASP:HB3	7:G:168:LEU:HD11	1.78	0.64
18:W:36:ILE:HG21	18:W:48:MET:HG2	1.80	0.64
4:D:32:LEU:HD12	4:D:36:GLU:CG	2.27	0.64
8:H:143:LEU:HD23	8:H:144:LEU:N	2.12	0.64
4:D:135:GLN:OE1	4:D:138:ARG:NH2	2.31	0.64
4:D:37:VAL:HG21	7:G:2:PHE:HD2	1.63	0.63
15:Q:24:LYS:HD2	16:R:97:THR:HB	1.78	0.63
15:Q:42:TRP:CH2	15:Q:102:VAL:HG22	2.32	0.63
16:R:128:LYS:O	16:R:132:ILE:HG12	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:34:ASN:O	4:D:68:THR:OG1	2.15	0.63
5:E:29:THR:HG23	5:E:32:GLU:H	1.63	0.63
5:E:67:ASP:OD2	5:E:69:THR:OG1	2.08	0.63
15:Q:160:ALA:HA	15:Q:163:GLU:OE2	1.97	0.63
17:T:30:DC:H2'	17:T:31:DC:C6	2.33	0.63
18:W:36:ILE:HD11	18:W:52:LEU:HD21	1.79	0.63
15:Q:99:LEU:HD21	15:Q:101:ARG:HE	1.63	0.63
19:X:122:GLU:OE2	19:X:126:ASN:ND2	2.32	0.63
15:Q:24:LYS:HD3	16:R:99:SER:CB	2.26	0.63
19:X:119:LEU:HA	19:X:123:ALA:HB3	1.81	0.63
10:J:57:GLU:OE1	10:J:57:GLU:N	2.31	0.63
18:W:113:ARG:HG2	19:X:219:LEU:HD21	1.81	0.63
1:A:595:ILE:HD11	1:A:675:VAL:HG11	1.81	0.63
5:E:133:GLN:OE1	5:E:133:GLN:N	2.31	0.63
6:F:52:ILE:O	6:F:53:THR:OG1	2.17	0.63
2:B:841:ARG:HH11	14:P:3:A:H1'	1.62	0.63
2:B:841:ARG:NH1	14:P:3:A:C1'	2.62	0.63
15:Q:15:VAL:HB	15:Q:134:ALA:CB	2.29	0.63
7:G:52:ASP:HB3	7:G:71:LYS:CG	2.27	0.62
1:A:663:ASP:OD1	1:A:666:ARG:NH2	2.31	0.62
7:G:21:ASN:OD1	7:G:24:ASN:HB2	1.98	0.62
4:D:41:LEU:HB2	4:D:65:LEU:HD13	1.82	0.62
1:A:352:GLY:HA2	2:B:1085:ARG:HH12	1.62	0.62
2:B:223:SER:OG	2:B:350:HIS:ND1	2.28	0.62
19:X:81:ILE:HD13	19:X:106:THR:HG21	1.81	0.62
2:B:105:PRO:HB3	16:R:148:VAL:HG11	1.82	0.62
4:D:64:THR:HG21	7:G:46:ILE:HG21	1.82	0.62
15:Q:42:TRP:HH2	15:Q:100:LEU:HD21	1.65	0.62
1:A:644:SER:O	1:A:651:SER:OG	2.15	0.61
14:P:12:C:H2'	14:P:13:A:H8	1.65	0.61
15:Q:118:VAL:HG23	15:Q:120:GLU:OE1	2.00	0.61
4:D:111:SER:OG	4:D:127:LEU:HD21	2.00	0.61
15:Q:44:GLN:HE22	15:Q:46:ARG:HG3	1.65	0.61
1:A:47:THR:OG1	1:A:51:ARG:O	2.08	0.61
19:X:145:VAL:HG11	19:X:151:LEU:HB2	1.82	0.61
16:R:122:GLU:HA	16:R:125:MET:CE	2.31	0.61
2:B:59:VAL:HG23	2:B:408:PHE:CZ	2.35	0.61
7:G:114:PRO:HD2	7:G:117:MET:CE	2.30	0.61
7:G:53:ASN:OD1	7:G:54:ILE:N	2.33	0.61
15:Q:30:ALA:HB3	15:Q:145:ASN:HD22	1.66	0.61
1:A:668:PHE:CZ	1:A:672:ILE:HD11	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:45:LYS:HE3	4:D:61:PHE:CZ	2.36	0.61
15:Q:114:LYS:HZ3	15:Q:115:LYS:HB3	1.65	0.61
1:A:1343:LEU:HD12	1:A:1359:SER:OG	2.01	0.61
18:W:171:LYS:O	18:W:175:THR:HG23	2.00	0.60
2:B:929:PRO:O	2:B:948:GLN:NE2	2.34	0.60
15:Q:44:GLN:HE21	16:R:6:GLU:HG2	1.65	0.60
18:W:42:CYS:SG	18:W:75:ARG:NH1	2.74	0.60
15:Q:121:ASN:HA	16:R:25:LYS:HD3	1.83	0.60
19:X:99:LEU:CD2	19:X:120:MET:HE3	2.30	0.60
4:D:44:ARG:NH2	7:G:47:ALA:HB1	2.16	0.60
5:E:29:THR:CG2	5:E:32:GLU:CD	2.70	0.60
1:A:499:ASP:OD1	14:P:14:A:H4'	2.02	0.60
1:A:1016:LEU:HD22	1:A:1045:LEU:HD21	1.83	0.60
7:G:27:LYS:HD3	7:G:51:ILE:HD13	1.84	0.60
8:H:58:LEU:HD11	8:H:143:LEU:HD21	1.82	0.60
4:D:60:VAL:CG1	7:G:103:PRO:HB3	2.29	0.60
9:I:93:GLU:OE1	9:I:93:GLU:N	2.35	0.60
4:D:41:LEU:HD13	4:D:65:LEU:HA	1.84	0.59
1:A:378:VAL:HG21	1:A:458:PHE:CZ	2.36	0.59
7:G:129:LYS:HD2	7:G:133:GLU:OE2	2.03	0.59
4:D:45:LYS:HE2	4:D:45:LYS:HA	1.84	0.59
12:L:21:GLU:OE1	12:L:21:GLU:N	2.35	0.59
15:Q:94:GLU:N	15:Q:94:GLU:OE1	2.34	0.59
1:A:671:ASN:O	1:A:675:VAL:HG12	2.01	0.59
4:D:37:VAL:HG11	7:G:2:PHE:CE2	2.37	0.59
4:D:132:ASP:O	4:D:136:THR:HG23	2.02	0.59
9:I:116:ALA:HB3	9:I:119:CYS:HB3	1.84	0.59
1:A:1166:LEU:O	1:A:1170:THR:HG22	2.02	0.59
1:A:691:ASP:OD2	1:A:765:ASN:ND2	2.35	0.59
19:X:81:ILE:HG22	19:X:85:MET:CE	2.33	0.59
11:K:11:LEU:O	11:K:37:LYS:NZ	2.32	0.58
18:W:165:GLU:HA	18:W:168:MET:HE1	1.84	0.58
7:G:85:VAL:HA	7:G:144:ARG:HH11	1.67	0.58
2:B:743:ARG:O	2:B:922:ARG:NH2	2.37	0.58
1:A:266:MET:HE1	14:P:5:C:N3	2.18	0.58
7:G:138:GLN:HG2	7:G:141:ASP:OD2	2.03	0.58
15:Q:31:PHE:HD2	15:Q:37:VAL:HG11	1.68	0.58
1:A:590:GLN:O	1:A:593:SER:OG	2.16	0.58
1:A:853:LYS:NZ	1:A:1100:THR:O	2.35	0.58
5:E:38:GLU:OE1	5:E:38:GLU:N	2.35	0.58
11:K:45:ILE:HG21	11:K:94:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:109:LYS:O	15:Q:149:LEU:N	2.37	0.58
1:A:904:GLN:NE2	1:A:981:CYS:O	2.36	0.58
4:D:33:LEU:HD13	4:D:101:ALA:HB1	1.85	0.58
7:G:45:VAL:HA	7:G:76:VAL:HG12	1.86	0.58
9:I:27:LYS:O	9:I:36:LEU:N	2.36	0.58
15:Q:33:ALA:HB2	16:R:91:GLN:HA	1.85	0.58
1:A:1307:VAL:HG22	1:A:1338:THR:HG22	1.84	0.58
1:A:564:LEU:HD13	1:A:567:LEU:HD12	1.85	0.58
11:K:100:LEU:HD21	11:K:104:ARG:HH11	1.69	0.58
15:Q:39:PHE:HA	15:Q:42:TRP:HD1	1.67	0.58
1:A:868:MET:SD	1:A:1404:THR:HG21	2.44	0.58
1:A:948:ILE:HG23	1:A:1007:ILE:CG2	2.34	0.57
10:J:31:GLU:OE1	10:J:31:GLU:N	2.36	0.57
15:Q:111:LYS:HB2	15:Q:149:LEU:HD11	1.85	0.57
2:B:161:CYS:SG	2:B:162:LEU:N	2.77	0.57
1:A:266:MET:SD	14:P:5:C:C2	2.97	0.57
15:Q:29:MET:HB2	16:R:94:THR:HG23	1.85	0.57
1:A:923:ASP:OD1	1:A:1052:ARG:NH2	2.37	0.57
1:A:1077:ASN:ND2	6:F:56:TYR:OH	2.36	0.57
2:B:282:ARG:NH2	15:Q:34:ALA:HB1	2.18	0.57
9:I:79:PRO:O	9:I:95:VAL:HG23	2.03	0.57
15:Q:163:GLU:OE1	15:Q:163:GLU:N	2.33	0.57
19:X:234:GLU:OE1	19:X:238:LYS:NZ	2.37	0.57
18:W:168:MET:HG2	18:W:169:PRO:CD	2.34	0.57
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.87	0.57
15:Q:13:GLU:OE2	16:R:42:LYS:HD3	2.05	0.57
15:Q:27:ASN:O	16:R:95:VAL:HG13	2.05	0.57
2:B:197:GLN:NE2	2:B:466:VAL:HG22	2.19	0.57
4:D:87:LEU:HB3	4:D:97:LEU:HD11	1.87	0.57
11:K:77:THR:OG1	11:K:81:TYR:O	2.17	0.57
1:A:368:THR:HG23	1:A:481:THR:HG21	1.87	0.57
7:G:120:ASP:OD1	7:G:122:ASN:ND2	2.37	0.57
7:G:38:CYS:HB3	7:G:155:ASN:O	2.05	0.57
13:N:58:DT:H1'	13:N:59:DT:H5''	1.86	0.57
15:Q:24:LYS:CD	16:R:97:THR:HB	2.34	0.57
4:D:133:ASP:O	4:D:137:LYS:HG2	2.05	0.57
7:G:118:GLU:OE1	7:G:118:GLU:N	2.37	0.57
19:X:180:LYS:O	19:X:183:LYS:HG2	2.05	0.57
1:A:542:LEU:HD21	1:A:772:SER:O	2.05	0.56
2:B:866:ILE:HD12	2:B:921:ILE:HD11	1.86	0.56
15:Q:30:ALA:HB1	16:R:91:GLN:NE2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:PHE:CD2	2:B:437:THR:HG21	2.40	0.56
15:Q:39:PHE:HA	15:Q:42:TRP:CD1	2.40	0.56
15:Q:163:GLU:O	15:Q:166:ARG:HG2	2.05	0.56
4:D:37:VAL:O	4:D:41:LEU:HG	2.05	0.56
7:G:150:THR:HG22	7:G:159:ALA:HB2	1.85	0.56
7:G:34:VAL:O	7:G:37:THR:HG22	2.05	0.56
19:X:131:GLU:HB2	19:X:140:LYS:CG	2.35	0.56
1:A:406:VAL:CG2	1:A:419:ILE:HD11	2.32	0.56
4:D:41:LEU:CD1	4:D:68:THR:HG21	2.36	0.56
15:Q:166:ARG:HA	15:Q:169:LYS:HE3	1.88	0.56
1:A:1138:SER:OG	1:A:1360:ASN:ND2	2.38	0.56
2:B:747:LEU:HD21	17:T:49:DG:P	2.46	0.56
2:B:1077:GLY:HA2	17:T:47:DC:OP2	2.06	0.56
15:Q:166:ARG:NE	15:Q:170:VAL:HG23	2.19	0.56
19:X:114:LYS:O	19:X:117:GLN:HG3	2.06	0.56
19:X:131:GLU:HB2	19:X:140:LYS:HG3	1.87	0.56
1:A:890:ARG:HE	1:A:1023:VAL:HG22	1.71	0.55
4:D:57:LEU:HD13	4:D:61:PHE:HE2	1.67	0.55
6:F:57:MET:HB2	6:F:123:LEU:HD13	1.88	0.55
9:I:30:LYS:O	9:I:33:ARG:NH1	2.38	0.55
1:A:1127:LEU:HD12	1:A:1378:LEU:CD1	2.37	0.55
6:F:73:ILE:HG21	6:F:92:ILE:HD11	1.87	0.55
16:R:96:PHE:HA	16:R:106:LEU:HA	1.89	0.55
3:C:56:SER:OG	3:C:158:GLU:N	2.39	0.55
11:K:45:ILE:CG2	11:K:94:LEU:HD21	2.37	0.55
18:W:176:LEU:HD11	18:W:179:ARG:HH11	1.71	0.55
1:A:460:ARG:NH1	1:A:493:ASN:O	2.39	0.55
1:A:1458:ILE:CD1	2:B:1107:LEU:HD12	2.35	0.55
5:E:29:THR:HG22	5:E:32:GLU:CG	2.32	0.55
16:R:130:LEU:HA	16:R:133:GLU:OE1	2.07	0.55
2:B:115:LEU:HD22	2:B:908:MET:HE1	1.87	0.55
15:Q:114:LYS:HD3	15:Q:142:ASN:HB3	1.89	0.55
2:B:1161:GLU:O	2:B:1164:SER:OG	2.17	0.55
8:H:8:ASP:OD1	8:H:9:ILE:N	2.39	0.55
15:Q:121:ASN:HA	16:R:25:LYS:CG	2.37	0.55
5:E:66:ASP:OD1	5:E:67:ASP:N	2.40	0.55
2:B:526:LEU:HD11	2:B:532:ILE:HD11	1.88	0.55
7:G:8:GLU:OE2	7:G:71:LYS:HE3	2.07	0.55
10:J:14:VAL:HG13	10:J:49:LEU:HD21	1.89	0.55
18:W:37:LEU:CD1	18:W:72:ILE:HG21	2.35	0.55
1:A:745:LEU:HD12	1:A:822:PHE:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:LYS:NZ	15:Q:171:LEU:HD23	2.21	0.55
15:Q:16:VAL:HG21	16:R:56:PHE:CE1	2.41	0.55
16:R:120:ALA:HB3	16:R:124:TYR:HB2	1.87	0.55
18:W:63:LEU:HD22	18:W:92:TYR:CE2	2.42	0.55
5:E:74:VAL:HG23	5:E:103:LEU:HB2	1.89	0.55
7:G:10:GLU:HB2	7:G:67:LEU:HD11	1.89	0.55
18:W:14:LEU:HD23	18:W:194:THR:HG22	1.89	0.55
8:H:31:GLU:OE1	8:H:31:GLU:N	2.40	0.54
15:Q:15:VAL:HG13	16:R:42:LYS:NZ	2.22	0.54
15:Q:44:GLN:NE2	16:R:6:GLU:HG2	2.22	0.54
3:C:242:GLU:OE1	3:C:242:GLU:N	2.40	0.54
16:R:93:LEU:HB2	16:R:110:VAL:HB	1.89	0.54
1:A:91:ALA:HB3	1:A:290:LEU:HD22	1.88	0.54
1:A:1232:ALA:O	1:A:1236:ASN:ND2	2.40	0.54
2:B:91:ILE:HD13	2:B:126:VAL:HG12	1.88	0.54
16:R:21:VAL:HA	16:R:114:ALA:O	2.07	0.54
18:W:129:CYS:HB2	18:W:132:CYS:SG	2.48	0.54
15:Q:46:ARG:HH22	15:Q:104:GLY:H	1.53	0.54
19:X:77:VAL:HG21	19:X:111:ILE:HD11	1.90	0.54
4:D:131:LEU:O	4:D:134:ILE:HG13	2.08	0.54
1:A:1316:ASN:OD1	1:A:1317:LYS:N	2.41	0.54
2:B:149:ILE:HA	2:B:437:THR:HG22	1.89	0.54
4:D:41:LEU:CB	4:D:65:LEU:HD13	2.38	0.54
15:Q:24:LYS:CG	16:R:97:THR:HB	2.38	0.54
16:R:97:THR:N	16:R:105:SER:O	2.40	0.54
4:D:59:GLU:N	4:D:59:GLU:OE1	2.38	0.54
1:A:266:MET:CE	14:P:5:C:N3	2.71	0.54
4:D:45:LYS:O	4:D:49:GLU:HG2	2.08	0.54
15:Q:15:VAL:HG22	16:R:42:LYS:HZ3	1.73	0.54
1:A:869:GLU:OE1	1:A:1455:SER:OG	2.23	0.54
4:D:85:SER:O	4:D:89:GLN:HG2	2.08	0.54
15:Q:30:ALA:HB3	15:Q:145:ASN:ND2	2.23	0.54
16:R:4:ARG:HA	16:R:4:ARG:NE	2.22	0.54
18:W:43:VAL:HB	18:W:48:MET:HE2	1.90	0.54
19:X:170:ASP:O	19:X:173:GLU:HG3	2.08	0.54
1:A:376:ASP:OD2	1:A:473:ARG:NE	2.40	0.53
4:D:33:LEU:HD22	4:D:101:ALA:HB3	1.90	0.53
4:D:119:GLU:N	4:D:119:GLU:OE1	2.41	0.53
19:X:168:LEU:N	19:X:199:LYS:O	2.37	0.53
19:X:185:LEU:HD12	19:X:189:ILE:HD11	1.90	0.53
19:X:231:GLU:O	19:X:234:GLU:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1365:ILE:HD11	5:E:144:LEU:HD13	1.89	0.53
2:B:939:HIS:NE2	2:B:983:GLU:OE1	2.40	0.53
4:D:71:PHE:HB3	4:D:73:ARG:HH22	1.73	0.53
1:A:606:HIS:HD2	1:A:608:THR:HG22	1.73	0.53
16:R:56:PHE:HB3	16:R:81:HIS:HB2	1.90	0.53
18:W:46:GLU:O	18:W:50:GLU:HG2	2.09	0.53
19:X:185:LEU:CD1	19:X:189:ILE:HD11	2.37	0.53
1:A:848:ILE:HD11	2:B:499:ARG:HD3	1.89	0.53
2:B:931:ILE:HG22	2:B:945:CYS:SG	2.49	0.53
1:A:91:ALA:CB	1:A:290:LEU:HD22	2.39	0.53
9:I:17:CYS:SG	9:I:22:ASN:N	2.80	0.53
1:A:145:TYR:OH	13:N:64:DG:OP1	2.23	0.53
1:A:1427:LEU:HD12	1:A:1459:MET:SD	2.49	0.53
2:B:1050:ARG:NH1	2:B:1054:MET:SD	2.82	0.53
6:F:112:ASP:OD1	6:F:113:GLY:N	2.41	0.53
16:R:135:SER:O	16:R:138:PRO:HD2	2.09	0.53
1:A:332:SER:OG	17:T:54:DG:OP2	2.27	0.53
7:G:114:PRO:HD2	7:G:117:MET:HE1	1.90	0.53
1:A:359:VAL:HG21	2:B:1106:ARG:HD3	1.90	0.53
4:D:35:SER:HB3	4:D:80:ILE:CD1	2.39	0.53
5:E:120:ASP:OD1	5:E:121:MET:N	2.41	0.53
18:W:129:CYS:SG	18:W:161:VAL:HG22	2.48	0.53
2:B:834:ARG:NH2	2:B:840:MET:SD	2.82	0.52
7:G:158:PHE:CE2	18:W:139:LEU:HD23	2.45	0.52
15:Q:18:VAL:CG1	16:R:40:VAL:HG11	2.36	0.52
16:R:58:LEU:HD23	16:R:63:ALA:HB2	1.91	0.52
4:D:48:ASN:HD22	4:D:57:LEU:HD12	1.74	0.52
4:D:87:LEU:HB3	4:D:97:LEU:CD1	2.40	0.52
16:R:31:TRP:CZ3	16:R:40:VAL:HB	2.44	0.52
16:R:130:LEU:HA	16:R:133:GLU:CD	2.30	0.52
7:G:25:THR:O	7:G:28:GLN:HG3	2.08	0.52
6:F:96:GLU:OE1	6:F:102:ILE:HD13	2.10	0.52
4:D:118:LEU:HD21	4:D:127:LEU:HD22	1.91	0.52
2:B:508:MET:HE1	2:B:621:ILE:HG23	1.91	0.52
4:D:77:ARG:HH11	4:D:80:ILE:CD1	2.22	0.52
9:I:50:ASN:OD1	9:I:51:SER:N	2.43	0.52
15:Q:111:LYS:O	15:Q:146:PHE:HA	2.10	0.52
7:G:40:GLY:HA2	7:G:157:ILE:CD1	2.40	0.52
17:T:32:DT:H2'	17:T:33:DC:C6	2.44	0.52
18:W:154:CYS:O	18:W:158:HIS:N	2.40	0.52
2:B:1060:HIS:NE2	2:B:1082:GLY:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:VAL:HG23	2:B:404:PHE:CE2	2.46	0.51
4:D:45:LYS:HE3	4:D:61:PHE:HZ	1.75	0.51
13:N:58:DT:H1'	13:N:59:DT:C5'	2.41	0.51
15:Q:44:GLN:HE22	15:Q:46:ARG:CG	2.23	0.51
1:A:596:ILE:HD13	1:A:668:PHE:CE1	2.46	0.51
7:G:82:GLY:CA	7:G:146:LYS:HE2	2.28	0.51
15:Q:46:ARG:HB3	15:Q:48:GLU:OE2	2.09	0.51
15:Q:124:TYR:HB3	16:R:20:LEU:HD11	1.92	0.51
1:A:685:HIS:NE2	1:A:769:MET:SD	2.83	0.51
16:R:21:VAL:HG11	16:R:83:PHE:CE2	2.45	0.51
2:B:146:LYS:HD3	16:R:149:VAL:HG21	1.91	0.51
7:G:4:HIS:HA	7:G:75:ILE:HD13	1.93	0.51
15:Q:26:TYR:CD1	16:R:97:THR:HG22	2.45	0.51
16:R:131:GLN:HA	16:R:134:GLU:OE1	2.10	0.51
17:T:59:DA:H2''	17:T:60:DG:C8	2.45	0.51
18:W:120:ASP:HA	18:W:123:ASN:HB2	1.93	0.51
4:D:71:PHE:HB3	4:D:73:ARG:NH2	2.25	0.51
9:I:119:CYS:SG	9:I:120:GLY:N	2.81	0.51
15:Q:163:GLU:HB2	15:Q:166:ARG:HD3	1.93	0.51
1:A:926:ASN:OD1	1:A:927:GLU:N	2.43	0.51
15:Q:18:VAL:HG13	15:Q:18:VAL:O	2.11	0.51
15:Q:29:MET:HG2	15:Q:146:PHE:CE1	2.45	0.51
15:Q:114:LYS:HD3	15:Q:144:TYR:HE1	1.76	0.51
18:W:125:ALA:O	18:W:128:LYS:NZ	2.41	0.51
1:A:492:TYR:O	1:A:494:ALA:N	2.44	0.51
9:I:36:LEU:HD12	9:I:46:GLN:O	2.11	0.51
18:W:113:ARG:HA	18:W:116:THR:OG1	2.11	0.51
1:A:201:GLU:OE2	1:A:213:LYS:NZ	2.44	0.51
18:W:172:ASP:O	18:W:176:LEU:HD23	2.10	0.51
2:B:596:ILE:HG22	16:R:129:ARG:HA	1.93	0.50
5:E:29:THR:HG22	5:E:32:GLU:OE1	2.11	0.50
15:Q:39:PHE:O	15:Q:42:TRP:HB2	2.11	0.50
19:X:103:LEU:HA	19:X:106:THR:HG1	1.76	0.50
1:A:475:ARG:NH1	11:K:68:GLU:OE2	2.43	0.50
4:D:38:HIS:HA	4:D:41:LEU:HD12	1.93	0.50
18:W:120:ASP:O	18:W:124:ARG:HG3	2.12	0.50
4:D:127:LEU:O	4:D:131:LEU:HG	2.12	0.50
17:T:57:DT:H2''	17:T:58:DG:N7	2.26	0.50
18:W:113:ARG:HD2	19:X:219:LEU:HD11	1.94	0.50
1:A:280:LEU:HA	1:A:283:ILE:HG22	1.93	0.50
1:A:360:ASP:OD1	2:B:1062:ARG:NE	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:728:MET:O	2:B:731:GLN:N	2.45	0.50
4:D:35:SER:HB3	4:D:80:ILE:HD11	1.94	0.50
5:E:48:PRO:O	5:E:49:SER:OG	2.28	0.50
1:A:1424:THR:O	1:A:1429:LYS:NZ	2.44	0.50
2:B:747:LEU:CD2	17:T:49:DG:P	2.95	0.50
4:D:37:VAL:HG11	7:G:2:PHE:HE2	1.76	0.50
5:E:71:GLN:HB2	5:E:99:ILE:HG22	1.92	0.50
9:I:82:GLU:OE1	9:I:82:GLU:N	2.39	0.50
16:R:37:ARG:NH2	16:R:61:ASP:OD2	2.45	0.50
1:A:873:VAL:HG22	1:A:879:VAL:HG22	1.92	0.50
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.47	0.50
14:P:5:C:H2'	14:P:6:C:C6	2.47	0.50
15:Q:162:GLU:O	15:Q:165:GLU:HG3	2.11	0.50
16:R:124:TYR:OH	16:R:128:LYS:HD3	2.11	0.50
19:X:99:LEU:HB2	19:X:120:MET:HE3	1.93	0.50
1:A:564:LEU:HD11	1:A:594:LEU:HD13	1.93	0.50
1:A:564:LEU:HD12	1:A:570:TRP:CD2	2.46	0.50
2:B:273:PHE:HB3	2:B:284:ILE:HD12	1.94	0.50
4:D:41:LEU:HD22	4:D:61:PHE:CE1	2.47	0.50
7:G:114:PRO:HD2	7:G:117:MET:HE2	1.93	0.50
15:Q:153:ARG:HH11	15:Q:177:MET:CE	2.25	0.50
1:A:550:LYS:O	1:A:553:VAL:HG12	2.12	0.50
1:A:1474:LEU:HD23	7:G:58:VAL:HA	1.94	0.50
2:B:455:ASP:OD1	2:B:456:GLN:N	2.45	0.50
15:Q:112:GLY:HA2	15:Q:145:ASN:O	2.12	0.50
2:B:797:ASN:HB3	2:B:800:ALA:HB3	1.93	0.50
4:D:29:ALA:HB2	7:G:5:ILE:HG22	1.94	0.50
2:B:1028:LEU:HD11	2:B:1043:ILE:HD11	1.93	0.49
2:B:1132:THR:OG1	2:B:1134:THR:HG22	2.12	0.49
3:C:67:ARG:NH1	3:C:149:LEU:O	2.45	0.49
7:G:1:MET:HA	7:G:77:PHE:HD1	1.76	0.49
18:W:107:LEU:HD22	18:W:188:TYR:CE1	2.47	0.49
1:A:1095:LEU:O	1:A:1095:LEU:HD23	2.12	0.49
2:B:285:LEU:HD21	2:B:305:LEU:HD21	1.95	0.49
1:A:904:GLN:OE1	1:A:1044:HIS:NE2	2.46	0.49
1:A:469:MET:O	2:B:1097:HIS:NE2	2.44	0.49
16:R:28:SER:HA	16:R:31:TRP:CD1	2.47	0.49
19:X:103:LEU:HA	19:X:106:THR:OG1	2.13	0.49
3:C:260:GLN:HG2	11:K:91:ILE:HG21	1.95	0.49
7:G:165:ASP:HB3	7:G:168:LEU:CD1	2.43	0.49
16:R:97:THR:HG21	16:R:107:GLU:OE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:R:97:THR:HG23	16:R:107:GLU:HG2	1.95	0.49
18:W:107:LEU:HD22	18:W:188:TYR:HE1	1.77	0.49
1:A:267:GLN:O	2:B:890:ARG:NH1	2.46	0.49
1:A:1038:THR:HG22	1:A:1038:THR:O	2.12	0.49
18:W:88:ARG:NH2	18:W:90:ASN:OD1	2.46	0.49
19:X:78:LEU:HD12	19:X:79:ALA:N	2.28	0.49
4:D:15:GLU:OE1	4:D:23:PRO:HD3	2.13	0.49
7:G:146:LYS:O	7:G:161:GLY:HA2	2.13	0.49
9:I:87:GLN:OE1	9:I:87:GLN:N	2.46	0.49
17:T:31:DC:H2'	17:T:32:DT:C6	2.47	0.49
1:A:481:THR:HG22	1:A:482:PHE:O	2.12	0.49
16:R:12:ALA:HB2	16:R:106:LEU:HD23	1.95	0.49
16:R:121:SER:O	16:R:125:MET:HE1	2.13	0.49
16:R:133:GLU:HA	16:R:136:SER:OG	2.13	0.49
1:A:1087:VAL:HG12	1:A:1400:LEU:HD22	1.95	0.48
15:Q:29:MET:HB2	16:R:94:THR:CG2	2.43	0.48
15:Q:156:THR:HG23	15:Q:158:GLU:HG2	1.95	0.48
7:G:30:LEU:O	7:G:34:VAL:HG22	2.13	0.48
8:H:91:VAL:HG22	8:H:144:LEU:HD13	1.96	0.48
11:K:65:HIS:HE1	11:K:67:LEU:HD12	1.78	0.48
1:A:930:LEU:HD23	1:A:939:VAL:HG12	1.95	0.48
2:B:547:GLU:OE2	16:R:118:PRO:HD3	2.12	0.48
15:Q:46:ARG:HG3	15:Q:46:ARG:HH21	1.77	0.48
2:B:546:GLU:OE2	15:Q:122:THR:HG21	2.13	0.48
2:B:715:ASP:N	2:B:715:ASP:OD1	2.47	0.48
2:B:834:ARG:NH2	2:B:841:ARG:O	2.44	0.48
7:G:96:GLY:HA3	7:G:108:ILE:O	2.14	0.48
7:G:105:SER:O	7:G:158:PHE:HB2	2.12	0.48
19:X:166:ILE:HG21	19:X:171:ILE:HD11	1.95	0.48
2:B:478:THR:O	2:B:482:LEU:HD23	2.14	0.48
2:B:1084:LEU:CD1	17:T:46:DG:H5''	2.44	0.48
4:D:36:GLU:O	4:D:40:LEU:HG	2.13	0.48
15:Q:42:TRP:HB3	16:R:9:LEU:HD13	1.96	0.48
19:X:155:LEU:HD22	19:X:203:PHE:N	2.28	0.48
8:H:28:LEU:N	8:H:41:LEU:O	2.43	0.48
1:A:514:GLU:OE2	2:B:1102:PHE:N	2.44	0.48
2:B:775:GLY:N	2:B:1047:TYR:OH	2.47	0.48
2:B:910:THR:N	2:B:918:PHE:O	2.40	0.48
16:R:46:ALA:HB3	16:R:53:GLU:HB3	1.95	0.48
16:R:126:ARG:O	16:R:130:LEU:HG	2.14	0.48
18:W:24:GLY:HA2	19:X:210:PHE:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:40:ASN:ND2	18:W:42:CYS:O	2.46	0.48
2:B:686:GLU:N	2:B:686:GLU:OE1	2.47	0.48
2:B:907:VAL:HG13	2:B:921:ILE:HG22	1.95	0.48
7:G:51:ILE:HG13	7:G:51:ILE:O	2.14	0.48
1:A:849:ASP:OD1	1:A:850:THR:N	2.46	0.48
2:B:508:MET:CE	2:B:621:ILE:HG23	2.44	0.48
2:B:149:ILE:CA	2:B:437:THR:HG22	2.44	0.47
2:B:610:ARG:CZ	9:I:69:ILE:HD12	2.44	0.47
7:G:35:GLU:OE2	7:G:47:ALA:HA	2.14	0.47
8:H:96:VAL:HG12	8:H:116:VAL:CG2	2.29	0.47
15:Q:114:LYS:NZ	15:Q:115:LYS:HB3	2.27	0.47
1:A:312:PHE:O	1:A:316:THR:HG22	2.14	0.47
15:Q:47:LEU:HD12	15:Q:99:LEU:O	2.15	0.47
15:Q:50:ASP:OD2	15:Q:97:PRO:HD2	2.14	0.47
16:R:18:VAL:HG23	16:R:110:VAL:HG22	1.94	0.47
17:T:59:DA:H2''	17:T:60:DG:H8	1.79	0.47
19:X:158:HIS:NE2	19:X:166:ILE:HD11	2.29	0.47
1:A:706:ILE:HD11	1:A:787:VAL:HG21	1.97	0.47
4:D:25:GLU:HG3	4:D:26:PHE:CD2	2.49	0.47
15:Q:175:SER:HA	15:Q:178:GLN:OE1	2.14	0.47
17:T:45:DT:H2'	17:T:46:DG:C8	2.49	0.47
18:W:110:MET:O	18:W:114:ILE:HG12	2.14	0.47
19:X:228:MET:SD	19:X:228:MET:N	2.87	0.47
1:A:1485:GLU:OE2	7:G:20:PRO:HD2	2.14	0.47
2:B:410:ASN:ND2	2:B:439:ILE:HD11	2.30	0.47
3:C:99:VAL:HG21	3:C:127:VAL:HG21	1.96	0.47
18:W:139:LEU:O	18:W:143:GLN:HG2	2.14	0.47
2:B:248:LYS:HZ1	15:Q:171:LEU:HD23	1.79	0.47
2:B:1040:GLN:OE1	2:B:1040:GLN:N	2.47	0.47
15:Q:31:PHE:HB2	16:R:92:THR:OG1	2.14	0.47
15:Q:173:HIS:O	15:Q:176:ILE:HG22	2.14	0.47
16:R:31:TRP:CE3	16:R:40:VAL:HB	2.49	0.47
17:T:45:DT:H2'	17:T:46:DG:H8	1.79	0.47
2:B:552:ASN:OD1	2:B:553:LEU:N	2.47	0.47
2:B:745:ASP:OD1	2:B:745:ASP:N	2.46	0.47
4:D:34:ASN:H	4:D:102:ASN:HD21	1.61	0.47
7:G:48:VAL:HG13	7:G:72:TYR:HD2	1.79	0.47
9:I:86:CYS:SG	9:I:87:GLN:N	2.88	0.47
1:A:935:GLN:O	1:A:939:VAL:HG13	2.14	0.47
2:B:819:SER:N	2:B:827:GLU:OE2	2.48	0.47
7:G:79:PRO:HB2	7:G:150:THR:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:P:6:C:H2'	14:P:7:A:H8	1.77	0.47
19:X:99:LEU:HB2	19:X:120:MET:CE	2.45	0.47
1:A:82:PRO:O	2:B:1160:GLN:NE2	2.45	0.47
1:A:567:LEU:HD21	1:A:595:ILE:HG12	1.97	0.47
15:Q:120:GLU:O	16:R:25:LYS:HD3	2.15	0.47
15:Q:121:ASN:HA	16:R:25:LYS:CD	2.45	0.47
2:B:114:ARG:NE	2:B:191:GLU:OE2	2.47	0.47
16:R:19:TRP:CD1	16:R:112:GLN:HB3	2.50	0.47
1:A:1049:LEU:HD13	1:A:1054:MET:CE	2.45	0.47
2:B:197:GLN:HE21	2:B:466:VAL:HG22	1.80	0.47
2:B:601:VAL:HG22	2:B:616:THR:HG23	1.96	0.47
18:W:108:ASP:O	18:W:112:ARG:HG2	2.15	0.47
2:B:433:LEU:HD23	2:B:433:LEU:O	2.15	0.46
2:B:910:THR:O	2:B:918:PHE:N	2.45	0.46
2:B:1134:THR:HG23	2:B:1134:THR:O	2.15	0.46
3:C:246:LEU:HD12	11:K:106:ARG:HH11	1.80	0.46
4:D:130:ILE:O	4:D:134:ILE:HG12	2.14	0.46
15:Q:152:HIS:CE1	15:Q:154:THR:HG22	2.50	0.46
17:T:43:DA:H2'	17:T:44:DT:C6	2.50	0.46
18:W:37:LEU:HD13	18:W:72:ILE:HG21	1.97	0.46
2:B:1085:ARG:CD	17:T:45:DT:OP1	2.63	0.46
16:R:97:THR:O	16:R:104:LEU:HA	2.14	0.46
4:D:80:ILE:HA	4:D:83:VAL:HG12	1.97	0.46
4:D:105:PRO:HG2	4:D:131:LEU:HD22	1.98	0.46
4:D:135:GLN:O	4:D:138:ARG:HB2	2.15	0.46
7:G:15:PRO:HA	7:G:18:PHE:CZ	2.51	0.46
11:K:24:ASP:OD1	11:K:26:LYS:N	2.44	0.46
19:X:82:VAL:O	19:X:85:MET:HG2	2.15	0.46
1:A:564:LEU:HD11	1:A:594:LEU:CD1	2.46	0.46
4:D:23:PRO:HG2	4:D:26:PHE:HD2	1.81	0.46
18:W:157:CYS:SG	18:W:159:THR:HG22	2.55	0.46
2:B:125:TYR:CE2	16:R:149:VAL:HB	2.51	0.46
2:B:931:ILE:HG21	2:B:947:ILE:HA	1.96	0.46
7:G:1:MET:SD	7:G:2:PHE:N	2.89	0.46
11:K:63:VAL:HG12	11:K:71:ILE:HG22	1.98	0.46
16:R:41:GLY:O	16:R:42:LYS:HE2	2.16	0.46
1:A:251:THR:HG23	1:A:252:VAL:HG23	1.97	0.46
4:D:41:LEU:O	4:D:45:LYS:HG2	2.15	0.46
7:G:1:MET:HA	7:G:77:PHE:CD1	2.50	0.46
18:W:107:LEU:HD21	18:W:184:ILE:CD1	2.40	0.46
1:A:1116:ASN:OD1	1:A:1117:VAL:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:78:ILE:HD11	3:C:127:VAL:CG2	2.46	0.46
4:D:63:LYS:NZ	7:G:100:GLU:OE2	2.48	0.46
4:D:112:LYS:HB3	4:D:119:GLU:OE2	2.16	0.46
7:G:43:GLY:HA2	7:G:157:ILE:HD12	1.98	0.46
7:G:80:PHE:O	7:G:147:ILE:HB	2.16	0.46
15:Q:114:LYS:CD	15:Q:142:ASN:HB3	2.45	0.46
1:A:1228:MET:HA	1:A:1231:ILE:HD12	1.98	0.46
2:B:270:ILE:HD11	2:B:305:LEU:HD22	1.97	0.46
2:B:510:CYS:SG	2:B:705:GLY:N	2.88	0.46
2:B:551:GLU:OE1	16:R:113:ARG:NH1	2.48	0.46
7:G:79:PRO:HG2	7:G:150:THR:HG21	1.98	0.46
10:J:9:THR:OG1	10:J:44:CYS:SG	2.73	0.46
13:N:58:DT:H2''	13:N:59:DT:H5'	1.96	0.46
16:R:28:SER:HA	16:R:31:TRP:HD1	1.80	0.46
19:X:114:LYS:HA	19:X:117:GLN:HG3	1.98	0.46
1:A:239:GLU:OE1	1:A:242:TYR:N	2.49	0.46
1:A:337:LYS:HE2	1:A:337:LYS:HA	1.98	0.46
1:A:1243:LEU:HD21	1:A:1259:ILE:HG23	1.97	0.46
7:G:3:TYR:O	7:G:75:ILE:HA	2.16	0.46
7:G:93:ASN:O	7:G:128:TYR:OH	2.17	0.46
15:Q:19:PRO:HG2	15:Q:138:PHE:HE1	1.81	0.46
2:B:928:ILE:HD12	2:B:928:ILE:H	1.81	0.46
6:F:73:ILE:HG21	6:F:92:ILE:CD1	2.46	0.46
2:B:912:ASN:OD1	2:B:916:TYR:N	2.45	0.45
4:D:17:ALA:O	4:D:20:LEU:HD23	2.16	0.45
4:D:127:LEU:HA	4:D:130:ILE:HG12	1.98	0.45
15:Q:101:ARG:HD3	15:Q:109:LYS:HD3	1.98	0.45
1:A:603:ILE:HD11	1:A:627:LYS:HE3	1.98	0.45
15:Q:27:ASN:ND2	16:R:98:GLU:OE2	2.50	0.45
4:D:17:ALA:HB1	4:D:95:PHE:CZ	2.51	0.45
16:R:124:TYR:CZ	16:R:128:LYS:HD3	2.50	0.45
2:B:344:GLN:O	2:B:361:LYS:NZ	2.45	0.45
3:C:105:VAL:HG11	3:C:115:VAL:HG22	1.97	0.45
4:D:44:ARG:HH22	7:G:48:VAL:N	2.15	0.45
5:E:29:THR:HG23	5:E:32:GLU:CG	2.33	0.45
13:N:41:DC:H2''	13:N:42:DA:C8	2.52	0.45
1:A:567:LEU:HD22	1:A:671:ASN:HD22	1.81	0.45
1:A:1211:LEU:HD23	1:A:1212:LEU:N	2.32	0.45
2:B:146:LYS:HD3	16:R:149:VAL:HG11	1.99	0.45
2:B:380:ARG:NH2	2:B:609:GLU:OE2	2.48	0.45
2:B:450:THR:HB	17:T:51:DT:H4'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:115:ILE:HG22	4:D:118:LEU:H	1.81	0.45
15:Q:99:LEU:HD21	15:Q:101:ARG:NE	2.30	0.45
18:W:107:LEU:HD12	18:W:191:LEU:HD11	1.98	0.45
19:X:235:GLU:HA	19:X:238:LYS:NZ	2.31	0.45
1:A:340:LYS:HE3	1:A:1436:VAL:HG11	1.98	0.45
4:D:64:THR:HG23	7:G:2:PHE:CZ	2.52	0.45
15:Q:28:ILE:HD12	16:R:94:THR:O	2.17	0.45
15:Q:38:ASN:OD1	15:Q:40:ALA:HB3	2.17	0.45
18:W:43:VAL:HB	18:W:48:MET:CE	2.45	0.45
1:A:279:LYS:NZ	1:A:316:THR:HG23	2.31	0.45
2:B:249:LYS:NZ	15:Q:168:ASN:HD21	2.14	0.45
7:G:13:LEU:HD11	7:G:17:TYR:HB2	1.99	0.45
8:H:30:CYS:O	8:H:39:LEU:N	2.42	0.45
15:Q:100:LEU:HD22	15:Q:110:PHE:CD2	2.46	0.45
15:Q:126:ILE:CG2	16:R:18:VAL:HB	2.46	0.45
1:A:114:CYS:O	1:A:227:ARG:NH1	2.49	0.45
1:A:595:ILE:CD1	1:A:675:VAL:HG11	2.45	0.45
1:A:823:VAL:HG22	1:A:835:GLU:HB2	1.99	0.45
1:A:978:VAL:O	1:A:979:LEU:HD22	2.16	0.45
4:D:23:PRO:CD	7:G:78:ARG:HH12	2.28	0.45
15:Q:166:ARG:CA	15:Q:169:LYS:HE3	2.47	0.45
17:T:33:DC:H2'	17:T:34:DG:C8	2.52	0.45
1:A:457:ILE:HD11	1:A:515:ILE:CD1	2.45	0.45
1:A:1361:ASP:OD1	1:A:1362:ILE:N	2.49	0.45
2:B:596:ILE:CG2	16:R:132:ILE:HG13	2.47	0.45
15:Q:25:LYS:HB2	16:R:98:GLU:HG3	1.99	0.45
15:Q:101:ARG:NH2	15:Q:109:LYS:HE2	2.32	0.45
2:B:356:PHE:CE2	15:Q:114:LYS:HB3	2.52	0.45
4:D:26:PHE:CE1	7:G:5:ILE:HG21	2.51	0.45
15:Q:28:ILE:HG22	15:Q:143:TRP:HA	1.99	0.45
17:T:44:DT:H2'	17:T:45:DT:C6	2.52	0.45
1:A:478:PRO:O	1:A:483:ARG:NH1	2.50	0.44
2:B:363:TYR:CD2	2:B:553:LEU:HD11	2.52	0.44
3:C:100:GLU:OE2	3:C:162:ARG:NH2	2.50	0.44
1:A:1301:ILE:HB	1:A:1304:ILE:HD12	2.00	0.44
2:B:567:ILE:HD13	2:B:612:ILE:HB	2.00	0.44
3:C:182:VAL:HG23	3:C:233:VAL:HG22	1.98	0.44
1:A:100:LEU:HD21	1:A:193:ARG:HD2	1.99	0.44
2:B:248:LYS:NZ	15:Q:170:VAL:O	2.43	0.44
2:B:934:LYS:NZ	14:P:14:A:OP1	2.41	0.44
5:E:189:GLN:O	5:E:209:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:62:VAL:O	18:W:66:LEU:HD23	2.18	0.44
18:W:148:MET:SD	18:W:149:THR:N	2.90	0.44
1:A:107:LEU:HD21	1:A:216:LEU:HD21	2.00	0.44
2:B:90:GLN:CB	16:R:140:ARG:HD3	2.48	0.44
4:D:32:LEU:HD23	7:G:4:HIS:HB2	1.99	0.44
2:B:369:VAL:O	2:B:373:LEU:HD23	2.18	0.44
2:B:540:PRO:HB3	16:R:132:ILE:HD12	1.99	0.44
4:D:131:LEU:HA	4:D:134:ILE:HG12	2.00	0.44
7:G:152:VAL:HA	7:G:156:ASP:O	2.17	0.44
9:I:116:ALA:HB3	9:I:119:CYS:CB	2.46	0.44
18:W:19:LYS:O	18:W:22:ILE:HG22	2.18	0.44
18:W:113:ARG:CG	19:X:219:LEU:HD11	2.48	0.44
1:A:969:ILE:HD12	5:E:201:GLY:O	2.17	0.44
2:B:590:LEU:CD2	16:R:125:MET:HG2	2.48	0.44
5:E:173:ILE:HG23	5:E:209:VAL:HG12	1.99	0.44
2:B:590:LEU:HD21	16:R:125:MET:HG2	2.00	0.44
4:D:77:ARG:HH11	4:D:80:ILE:HD12	1.81	0.44
15:Q:26:TYR:HD2	15:Q:138:PHE:HB3	1.83	0.44
18:W:128:LYS:HE3	18:W:135:THR:HG22	1.98	0.44
2:B:97:THR:HG21	16:R:148:VAL:HB	1.99	0.44
8:H:74:GLU:N	8:H:74:GLU:OE1	2.50	0.44
19:X:171:ILE:HG13	19:X:201:LEU:HD12	1.98	0.44
19:X:194:ARG:HD2	19:X:200:ILE:HD11	2.00	0.44
8:H:26:SER:CB	8:H:45:ILE:HD11	2.47	0.44
10:J:10:CYS:SG	10:J:11:GLY:N	2.91	0.44
15:Q:125:TYR:HD1	15:Q:139:PRO:HA	1.83	0.44
15:Q:156:THR:CG2	15:Q:159:GLU:HG3	2.47	0.44
16:R:30:GLN:O	16:R:62:LEU:HD11	2.18	0.44
18:W:108:ASP:OD1	18:W:109:HIS:N	2.51	0.44
4:D:32:LEU:HD12	4:D:36:GLU:HG3	1.99	0.43
16:R:30:GLN:OE1	16:R:62:LEU:HG	2.17	0.43
1:A:354:LEU:HD13	1:A:1459:MET:HG3	2.01	0.43
2:B:896:LEU:HD23	2:B:897:ARG:O	2.18	0.43
15:Q:31:PHE:CD2	15:Q:37:VAL:HG21	2.53	0.43
1:A:1016:LEU:HD22	1:A:1045:LEU:CD2	2.47	0.43
5:E:29:THR:HG23	5:E:32:GLU:CB	2.48	0.43
18:W:105:TYR:HA	18:W:108:ASP:OD2	2.17	0.43
1:A:864:LEU:HD21	1:A:1128:ILE:HD12	2.00	0.43
1:A:936:GLU:HA	1:A:939:VAL:HG22	2.00	0.43
2:B:717:ASN:OD1	2:B:939:HIS:ND1	2.52	0.43
2:B:794:VAL:HG13	2:B:965:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:15:VAL:HB	15:Q:134:ALA:HB1	2.00	0.43
15:Q:33:ALA:HB2	16:R:91:GLN:CA	2.46	0.43
15:Q:158:GLU:HG2	15:Q:159:GLU:H	1.84	0.43
18:W:113:ARG:CD	19:X:219:LEU:HD11	2.48	0.43
1:A:37:THR:OG1	1:A:61:ARG:NH1	2.51	0.43
1:A:521:VAL:HG13	1:A:522:PRO:HD3	2.00	0.43
1:A:745:LEU:HD12	1:A:822:PHE:CD1	2.54	0.43
1:A:1101:GLN:N	1:A:1101:GLN:OE1	2.52	0.43
2:B:369:VAL:HG22	2:B:373:LEU:HD23	2.01	0.43
4:D:37:VAL:HG11	7:G:2:PHE:CD2	2.54	0.43
15:Q:15:VAL:HG22	16:R:42:LYS:NZ	2.34	0.43
1:A:1136:THR:O	1:A:1136:THR:OG1	2.32	0.43
3:C:37:VAL:O	3:C:42:VAL:HG23	2.19	0.43
7:G:120:ASP:HB2	7:G:129:LYS:HZ2	1.83	0.43
1:A:386:ALA:O	1:A:449:HIS:ND1	2.50	0.43
1:A:1480:CYS:SG	7:G:19:GLY:HA2	2.58	0.43
2:B:114:ARG:NH1	2:B:184:TYR:OH	2.48	0.43
2:B:262:TYR:O	2:B:263:ILE:HD13	2.19	0.43
3:C:14:LEU:HD12	3:C:19:VAL:HG22	2.00	0.43
3:C:256:LEU:HB3	11:K:95:ILE:HD11	1.99	0.43
6:F:86:GLU:N	6:F:86:GLU:OE1	2.52	0.43
1:A:587:THR:HG21	8:H:119:GLY:O	2.18	0.43
1:A:1123:ARG:NE	1:A:1381:GLU:OE2	2.51	0.43
7:G:109:SER:O	7:G:113:ILE:HG13	2.19	0.43
7:G:110:ARG:NH1	7:G:113:ILE:HG21	2.34	0.43
1:A:353:ASN:OD1	2:B:1071:ASN:ND2	2.52	0.43
1:A:1307:VAL:HG22	1:A:1338:THR:CG2	2.49	0.43
1:A:790:GLN:NE2	1:A:791:GLN:O	2.52	0.42
2:B:90:GLN:HA	16:R:140:ARG:HD3	2.00	0.42
2:B:393:LEU:HD13	2:B:485:LEU:HD22	2.01	0.42
7:G:7:LEU:HD22	7:G:72:TYR:OH	2.20	0.42
16:R:134:GLU:O	16:R:137:LYS:HB2	2.19	0.42
18:W:73:LYS:HB2	18:W:93:PHE:CE2	2.54	0.42
18:W:111:ARG:O	18:W:114:ILE:HB	2.19	0.42
19:X:82:VAL:HA	19:X:85:MET:HG2	2.00	0.42
1:A:827:TYR:O	2:B:716:HIS:ND1	2.52	0.42
19:X:97:LEU:HB2	19:X:102:ILE:HD11	2.02	0.42
19:X:111:ILE:HG23	19:X:116:LYS:HE2	2.01	0.42
19:X:131:GLU:HB2	19:X:140:LYS:HG2	2.01	0.42
1:A:340:LYS:CD	1:A:1436:VAL:HG11	2.49	0.42
15:Q:15:VAL:HG13	16:R:42:LYS:HZ1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:115:LYS:HB2	15:Q:143:TRP:HB2	2.01	0.42
18:W:184:ILE:O	18:W:184:ILE:HG13	2.20	0.42
19:X:158:HIS:ND1	19:X:163:LEU:HD12	2.34	0.42
1:A:74:CYS:SG	1:A:84:HIS:CE1	3.12	0.42
1:A:668:PHE:CE1	1:A:672:ILE:HD11	2.54	0.42
2:B:952:GLU:HA	3:C:39:ILE:HD11	2.02	0.42
15:Q:99:LEU:CD2	15:Q:101:ARG:HE	2.31	0.42
15:Q:125:TYR:HA	15:Q:138:PHE:O	2.19	0.42
18:W:165:GLU:O	18:W:168:MET:HE3	2.18	0.42
7:G:104:MET:HG2	7:G:158:PHE:HA	2.02	0.42
3:C:70:LEU:O	10:J:6:ARG:NH2	2.49	0.42
7:G:90:THR:HG21	7:G:100:GLU:HB2	2.01	0.42
18:W:106:LYS:NZ	19:X:225:VAL:HG11	2.35	0.42
1:A:606:HIS:CD2	1:A:608:THR:HG22	2.53	0.42
4:D:30:GLU:HG2	7:G:4:HIS:HB3	2.02	0.42
15:Q:124:TYR:OH	16:R:22:LYS:HE2	2.19	0.42
16:R:4:ARG:HA	16:R:4:ARG:CZ	2.50	0.42
2:B:411:LEU:HD22	2:B:440:ILE:HD11	2.02	0.42
3:C:113:ARG:NH1	3:C:119:ASP:OD2	2.51	0.42
7:G:4:HIS:NE2	7:G:73:LYS:HB3	2.34	0.42
15:Q:17:ARG:N	15:Q:135:PHE:O	2.48	0.42
16:R:29:GLN:OE1	16:R:29:GLN:HA	2.19	0.42
16:R:115:GLU:HA	16:R:115:GLU:OE1	2.19	0.42
16:R:122:GLU:HA	16:R:125:MET:HE2	2.01	0.42
2:B:105:PRO:CB	16:R:148:VAL:HG11	2.49	0.42
2:B:1062:ARG:NH2	2:B:1066:PRO:O	2.50	0.42
15:Q:42:TRP:CZ3	15:Q:102:VAL:HG22	2.54	0.42
15:Q:102:VAL:HG21	15:Q:108:ARG:HG2	2.02	0.42
19:X:95:HIS:ND1	19:X:96:PRO:O	2.51	0.42
1:A:680:LEU:O	1:A:684:GLY:N	2.53	0.42
1:A:1210:TRP:CZ3	9:I:53:ILE:HD13	2.55	0.42
1:A:1372:GLU:OE2	5:E:207:ARG:NH1	2.52	0.42
2:B:954:MET:HB3	2:B:955:PRO:HD2	2.02	0.42
4:D:75:LYS:HG2	4:D:141:GLN:NE2	2.34	0.42
15:Q:124:TYR:HD2	15:Q:143:TRP:HZ2	1.68	0.42
18:W:176:LEU:CD1	18:W:179:ARG:HH11	2.33	0.42
19:X:155:LEU:CD1	19:X:189:ILE:HG12	2.50	0.42
2:B:198:GLU:OE1	2:B:388:TYR:OH	2.31	0.41
2:B:906:GLN:OE1	2:B:922:ARG:NH1	2.53	0.41
7:G:97:LEU:HG	7:G:128:TYR:CE2	2.55	0.41
15:Q:153:ARG:HB2	15:Q:180:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:169:LYS:HD2	15:Q:169:LYS:O	2.20	0.41
19:X:118:TRP:HA	19:X:121:THR:HG22	2.02	0.41
1:A:253:LEU:HD23	1:A:254:PRO:O	2.20	0.41
1:A:937:ASP:OD1	1:A:937:ASP:N	2.53	0.41
2:B:912:ASN:OD1	2:B:915:GLY:N	2.53	0.41
7:G:23:LEU:HD23	7:G:23:LEU:H	1.85	0.41
8:H:147:LYS:O	8:H:148:LEU:HD22	2.20	0.41
1:A:766:PHE:HB3	1:A:781:ILE:HD12	2.00	0.41
4:D:26:PHE:HE1	7:G:5:ILE:HD13	1.85	0.41
11:K:82:SER:OG	11:K:84:GLN:OE1	2.38	0.41
15:Q:166:ARG:HE	15:Q:170:VAL:HA	1.86	0.41
1:A:1433:GLU:OE1	17:T:41:DA:H4'	2.20	0.41
2:B:485:LEU:HD21	2:B:526:LEU:HD21	2.01	0.41
7:G:7:LEU:HD22	7:G:72:TYR:CE1	2.54	0.41
7:G:34:VAL:HG21	7:G:48:VAL:CG2	2.50	0.41
15:Q:19:PRO:HG2	15:Q:138:PHE:CE1	2.55	0.41
15:Q:28:ILE:HD13	16:R:95:VAL:HG22	2.03	0.41
16:R:18:VAL:CG2	16:R:110:VAL:HA	2.50	0.41
18:W:63:LEU:HD22	18:W:92:TYR:CZ	2.56	0.41
2:B:418:TYR:OH	2:B:433:LEU:HD22	2.21	0.41
2:B:1165:MET:O	2:B:1166:SER:OG	2.26	0.41
4:D:29:ALA:O	4:D:94:LYS:NZ	2.34	0.41
7:G:152:VAL:HB	7:G:157:ILE:HG12	2.02	0.41
15:Q:24:LYS:HD3	16:R:99:SER:CA	2.50	0.41
18:W:36:ILE:HD11	18:W:52:LEU:CD2	2.49	0.41
2:B:1035:ARG:NH2	2:B:1036:LYS:O	2.53	0.41
9:I:49:ASP:OD1	9:I:49:ASP:N	2.54	0.41
1:A:1191:GLU:O	1:A:1195:VAL:HG23	2.20	0.41
1:A:1191:GLU:OE1	1:A:1191:GLU:N	2.53	0.41
2:B:690:CYS:SG	2:B:691:SER:N	2.94	0.41
3:C:78:ILE:HD11	3:C:127:VAL:HG23	2.03	0.41
4:D:75:LYS:N	4:D:75:LYS:HD3	2.34	0.41
1:A:564:LEU:HD12	1:A:570:TRP:CE2	2.56	0.41
1:A:737:PHE:O	1:A:741:VAL:HG23	2.21	0.41
4:D:26:PHE:CE1	7:G:5:ILE:HD13	2.55	0.41
18:W:22:ILE:O	18:W:26:TYR:HB2	2.21	0.41
1:A:603:ILE:HG23	1:A:603:ILE:O	2.21	0.41
2:B:90:GLN:HB2	16:R:140:ARG:HD3	2.03	0.41
2:B:248:LYS:NZ	15:Q:171:LEU:HA	2.35	0.41
2:B:354:SER:O	2:B:356:PHE:N	2.49	0.41
2:B:596:ILE:CG2	16:R:129:ARG:HA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:7:LEU:HD23	7:G:8:GLU:N	2.36	0.41
8:H:88:PHE:HB2	8:H:144:LEU:HD12	2.03	0.41
15:Q:105:LYS:HD3	15:Q:105:LYS:N	2.35	0.41
16:R:133:GLU:O	16:R:137:LYS:HG3	2.20	0.41
18:W:18:ALA:HA	18:W:21:VAL:HG22	2.02	0.41
18:W:168:MET:N	18:W:169:PRO:HD2	2.36	0.41
19:X:114:LYS:HA	19:X:117:GLN:CG	2.51	0.41
1:A:75:ALA:HB2	2:B:1131:ARG:NE	2.36	0.41
1:A:1026:ASP:OD1	1:A:1031:ARG:NH1	2.54	0.41
2:B:83:ARG:N	2:B:133:ILE:O	2.48	0.41
3:C:267:ILE:HD12	11:K:84:GLN:HB3	2.02	0.41
4:D:22:PHE:HB3	4:D:23:PRO:HD2	2.03	0.41
7:G:16:ARG:HB3	7:G:16:ARG:NH2	2.36	0.41
14:P:1:A:N3	14:P:1:A:H2'	2.35	0.41
15:Q:16:VAL:HA	15:Q:135:PHE:O	2.21	0.41
15:Q:22:THR:HG21	15:Q:26:TYR:CZ	2.56	0.41
15:Q:28:ILE:CD1	16:R:95:VAL:HG22	2.51	0.41
17:T:29:DC:H2''	17:T:30:DC:O4'	2.21	0.41
19:X:81:ILE:HG23	19:X:102:ILE:HG21	2.03	0.41
19:X:124:LEU:HD13	19:X:137:TYR:CD2	2.55	0.41
19:X:167:LEU:HD23	19:X:198:LYS:HD3	2.03	0.41
2:B:549:SER:HB3	16:R:117:ARG:HH21	1.86	0.40
7:G:92:VAL:HB	7:G:126:PRO:HG2	2.03	0.40
18:W:127:PHE:HD1	18:W:161:VAL:HG11	1.85	0.40
19:X:84:TYR:HD2	19:X:102:ILE:HG23	1.87	0.40
10:J:20:ALA:O	10:J:24:LEU:HD23	2.20	0.40
3:C:4:ALA:HB2	11:K:93:ASP:HB3	2.02	0.40
3:C:74:THR:HG22	3:C:128:ILE:O	2.21	0.40
4:D:30:GLU:HG2	4:D:30:GLU:O	2.21	0.40
4:D:41:LEU:HD22	4:D:61:PHE:HE1	1.86	0.40
7:G:85:VAL:HA	7:G:144:ARG:NH1	2.32	0.40
13:N:57:DT:H2''	13:N:58:DT:H5'	2.03	0.40
15:Q:156:THR:HG22	15:Q:159:GLU:HG3	2.03	0.40
18:W:118:GLU:OE2	18:W:177:LEU:HD13	2.21	0.40
19:X:206:LYS:HA	19:X:209:GLN:OE1	2.21	0.40
1:A:948:ILE:HD12	1:A:1007:ILE:HD13	2.03	0.40
1:A:1206:ARG:NH1	1:A:1262:MET:O	2.55	0.40
2:B:356:PHE:CD2	15:Q:114:LYS:HB3	2.56	0.40
2:B:653:TRP:CZ2	2:B:662:VAL:HG11	2.56	0.40
2:B:1053:HIS:NE2	14:P:13:A:H4'	2.36	0.40
7:G:152:VAL:HG23	7:G:157:ILE:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:165:ASP:O	7:G:168:LEU:HD12	2.22	0.40
1:A:930:LEU:CD2	1:A:939:VAL:HG12	2.52	0.40
1:A:1226:LEU:HD23	1:A:1226:LEU:H	1.86	0.40
1:A:1416:ARG:NH1	17:T:41:DA:O4'	2.55	0.40
7:G:27:LYS:HD3	7:G:51:ILE:CD1	2.50	0.40
10:J:14:VAL:HG13	10:J:49:LEU:CD2	2.51	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	1405/1984 (71%)	1316 (94%)	88 (6%)	1 (0%)	51	82
2	B	1122/1300 (86%)	1045 (93%)	77 (7%)	0	100	100
3	C	253/275 (92%)	238 (94%)	15 (6%)	0	100	100
4	D	126/184 (68%)	124 (98%)	2 (2%)	0	100	100
5	E	207/210 (99%)	189 (91%)	17 (8%)	1 (0%)	29	61
6	F	80/127 (63%)	74 (92%)	6 (8%)	0	100	100
7	G	169/172 (98%)	167 (99%)	2 (1%)	0	100	100
8	H	146/150 (97%)	139 (95%)	7 (5%)	0	100	100
9	I	112/125 (90%)	95 (85%)	17 (15%)	0	100	100
10	J	65/67 (97%)	60 (92%)	5 (8%)	0	100	100
11	K	112/117 (96%)	109 (97%)	3 (3%)	0	100	100
12	L	42/58 (72%)	37 (88%)	5 (12%)	0	100	100
15	Q	134/517 (26%)	126 (94%)	8 (6%)	0	100	100
16	R	133/249 (53%)	131 (98%)	2 (2%)	0	100	100
18	W	185/439 (42%)	185 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	X	169/291 (58%)	167 (99%)	2 (1%)	0	100	100
All	All	4460/6265 (71%)	4202 (94%)	256 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	345	GLY
5	E	84	ILE

### 5.3.2 Protein sidechains [i](#)

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	1249/1763 (71%)	1248 (100%)	1 (0%)	93	98
2	B	990/1127 (88%)	988 (100%)	2 (0%)	93	98
3	C	234/252 (93%)	234 (100%)	0	100	100
4	D	118/160 (74%)	117 (99%)	1 (1%)	81	91
5	E	191/192 (100%)	190 (100%)	1 (0%)	88	94
6	F	71/111 (64%)	71 (100%)	0	100	100
7	G	152/153 (99%)	152 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	103/112 (92%)	103 (100%)	0	100	100
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	41/55 (74%)	41 (100%)	0	100	100
15	Q	121/448 (27%)	120 (99%)	1 (1%)	81	91
16	R	118/218 (54%)	118 (100%)	0	100	100
18	W	169/373 (45%)	167 (99%)	2 (1%)	71	85
19	X	154/261 (59%)	154 (100%)	0	100	100
All	All	4000/5518 (72%)	3992 (100%)	8 (0%)	93	98



All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	853	LYS
2	B	332	LYS
2	B	1131	ARG
4	D	24	LYS
5	E	47	LYS
15	Q	169	LYS
18	W	56	ARG
18	W	153	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	296	ASN
1	A	601	ASN
1	A	671	ASN
1	A	703	GLN
1	A	791	GLN
1	A	825	ASN
1	A	1077	ASN
1	A	1146	GLN
1	A	1360	ASN
2	B	344	GLN
2	B	503	ASN
2	B	654	GLN
2	B	699	HIS
2	B	1071	ASN
2	B	1094	GLN
4	D	34	ASN
4	D	102	ASN
7	G	122	ASN
9	I	91	HIS
11	K	2	ASN
15	Q	44	GLN
15	Q	53	ASN
15	Q	145	ASN
15	Q	168	ASN
16	R	91	GLN
18	W	109	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	13/14 (92%)	3 (23%)	2 (15%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	2	C
14	P	3	A
14	P	7	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	P	2	C
14	P	6	C

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 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.

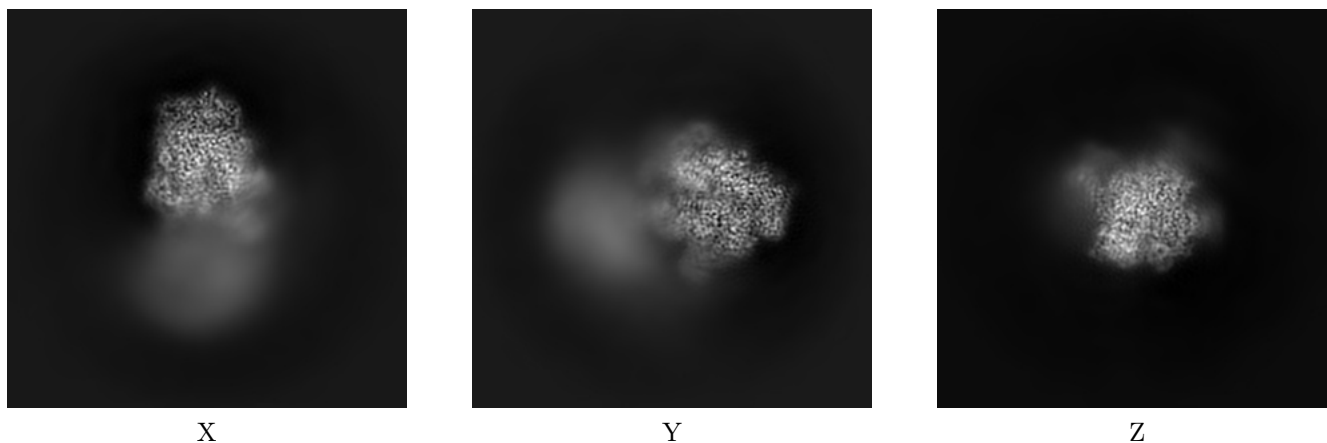
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19726. 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](#)

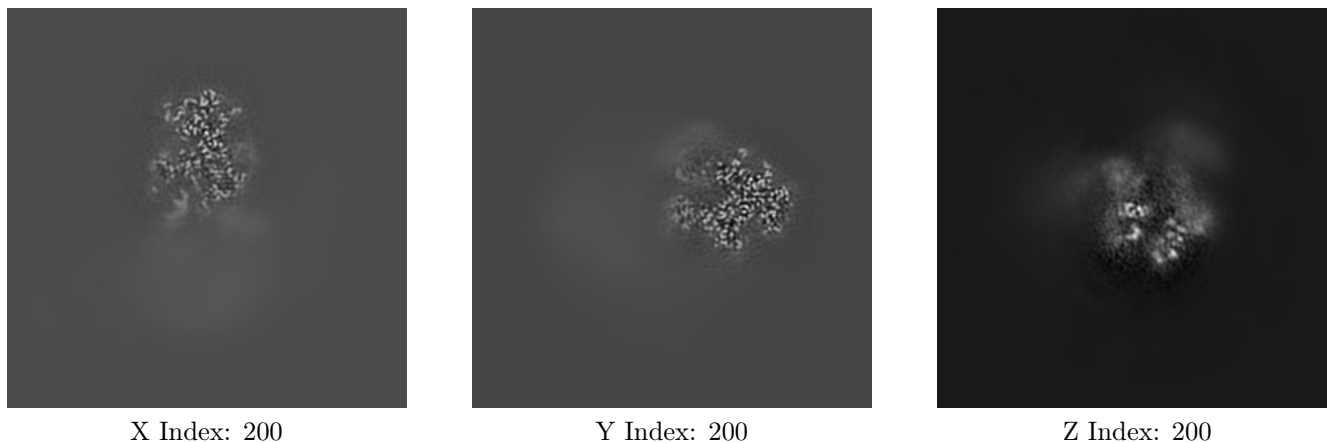
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

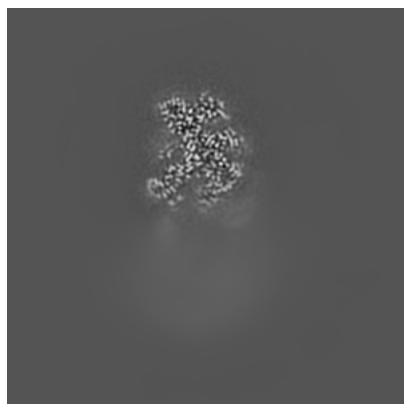
#### 6.2.1 Primary map



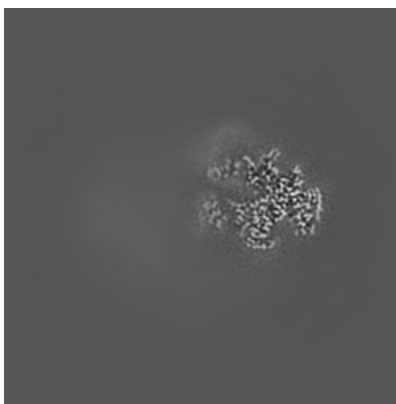
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

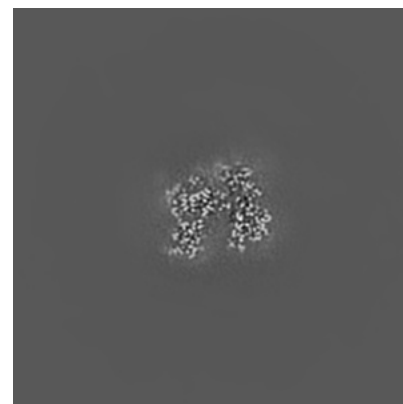
### 6.3.1 Primary map



X Index: 187



Y Index: 198

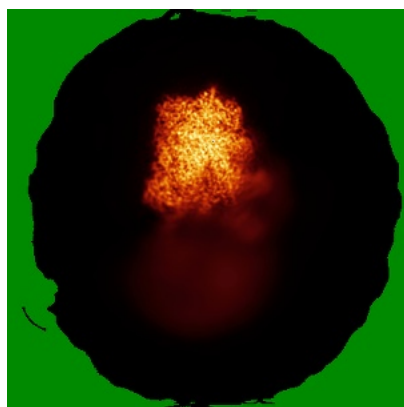


Z Index: 260

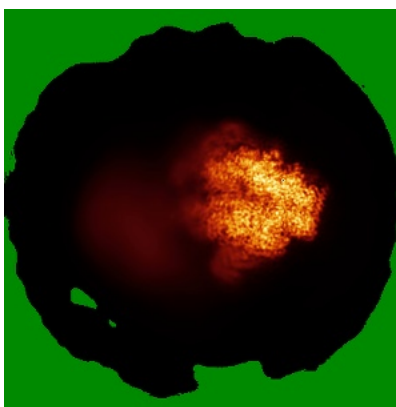
The images above show the largest variance slices of the map in three orthogonal directions.

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

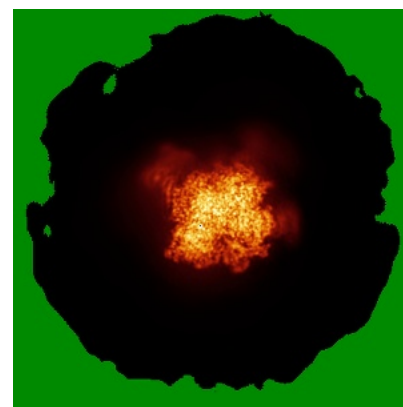
### 6.4.1 Primary map



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 3.37. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

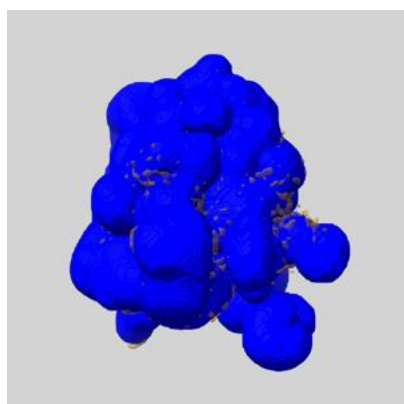
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

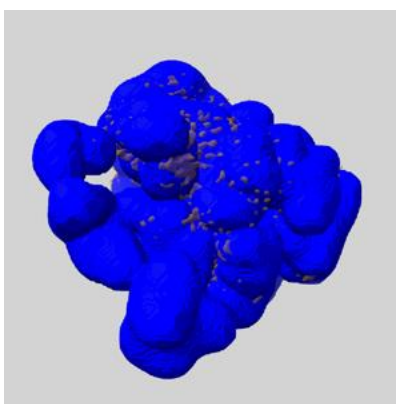
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

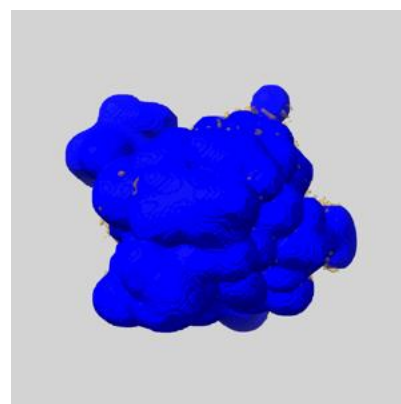
### 6.6.1 emd\_19726\_msk\_1.map [i](#)



X



Y

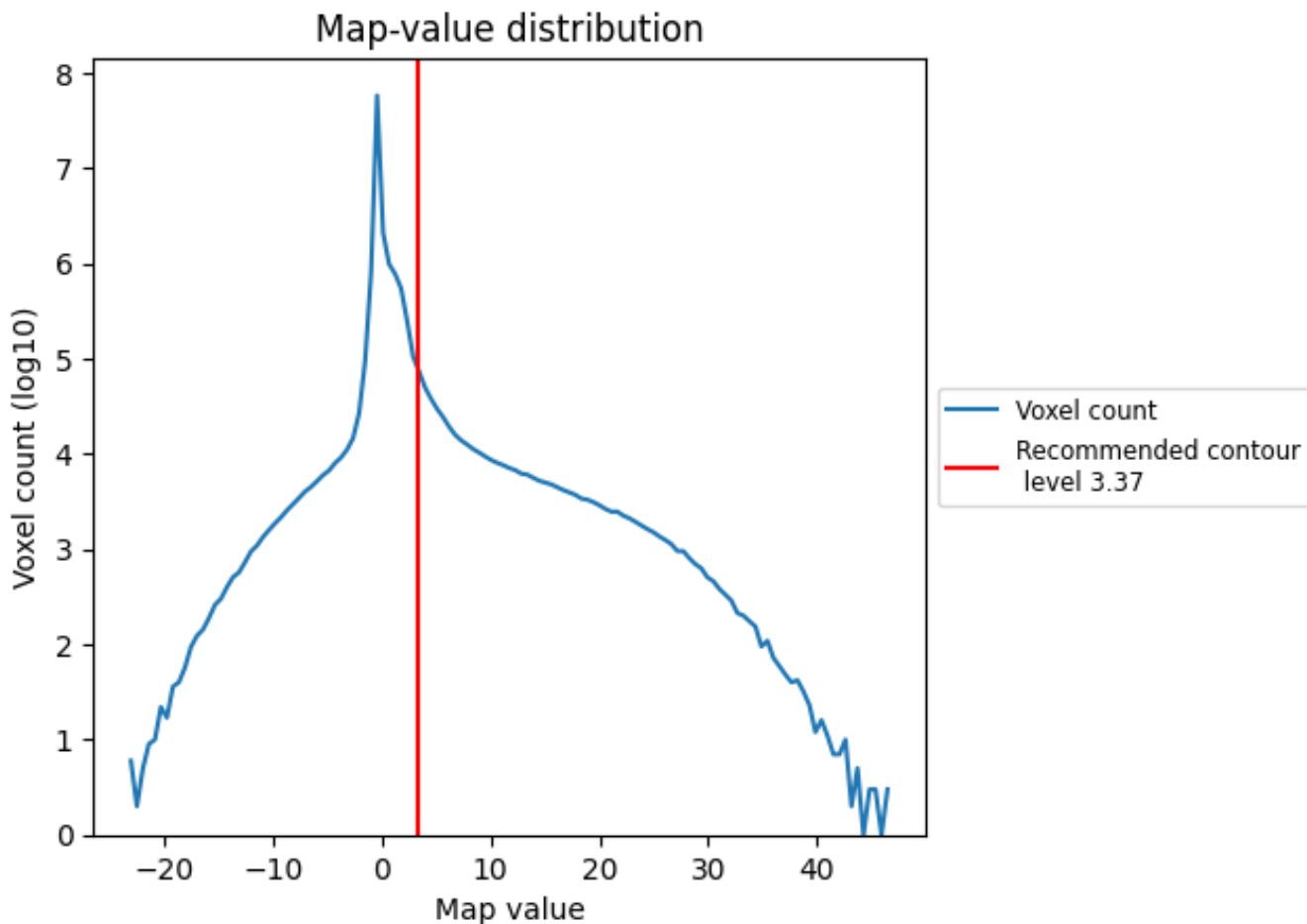


Z

## 7 Map analysis [i](#)

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

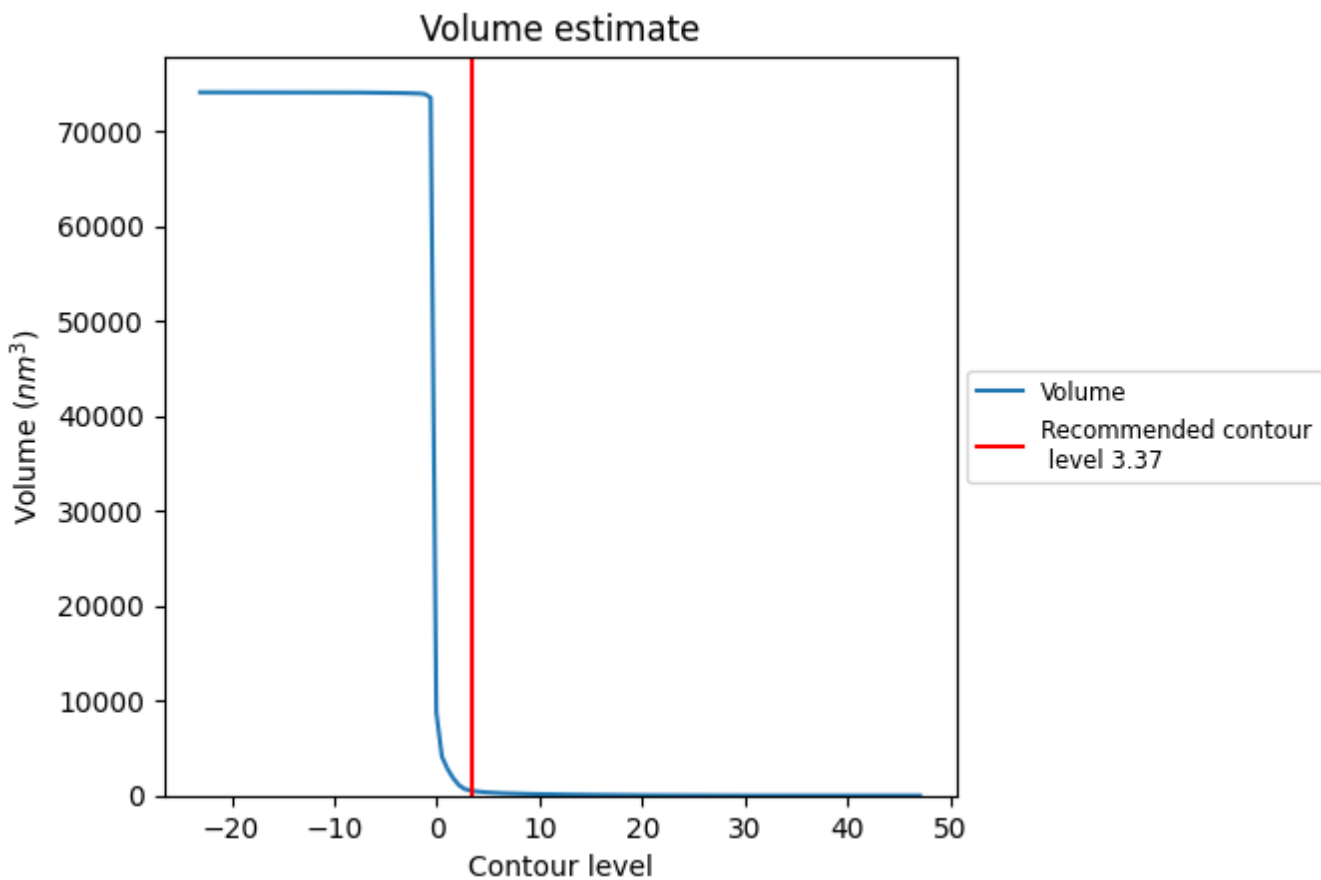
### 7.1 Map-value distribution [i](#)



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.



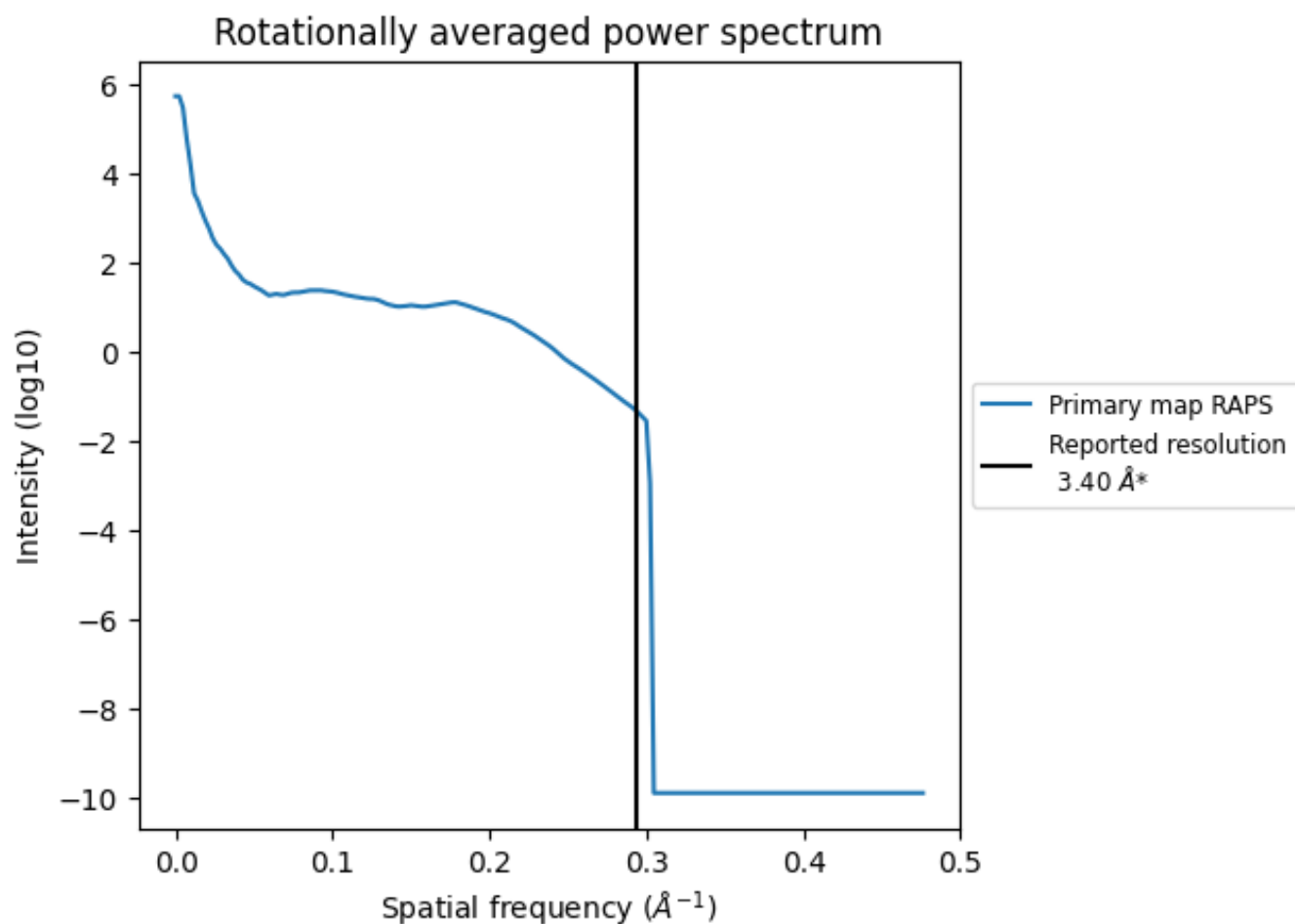
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 521 nm<sup>3</sup>; this corresponds to an approximate mass of 470 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 [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

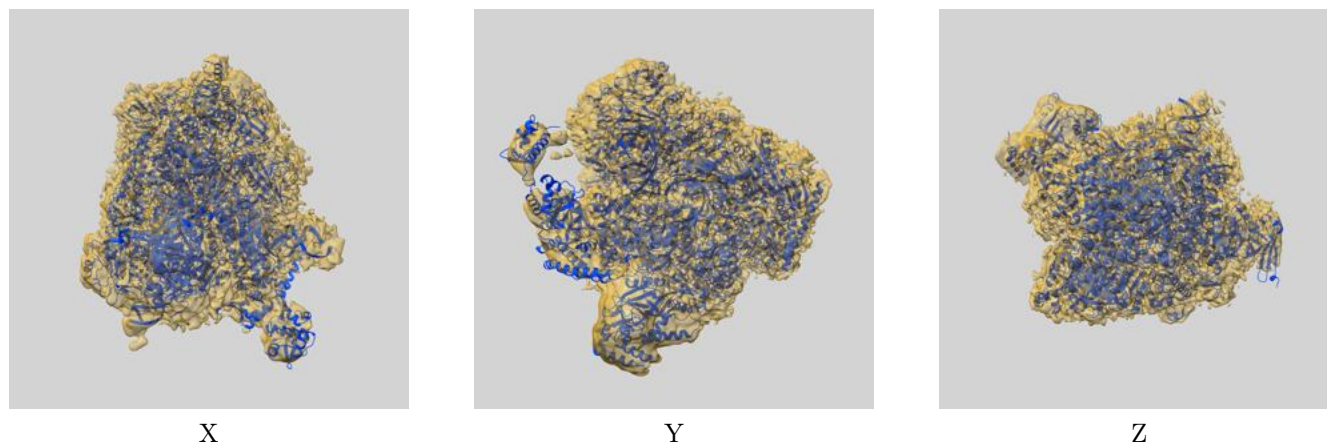
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

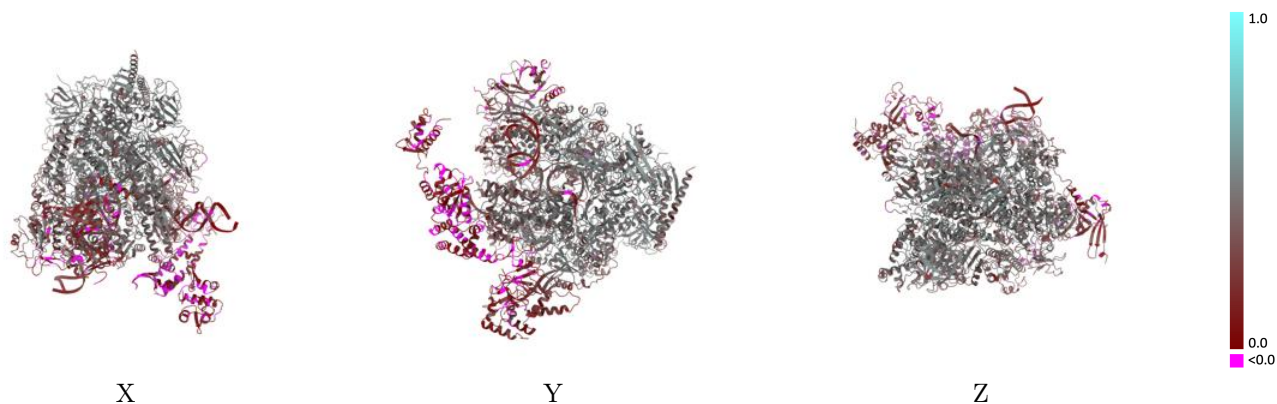
This section contains information regarding the fit between EMDB map EMD-19726 and PDB model 8S55. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlay [i](#)



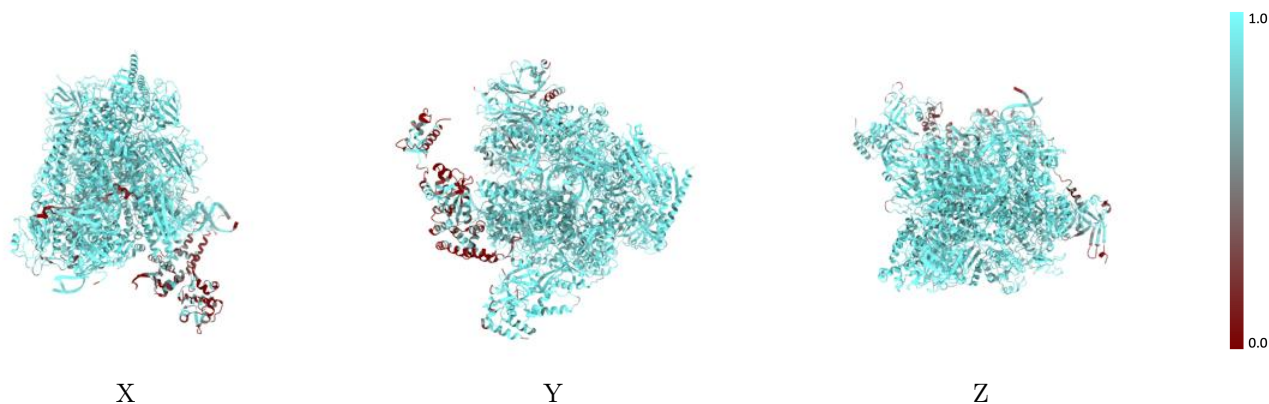
The images above show the 3D surface view of the map at the recommended contour level 3.37 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



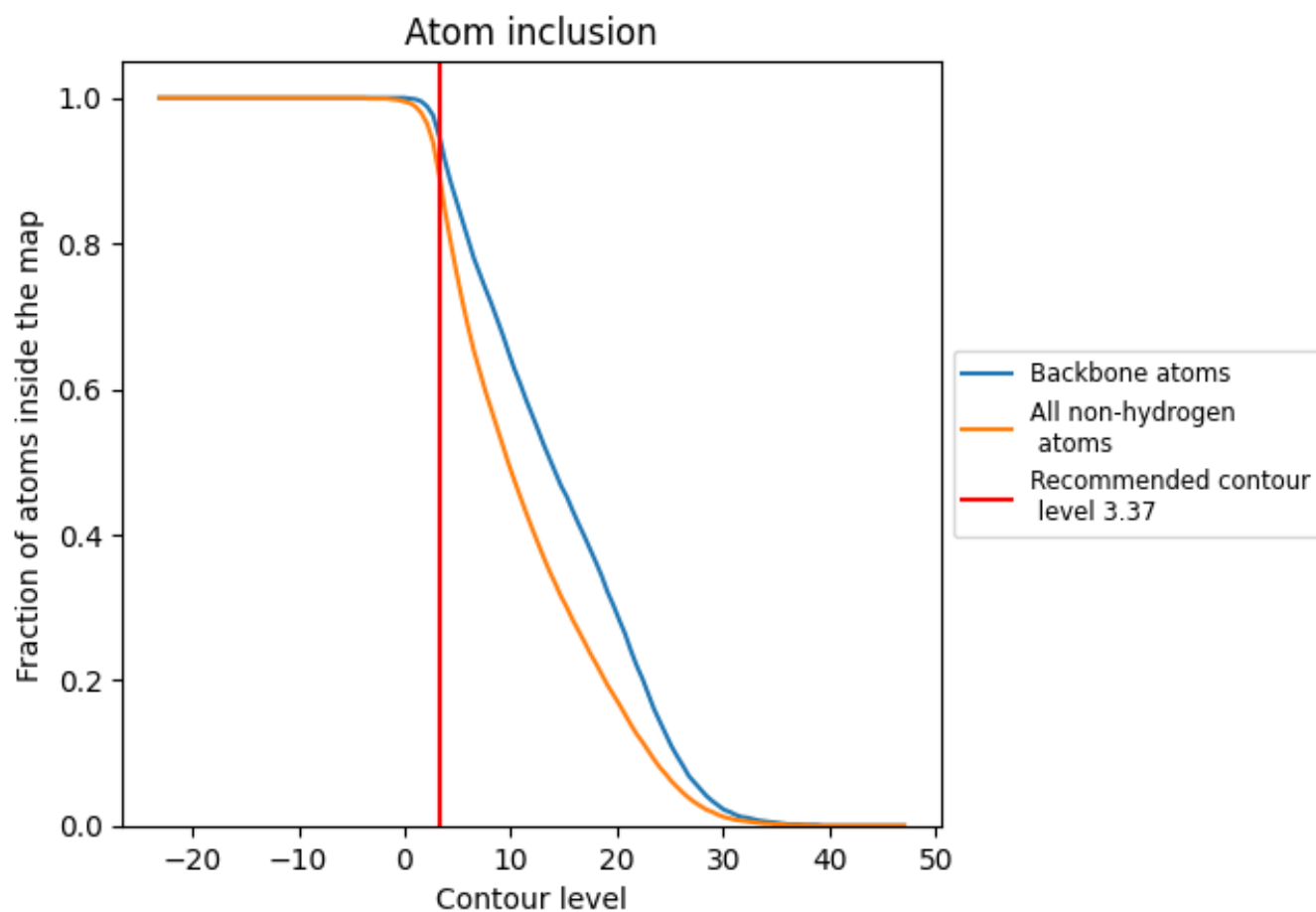
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.37).









































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 88% 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 (3.37) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8850	 0.3650
A	 0.9340	 0.4260
B	 0.9370	 0.4420
C	 0.9550	 0.4700
D	 0.8780	 0.1750
E	 0.9370	 0.3990
F	 0.9180	 0.3850
G	 0.9150	 0.2250
H	 0.9420	 0.4470
I	 0.8540	 0.2650
J	 0.9520	 0.4640
K	 0.9600	 0.4580
L	 0.9520	 0.3970
N	 0.8950	 0.2410
P	 0.9020	 0.3340
Q	 0.8360	 0.2260
R	 0.7070	 0.1660
T	 0.9390	 0.2820
W	 0.4840	 0.0450
X	 0.4050	 0.0820

