

#### Mar 10, 2024 – 11:12 PM EDT

I	PDB ID	:	6OJ5
$\mathrm{EN}$	IDB ID	:	EMD-20088
	Title	:	In situ structure of rotavirus VP1 RNA-dependent RNA polymerase $({\rm TLP\_RNA})$
1	Authors	:	Jenni, S.; Salgado, E.N.; Herrmann, T.; Li, Z.; Grant, T.; Grigorieff, N.; Trapani, S.; Estrozi, L.F.; Harrison, S.C.
Depos	sited on	:	2019-04-10
Res	solution	:	5.20  Å(reported)
	This is	a F	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 (i) 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 (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev70
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 5.20 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.



Whole archive	EM structures (#Entries)	
158037	(#Entries)	
15/571	4237	
154315	3826	
	Whole archive   (#Entries)   158937   154571   154315	

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 <=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		
			52%		
1	A	887	76%	12%	12%
			46%		
1	В	887	75%	13%	12%
			41%		
1	C	887	75%	13%	12%
			50%		
1	D	887	81%	12%	7%
			50%		
1	Ε	887	78%	11% •	10%
			53%		
1	F	887	81%	8% •	10%
			44%		
1	G	887	81%	9%	10%
			42%		
1	Н	887	78%	12%	10%



Mol	Chain	Length	Quality of chain		
			50%		
1	Ι	887	79%	11%	10%
			55%		
1	J	887	78%	13%	8%
			53%		
2	Р	1088	87%		13%



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 148557 atoms, of which 74462 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.

Mol	Chain	Residues			Aton	ns			AltConf	Trace				
1	Λ	781	Total	С	Η	Ν	Ο	S	0	0				
1		101	12787	4052	6408	1101	1190	36	0	0				
1	Р	781	Total	С	Η	Ν	Ο	S	0	0				
1	D	101	12787	4052	6408	1101	1190	36	0	0				
1	C	780	Total	С	Η	Ν	Ο	S	0	0				
	U	180	12772	4047	6400	1100	1189	36	0	0				
1	Л	827	Total	С	Η	Ν	Ο	$\mathbf{S}$	0	0				
1	D	021	13574	4297	6809	1163	1269	36	0					
1	F	705	Total	С	Η	Ν	Ο	$\mathbf{S}$	0	0				
1	Ľ	795	13028	4132	6529	1118	1213	36		0				
1	F	802	Total	С	Η	Ν	Ο	$\mathbf{S}$	0	0				
1	Ľ	802	13151	4170	6588	1130	1227	36	0	0				
1	C	802	Total	С	Η	Ν	Ο	$\mathbf{S}$	0	0				
1	0	G	ŭ	ŭ	G	802	13151	4170	6588	1130	1227	36	0	0
1	Ц	802	Total	С	Η	Ν	Ο	S	0	0				
1	11	802	13151	4170	6588	1130	1227	36	0	0				
1	Т	800	Total	С	Η	Ν	Ο	S	0	0				
	1	800	13114	4159	6569	1127	1223	36	0	0				
1	т	816	Total	С	Н	Ν	Ο	S	0	0				
	J	610	13391	4242	6713	1149	1251	36	0	0				

• Molecule 1 is a protein called Inner capsid protein VP2.

• Molecule 2 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	Р	1086	Total	С	Н	N 1 455	0	S	0	0
		1000	17051	5633	8862	1455	1062	39		



# 3 Residue-property plots (i)

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

• Molecule 1: Inner capsid protein VP2

























M884 N885 E886 L887

• Molecule 1: Inner capsid protein VP2



PROTEIN DATA BANK













• Molecule 2: RNA-directed RNA polymerase







# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	82008	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT $(4k \ge 4k)$	Depositor
Maximum map value	10.245	Depositor
Minimum map value	-6.056	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.486	Depositor
Recommended contour level	2.0	Depositor
Map size (Å)	369.0, 369.0, 369.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.23, 1.23, 1.23	Depositor



# 5 Model quality (i)

# 5.1 Standard geometry (i)

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	Bo	nd lengths	Bond angles		
		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.50	0/6495	0.91	16/8810~(0.2%)	
1	В	0.48	0/6495	0.90	18/8810~(0.2%)	
1	С	0.49	1/6487~(0.0%)	0.90	15/8799~(0.2%)	
1	D	0.48	0/6885	0.89	15/9332~(0.2%)	
1	Е	0.49	0/6618	0.91	16/8979~(0.2%)	
1	F	0.48	0/6683	0.88	12/9064~(0.1%)	
1	G	0.47	0/6683	0.86	9/9064~(0.1%)	
1	Н	0.48	0/6683	0.88	8/9064~(0.1%)	
1	Ι	0.48	0/6665	0.87	14/9041~(0.2%)	
1	J	0.48	0/6798	0.87	9/9217~(0.1%)	
2	Р	0.48	0/8963	0.85	8/12120 (0.1%)	
All	All	0.48	1/75455~(0.0%)	0.88	140/102300~(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	А	0	1
1	В	0	1
1	С	0	1
1	D	0	2
1	F	0	1
1	G	0	3
1	Н	0	1
1	Ι	0	3
1	J	0	3
2	Р	0	2
All	All	0	18

All (1) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	С	306	ILE	C-N	-5.05	1.22	1.34

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	882	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	С	671	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	В	671	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	D	882	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	G	397	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	D	671	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	Е	671	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	Н	514	MET	CG-SD-CE	6.72	110.95	100.20
1	F	451	ARG	NE-CZ-NH1	6.65	123.63	120.30
2	Р	614	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	Е	534	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	С	882	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	F	397	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	F	451	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	А	759	LEU	CA-CB-CG	6.26	129.69	115.30
1	Е	176	LEU	CA-CB-CG	6.21	129.57	115.30
1	Е	882	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	Ι	451	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	А	389	LEU	CA-CB-CG	6.10	129.33	115.30
2	Р	1077	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	Н	451	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	В	882	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	В	550	LEU	CA-CB-CG	5.99	129.08	115.30
1	В	747	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	D	747	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	В	522	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	Е	685	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	А	337	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	А	747	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	А	229	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	Н	673	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	С	747	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	Е	715	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	В	546	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	В	685	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	F	797	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	В	715	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	А	671	ARG	NE-CZ-NH1	5.70	123.15	120.30



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Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	D	546	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	Ι	685	ARG	NE-CZ-NH1	5.68	123.14	120.30
2	Р	829	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	J	150	ARG	CB-CA-C	5.66	121.72	110.40
1	G	304	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	С	229	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	D	685	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	С	685	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	В	455	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	Е	747	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	С	677	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	С	505	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	С	721	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	В	397	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	J	451	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	А	505	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	Ι	337	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	Е	142	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	D	304	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	F	131	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	F	131	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	Ι	671	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	J	534	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	D	284	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	J	732	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	G	663	ARG	NE-CZ-NH1	5.39	123.00	120.30
2	Р	783	TYR	CA-CB-CG	5.38	123.61	113.40
1	F	721	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	F	685	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	А	546	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	Ι	534	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	Ε	671	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	Ι	732	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	Н	286	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	J	721	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	G	131	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	Е	229	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	J	131	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	В	284	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	D	715	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	D	$15\overline{0}$	ARG	NE-CZ-NH1	$5.2\overline{5}$	122.93	120.30
1	С	715	ARG	NE-CZ-NH1	5.25	122.93	120.30



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Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Ι	655	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	С	297	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	С	131	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	D	131	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	Н	882	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	Ι	131	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	G	229	ARG	NE-CZ-NH1	5.21	122.91	120.30
2	Р	627	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	F	304	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	Ι	230	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	F	286	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	D	677	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	F	534	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	Ι	451	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	D	663	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	А	522	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	Ι	152	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	С	201	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	Е	505	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	J	337	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	А	685	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	Е	149	LEU	CA-CB-CG	5.16	127.17	115.30
1	А	397	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	D	721	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	С	337	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	D	675	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	G	286	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	А	882	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	В	142	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	Н	546	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	В	555	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	Ι	673	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	Е	397	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	Е	621	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	В	229	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	G	505	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	F	428	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	Ι	663	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	P	98	LEU	CB-CG-CD1	5.08	119.63	111.00
1	С	170	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	721	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	Ι	286	ARG	NE-CZ-NH1	5.06	122.83	120.30



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	397	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	J	286	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	В	337	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	G	732	ARG	NE-CZ-NH1	5.05	122.83	120.30
2	Р	661	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	D	297	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	А	150	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	Р	368	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	В	155	TRP	CA-CB-CG	5.03	123.25	113.70
1	Н	677	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	В	759	LEU	CA-CB-CG	5.02	126.84	115.30
1	Н	671	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	J	488	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	А	715	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	Е	150	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	Е	373	PHE	CB-CG-CD1	5.01	124.31	120.80
1	G	397	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	С	591	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (18) planarity outliers are listed below:

$\mathbf{Mol}$	Chain	$\mathbf{Res}$	Type	Group
1	А	371	THR	Peptide
1	В	143	ALA	Peptide
1	С	143	ALA	Peptide
1	D	102	ILE	Peptide
1	D	143	ALA	Peptide
1	F	106	GLU	Peptide
1	G	106	GLU	Peptide
1	G	450	GLN	Peptide
1	G	525	PHE	Peptide
1	Н	106	GLU	Peptide
1	Ι	106	GLU	Peptide
1	Ι	143	ALA	Peptide
1	Ι	579	THR	Peptide
1	J	106	GLU	Peptide
1	J	650	GLU	Mainchain
1	J	828	SER	Peptide
2	Р	328	TRP	Mainchain
2	Р	941	LYS	Peptide



### 5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	6379	6408	6408	56	0
1	В	6379	6408	6408	62	0
1	С	6372	6400	6399	63	0
1	D	6765	6809	6809	57	0
1	Е	6499	6529	6529	59	0
1	F	6563	6588	6588	50	0
1	G	6563	6588	6588	44	0
1	Н	6563	6588	6588	59	0
1	Ι	6545	6569	6569	50	0
1	J	6678	6713	6713	67	0
2	Р	8789	8862	8861	77	0
All	All	74095	74462	74460	597	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 4.

All (597) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:P:359:MET:SD	2:P:614:ARG:NH2	2.61	0.73
1:F:744:GLU:O	1:F:748:THR:OG1	2.06	0.72
1:G:281:ILE:O	1:G:286:ARG:NH1	2.23	0.72
1:F:281:ILE:O	1:F:286:ARG:NH1	2.23	0.71
1:F:309:ASN:O	1:F:622:ASN:ND2	2.23	0.71
1:H:326:ASP:OD1	1:H:397:ARG:NH1	2.24	0.71
1:B:219:PHE:O	1:F:797:ARG:NH2	2.24	0.70
2:P:998:SER:OG	2:P:1001:TYR:O	2.08	0.70
1:E:114:LYS:NZ	2:P:549:THR:O	2.24	0.70
1:C:294:ASN:OD1	1:C:866:SER:OG	2.07	0.70
1:I:281:ILE:O	1:I:286:ARG:NH1	2.25	0.70
1:C:360:LEU:O	1:C:538:ARG:NH1	2.25	0.70
1:J:744:GLU:O	1:J:748:THR:OG1	2.08	0.70
1:E:219:PHE:O	1:I:797:ARG:NH2	2.25	0.69
1:B:523:GLN:O	1:B:533:LYS:NZ	2.25	0.69
2:P:131:ASP:O	2:P:336:LYS:NZ	2.25	0.69



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:546:ARG:NH2	1:A:595:ILE:O	2.26	0.69
1:C:366:THR:O	1:D:86:LYS:NZ	2.24	0.69
1:B:366:THR:O	2:P:1060:LYS:NZ	2.26	0.69
1:J:281:ILE:O	1:J:286:ARG:NH1	2.26	0.69
1:A:584:GLN:O	1:A:587:SER:OG	2.08	0.68
1:A:294:ASN:OD1	1:A:866:SER:OG	2.10	0.68
2:P:293:ASP:OD1	2:P:296:ARG:NH2	2.26	0.68
1:H:281:ILE:O	1:H:286:ARG:NH1	2.26	0.68
1:D:294:ASN:OD1	1:D:866:SER:OG	2.11	0.68
1:E:294:ASN:OD1	1:E:866:SER:OG	2.11	0.67
1:I:474:GLN:OE1	1:I:512:GLN:NE2	2.28	0.67
1:J:326:ASP:OD1	1:J:397:ARG:NH1	2.27	0.67
2:P:249:SER:O	2:P:518:TYR:OH	2.13	0.67
1:B:154:TYR:OH	1:B:723:GLU:OE2	2.13	0.67
1:I:744:GLU:O	1:I:748:THR:OG1	2.12	0.67
1:G:519:GLN:OE1	1:G:522:ARG:NH2	2.27	0.67
1:F:440:ASN:O	1:F:451:ARG:NH2	2.28	0.67
1:J:134:GLU:OE2	1:J:136:ARG:NH2	2.26	0.67
1:A:379:SER:OG	2:P:268:GLU:OE1	2.12	0.67
1:E:731:ALA:N	1:E:832:VAL:O	2.28	0.66
1:I:624:ARG:NH2	1:I:627:ASP:OD2	2.29	0.66
1:E:440:ASN:O	1:E:451:ARG:NH1	2.27	0.66
1:D:244:ASN:OD1	1:H:671:ARG:NH1	2.29	0.66
1:I:326:ASP:OD1	1:I:397:ARG:NH1	2.29	0.66
1:C:294:ASN:ND2	1:G:401:LEU:O	2.29	0.66
1:B:294:ASN:OD1	1:B:866:SER:OG	2.12	0.66
1:C:523:GLN:O	1:C:533:LYS:NZ	2.28	0.66
1:D:523:GLN:O	1:D:533:LYS:NZ	2.27	0.66
1:H:316:ASN:O	1:H:675:ARG:NH1	2.28	0.65
1:H:751:TYR:OH	1:H:797:ARG:O	2.13	0.65
1:B:603:SER:OG	1:B:605:GLN:OE1	2.14	0.65
1:C:270:GLU:OE1	1:C:307:ARG:NH2	2.29	0.65
1:F:751:TYR:OH	1:F:797:ARG:O	2.11	0.65
1:F:326:ASP:OD1	1:F:397:ARG:NH1	2.29	0.65
1:E:467:GLU:OE1	1:E:483:ASN:ND2	2.29	0.65
2:P:460:ARG:NH1	2:P:631:ASP:OD1	2.30	0.65
2:P:922:GLU:OE1	2:P:926:SER:OG	2.13	0.65
1:C:599:THR:OG1	1:C:884:MET:SD	2.53	0.65
2:P:109:TYR:OH	2:P:341:ASP:OD2	2.15	0.65
1:D:376:GLY:O	1:D:590:SER:OG	2.15	0.65
1:C:441:THR:O	1:C:532:TYR:OH	2.14	0.64



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:270:GLU:OE1	1:E:307:ARG:NH2	2.30	0.64
1:F:584:GLN:O	1:F:587:SER:OG	2.12	0.64
1:J:270:GLU:OE2	1:J:307:ARG:NH1	2.30	0.64
1:I:697:GLU:OE2	1:I:701:ARG:NE	2.28	0.64
2:P:344:LEU:O	2:P:348:LYS:NZ	2.29	0.64
1:C:546:ARG:NH2	1:C:595:ILE:O	2.30	0.64
1:D:426:PHE:O	1:D:576:GLN:NE2	2.31	0.64
1:B:603:SER:O	1:B:606:THR:OG1	2.15	0.64
1:C:603:SER:O	1:C:606:THR:OG1	2.14	0.64
2:P:461:ILE:O	2:P:591:SER:OG	2.15	0.64
1:C:131:ARG:NH2	1:C:211:THR:OG1	2.31	0.64
1:E:505:ARG:NH2	1:E:562:GLU:OE1	2.31	0.63
1:G:603:SER:O	1:G:606:THR:OG1	2.12	0.63
1:J:343:LEU:HD13	1:J:346:LEU:HD21	1.79	0.63
1:B:584:GLN:O	1:B:587:SER:OG	2.11	0.63
1:H:519:GLN:OE1	1:H:522:ARG:NH2	2.31	0.63
1:A:241:ALA:HB1	1:J:671:ARG:HG2	1.81	0.63
1:E:342:ASP:OD1	1:E:383:ASN:ND2	2.32	0.63
1:J:599:THR:OG1	1:J:884:MET:SD	2.53	0.63
1:E:810:ASN:OD1	1:E:813:SER:OG	2.15	0.63
1:I:309:ASN:O	1:I:622:ASN:ND2	2.32	0.62
1:J:246:VAL:HG11	1:J:853:LEU:HD21	1.80	0.62
2:P:922:GLU:O	2:P:991:SER:OG	2.16	0.62
1:G:697:GLU:OE2	1:G:701:ARG:NE	2.33	0.62
2:P:447:ILE:O	2:P:574:GLN:N	2.32	0.62
1:J:309:ASN:O	1:J:622:ASN:ND2	2.33	0.61
1:J:751:TYR:OH	1:J:797:ARG:O	2.17	0.61
1:I:401:LEU:HD22	1:I:585:LEU:HD21	1.81	0.61
2:P:843:ALA:O	2:P:846:SER:OG	2.11	0.61
1:F:401:LEU:HD22	1:F:585:LEU:HD21	1.82	0.61
1:F:731:ALA:N	1:F:832:VAL:O	2.33	0.61
1:J:142:ARG:NH1	1:J:147:LYS:O	2.33	0.61
1:J:224:THR:O	1:J:229:ARG:NH1	2.34	0.61
1:B:441:THR:HG1	1:B:532:TYR:HH	1.48	0.61
1:C:467:GLU:OE1	1:C:483:ASN:ND2	2.34	0.61
1:D:360:LEU:HD11	1:D:542:LEU:HD11	1.83	0.60
1:D:180:VAL:O	1:D:184:MET:N	2.34	0.60
1:J:412:ILE:HG22	1:J:543:LEU:HD22	1.83	0.60
1:J:478:TRP:O	1:J:482:VAL:HG23	2.01	0.60
1:A:361:GLN:OE1	1:E:534:ARG:NH2	2.34	0.60
1:F:713:ALA:O	1:F:829:THR:OG1	2.15	0.60



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:P:729:ARG:NH2	2:P:767:ASP:O	2.34	0.60
1:G:397:ARG:HH22	1:G:579:THR:HG23	1.65	0.60
1:B:716:ASP:OD1	1:B:827:THR:OG1	2.10	0.60
2:P:14:PHE:O	2:P:17:ASN:ND2	2.34	0.60
2:P:331:HIS:NE2	2:P:691:ALA:O	2.35	0.60
1:C:603:SER:OG	1:C:605:GLN:OE1	2.19	0.59
1:A:315:LEU:O	1:A:675:ARG:NH1	2.34	0.59
1:A:717:MET:N	1:A:828:SER:O	2.35	0.59
1:A:376:GLY:O	1:A:590:SER:OG	2.20	0.59
1:A:381:ALA:HB1	1:A:587:SER:HB3	1.83	0.59
2:P:488:ARG:NH2	2:P:505:ASP:OD2	2.36	0.59
1:H:650:GLU:O	1:H:654:LYS:N	2.35	0.59
1:B:272:LEU:HD11	1:B:277:ILE:HD11	1.84	0.59
1:B:717:MET:O	1:B:827:THR:OG1	2.21	0.59
1:D:717:MET:O	1:D:827:THR:OG1	2.20	0.58
1:B:261:GLU:OE2	1:B:265:GLN:NE2	2.36	0.58
1:E:792:GLN:NE2	1:E:801:THR:O	2.35	0.58
1:B:131:ARG:NH2	1:B:211:THR:OG1	2.37	0.58
1:C:584:GLN:O	1:C:587:SER:OG	2.18	0.58
1:C:717:MET:N	1:C:828:SER:O	2.36	0.58
1:H:244:ASN:OD1	1:H:853:LEU:N	2.37	0.58
2:P:786:ARG:NE	2:P:871:LYS:O	2.36	0.58
1:I:314:ARG:NH2	1:I:626:ASN:OD1	2.37	0.58
1:H:697:GLU:OE2	1:H:701:ARG:NE	2.37	0.58
1:J:624:ARG:NH2	1:J:627:ASP:OD2	2.37	0.57
2:P:351:TYR:OH	2:P:526:SER:O	2.20	0.57
1:A:478:TRP:O	1:A:482:VAL:HG23	2.05	0.57
1:H:309:ASN:O	1:H:622:ASN:ND2	2.35	0.57
1:I:444:TYR:O	1:I:448:GLY:N	2.37	0.57
1:I:713:ALA:O	1:I:829:THR:OG1	2.12	0.57
1:D:129:LEU:HD11	1:D:207:VAL:HG21	1.85	0.57
1:D:478:TRP:O	1:D:482:VAL:HG23	2.04	0.57
1:E:129:LEU:HD11	1:E:207:VAL:HG22	1.87	0.57
1:I:397:ARG:NH1	1:I:579:THR:O	2.37	0.57
1:J:316:ASN:O	1:J:675:ARG:NH1	2.38	0.57
1:J:349:THR:OG1	2:P:362:GLU:OE2	2.13	0.57
1:A:603:SER:O	1:A:606:THR:OG1	2.19	0.57
1:G:252:LEU:O	1:G:845:SER:OG	2.18	0.57
1:G:720:GLU:OE2	1:G:732:ARG:NE	2.38	0.57
2:P:632:ASP:OD1	2:P:632:ASP:N	2.37	0.57
1:H:624:ARG:NH2	1:H:627:ASP:OD2	2.38	0.57



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:I:283:GLU:OE1	1:I:286:ARG:NH2	2.37	0.57
1:E:785:LEU:O	1:E:788:THR:OG1	2.17	0.57
1:C:261:GLU:OE2	1:C:265:GLN:NE2	2.38	0.56
2:P:2:GLY:N	2:P:754:GLU:OE2	2.38	0.56
1:D:219:PHE:O	1:H:797:ARG:NH2	2.38	0.56
1:A:719:LEU:HD11	1:A:828:SER:HB3	1.88	0.56
1:D:717:MET:N	1:D:828:SER:O	2.38	0.56
1:A:261:GLU:OE2	1:A:265:GLN:NE2	2.39	0.56
1:E:546:ARG:NH2	1:E:595:ILE:O	2.37	0.56
1:F:474:GLN:O	1:F:512:GLN:NE2	2.38	0.56
2:P:439:PRO:O	2:P:469:TYR:OH	2.23	0.56
1:D:863:ALA:O	1:H:91:LYS:NZ	2.37	0.56
1:E:311:LEU:O	1:E:618:HIS:NE2	2.38	0.56
1:D:751:TYR:O	1:D:755:THR:OG1	2.13	0.56
1:A:785:LEU:O	1:A:788:THR:OG1	2.16	0.56
1:B:860:ASP:OD2	1:F:90:GLN:NE2	2.39	0.56
1:C:700:GLU:O	1:C:708:GLN:NE2	2.39	0.56
1:C:810:ASN:OD1	1:C:813:SER:OG	2.17	0.56
1:H:124:LYS:NZ	1:H:182:THR:O	2.38	0.56
1:E:441:THR:O	1:E:532:TYR:OH	2.24	0.56
1:H:599:THR:OG1	1:H:884:MET:SD	2.50	0.56
1:A:201:ARG:O	1:J:642:GLN:NE2	2.39	0.56
1:H:343:LEU:HA	1:H:600:VAL:HG11	1.88	0.56
1:B:373:PHE:O	1:B:377:ILE:HD11	2.06	0.55
1:A:282:PRO:HD2	1:A:285:ILE:HD12	1.87	0.55
2:P:274:LYS:NZ	2:P:508:ARG:O	2.38	0.55
1:A:320:ASN:O	1:A:671:ARG:NH1	2.39	0.55
1:B:343:LEU:HA	1:B:600:VAL:HG11	1.88	0.55
1:B:450:GLN:NE2	1:C:518:MET:SD	2.79	0.55
1:E:627:ASP:O	1:E:631:ILE:HD12	2.07	0.55
1:F:316:ASN:O	1:F:675:ARG:NH1	2.40	0.55
1:G:706:ILE:O	1:G:834:LYS:NZ	2.37	0.55
1:D:177:TYR:CZ	1:D:181:LEU:HD11	2.41	0.55
1:J:603:SER:O	1:J:606:THR:OG1	2.20	0.55
1:E:603:SER:O	1:E:606:THR:OG1	2.22	0.55
1:I:240:GLN:OE1	1:I:243:ARG:NH2	2.41	0.54
1:J:478:TRP:NE1	1:J:513:LEU:HD13	2.23	0.54
1:C:272:LEU:HD13	1:C:305:TYR:CD1	2.42	0.54
1:E:478:TRP:O	1:E:482:VAL:HG23	2.06	0.54
1:C:717:MET:O	1:C:827:THR:OG1	2.17	0.54
1:B:674:ASP:OD1	1:B:677:ARG:NH1	2.39	0.54



	ous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:420:VAL:HG23	1:D:421:VAL:HG23	1.88	0.54
2:P:174:ALA:HA	2:P:177:VAL:HG22	1.88	0.54
1:H:343:LEU:HD13	1:H:346:LEU:HD21	1.89	0.54
1:C:333:TYR:OH	1:C:388:THR:HG23	2.08	0.54
1:E:141:TYR:OH	1:E:812:ASP:OD2	2.19	0.54
1:F:177:TYR:OH	1:F:685:ARG:O	2.26	0.54
1:B:441:THR:OG1	1:B:532:TYR:OH	2.21	0.54
1:G:165:GLY:O	1:G:169:VAL:HG23	2.07	0.54
2:P:908:GLN:O	2:P:912:GLN:N	2.40	0.54
1:A:751:TYR:O	1:A:755:THR:OG1	2.16	0.54
1:C:429:GLU:OE1	1:H:534:ARG:NH1	2.41	0.54
1:J:700:GLU:O	1:J:708:GLN:NE2	2.41	0.54
1:D:241:ALA:HB1	1:H:671:ARG:HG2	1.88	0.53
1:H:335:LEU:HD11	1:H:613:VAL:HG11	1.90	0.53
1:I:599:THR:OG1	1:I:884:MET:SD	2.59	0.53
2:P:238:SER:O	2:P:335:ARG:NH1	2.41	0.53
1:C:200:SER:O	1:G:642:GLN:NE2	2.41	0.53
1:G:751:TYR:O	1:G:755:THR:HG23	2.07	0.53
1:H:721:ARG:NH2	1:H:727:TYR:OH	2.41	0.53
1:A:555:ARG:NH1	1:A:882:ARG:O	2.42	0.53
1:J:728:VAL:HG23	1:J:730:ILE:HG22	1.91	0.53
1:D:131:ARG:NH2	1:D:211:THR:OG1	2.40	0.53
1:B:360:LEU:O	1:B:538:ARG:NH1	2.41	0.53
1:G:537:GLN:HA	1:G:540:ILE:HD12	1.90	0.53
1:I:721:ARG:NH2	1:I:727:TYR:OH	2.42	0.53
1:C:201:ARG:O	1:G:642:GLN:NE2	2.42	0.53
1:J:719:LEU:HD21	1:J:828:SER:HB3	1.89	0.53
1:H:246:VAL:HG11	1:H:853:LEU:HD21	1.91	0.53
1:H:514:MET:CG	1:H:547:LEU:HD13	2.39	0.53
1:J:180:VAL:O	1:J:184:MET:N	2.41	0.53
1:F:262:TYR:CD2	1:F:688:ILE:HD11	2.44	0.53
1:B:478:TRP:O	1:B:482:VAL:HG23	2.09	0.52
1:E:134:GLU:OE1	1:E:134:GLU:N	2.42	0.52
1:G:184:MET:SD	1:G:684:ARG:NH2	2.82	0.52
1:D:237:GLN:OE1	1:D:239:VAL:HG13	2.10	0.52
1:G:757:MET:O	1:G:761:ASN:N	2.43	0.52
1:I:343:LEU:HD13	1:I:346:LEU:HD21	1.90	0.52
1:F:757:MET:O	1:F:761:ASN:N	2.43	0.52
1:I:731:ALA:N	1:I:832:VAL:O	2.43	0.52
1:J:419:THR:HG21	1:J:513:LEU:HD22	1.91	0.52
1:I:397:ARG:HH22	1:I:579:THR:HG23	1.75	0.52



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:I:478:TRP:O	1:I:482:VAL:HG23	2.10	0.52	
1:J:349:THR:HG22	1:J:594:LEU:HD11	1.91	0.52	
1:C:478:TRP:NE1	1:C:513:LEU:HD13	2.25	0.52	
1:C:611:TYR:O	1:C:615:VAL:HG23	2.10	0.52	
1:E:335:LEU:O	1:E:338:SER:OG	2.21	0.52	
1:F:126:GLN:N	1:F:126:GLN:OE1	2.43	0.52	
1:H:207:VAL:HG12	1:H:211:THR:HG21	1.92	0.52	
1:D:134:GLU:N	1:D:134:GLU:OE1	2.42	0.52	
2:P:834:THR:CG2	2:P:965:LEU:HD23	2.40	0.52	
1:B:751:TYR:O	1:B:755:THR:OG1	2.14	0.51	
1:G:729:ASN:OD1	1:G:806:LEU:HD12	2.10	0.51	
1:H:444:TYR:O	1:H:448:GLY:N	2.43	0.51	
1:A:165:GLY:O	1:A:169:VAL:HG23	2.11	0.51	
1:H:89:HIS:O	1:H:93:VAL:HG23	2.10	0.51	
1:B:177:TYR:CZ	1:B:181:LEU:HD11	2.45	0.51	
1:B:312:GLN:OE1	1:B:571:ASN:N	2.43	0.51	
1:F:875:ALA:O	1:F:883:ILE:HG22	2.10	0.51	
1:D:584:GLN:O	1:D:587:SER:OG	2.12	0.51	
1:J:713:ALA:HB1	1:J:715:ARG:NH1	2.25	0.51	
1:C:134:GLU:N	1:C:134:GLU:OE1	2.44	0.51	
1:C:177:TYR:CE2	1:C:181:LEU:HD11	2.46	0.51	
1:C:625:ILE:O	1:C:629:VAL:HG23	2.10	0.51	
1:J:353:ILE:O	1:J:357:SER:OG	2.18	0.51	
2:P:775:TYR:OH	2:P:1040:GLU:OE2	2.26	0.51	
2:P:917:ARG:NH2	2:P:1004:TYR:O	2.42	0.51	
1:D:69:LYS:HA	1:D:80:LEU:HD21	1.92	0.51	
1:G:553:LEU:HD13	1:G:595:ILE:HD13	1.91	0.51	
1:H:875:ALA:O	1:H:883:ILE:HG22	2.10	0.51	
1:E:177:TYR:CZ	1:E:181:LEU:HD11	2.45	0.51	
1:B:290:ASN:ND2	1:B:876:VAL:O	2.43	0.50	
2:P:127:ASP:O	2:P:131:ASP:N	2.43	0.50	
1:B:372:GLN:O	1:B:407:ASN:ND2	2.45	0.50	
1:D:291:TYR:CE1	1:D:869:THR:HG22	2.45	0.50	
1:F:333:TYR:OH	1:F:388:THR:HG23	2.11	0.50	
1:G:744:GLU:O	1:G:748:THR:OG1	2.09	0.50	
1:H:165:GLY:O	1:H:169:VAL:HG23	2.11	0.50	
1:H:510:VAL:HG11	1:H:551:VAL:HG22	1.92	0.50	
1:H:610:TYR:O	1:H:614:ASN:ND2	2.44	0.50	
1:H:815:ASP:HB2	1:H:818:LEU:HD12	1.93	0.50	
1:C:610:TYR:O	1:C:614:ASN:ND2	2.44	0.50	
2:P:1029:VAL:HG11	2:P:1063:MET:SD	2.52	0.50	



	the second	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:344:LYS:O	2:P:508:ARG:NH1	2.45	0.50	
1:D:85:THR:OG1	2:P:1068:LYS:NZ	2.44	0.50	
1:H:713:ALA:O	1:H:829:THR:OG1	2.14	0.50	
1:I:875:ALA:O	1:I:883:ILE:HG22	2.11	0.50	
1:C:478:TRP:O	1:C:482:VAL:HG23	2.12	0.50	
2:P:744:ILE:HD13	2:P:748:LEU:HD22	1.94	0.50	
1:B:869:THR:O	1:F:405:THR:OG1	2.29	0.50	
1:F:301:SER:O	1:F:304:ARG:NH1	2.45	0.50	
2:P:760:ASN:O	2:P:785:GLN:NE2	2.45	0.50	
1:B:343:LEU:HD13	1:B:346:LEU:HD21	1.93	0.50	
1:D:156:LYS:NZ	1:D:704:ASP:OD2	2.45	0.50	
1:J:91:LYS:NZ	2:P:642:GLU:O	2.26	0.50	
2:P:140:SER:OG	2:P:738:GLN:OE1	2.17	0.50	
1:B:224:THR:OG1	1:B:229:ARG:NH2	2.44	0.49	
1:D:531:ASP:OD2	1:E:538:ARG:NH2	2.45	0.49	
1:E:713:ALA:O	1:E:829:THR:HG23	2.12	0.49	
1:H:416:TRP:O	1:H:420:VAL:HG22	2.12	0.49	
1:H:611:TYR:O	1:H:615:VAL:HG23	2.12	0.49	
2:P:678:ALA:O	2:P:690:ARG:NE	2.36	0.49	
1:I:610:TYR:O	1:I:614:ASN:ND2	2.45	0.49	
1:J:553:LEU:HD13	1:J:595:ILE:HD13	1.95	0.49	
1:D:406:THR:HG22	1:E:355:LYS:HG3	1.94	0.49	
1:E:729:ASN:O	1:E:832:VAL:N	2.42	0.49	
1:D:416:TRP:O	1:D:419:THR:OG1	2.30	0.49	
1:A:392:ALA:O	1:A:396:GLN:N	2.45	0.49	
1:B:177:TYR:CE1	1:B:181:LEU:HD11	2.48	0.49	
1:A:797:ARG:NH1	1:F:296:ASP:OD2	2.45	0.49	
1:A:871:GLU:HG2	1:A:873:ILE:HG22	1.95	0.49	
1:D:828:SER:OG	1:D:829:THR:N	2.46	0.49	
1:J:393:MET:O	1:J:396:GLN:NE2	2.46	0.49	
1:H:744:GLU:O	1:H:748:THR:OG1	2.15	0.49	
1:A:728:VAL:HG23	1:A:730:ILE:HG22	1.95	0.49	
1:A:109:GLU:O	2:P:258:ASN:ND2	2.46	0.48	
1:E:724:MET:SD	1:E:724:MET:N	2.86	0.48	
1:F:815:ASP:HB2	1:F:818:LEU:HD12	1.94	0.48	
1:G:397:ARG:NH1	1:G:579:THR:O	2.46	0.48	
1:I:792:GLN:O	1:I:796:LEU:N	2.45	0.48	
1:G:283:GLU:OE1	1:G:286:ARG:NH2	2.47	0.48	
1:H:281:ILE:HG22	1:H:282:PRO:O	2.14	0.48	
1:I:751:TYR:O	1:I:755:THR:HG23	2.13	0.48	
1:J:312:GLN:OE1	1:J:571:ASN:ND2	2.47	0.48	



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:797:ARG:NH1	1:G:296:ASP:OD2	2.45	0.48
1:E:673:ARG:NH2	1:J:886:GLU:OE2	2.46	0.48
1:C:389:LEU:HD23	1:C:399:MET:CE	2.44	0.48
1:E:478:TRP:NE1	1:E:513:LEU:HD13	2.28	0.48
1:B:728:VAL:HG23	1:B:730:ILE:HG22	1.95	0.48
1:D:412:ILE:HG22	1:D:543:LEU:HD22	1.95	0.48
1:F:397:ARG:HH22	1:F:579:THR:HG23	1.77	0.48
1:G:312:GLN:NE2	1:G:569:THR:O	2.45	0.48
1:H:488:ARG:O	1:H:499:VAL:HG22	2.14	0.48
1:G:611:TYR:O	1:G:615:VAL:HG23	2.14	0.48
1:C:154:TYR:OH	1:C:723:GLU:OE2	2.26	0.48
1:E:555:ARG:NH2	1:E:879:ASP:OD2	2.46	0.48
1:G:419:THR:HG21	1:G:513:LEU:HD22	1.95	0.48
1:A:381:ALA:HB1	1:A:587:SER:CB	2.44	0.48
1:H:115:LEU:HD23	1:H:118:ILE:HD12	1.96	0.48
1:H:346:LEU:HD22	1:H:594:LEU:O	2.14	0.48
1:J:610:TYR:O	1:J:614:ASN:ND2	2.47	0.48
1:A:423:ASN:HB3	1:A:431:LEU:HD11	1.95	0.47
1:D:311:LEU:O	1:D:618:HIS:NE2	2.46	0.47
1:J:397:ARG:NH1	1:J:579:THR:O	2.47	0.47
1:B:731:ALA:N	1:B:832:VAL:O	2.47	0.47
1:C:398:THR:OG1	1:C:577:THR:OG1	2.21	0.47
1:D:666:ASP:OD2	1:I:347:VAL:HG22	2.13	0.47
1:E:131:ARG:NH2	1:E:211:THR:OG1	2.47	0.47
1:E:611:TYR:O	1:E:615:VAL:HG23	2.14	0.47
1:F:130:PHE:CZ	1:F:132:ILE:HD11	2.49	0.47
1:I:346:LEU:HD22	1:I:594:LEU:O	2.14	0.47
2:P:80:ASP:OD1	2:P:81:LYS:N	2.45	0.47
1:B:415:MET:O	1:B:419:THR:HG23	2.14	0.47
1:B:757:MET:O	1:B:761:ASN:N	2.47	0.47
1:F:483:ASN:O	1:F:486:GLN:NE2	2.46	0.47
1:C:244:ASN:O	1:C:853:LEU:N	2.47	0.47
1:E:320:ASN:ND2	1:J:545:ASN:OD1	2.48	0.47
1:E:682:GLU:OE2	1:E:685:ARG:NE	2.45	0.47
1:J:84:LYS:NZ	2:P:282:ASP:OD1	2.48	0.47
1:A:745:LEU:HD21	1:A:751:TYR:CE1	2.49	0.47
1:F:319:ASP:O	1:F:675:ARG:NH2	2.46	0.47
1:A:177:TYR:CE2	1:A:181:LEU:HD11	2.49	0.47
1:B:322:GLU:HB3	1:B:578:LEU:HD11	1.94	0.47
1:C:312:GLN:NE2	1:C:494:GLY:O	2.48	0.47
1:A:674:ASP:OD1	1:A:677:ARG:NH1	2.46	0.47



Atom-1	Atom-2	Interatomic	Clash	
1100111-1	1100111-2	distance $(Å)$	overlap (Å)	
1:B:241:ALA:HB1	1:F:671:ARG:HG2	1.96	0.47	
1:B:312:GLN:NE2	1:B:569:THR:O	2.47	0.47	
1:B:397:ARG:HA	1:B:577:THR:HG21	1.96	0.47	
1:D:603:SER:O	1:D:606:THR:OG1	2.27	0.47	
1:E:415:MET:O	1:E:419:THR:HG23	2.15	0.47	
2:P:208:ASN:O	2:P:696:LEU:HD12	2.14	0.47	
1:H:584:GLN:O	1:H:587:SER:OG	2.13	0.47	
1:A:142:ARG:NE	1:A:148:GLU:OE2	2.47	0.47	
1:C:280:TYR:CD2	1:C:861:LEU:HD23	2.50	0.47	
1:C:416:TRP:O	1:C:419:THR:OG1	2.28	0.47	
1:E:643:LYS:HE3	1:E:648:ILE:HD11	1.97	0.47	
1:H:688:ILE:HG22	1:H:692:ILE:HD12	1.97	0.47	
1:J:519:GLN:OE1	1:J:522:ARG:NH2	2.48	0.47	
2:P:691:ALA:HB2	2:P:723:ARG:HB2	1.96	0.47	
1:A:137:GLN:NE2	1:A:221:ASP:OD2	2.48	0.47	
1:B:599:THR:OG1	1:B:884:MET:SD	2.62	0.47	
1:D:244:ASN:O	1:D:853:LEU:N	2.47	0.47	
1:E:301:SER:O	1:E:304:ARG:NH1	2.45	0.47	
1:G:609:HIS:O	1:G:613:VAL:HG23	2.15	0.47	
1:G:728:VAL:HG23	1:G:730:ILE:HG22	1.97	0.47	
1:C:730:ILE:O	1:C:831:LYS:NZ	2.31	0.46	
1:E:882:ARG:NH1	1:I:527:THR:O	2.48	0.46	
1:C:649:VAL:HG11	1:C:669:MET:HG2	1.95	0.46	
1:E:719:LEU:HD11	1:E:828:SER:HB3	1.96	0.46	
1:J:453:HIS:O	1:J:455:ARG:NH1	2.48	0.46	
1:J:713:ALA:HB3	1:J:717:MET:CE	2.46	0.46	
1:D:611:TYR:O	1:D:615:VAL:HG23	2.15	0.46	
2:P:495:SER:OG	2:P:499:GLN:O	2.27	0.46	
1:G:623:GLU:OE1	1:G:685:ARG:NH2	2.48	0.46	
1:I:505:ARG:NH2	1:I:562:GLU:OE2	2.47	0.46	
1:F:565:MET:HA	1:F:568:ILE:HD12	1.97	0.46	
2:P:611:VAL:HG21	2:P:659:TYR:CE1	2.51	0.46	
2:P:651:VAL:O	2:P:655:VAL:HG23	2.16	0.46	
1:B:314:ARG:HB3	1:B:679:LEU:HD21	1.98	0.46	
1:B:745:LEU:HD12	1:B:750:ASP:H	1.81	0.46	
1:E:316:ASN:O	1:E:675:ARG:NH1	2.44	0.46	
1:J:165:GLY:O	1:J:169:VAL:HG23	2.15	0.46	
1:J:713:ALA:HB3	1:J:717:MET:HE1	1.97	0.46	
2:P:105:ASN:ND2	2:P:235:SER:O	2.48	0.46	
1:C:716:ASP:OD1	1:C:827:THR:OG1	2.34	0.46	
1:C:828:SER:OG	1:C:829:THR:N	2.49	0.46	



Atom 1	Atom 0	Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
1:D:416:TRP:O	1:D:420:VAL:HG22	2.16	0.46	
1:F:397:ARG:NH1	1:F:579:THR:O	2.48	0.46	
1:F:479:LEU:O	1:F:483:ASN:ND2	2.49	0.46	
1:G:177:TYR:OH	1:G:685:ARG:O	2.31	0.46	
1:I:167:TYR:OH	1:I:642:GLN:N	2.47	0.46	
2:P:629:ASP:OD1	2:P:629:ASP:N	2.46	0.46	
1:A:611:TYR:O	1:A:615:VAL:HG23	2.16	0.46	
1:E:719:LEU:HD11	1:E:828:SER:CB	2.45	0.46	
1:E:777:SER:OG	1:E:778:VAL:N	2.49	0.46	
2:P:420:LYS:O	2:P:424:VAL:HG23	2.15	0.46	
1:A:285:ILE:HD11	1:A:567:CYS:SG	2.56	0.46	
1:G:376:GLY:O	1:G:590:SER:OG	2.34	0.46	
2:P:816:SER:O	2:P:820:LEU:N	2.48	0.46	
1:E:127:THR:HG22	1:E:128:LYS:H	1.81	0.45	
2:P:260:THR:N	2:P:272:SER:O	2.46	0.45	
1:C:731:ALA:HB2	1:C:831:LYS:HE3	1.98	0.45	
1:J:178:ASP:OD1	1:J:179:GLN:N	2.50	0.45	
1:J:828:SER:OG	1:J:829:THR:O	2.21	0.45	
1:A:420:VAL:HG23	1:A:421:VAL:HG23	1.99	0.45	
1:C:415:MET:O	1:C:419:THR:HG23	2.16	0.45	
1:C:728:VAL:HG23	1:C:730:ILE:HG22	1.98	0.45	
1:D:360:LEU:HD23	1:D:538:ARG:HB3	1.99	0.45	
1:G:272:LEU:HD13	1:G:305:TYR:CD1	2.51	0.45	
1:G:547:LEU:O	1:G:551:VAL:HG23	2.16	0.45	
1:H:609:HIS:O	1:H:613:VAL:HG23	2.17	0.45	
1:J:547:LEU:O	1:J:551:VAL:HG23	2.16	0.45	
1:B:165:GLY:O	1:B:169:VAL:HG23	2.17	0.45	
1:F:283:GLU:OE1	1:F:286:ARG:NH2	2.49	0.45	
1:A:401:LEU:HD23	1:A:585:LEU:HD21	1.99	0.45	
1:E:666:ASP:OD2	1:J:347:VAL:HG22	2.17	0.45	
1:H:745:LEU:HD11	1:H:751:TYR:CD1	2.51	0.45	
1:I:719:LEU:HD22	1:I:728:VAL:C	2.37	0.45	
1:J:609:HIS:O	1:J:613:VAL:HG23	2.17	0.45	
2:P:337:GLN:O	2:P:451:ARG:NH1	2.49	0.45	
1:C:868:ASP:OD2	1:G:405:THR:HG22	2.16	0.45	
1:J:584:GLN:O	1:J:587:SER:OG	2.15	0.45	
1:A:707:ALA:N	1:A:770:LEU:O	2.47	0.45	
1:D:475:VAL:HG22	1:D:516:ALA:HB1	1.98	0.45	
1:J:129:LEU:HD12	1:J:208:ASP:HB2	1.99	0.45	
2:P:6:LEU:O	2:P:9:SER:OG	2.29	0.45	
1:A:667:ASP:OD1	1:A:668:GLN:N	2.49	0.45	



	• • • • •	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:208:ASP:OD1	1:B:209:SER:N	2.49	0.45	
1:F:177:TYR:CZ	1:F:181:LEU:HD11	2.51	0.45	
1:H:283:GLU:OE1	1:H:286:ARG:NH2	2.50	0.45	
1:I:315:LEU:CD2	1:I:679:LEU:HD11	2.47	0.45	
1:C:505:ARG:NH2	1:C:562:GLU:OE1	2.50	0.44	
1:D:775:ASP:OD1	1:D:776:SER:N	2.48	0.44	
1:J:706:ILE:O	1:J:834:LYS:NZ	2.48	0.44	
1:A:416:TRP:O	1:A:420:VAL:HG22	2.18	0.44	
1:C:195:VAL:O	1:C:206:VAL:N	2.50	0.44	
1:G:517:LEU:HD23	1:G:520:LEU:HD12	1.98	0.44	
1:H:376:GLY:O	1:H:590:SER:OG	2.34	0.44	
1:C:275:ASP:O	1:C:279:ASN:ND2	2.50	0.44	
1:C:663:ARG:NH1	1:H:358:GLN:OE1	2.50	0.44	
1:H:456:ASN:OD1	1:H:457:GLY:N	2.50	0.44	
1:A:609:HIS:O	1:A:613:VAL:HG23	2.17	0.44	
1:B:244:ASN:OD1	1:F:671:ARG:NH1	2.51	0.44	
1:J:79:LEU:HA	1:J:82:VAL:HG22	1.99	0.44	
1:J:92:GLU:OE2	2:P:645:LYS:N	2.44	0.44	
1:J:130:PHE:CZ	1:J:132:ILE:HD11	2.53	0.44	
1:C:731:ALA:N	1:C:832:VAL:O	2.48	0.44	
1:B:416:TRP:O	1:B:419:THR:OG1	2.30	0.44	
1:D:372:GLN:O	1:D:407:ASN:ND2	2.50	0.44	
1:D:868:ASP:OD2	1:H:405:THR:HG22	2.18	0.44	
1:J:246:VAL:CG1	1:J:853:LEU:HD21	2.45	0.44	
1:G:240:GLN:OE1	1:G:243:ARG:NH2	2.47	0.44	
1:G:851:SER:OG	1:G:852:ASN:N	2.51	0.44	
1:I:611:TYR:O	1:I:615:VAL:HG23	2.17	0.44	
1:J:138:LEU:HD12	1:J:154:TYR:HB2	2.00	0.44	
1:J:401:LEU:HD22	1:J:585:LEU:HD21	2.00	0.44	
2:P:744:ILE:HB	2:P:748:LEU:HD22	1.99	0.44	
1:D:441:THR:HG23	1:D:442:ILE:HD12	2.00	0.44	
1:J:851:SER:OG	1:J:852:ASN:N	2.50	0.44	
2:P:906:ASN:OD1	2:P:907:VAL:N	2.51	0.44	
1:B:649:VAL:HG11	1:B:669:MET:HG2	2.00	0.44	
1:A:731:ALA:N	1:A:832:VAL:O	2.51	0.43	
1:B:501:ASN:HB2	1:B:504:ILE:HD12	2.00	0.43	
1:H:608:PHE:CG	1:H:862:LEU:HD13	2.53	0.43	
1:B:436:LEU:HD22	1:C:887:LEU:OXT	2.18	0.43	
1:D:241:ALA:HB1	1:H:671:ARG:CG	2.49	0.43	
1:E:602:PRO:HB2	1:E:607:LEU:HD21	1.99	0.43	
1:I:282:PRO:HB2	1:I:285:ILE:HD12	2.00	0.43	



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Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:G:625:ILE:O	1:G:629:VAL:HG23	2.19	0.43	
1:J:472:ASN:HB3	1:J:475:VAL:HG12	2.00	0.43	
1:F:180:VAL:O	1:F:184:MET:N	2.51	0.43	
1:C:437:ALA:O	1:C:441:THR:HG22	2.19	0.43	
1:F:446:ALA:HB2	1:F:525:PHE:CE1	2.54	0.43	
1:C:392:ALA:O	1:C:396:GLN:N	2.51	0.43	
1:A:349:THR:HG22	1:A:594:LEU:CD1	2.49	0.43	
1:F:252:LEU:O	1:F:845:SER:OG	2.29	0.43	
1:F:729:ASN:O	1:F:832:VAL:N	2.49	0.43	
1:I:470:ILE:HG21	1:I:475:VAL:HG11	2.00	0.43	
1:F:456:ASN:OD1	1:F:457:GLY:N	2.52	0.43	
1:A:177:TYR:CZ	1:A:181:LEU:HD11	2.53	0.43	
1:B:713:ALA:O	1:B:715:ARG:N	2.52	0.43	
1:E:716:ASP:OD1	1:E:827:THR:OG1	2.36	0.43	
1:F:721:ARG:NH2	1:F:727:TYR:OH	2.51	0.43	
1:G:364:ALA:C	1:G:365:LEU:HD12	2.39	0.43	
1:G:744:GLU:N	1:G:744:GLU:OE1	2.52	0.43	
1:H:329:THR:HG23	1:H:395:SER:O	2.19	0.43	
2:P:282:ASP:OD1	2:P:645:LYS:NZ	2.45	0.43	
1:D:268:LEU:HD12	1:D:268:LEU:O	2.19	0.42	
1:I:727:TYR:CD2	1:I:809:ILE:HD11	2.54	0.42	
1:A:415:MET:O	1:A:419:THR:HG23	2.19	0.42	
1:A:565:MET:HA	1:A:568:ILE:HD12	2.02	0.42	
1:B:631:ILE:HG21	1:B:648:ILE:HD13	2.00	0.42	
1:D:89:HIS:CE1	1:D:364:ALA:HB2	2.54	0.42	
1:D:314:ARG:HB3	1:D:679:LEU:HD21	2.01	0.42	
1:D:731:ALA:HB2	1:D:831:LYS:HE3	2.01	0.42	
1:I:290:ASN:O	1:I:869:THR:OG1	2.34	0.42	
2:P:834:THR:HG23	2:P:965:LEU:HD23	2.01	0.42	
1:A:208:ASP:OD1	1:A:209:SER:N	2.52	0.42	
1:I:216:ASP:OD1	1:I:217:ALA:N	2.52	0.42	
1:A:856:THR:HG1	1:A:858:TYR:HE2	1.66	0.42	
1:E:292:ILE:CG2	1:I:433:ALA:HB1	2.49	0.42	
1:I:711:ILE:HD11	1:I:734:LEU:HD12	2.01	0.42	
2:P:671:SER:OG	2:P:672:THR:N	2.51	0.42	
1:D:609:HIS:O	1:D:613:VAL:HG23	2.20	0.42	
1:D:667:ASP:OD1	1:D:668:GLN:N	2.52	0.42	
1:E:320:ASN:O	1:E:671:ARG:NH1	2.49	0.42	
2:P:843:ALA:HB3	2:P:844:PRO:HD3	2.02	0.42	
1:A:689:PHE:CZ	1:A:693:LEU:HD21	2.55	0.42	
1:D:555:ARG:NH1	1:D:882:ARG:O	2.51	0.42	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:E:713:ALA:O	1:E:715:ARG:N	2.53	0.42	
1:G:178:ASP:OD1	1:G:179:GLN:N	2.52	0.42	
1:G:505:ARG:NE	1:G:562:GLU:OE1	2.49	0.42	
2:P:48:ASN:HB3	2:P:55:LEU:HD23	2.00	0.42	
2:P:141:ASN:O	2:P:145:VAL:HG23	2.20	0.42	
1:B:871:GLU:HG2	1:B:873:ILE:HG22	2.01	0.42	
1:I:198:LYS:NZ	1:I:212:ALA:HB1	2.35	0.42	
1:J:625:ILE:O	1:J:629:VAL:HG23	2.19	0.42	
2:P:961:TYR:O	2:P:964:SER:OG	2.34	0.42	
1:F:428:ARG:O	1:F:432:VAL:HG23	2.19	0.42	
1:F:611:TYR:O	1:F:615:VAL:HG23	2.19	0.42	
1:J:531:ASP:OD1	1:J:532:TYR:N	2.51	0.42	
2:P:805:SER:OG	2:P:806:SER:N	2.52	0.42	
1:A:272:LEU:HD11	1:A:277:ILE:HD11	2.01	0.42	
1:D:208:ASP:OD1	1:D:209:SER:N	2.53	0.42	
1:E:726:GLY:N	1:E:809:ILE:O	2.52	0.42	
1:I:609:HIS:O	1:I:613:VAL:HG23	2.20	0.42	
2:P:607:LEU:O	2:P:611:VAL:HG23	2.19	0.42	
1:D:344:LYS:HG2	1:D:600:VAL:HG12	2.01	0.41	
1:I:757:MET:O	1:I:761:ASN:N	2.53	0.41	
1:J:290:ASN:ND2	1:J:559:TYR:OH	2.49	0.41	
2:P:367:ILE:O	2:P:371:VAL:HG23	2.20	0.41	
1:A:700:GLU:O	1:A:708:GLN:NE2	2.53	0.41	
1:B:393:MET:O	1:B:396:GLN:NE2	2.49	0.41	
1:C:400:SER:C	1:C:401:LEU:HD12	2.41	0.41	
1:F:609:HIS:O	1:F:613:VAL:HG23	2.20	0.41	
1:C:713:ALA:O	1:C:715:ARG:N	2.53	0.41	
1:D:674:ASP:OD1	1:D:677:ARG:NH1	2.53	0.41	
1:E:733:ASN:OD1	1:E:734:LEU:N	2.53	0.41	
1:F:326:ASP:OD2	1:F:579:THR:HG22	2.20	0.41	
1:H:333:TYR:OH	1:H:388:THR:HG23	2.20	0.41	
1:I:315:LEU:HD21	1:I:679:LEU:HD11	2.02	0.41	
1:J:320:ASN:O	1:J:671:ARG:NE	2.54	0.41	
2:P:335:ARG:O	2:P:337:GLN:N	2.53	0.41	
1:D:441:THR:OG1	1:D:532:TYR:OH	2.10	0.41	
1:E:156:LYS:NZ	1:E:704:ASP:OD2	2.53	0.41	
1:F:751:TYR:O	1:F:755:THR:HG23	2.20	0.41	
1:H:514:MET:HG3	1:H:547:LEU:HD13	2.02	0.41	
1:H:603:SER:O	1:H:606:THR:OG1	2.34	0.41	
1:I:851:SER:OG	1:I:852:ASN:N	2.53	0.41	
1:E:667:ASP:OD1	1:E:668:GLN:N	2.53	0.41	



	ous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:I:124:LYS:NZ	1:I:181:LEU:O	2.53	0.41
1:I:329:THR:HG23	1:I:395:SER:O	2.21	0.41
1:J:611:TYR:O	1:J:615:VAL:HG23	2.21	0.41
1:B:565:MET:HA	1:B:568:ILE:HD12	2.01	0.41
1:B:611:TYR:O	1:B:615:VAL:HG23	2.21	0.41
1:F:272:LEU:HD13	1:F:305:TYR:CD1	2.55	0.41
1:H:717:MET:O	1:H:828:SER:N	2.49	0.41
2:P:122:ALA:HB2	2:P:193:TYR:CD2	2.54	0.41
1:C:255:ILE:O	1:C:258:ALA:HB3	2.21	0.41
1:C:441:THR:HG23	1:C:442:ILE:HD12	2.02	0.41
1:F:531:ASP:OD1	1:F:532:TYR:N	2.54	0.41
1:G:440:ASN:O	1:G:451:ARG:NE	2.54	0.41
1:H:453:HIS:O	1:H:455:ARG:NH1	2.50	0.41
1:J:688:ILE:HG22	1:J:692:ILE:HD12	2.03	0.41
1:A:224:THR:OG1	1:A:229:ARG:NH2	2.54	0.41
1:A:740:ILE:HD12	1:A:764:VAL:HG21	2.03	0.41
1:B:474:GLN:HB3	1:B:516:ALA:HB2	2.03	0.41
1:C:208:ASP:OD1	1:C:209:SER:N	2.53	0.41
1:E:304:ARG:N	1:E:856:THR:O	2.53	0.41
1:G:731:ALA:HB2	1:G:831:LYS:HB3	2.02	0.41
1:D:673:ARG:NH1	1:I:887:LEU:OXT	2.53	0.41
1:B:189:LEU:HD11	1:B:855:PHE:CZ	2.56	0.40
1:B:733:ASN:OD1	1:B:734:LEU:N	2.54	0.40
1:D:429:GLU:OE1	1:I:534:ARG:NH2	2.48	0.40
1:E:441:THR:HG23	1:E:442:ILE:HD12	2.03	0.40
1:F:627:ASP:OD1	1:F:685:ARG:NH2	2.54	0.40
1:B:428:ARG:O	1:B:432:VAL:HG23	2.21	0.40
1:B:724:MET:SD	1:B:724:MET:N	2.94	0.40
1:C:742:LEU:HD13	1:C:767:VAL:O	2.21	0.40
1:E:268:LEU:HD12	1:E:268:LEU:O	2.20	0.40
1:H:383:ASN:OD1	1:H:384:ASP:N	2.54	0.40
1:H:757:MET:O	1:H:761:ASN:N	2.54	0.40
2:P:102:LEU:O	2:P:111:ASN:ND2	2.55	0.40
2:P:492:GLU:OE2	2:P:679:LYS:NZ	2.52	0.40
2:P:591:SER:HA	2:P:596:THR:HG21	2.03	0.40
1:C:311:LEU:O	1:C:618:HIS:NE2	2.53	0.40
1:I:719:LEU:HD22	1:I:729:ASN:N	2.37	0.40
1:J:216:ASP:OD1	1:J:217:ALA:N	2.54	0.40
1:A:244:ASN:OD1	1:J:671:ARG:NH1	2.54	0.40
1:A:733:ASN:OD1	1:A:734:LEU:N	2.54	0.40
1:F:559:TYR:O	1:F:563:THR:HG23	2.21	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:727:TYR:CD2	1:G:809:ILE:HD11	2.57	0.40
1:H:240:GLN:OE1	1:H:243:ARG:NH2	2.50	0.40
2:P:613:SER:OG	2:P:614:ARG:NH1	2.55	0.40
2:P:715:SER:O	2:P:719:VAL:HG23	2.21	0.40
1:B:225:GLU:O	1:B:229:ARG:NH1	2.54	0.40
1:C:783:ALA:HB3	1:C:785:LEU:CD1	2.52	0.40
1:E:478:TRP:CE2	1:E:513:LEU:HD13	2.56	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	Perce	ntiles
1	А	779/887~(88%)	712 (91%)	67~(9%)	0	100	100
1	В	779/887~(88%)	714 (92%)	65~(8%)	0	100	100
1	С	778/887~(88%)	706 (91%)	72 (9%)	0	100	100
1	D	825/887~(93%)	752 (91%)	72 (9%)	1 (0%)	51	85
1	Е	793/887~(89%)	720 (91%)	73 (9%)	0	100	100
1	F	800/887~(90%)	720 (90%)	80 (10%)	0	100	100
1	G	800/887~(90%)	721 (90%)	79 (10%)	0	100	100
1	Н	800/887~(90%)	722 (90%)	77 (10%)	1 (0%)	51	85
1	Ι	798/887~(90%)	724 (91%)	74 (9%)	0	100	100
1	J	814/887~(92%)	739~(91%)	75 (9%)	0	100	100
2	Р	1084/1088~(100%)	985 (91%)	96 (9%)	3 (0%)	41	76
All	All	9050/9958~(91%)	8215 (91%)	830 (9%)	5 (0%)	54	85

All (5) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
2	Р	82	TYR
2	Р	84	ALA
2	Р	942	PRO
1	Н	107	PRO
1	D	103	PRO

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric Outliers H		Perce	Percentiles	
1	А	717/818~(88%)	715 (100%)	2(0%)	92	95	
1	В	717/818 (88%)	716 (100%)	1 (0%)	93	97	
1	С	716/818 (88%)	716 (100%)	0	100	100	
1	D	762/818~(93%)	762 (100%)	0	100	100	
1	Е	731/818 (89%)	729 (100%)	2 (0%)	92	95	
1	F	738/818 (90%)	737 (100%)	1 (0%)	93	97	
1	G	738/818 (90%)	737 (100%)	1 (0%)	93	97	
1	Н	738/818~(90%)	737 (100%)	1 (0%)	93	97	
1	Ι	736/818~(90%)	735 (100%)	1 (0%)	93	97	
1	J	752/818~(92%)	751 (100%)	1 (0%)	93	97	
2	Р	986/989~(100%)	985 (100%)	1 (0%)	93	97	
All	All	8331/9169~(91%)	8320 (100%)	11 (0%)	93	97	

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	314	ARG
1	А	383	ASN
1	В	320	ASN
1	Е	314	ARG
1	Е	320	ASN
1	F	732	ARG
1	G	732	ARG



Continued from previous page...

Mol	Chain	Res	Type
1	Н	732	ARG
1	Ι	732	ARG
1	J	732	ARG
2	Р	130	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	614	ASN
1	В	287	ASN
1	В	690	ASN
1	С	497	ASN
1	С	614	ASN
1	D	545	ASN
1	Ε	571	ASN
1	F	622	ASN
1	Н	549	GLN
1	Ι	614	ASN
1	J	614	ASN
1	J	636	ASN
2	Р	785	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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

There are no ligands in this entry.



# 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-20088. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

# 6.1 Orthogonal projections (i)

#### 6.1.1 Primary map



6.1.2 Raw map



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



### 6.2 Central slices (i)

#### 6.2.1 Primary map



X Index: 150





Z Index: 150

#### 6.2.2 Raw map



X Index: 150

Y Index: 150



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: 146





Z Index: 147

#### 6.3.2 Raw map



X Index: 152

Y Index: 155



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



#### 6.4.2 Raw map



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

#### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.



#### Mask visualisation (i) 6.6

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

#### $emd_{20088}msk_{1.map}$ (i) 6.6.1





# 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 523  $\rm nm^3;$  this corresponds to an approximate mass of 473 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 0.192  ${\rm \AA^{-1}}$ 



# 8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

#### 8.1 FSC (i)



\*Reported resolution corresponds to spatial frequency of 0.192  ${\rm \AA^{-1}}$ 



# 8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	5.20	-	-
Author-provided FSC curve	5.20	5.63	5.24
Unmasked-calculated*	5.34	6.00	5.40

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20088 and PDB model 6OJ5. Per-residue inclusion information can be found in section 3 on page 5.

# 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 2.0 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 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 (2.0).



### 9.4 Atom inclusion (i)



At the recommended contour level, 39% of all backbone atoms, 39% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.3920	0.0760	1.0
А	0.3660	0.0520	
В	0.4110	0.0810	
С	0.4340	0.1090	
D	0.4070	0.0890	
Е	0.3840	0.0650	
F	0.3660	0.0470	
G	0.4380	0.1050	
Н	0.4320	0.1090	
Ι	0.3870	0.0660	0.0 <
J	0.3460	0.0360	
Р	0.4040	0.0770	

