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PDB ID	:	8W9F
EMDB ID	:	EMD-37367
Title	:	Cryo-EM structure of the Rpd3S-nucleosome complex from budding yeast in
		State 3
Authors	:	Wang, C.; Zhan, X.
Deposited on	:	2023-09-05
Resolution	:	4.40  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* 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. dev 92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{MapQ}$	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

# 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 4.40 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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		Qua	ality o	f chain		
1	А	1536	22%	13% •		61%		
2	Е	684	37% 29%	16%	5%•	48%		
2	F	684	20% 16% 7%			77%		
3	В	433	23%	59%		24%	5%	11%
4	С	401	21%	9%	•	54%		
4	D	401	40% 32%	13%	•	54%		
4	G	401	17% 16% •			83%		
5	a	136	7%	65%		••	29%	



Mol	Chain	Length	Quality of chain		
5	е	136	68%	••	27%
6	b	103	<b>•</b> 74%		23%
6	f	103	5%	•	20%
7	с	130	<b>•</b> 78%		• 18%
7	g	130	8%		• 18%
8	d	126	<b>•</b> 70%	• •	25%
8	h	126		•	25%
9	i	147	• 100%		
10	j	147	• 99%		



# 2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 27868 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 Transcriptional regulatory protein SIN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	А	606	Total 5066	C 3253	N 860	O 938	${ m S}$ 15	0	0

• Molecule 2 is a protein called Transcriptional regulatory protein RCO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2 E	353	Total	С	Ν	Ο	$\mathbf{S}$	0	0
	Ľ		2884	1837	493	536	18		0
2	2 F	F 156	Total	С	Ν	0	$\mathbf{S}$	0	0
			1282	822	211	239	10	0	U

• Molecule 3 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	В	385	Total 3057	C 1948	N 513	0 571	$\begin{array}{c} \mathrm{S} \\ \mathrm{25} \end{array}$	0	0

• Molecule 4 is a protein called Chromatin modification-related protein EAF3.

Mol	Chain	Residues	Atoms	AltConf Trace
4 C	183	Total C N O S	0 0	
	105	1483  950  239  285  9	0 0	
4	Л	185	Total C N O S	
	D	100	1497  959  241  288  9	
4	4 C	60	Total C N O S	0 0
4	G	09	570 $371$ $98$ $97$ $4$	0 0

• Molecule 5 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	97	Total 801	C 505	N 155	0 137	$\frac{S}{4}$	0	0



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Mol	Chain	Residues	Atoms					AltConf	Trace
5	е	99	Total 816	C 514	N 158	0 140	$\frac{S}{4}$	0	0

• Molecule 6 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	3 h	70	Total	С	Ν	0	S	0	0
d U	U	19	627	395	121	110	1		
6	f	80	Total	С	Ν	0	S	0	0
0	1	1 02	653	412	127	113	1		0

• Molecule 7 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	7 с	107	Total	С	Ν	0	0	0
		101	817	516	158	143	0	0
7	7 g	g 107	Total	С	Ν	Ο	0	0
1			817	516	158	143		0

• Molecule 8 is a protein called Histone H2B type 1-K.

Mol	Chain	Residues	Atoms				AltConf	Trace	
8	8 4	94	Total	С	Ν	0	S	0	0
o u	u		735	461	134	138	2		
0	8 h	h 94	Total	С	Ν	0	S	0	0
0			735	461	134	138	2	0	U

• Molecule 9 is a DNA chain called 5-DNA.

Mol	Chain	Residues	Atoms				AltConf	Trace	
9	i	147	Total 3011	C 1440	N 546	O 879	Р 146	0	0

• Molecule 10 is a DNA chain called 3-DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	147	Total 3010	C 1440	N 543	0 881	Р 146	0	0

• Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).



Mol	Chain	Residues	Atoms	AltConf
11	Е	4	Total Zn 4 4	0
11	В	1	Total Zn 1 1	0
11	F	2	Total Zn 2 2	0



# 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: Transcriptional regulatory protein SIN3













• Molecule 4: Chromatin modification-related protein EAF3







Chain f:	77%	• 20%
TEM TEM TEM TEM TEM TEM TEM TEM TEM TEM	ARC ARC 1/27 1/22 1/22 1/22 1/22 1/22 1/22 1/22	
• Molecule 7: Histone I	H2A type $1-B/E$	
Chain c:	78%	• 18%
MET SER GLY ARG CLY CLY CLY CLY CLY CLY ALA ALA ALA ALA ALA ALA ALA ALA ALA	176 L116 P117 A116 P117 K118 L18 H118 H118 H118 L18 L18 G17 L18 L18 L18	
• Molecule 7: Histone	H2A type $1-B/E$	
Chain g:	78%	• 18%
• • • • • • • • • • • • • • • • • • •		
MET SER GLY GLY GLY GLY GLY GLN GLY CLY GLY A12 A12 A12 A12 A12 K15 K15 K15 K15	T16 H31 F35 F36 F376 T76 T111 T111 T111 T111 T111 T115 T115 T11	THR GLU SER HIS HIS LYS CLYS CLYS CLYS CLYS
• Molecule 8: Histone	H2B type 1-K	
Chain d:	70%	• • 25%
MET PR.O PR.O GLU PR.O ALA ALA ALA ALA ALA ALA ALA ALA CYS CLYS GLY SER LYS CLYS CLYS CLYS CLYS CLYS CLYS CLYS	ALA VAL THR LLYS ALA GLN LLYS LLYS ALA GLN CLY CLYS ALS ALS ALS ALS ALS ALS ALS ALS ALS AL	1051 A107 €113 A124 LYS
• Molecule 8: Histone	H2B type 1-K	
Chain h:	71%	. 25%
		•
MET PRO GIU PRO ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	ALA THE THE THE THE THE THE THE THE THE THE	L106
• Molecule 9: 5-DNA		
Chain i:	100%	
A-73 A72 ∓73		
• Molecule 10: 3-DNA		
Chain it		
Unam j.	99%	
A-73 T-72 C-71 A-46 T/3		



# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	213127	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	50	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 $(6k \ge 4k)$	Depositor
Maximum map value	0.056	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	304.36002, 304.36002, 304.36002	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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: 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	Bo	ond lengths	В	ond angles
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.26	0/5180	0.41	0/6984
2	Е	0.55	2/2952~(0.1%)	0.86	12/3978~(0.3%)
2	F	2.28	3/1313~(0.2%)	0.70	5/1763~(0.3%)
3	В	0.43	2/3137~(0.1%)	0.63	4/4246~(0.1%)
4	С	0.27	0/1509	0.48	0/2039
4	D	1.84	6/1524~(0.4%)	0.49	1/2061~(0.0%)
4	G	0.70	0/583	0.97	3/777~(0.4%)
5	a	0.52	0/813	0.63	2/1090~(0.2%)
5	е	0.51	0/828	0.58	1/1109~(0.1%)
6	b	0.50	0/634	0.50	0/848
6	f	0.46	0/660	0.46	0/883
7	с	0.67	2/827~(0.2%)	0.55	1/1116~(0.1%)
7	g	0.40	0/827	0.49	0/1116
8	d	0.46	0/746	0.55	1/1003~(0.1%)
8	h	0.43	0/746	0.50	0/1003
9	i	0.77	0/3378	0.98	0/5212
10	j	0.77	0/3376	0.99	1/5209~(0.0%)
All	All	0.83	$15/2903\overline{3}\ (0.1\%)$	0.72	31/40437~(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
2	Е	0	1
3	В	0	1
All	All	0	3

All (15) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	F	372	TYR	CB-CG	80.40	2.72	1.51
4	D	236	TRP	CE3-CZ3	52.29	2.27	1.38
4	D	236	TRP	CZ3-CH2	28.56	1.85	1.40
4	D	236	TRP	CE2-CZ2	25.32	1.82	1.39
4	D	236	TRP	CD2-CE2	21.01	1.66	1.41
4	D	236	TRP	CZ2-CH2	14.53	1.65	1.37
4	D	236	TRP	CD2-CE3	14.49	1.62	1.40
7	с	117	PRO	N-CA	13.06	1.69	1.47
2	F	372	TYR	CG-CD1	11.65	1.54	1.39
2	F	372	TYR	CG-CD2	10.20	1.52	1.39
3	В	67	LYS	C-N	8.78	1.50	1.34
3	В	41	LYS	C-N	8.52	1.50	1.34
2	Е	179	SER	CA-CB	-6.39	1.43	1.52
7	с	116	LEU	C-N	5.41	1.44	1.34
2	Е	109	SER	CA-CB	-5.36	1.45	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Е	384	ARG	CB-CA-C	15.82	142.05	110.40
2	F	372	TYR	CA-CB-CG	12.40	136.95	113.40
2	F	372	TYR	CB-CG-CD2	11.70	128.02	121.00
2	F	372	TYR	CD1-CG-CD2	-11.38	105.38	117.90
2	F	372	TYR	CB-CG-CD1	9.19	126.51	121.00
3	В	85	PHE	CB-CA-C	-8.94	92.53	110.40
5	a	133	GLU	CB-CA-C	-7.58	95.23	110.40
2	Е	383	ASP	CB-CA-C	7.54	125.48	110.40
2	Е	182	ARG	CB-CG-CD	-7.40	92.35	111.60
4	D	236	TRP	CE3-CZ3-CH2	-7.40	113.06	121.20
2	Е	184	THR	OG1-CB-CG2	-7.28	93.25	110.00
7	с	117	PRO	CA-N-CD	-6.99	101.72	111.50
2	Е	387	PHE	N-CA-CB	6.66	122.58	110.60
2	Е	125	ARG	CB-CA-C	-6.42	97.56	110.40
3	В	42	PRO	N-CD-CG	-6.27	93.79	103.20
4	G	96	ARG	NE-CZ-NH1	6.25	123.42	120.30
8	d	34	LYS	CB-CA-C	-6.16	98.08	110.40
4	G	98	ARG	NE-CZ-NH1	6.13	123.37	120.30
2	Е	172	THR	CA-CB-OG1	5.76	121.10	109.00
10	j	-46	DA	O4'-C1'-N9	5.68	111.98	108.00
3	В	161	CYS	CA-CB-SG	5.53	123.95	114.00
2	Е	384	ARG	CB-CG-CD	5.38	125.59	111.60
2	Е	110	VAL	CG1-CB-CG2	-5.28	102.45	110.90
2	F	372	TYR	CG-CD2-CE2	5.28	125.53	121.30



Mol	Chain	$\operatorname{Res}$	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
5	е	90	MET	CB-CG-SD	5.28	128.22	112.40
5	a	90	MET	CB-CG-SD	5.27	128.21	112.40
3	В	41	LYS	C-N-CD	-5.17	109.23	120.60
2	Е	182	ARG	CB-CA-C	-5.16	100.07	110.40
4	G	110	ARG	NE-CZ-NH2	-5.16	117.72	120.30
2	Ε	174	ASN	CB-CA-C	-5.05	100.29	110.40
2	E	389	THR	CB-CA-C	5.04	125.21	111.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	1232	TYR	Peptide
3	В	157	ALA	Mainchain
2	Е	470	SER	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	5066	0	5024	202	0
2	Е	2884	0	2831	196	0
2	F	1282	0	1239	65	0
3	В	3057	0	2930	155	0
4	С	1483	0	1510	31	0
4	D	1497	0	1524	74	0
4	G	570	0	563	0	0
5	a	801	0	839	0	0
5	е	816	0	856	0	0
6	b	627	0	663	0	0
6	f	653	0	696	0	0
7	с	817	0	872	0	0
7	g	817	0	872	0	0
8	d	735	0	756	0	0
8	h	735	0	756	0	0
9	i	3011	0	1662	0	0
10	j	3010	0	1663	0	0



	J = J = J					
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	В	1	0	0	0	0
11	Е	4	0	0	0	0
11	F	2	0	0	0	0
All	All	27868	0	25256	563	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 16.

All (563) 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)
4:D:236:TRP:CE2	4:D:236:TRP:CZ2	1.82	1.65
4:D:236:TRP:CH2	4:D:236:TRP:CZ3	1.85	1.59
1:A:922:LYS:CE	2:E:129:TRP:CZ2	1.96	1.48
1:A:922:LYS:HE3	2:E:129:TRP:CE2	1.49	1.44
2:E:379:ILE:HD12	2:E:380:PRO:CD	1.53	1.39
1:A:798:HIS:CG	3:B:283:CYS:SG	2.17	1.38
1:A:819:PHE:CD2	3:B:33:ALA:HB2	1.61	1.34
1:A:922:LYS:HE3	2:E:129:TRP:CZ2	1.57	1.34
1:A:1190:GLN:NE2	2:E:129:TRP:CE3	1.95	1.33
4:D:236:TRP:CZ3	2:F:372:TYR:CG	2.16	1.33
3:B:152:ALA:HB2	3:B:161:CYS:O	1.27	1.32
4:D:236:TRP:CE3	2:F:372:TYR:CG	2.17	1.31
4:D:236:TRP:CE3	2:F:372:TYR:CB	2.15	1.28
3:B:151:HIS:N	3:B:161:CYS:SG	2.06	1.26
1:A:798:HIS:CD2	3:B:283:CYS:SG	2.28	1.26
1:A:922:LYS:NZ	2:E:129:TRP:CZ2	2.02	1.26
1:A:1190:GLN:OE1	2:E:129:TRP:CH2	1.90	1.24
1:A:922:LYS:CE	2:E:129:TRP:CE2	2.16	1.22
4:D:236:TRP:CZ3	2:F:372:TYR:CB	2.22	1.22
4:D:236:TRP:CZ3	4:D:236:TRP:CE3	2.27	1.21
4:D:236:TRP:CH2	2:F:372:TYR:CG	2.29	1.21
4:D:236:TRP:CD2	2:F:372:TYR:CG	2.28	1.21
1:A:918:GLU:OE2	2:E:128:LEU:HA	1.33	1.21
4:D:236:TRP:CE3	2:F:372:TYR:HB3	1.76	1.18
4:D:236:TRP:CE2	2:F:372:TYR:CG	2.32	1.18
1:A:819:PHE:CE2	3:B:33:ALA:HB2	1.75	1.18
4:D:236:TRP:CE2	2:F:372:TYR:CB	2.27	1.17
4:D:236:TRP:CD2	2:F:372:TYR:CB	2.26	1.17
1:A:922:LYS:CE	2:E:129:TRP:HZ2	1.43	1.17
1:A:812:GLU:OE2	3:B:37:GLY:HA2	1.44	1.16



	h i o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:D:236:TRP:CE2	2:F:372:TYR:HB2	1.81	1.15
1:A:922:LYS:CE	2:E:129:TRP:NE1	2.09	1.14
1:A:819:PHE:CE2	3:B:33:ALA:CB	2.32	1.12
1:A:904:GLU:HG2	2:E:116:ASN:HB2	1.29	1.12
4:D:236:TRP:CZ2	2:F:372:TYR:CG	2.37	1.12
2:E:381:LEU:HB3	2:E:384:ARG:HB2	1.33	1.07
1:A:819:PHE:HE2	3:B:33:ALA:N	1.52	1.07
2:E:179:SER:O	3:B:129:GLU:OE2	1.73	1.06
2:E:379:ILE:CD1	2:E:380:PRO:CD	2.33	1.05
2:E:379:ILE:CD1	2:E:380:PRO:HD3	1.84	1.05
1:A:922:LYS:CD	2:E:129:TRP:HZ2	1.71	1.04
1:A:922:LYS:NZ	2:E:129:TRP:CE2	2.24	1.04
1:A:813:GLU:OE1	2:E:110:VAL:HG12	1.56	1.03
4:D:236:TRP:CZ3	2:F:372:TYR:CD1	2.45	1.03
4:D:236:TRP:CZ2	2:F:372:TYR:CB	2.42	1.03
1:A:922:LYS:HE3	2:E:129:TRP:NE1	1.70	1.02
1:A:922:LYS:CE	2:E:129:TRP:HE1	1.70	1.01
4:D:236:TRP:CE2	2:F:372:TYR:CD2	2.48	1.01
4:D:236:TRP:CH2	2:F:372:TYR:CB	2.45	0.99
2:E:189:GLY:HA2	3:B:72:GLN:HB2	1.41	0.98
1:A:798:HIS:CB	3:B:283:CYS:SG	2.51	0.98
1:A:1190:GLN:OE1	2:E:129:TRP:CZ2	2.17	0.97
1:A:798:HIS:HB2	3:B:283:CYS:SG	2.05	0.97
3:B:149:LEU:HB3	3:B:161:CYS:HB2	1.46	0.97
1:A:798:HIS:CG	3:B:283:CYS:HG	1.79	0.96
1:A:918:GLU:OE2	2:E:128:LEU:CA	2.14	0.96
3:B:151:HIS:CB	3:B:161:CYS:SG	2.46	0.95
1:A:1190:GLN:NE2	2:E:129:TRP:CZ3	2.26	0.95
3:B:150:HIS:CE1	3:B:270:GLN:NE2	2.35	0.94
3:B:151:HIS:HB2	3:B:161:CYS:SG	2.07	0.94
1:A:918:GLU:OE2	2:E:127:SER:O	1.87	0.93
3:B:114:ASP:O	3:B:116:LEU:N	2.02	0.93
4:D:236:TRP:CD2	2:F:372:TYR:HB2	1.99	0.93
4:D:236:TRP:CZ2	2:F:372:TYR:CD2	2.57	0.92
1:A:819:PHE:HE2	3:B:33:ALA:H	0.93	0.91
1:A:904:GLU:CG	2:E:116:ASN:HB2	2.01	0.90
1:A:918:GLU:OE2	2:E:128:LEU:HD12	1.72	0.90
2:E:379:ILE:CD1	2:E:380:PRO:HD2	2.02	0.89
1:A:918:GLU:CD	2:E:128:LEU:HD12	1.93	0.89
4:D:236:TRP:CE3	2:F:372:TYR:CD1	2.60	0.88
3:B:28:ASP:HA	3:B:31:ASN:HD21	1.39	0.87



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:E:379:ILE:HD12	2:E:380:PRO:HD3	0.89	0.87
1:A:819:PHE:CE2	3:B:33:ALA:N	2.42	0.87
3:B:136:ARG:HG2	3:B:136:ARG:HH21	1.40	0.86
1:A:911:GLU:OE1	2:E:118:GLY:HA3	1.75	0.86
1:A:813:GLU:OE1	2:E:110:VAL:CG1	2.26	0.84
1:A:922:LYS:HE2	2:E:129:TRP:HE1	1.43	0.84
1:A:918:GLU:OE1	2:E:128:LEU:HD12	1.78	0.82
4:D:255:GLU:HG2	4:D:323:ILE:HG12	1.61	0.82
3:B:31:ASN:HD22	3:B:31:ASN:H	1.25	0.82
3:B:114:ASP:C	3:B:116:LEU:H	1.83	0.81
1:A:922:LYS:HD2	2:E:129:TRP:HZ2	1.44	0.81
1:A:819:PHE:CD2	3:B:33:ALA:CB	2.55	0.79
4:C:240:THR:O	4:C:242:ASP:N	2.14	0.79
1:A:812:GLU:OE2	3:B:37:GLY:CA	2.30	0.79
2:E:515:GLN:HG3	2:E:516:ASN:H	1.48	0.79
3:B:28:ASP:O	3:B:31:ASN:ND2	2.16	0.79
1:A:922:LYS:CD	2:E:129:TRP:CZ2	2.55	0.78
1:A:1190:GLN:OE1	2:E:129:TRP:CZ3	2.37	0.78
2:E:517:ASN:HB3	2:E:519:ASN:H	1.47	0.78
3:B:88:ARG:HG3	3:B:88:ARG:HH11	1.49	0.78
1:A:921:GLN:NE2	1:A:1186:LEU:O	2.17	0.78
3:B:136:ARG:HG2	3:B:136:ARG:NH2	1.98	0.78
3:B:28:ASP:HA	3:B:31:ASN:ND2	1.99	0.77
1:A:911:GLU:OE1	2:E:119:PRO:CD	2.32	0.77
1:A:922:LYS:NZ	2:E:129:TRP:NE1	2.29	0.77
1:A:868:ARG:HD2	1:A:873:LYS:HE3	1.66	0.77
2:E:384:ARG:HA	2:E:387:PHE:HB3	1.65	0.77
2:F:260:GLU:HG3	2:F:262:PHE:H	1.48	0.77
2:E:491:VAL:HG12	2:E:492:TRP:HD1	1.51	0.75
4:D:293:LEU:HD23	4:D:322:PRO:HB3	1.68	0.74
1:A:1190:GLN:NE2	2:E:129:TRP:CD2	2.54	0.74
3:B:280:ARG:HB2	3:B:313:TYR:HB2	1.69	0.73
3:B:350:ASP:N	3:B:350:ASP:OD1	2.16	0.73
3:B:78:HIS:HD1	3:B:82:TYR:HD1	1.37	0.73
2:F:372:TYR:CG	2:F:372:TYR:CB	2.72	0.73
4:C:288:TYR:O	4:C:292:CYS:HB2	1.89	0.72
1:A:1318:ALA:HB3	1:A:1321:ASP:HB2	1.72	0.72
1:A:911:GLU:OE1	2:E:119:PRO:HD3	1.90	0.71
2:E:404:ASP:N	2:E:404:ASP:OD2	2.19	0.71
3:B:152:ALA:CB	3:B:161:CYS:O	2.23	0.71
4:D:236:TRP:CE2	2:F:372:TYR:HD2	2.07	0.71



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:F:354:PRO:HD2	2:F:357:ILE:HD12	1.72	0.71
2:E:113:LEU:HD12	2:E:113:LEU:N	2.07	0.70
1:A:1190:GLN:CD	2:E:129:TRP:CZ3	2.64	0.70
2:E:570:GLN:HB2	2:F:564:ARG:HH22	1.56	0.70
3:B:149:LEU:HB3	3:B:161:CYS:CB	2.21	0.70
2:E:371:GLN:HA	4:C:240:THR:HG21	1.74	0.69
1:A:922:LYS:NZ	2:E:129:TRP:HZ2	1.65	0.69
3:B:2:VAL:N	3:B:370:ASP:OD1	2.26	0.69
2:E:187:TRP:HE3	2:E:187:TRP:N	1.91	0.69
2:E:372:TYR:OH	2:E:496:ARG:NH1	2.24	0.69
1:A:922:LYS:HD2	2:E:129:TRP:CZ2	2.25	0.69
2:E:384:ARG:HG3	2:E:387:PHE:HB3	1.75	0.68
1:A:812:GLU:CD	3:B:37:GLY:HA2	2.14	0.68
1:A:918:GLU:CD	2:E:128:LEU:HA	2.11	0.68
2:E:414:PHE:HB3	2:E:423:THR:HG21	1.76	0.67
2:E:184:THR:O	3:B:73:GLU:OE1	2.13	0.67
4:D:236:TRP:CH2	2:F:372:TYR:CA	2.79	0.66
2:E:384:ARG:HB3	2:E:387:PHE:HD2	1.61	0.66
3:B:299:LYS:NZ	3:B:331:ASN:OD1	2.28	0.66
2:E:181:ILE:HG13	3:B:136:ARG:HD2	1.77	0.66
3:B:88:ARG:HH11	3:B:88:ARG:CG	2.08	0.66
2:E:180:ASN:HB2	2:E:185:ILE:HD12	1.78	0.65
4:C:293:LEU:HD22	4:C:322:PRO:HB3	1.78	0.65
2:E:440:CYS:SG	2:E:441:ASP:N	2.70	0.65
3:B:91:PRO:HD2	3:B:114:ASP:OD1	1.97	0.65
3:B:28:ASP:C	3:B:31:ASN:ND2	2.50	0.64
2:E:379:ILE:CG1	2:E:380:PRO:HD2	2.26	0.64
3:B:150:HIS:CE1	3:B:270:GLN:HE22	2.13	0.64
4:D:236:TRP:CZ3	2:F:372:TYR:HB3	2.28	0.64
1:A:819:PHE:CE2	3:B:33:ALA:HB3	2.32	0.64
2:E:124:LYS:O	2:E:124:LYS:HG3	1.98	0.64
2:E:381:LEU:CB	2:E:384:ARG:HB2	2.20	0.63
2:E:424:ARG:HD3	2:E:435:ARG:HG3	1.80	0.63
4:D:236:TRP:CH2	2:F:372:TYR:HA	2.33	0.63
1:A:929:ASP:OD1	3:B:359:ASN:ND2	2.26	0.63
3:B:209:HIS:HE1	3:B:235:ASN:HB3	1.61	0.63
2:E:121:GLU:O	2:E:125:ARG:HG2	1.98	0.63
4:D:308:GLU:HA	4:D:311:LYS:HE2	1.81	0.63
3:B:285:ASN:OD1	3:B:358:SER:OG	2.14	0.62
3:B:81:GLU:CG	3:B:104:PHE:HZ	2.11	0.62
2:E:189:GLY:HA3	3:B:70:THR:HB	1.82	0.62



Atom-1	Atom-2	Interatomic	Clash
1100III-1	1100111-2	distance (Å)	overlap (Å)
2:E:180:ASN:C	2:E:180:ASN:HD22	2.00	0.62
1:A:912:TRP:CH2	2:E:111:THR:HG23	2.34	0.62
1:A:1007:LYS:O	1:A:1011:LYS:HG3	1.99	0.62
3:B:90:THR:HG23	3:B:92:ASP:H	1.63	0.62
2:E:179:SER:C	3:B:129:GLU:OE2	2.38	0.62
2:E:507:GLU:HB2	2:E:541:GLN:HE21	1.63	0.62
3:B:106:VAL:HG12	3:B:106:VAL:O	2.00	0.61
3:B:136:ARG:HH21	3:B:136:ARG:CG	2.13	0.61
3:B:28:ASP:CA	3:B:31:ASN:ND2	2.62	0.61
1:A:901:LYS:HZ1	2:E:105:ASP:N	1.99	0.61
3:B:44:ARG:HB3	3:B:315:MET:HG2	1.83	0.61
3:B:81:GLU:CG	3:B:104:PHE:CZ	2.83	0.61
3:B:149:LEU:CB	3:B:161:CYS:HB2	2.28	0.61
1:A:663:ASN:HB3	2:F:547:ILE:HG23	1.81	0.61
1:A:812:GLU:CD	3:B:37:GLY:CA	2.68	0.61
1:A:813:GLU:CD	2:E:110:VAL:HG12	2.19	0.61
2:E:516:ASN:ND2	2:E:540:THR:OG1	2.34	0.61
4:D:253:THR:OG1	4:D:323:ILE:O	2.19	0.61
3:B:81:GLU:HG3	3:B:104:PHE:CZ	2.36	0.60
2:E:367:GLY:HA3	2:E:371:GLN:HG3	1.83	0.60
1:A:665:GLU:HB3	2:E:552:PHE:CZ	2.36	0.60
1:A:808:PHE:CZ	3:B:280:ARG:HA	2.36	0.60
2:E:416:ILE:HA	2:E:423:THR:HG22	1.83	0.60
1:A:1181:ALA:HB1	1:A:1186:LEU:HB2	1.84	0.60
4:D:300:ARG:NH2	4:D:397:VAL:O	2.34	0.60
1:A:1076:LYS:HG2	1:A:1079:ARG:HH22	1.66	0.59
3:B:326:THR:O	3:B:330:ASN:ND2	2.35	0.59
2:E:543:ASP:O	2:E:546:SER:OG	2.21	0.59
1:A:911:GLU:OE1	2:E:118:GLY:CA	2.51	0.59
2:E:379:ILE:HG13	2:E:380:PRO:HD2	1.83	0.59
3:B:150:HIS:HE1	3:B:270:GLN:NE2	1.97	0.59
3:B:31:ASN:H	3:B:31:ASN:ND2	1.98	0.59
2:E:171:LEU:O	2:E:173:GLU:N	2.36	0.58
1:A:959:GLN:NE2	1:A:972:LYS:O	2.27	0.58
2:E:172:THR:HG22	3:B:63:ILE:HD13	1.86	0.58
3:B:31:ASN:HD22	3:B:31:ASN:N	2.00	0.58
2:E:187:TRP:N	2:E:187:TRP:CE3	2.71	0.58
1:A:819:PHE:CE2	3:B:33:ALA:CA	2.86	0.57
1:A:952:ILE:HA	1:A:955:ILE:HD12	1.86	0.57
1:A:911:GLU:OE1	2:E:119:PRO:HD2	2.04	0.57
2:E:107:LYS:HG3	2:E:107:LYS:O	2.05	0.57



	h i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:E:317:ALA:O	2:E:321:LYS:HG3	2.04	0.57
2:E:181:ILE:HG21	3:B:133:ARG:HG2	1.87	0.57
4:D:253:THR:HG23	4:D:256:MET:H	1.69	0.57
2:E:543:ASP:OD1	2:E:543:ASP:N	2.38	0.57
2:E:172:THR:HG22	3:B:63:ILE:CD1	2.34	0.57
2:E:443:CYS:HB2	2:E:445:THR:HG22	1.86	0.57
4:D:304:LEU:HD22	4:D:397:VAL:HG21	1.86	0.57
2:E:180:ASN:ND2	2:E:180:ASN:O	2.35	0.57
3:B:32:TYR:CD2	3:B:32:TYR:N	2.72	0.57
1:A:1206:GLN:OE1	1:A:1209:ARG:NH2	2.37	0.56
1:A:675:TYR:CZ	1:A:713:ASN:HB2	2.40	0.56
4:D:303:ARG:HH21	2:F:350:GLN:HA	1.70	0.56
1:A:918:GLU:OE1	2:E:128:LEU:CD1	2.53	0.56
4:C:244:LYS:HE2	4:C:379:PRO:HG2	1.88	0.56
1:A:696:ILE:HG21	2:E:493:LYS:HB2	1.86	0.56
1:A:812:GLU:OE1	3:B:280:ARG:NH1	2.19	0.56
3:B:297:TYR:O	3:B:300:SER:OG	2.21	0.56
1:A:912:TRP:CZ3	2:E:111:THR:HG23	2.41	0.56
2:E:402:ASN:HA	2:E:405:THR:HB	1.87	0.56
2:E:562:GLN:HA	2:E:565:LYS:HD3	1.88	0.56
2:F:302:HIS:HB2	2:F:307:LYS:HD3	1.88	0.56
2:E:379:ILE:CG1	2:E:380:PRO:CD	2.82	0.56
2:F:355:ASN:HA	2:F:358:LYS:HG3	1.88	0.56
3:B:91:PRO:HG2	3:B:113:PHE:O	2.06	0.56
1:A:1075:GLN:HA	1:A:1078:LYS:HG2	1.87	0.55
4:C:255:GLU:HB2	4:C:323:ILE:HG12	1.88	0.55
1:A:755:TYR:OH	3:B:194:GLU:OE1	2.24	0.55
1:A:1194:MET:HB2	1:A:1196:LEU:HG	1.88	0.55
1:A:1229:ARG:O	1:A:1233:ASN:HA	2.06	0.55
2:E:106:SER:O	2:E:106:SER:OG	2.18	0.55
1:A:999:THR:HG22	1:A:1001:ALA:H	1.71	0.55
1:A:1219:LEU:HD11	1:A:1223:TRP:HB2	1.89	0.55
3:B:81:GLU:HG2	3:B:104:PHE:HZ	1.71	0.55
4:D:305:GLN:O	4:D:308:GLU:HB3	2.06	0.55
1:A:886:HIS:O	1:A:890:THR:OG1	2.23	0.55
1:A:913:ASN:ND2	3:B:345:GLU:OE2	2.39	0.55
2:E:449:LEU:HD11	2:E:457:PHE:HE1	1.72	0.54
1:A:904:GLU:CD	2:E:116:ASN:HB2	2.28	0.54
2:E:327:ILE:HG22	2:E:337:ALA:HB1	1.88	0.54
2:E:491:VAL:HG12	2:E:492:TRP:CD1	2.38	0.54
2:E:452:VAL:HG21	2:E:464:TRP:HZ2	1.71	0.54



	jus puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:C:290:ASP:HA	4:C:322:PRO:HD2	1.89	0.54
1:A:851:LEU:HD13	1:A:855:LEU:HG	1.89	0.54
1:A:1178:VAL:HG12	1:A:1181:ALA:H	1.73	0.54
2:E:402:ASN:H	2:E:428:TRP:HZ2	1.54	0.54
2:E:184:THR:O	2:E:184:THR:OG1	2.15	0.54
2:E:492:TRP:HD1	2:E:492:TRP:H	1.55	0.54
3:B:67:LYS:HB2	3:B:67:LYS:HZ2	1.72	0.54
4:D:236:TRP:HH2	2:F:366:THR:HA	1.73	0.54
2:E:184:THR:HG21	3:B:76:GLN:HE22	1.72	0.54
3:B:70:THR:OG1	3:B:73:GLU:OE2	2.26	0.54
4:D:307:ASP:O	4:D:310:LEU:HB2	2.07	0.54
1:A:1190:GLN:CD	2:E:129:TRP:CE3	2.77	0.54
4:D:378:ASP:OD2	4:D:381:ARG:NH2	2.34	0.54
1:A:990:CYS:O	1:A:994:THR:HG23	2.08	0.54
4:D:335:ILE:HG21	4:D:363:LEU:HD21	1.89	0.53
1:A:954:SER:HA	2:E:414:PHE:CE2	2.44	0.53
3:B:28:ASP:O	3:B:32:TYR:CE2	2.62	0.53
2:E:189:GLY:CA	3:B:72:GLN:HB2	2.27	0.53
3:B:8:PHE:HD2	3:B:248:ARG:HD2	1.74	0.53
1:A:666:VAL:O	1:A:670:GLU:HG2	2.09	0.53
2:E:498:ILE:HG21	4:C:226:ILE:HD13	1.90	0.53
3:B:150:HIS:O	3:B:192:GLY:HA3	2.09	0.53
4:D:293:LEU:HD12	4:D:297:LEU:HB3	1.91	0.53
2:E:387:PHE:CD1	2:E:387:PHE:C	2.82	0.52
4:D:236:TRP:CZ3	2:F:372:TYR:HD1	2.20	0.52
3:B:307:VAL:HG21	3:B:329:LEU:HD11	1.90	0.52
4:C:342:ILE:O	4:C:345:THR:OG1	2.20	0.52
4:D:244:LYS:HB3	4:D:387:TYR:HB3	1.90	0.52
1:A:1280:ALA:O	1:A:1284:ILE:HG13	2.10	0.52
2:F:263:CYS:O	2:F:267:ASN:N	2.43	0.52
1:A:1287:ARG:HD2	1:A:1323:THR:HG22	1.90	0.52
2:E:126:GLU:O	2:E:126:GLU:HG3	2.08	0.52
2:E:384:ARG:HA	2:E:387:PHE:CB	2.38	0.52
1:A:917:ARG:CZ	1:A:1186:LEU:HD22	2.40	0.52
2:E:317:ALA:O	2:E:320:LYS:HG3	2.10	0.52
4:D:312:LYS:O	4:D:315:LYS:HG3	2.09	0.52
3:B:50:SER:O	3:B:54:ASN:ND2	2.40	0.52
3:B:274:ASP:OD1	3:B:274:ASP:N	2.34	0.52
2:E:470:SER:HB2	2:E:471:PRO:CD	2.40	0.52
3:B:167:VAL:HG22	3:B:197:PHE:HE2	1.73	0.52
2:F:562:GLN:O	2:F:566:LEU:HG	2.09	0.52



	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:875:ARG:O	1:A:879:ILE:HG12	2.10	0.51
3:B:377:PHE:O	3:B:381:GLU:HG2	2.10	0.51
3:B:150:HIS:HB3	3:B:166:ILE:HD12	1.91	0.51
4:C:222:LEU:HD21	4:C:363:LEU:HD11	1.92	0.51
1:A:782:TRP:CE2	3:B:226:VAL:HG21	2.46	0.51
1:A:1300:MET:O	1:A:1317:ILE:HB	2.10	0.51
1:A:794:GLY:HA2	2:E:460:LEU:HD13	1.92	0.51
3:B:78:HIS:ND1	3:B:82:TYR:CD1	2.77	0.51
2:E:449:LEU:HD11	2:E:457:PHE:CE1	2.46	0.51
3:B:38:HIS:C	3:B:38:HIS:CD2	2.85	0.51
3:B:294:CYS:O	3:B:298:VAL:HG23	2.11	0.51
3:B:338:LEU:HD21	3:B:353:LEU:HD13	1.93	0.51
2:E:308:PHE:O	2:E:312:ILE:HG12	2.11	0.51
2:E:169:THR:HG22	3:B:53:MET:CE	2.41	0.50
3:B:26:ASP:HB3	3:B:29:VAL:HG13	1.93	0.50
1:A:874:GLU:O	1:A:878:GLU:HG3	2.11	0.50
1:A:1140:ALA:HB1	1:A:1144:ILE:HB	1.92	0.50
2:E:504:LEU:HB3	2:E:538:LYS:HG3	1.92	0.50
2:E:558:SER:O	2:E:562:GLN:HG3	2.10	0.50
3:B:281:LEU:HB2	3:B:313:TYR:CD2	2.46	0.50
4:D:236:TRP:CZ3	2:F:372:TYR:CA	2.94	0.50
1:A:864:LYS:HG2	1:A:880:ILE:HD13	1.94	0.50
1:A:1184:LEU:HB2	1:A:1186:LEU:HG	1.93	0.50
2:F:559:LYS:O	2:F:563:LYS:HG2	2.11	0.50
3:B:279:ASP:OD2	3:B:314:THR:HG22	2.12	0.50
2:E:111:THR:HG22	2:E:113:LEU:H	1.77	0.49
1:A:842:THR:HG23	1:A:845:GLU:H	1.77	0.49
1:A:951:GLU:HG2	2:E:427:SER:HA	1.93	0.49
3:B:50:SER:HG	3:B:343:TYR:HE2	1.59	0.49
3:B:246:THR:O	3:B:250:VAL:HG23	2.12	0.49
4:D:236:TRP:CH2	2:F:366:THR:HA	2.47	0.49
2:F:302:HIS:HB3	2:F:306:CYS:HB2	1.94	0.49
1:A:862:ILE:HG13	1:A:863:TYR:N	2.28	0.49
2:E:326:PHE:CD1	2:E:341:PHE:HB2	2.46	0.49
2:E:385:GLN:OE1	2:E:385:GLN:HA	2.12	0.49
2:E:510:GLN:HG3	4:D:354:LEU:HD22	1.94	0.49
2:E:521:GLN:HB2	2:E:539:ILE:HD11	1.93	0.49
2:E:560:MET:HG2	2:F:557:LYS:HE3	1.93	0.49
1:A:1018:ILE:HD12	1:A:1022:PHE:HE2	1.77	0.49
2:F:259:ASN:ND2	2:F:274:CYS:SG	2.86	0.49
1:A:1139:PHE:CE1	1:A:1287:ARG:HG3	2.47	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:E:362:PRO:HG3	2:E:499:ASN:HB2	1.94	0.49
1:A:1203:ALA:O	1:A:1207:VAL:HG23	2.12	0.49
3:B:40:MET:SD	3:B:313:TYR:HE1	2.36	0.49
4:D:254:VAL:HA	4:D:257:VAL:HG12	1.94	0.49
2:E:571:GLU:HA	2:E:574:ILE:HG22	1.95	0.49
1:A:1202:ASP:OD2	1:A:1205:LYS:NZ	2.39	0.48
2:E:372:TYR:CZ	2:E:374:ASP:HB3	2.48	0.48
1:A:981:ASP:OD2	1:A:984:ILE:HG13	2.14	0.48
3:B:155:SER:HB3	4:C:393:GLN:HE22	1.79	0.48
2:E:437:ILE:HG12	2:E:448:HIS:CD2	2.48	0.48
1:A:1063:MET:HE1	1:A:1074:TYR:CD2	2.48	0.48
4:D:229:LYS:HD3	2:F:360:THR:HG21	1.96	0.48
1:A:675:TYR:CE2	1:A:713:ASN:HB2	2.49	0.48
4:D:236:TRP:CZ2	2:F:372:TYR:HD2	2.25	0.48
4:D:288:TYR:OH	2:F:339:LEU:HB3	2.14	0.48
2:F:316:MET:N	2:F:316:MET:SD	2.85	0.48
1:A:770:ARG:HH12	3:B:154:LYS:HZ3	1.60	0.48
4:C:393:GLN:O	4:C:397:VAL:HG23	2.13	0.48
3:B:11:ILE:HD13	3:B:11:ILE:H	1.78	0.48
2:F:327:ILE:HD11	2:F:338:LYS:HD2	1.96	0.48
1:A:872:ASP:O	1:A:874:GLU:N	2.47	0.48
1:A:1137:ASN:HD22	1:A:1283:GLN:NE2	2.13	0.47
2:E:180:ASN:ND2	2:E:180:ASN:N	2.58	0.47
3:B:28:ASP:CA	3:B:31:ASN:HD21	2.17	0.47
4:D:222:LEU:HG	4:D:339:PRO:HG3	1.95	0.47
1:A:1168:VAL:HG21	1:A:1232:TYR:CE1	2.48	0.47
1:A:937:GLN:O	1:A:941:LYS:HE2	2.14	0.47
1:A:1021:PHE:HE1	1:A:1305:PHE:HB2	1.79	0.47
3:B:281:LEU:HB2	3:B:313:TYR:CE2	2.49	0.47
1:A:978:ASP:OD1	1:A:1311:HIS:ND1	2.47	0.47
1:A:1131:GLN:HG3	1:A:1132:ASN:OD1	2.15	0.47
1:A:1261:LYS:HA	1:A:1261:LYS:HD3	1.71	0.47
3:B:114:ASP:C	3:B:116:LEU:N	2.54	0.47
1:A:1189:SER:O	1:A:1193:GLU:N	2.46	0.47
2:E:178:GLU:HG2	3:B:67:LYS:HZ1	1.79	0.47
3:B:31:ASN:ND2	3:B:31:ASN:N	2.58	0.47
3:B:296:ASN:HB2	3:B:328:LEU:HD21	1.97	0.47
1:A:901:LYS:NZ	2:E:105:ASP:HB3	2.30	0.47
3:B:30:GLY:HA2	3:B:42:PRO:HB2	1.95	0.47
3:B:34:TYR:CE1	3:B:113:PHE:HE1	2.33	0.47
3:B:285:ASN:ND2	3:B:285:ASN:O	2.48	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:C:245:ILE:HG12	4:C:390:THR:HG23	1.95	0.47
4:D:321:VAL:HG21	4:D:324:ARG:HD2	1.96	0.47
1:A:696:ILE:O	2:E:474:VAL:HG11	2.14	0.47
3:B:332:VAL:HG12	3:B:334:LEU:HD12	1.96	0.47
1:A:1343:LEU:HG	1:A:1344:PRO:HD2	1.97	0.47
2:E:556:TYR:HD2	2:F:557:LYS:HE2	1.79	0.47
1:A:1161:ILE:HG22	1:A:1204:TYR:HD2	1.80	0.47
3:B:149:LEU:HD22	3:B:161:CYS:HA	1.97	0.47
4:D:232:LEU:HD13	2:F:353:LEU:HD22	1.97	0.46
2:E:517:ASN:HB3	2:E:519:ASN:N	2.21	0.46
4:C:333:ARG:O	4:C:337:VAL:HG23	2.15	0.46
1:A:867:ILE:O	1:A:871:TYR:HB2	2.14	0.46
1:A:922:LYS:NZ	2:E:129:TRP:HE1	2.06	0.46
1:A:979:PHE:HZ	1:A:1152:THR:HG22	1.81	0.46
1:A:1034:TYR:O	1:A:1038:GLN:HG3	2.16	0.46
2:E:351:PHE:CD1	4:C:333:ARG:HD3	2.51	0.46
2:E:417:CYS:HA	2:E:446:PRO:O	2.14	0.46
2:E:576:LYS:O	2:E:580:ASN:ND2	2.48	0.46
2:F:287:LEU:HD12	2:F:288:ASP:H	1.81	0.46
2:E:398:LEU:HD12	2:E:457:PHE:CE2	2.51	0.46
2:E:423:THR:O	2:E:423:THR:OG1	2.33	0.46
3:B:28:ASP:HB3	3:B:32:TYR:OH	2.15	0.46
2:E:383:ASP:HA	2:E:386:LEU:HB2	1.97	0.46
1:A:799:ARG:HD2	1:A:799:ARG:HA	1.53	0.46
3:B:240:ASP:OD1	3:B:240:ASP:N	2.48	0.46
2:F:353:LEU:HB2	2:F:372:TYR:OH	2.15	0.46
1:A:770:ARG:HH22	3:B:154:LYS:HZ1	1.64	0.45
1:A:1252:HIS:O	1:A:1255:THR:HB	2.16	0.45
3:B:191:ASP:OD1	3:B:191:ASP:N	2.34	0.45
1:A:767:CYS:SG	1:A:770:ARG:HD2	2.56	0.45
2:E:189:GLY:CA	3:B:72:GLN:OE1	2.65	0.45
3:B:186:ASP:OD1	3:B:187:VAL:N	2.50	0.45
1:A:1324:LEU:HD12	1:A:1325:LYS:H	1.81	0.45
2:E:384:ARG:CG	2:E:387:PHE:HB3	2.44	0.45
3:B:224:ILE:HG12	3:B:224:ILE:O	2.16	0.45
2:E:260:GLU:HG2	2:E:262:PHE:H	1.80	0.45
2:E:450:ASP:N	2:E:450:ASP:OD1	2.50	0.45
3:B:41:LYS:HA	3:B:42:PRO:HD3	1.74	0.45
4:C:285:LEU:HD23	4:C:285:LEU:HA	1.80	0.45
4:D:299:TYR:O	4:D:303:ARG:HG3	2.16	0.45
1:A:941:LYS:HG2	1:A:942:LEU:HD23	1.99	0.45



	las puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1289:GLN:O	1:A:1292:SER:OG	2.35	0.45
2:E:472:THR:O	2:E:473:LYS:HG3	2.17	0.45
2:E:189:GLY:N	3:B:72:GLN:OE1	2.50	0.45
2:E:470:SER:HB2	2:E:471:PRO:HD2	1.98	0.45
1:A:972:LYS:HE3	1:A:972:LYS:HB2	1.79	0.45
1:A:1129:ILE:HG12	1:A:1279:SER:HB2	1.99	0.45
2:E:385:GLN:N	2:E:385:GLN:CD	2.71	0.44
4:D:293:LEU:HA	4:D:297:LEU:HB2	2.00	0.44
1:A:770:ARG:CG	1:A:774:CYS:HB2	2.47	0.44
1:A:827:THR:HG21	1:A:866:VAL:HG21	1.98	0.44
2:E:187:TRP:HB3	3:B:72:GLN:HB3	1.98	0.44
1:A:1175:ARG:NH2	1:A:1230:GLN:O	2.46	0.44
1:A:1142:THR:O	1:A:1146:ILE:HG12	2.18	0.44
1:A:1171:GLU:O	1:A:1174:THR:HG22	2.17	0.44
1:A:1340:SER:HB3	1:A:1347:THR:HG23	1.98	0.44
4:C:348:ASP:OD2	4:C:350:GLN:HG3	2.18	0.44
2:E:381:LEU:HB3	2:E:384:ARG:CB	2.25	0.44
2:E:554:LYS:HE3	2:E:554:LYS:HB3	1.65	0.44
2:F:556:TYR:OH	2:F:560:MET:SD	2.68	0.44
1:A:872:ASP:O	1:A:875:ARG:N	2.50	0.44
1:A:931:LEU:HD12	1:A:931:LEU:HA	1.83	0.44
1:A:965:HIS:CE1	1:A:967:LEU:HB2	2.53	0.44
2:E:180:ASN:ND2	2:E:180:ASN:H	2.16	0.44
2:E:452:VAL:O	2:E:454:ARG:N	2.51	0.44
3:B:14:LYS:H	3:B:14:LYS:HD2	1.83	0.44
3:B:274:ASP:O	3:B:282:GLY:HA3	2.18	0.44
3:B:279:ASP:CG	3:B:314:THR:HG22	2.38	0.44
4:C:395:GLU:OE1	4:C:395:GLU:N	2.50	0.44
4:D:254:VAL:HG21	4:D:289:PHE:CZ	2.53	0.44
1:A:942:LEU:HD13	2:E:428:TRP:CG	2.53	0.43
2:E:176:THR:HG22	3:B:63:ILE:HG12	2.01	0.43
2:F:576:LYS:HD3	2:F:576:LYS:HA	1.85	0.43
1:A:945:THR:O	1:A:949:ILE:HG12	2.18	0.43
4:C:382:SER:O	4:C:383:ASP:HB2	2.17	0.43
1:A:698:ASP:OD2	1:A:699:LEU:N	2.48	0.43
1:A:871:TYR:HE2	1:A:894:VAL:HG23	1.83	0.43
1:A:1020:LEU:HG	1:A:1273:ARG:HG2	2.00	0.43
2:E:397:LYS:HA	2:E:397:LYS:HD3	1.73	0.43
3:B:86:LEU:HD21	3:B:116:LEU:HG	2.00	0.43
4:C:355:LEU:O	4:C:359:THR:HG23	2.19	0.43
1:A:871:TYR:CE2	1:A:894:VAL:HG23	2.53	0.43



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:E:372:TYR:HD1	4:C:241:LYS:HE3	1.84	0.43	
4:C:257:VAL:HG22	4:C:373:TYR:CZ	2.54	0.43	
1:A:663:ASN:HA	2:F:547:ILE:HG12	1.99	0.43	
1:A:866:VAL:O	1:A:870:VAL:HG23	2.18	0.43	
3:B:82:TYR:C	3:B:82:TYR:CD2	2.85	0.43	
4:C:345:THR:HB	4:C:347:MET:H	1.84	0.43	
1:A:928:LEU:HD21	3:B:356:ARG:HB2	2.01	0.43	
2:E:381:LEU:N	2:E:381:LEU:HD23	2.32	0.43	
3:B:150:HIS:O	3:B:164:ASN:ND2	2.48	0.43	
3:B:197:PHE:CD1	3:B:203:VAL:HG21	2.54	0.43	
4:D:285:LEU:HD21	4:D:335:ILE:HD11	1.99	0.43	
1:A:1037:LYS:HA	1:A:1037:LYS:HD3	1.69	0.43	
1:A:1315:GLN:HE22	1:A:1325:LYS:HD3	1.83	0.43	
1:A:930:HIS:HD2	2:E:393:GLN:NE2	2.17	0.43	
3:B:112:VAL:O	3:B:112:VAL:HG13	2.18	0.43	
4:D:236:TRP:CZ2	2:F:372:TYR:CA	3.00	0.43	
1:A:984:ILE:O	1:A:988:ILE:HG13	2.18	0.43	
2:E:388:ASN:HD22	2:E:388:ASN:HA	1.37	0.43	
4:D:240:THR:HG21	2:F:371:GLN:HA	2.01	0.43	
4:D:309:LEU:HD13	4:D:309:LEU:HA	1.91	0.43	
4:D:395:GLU:HA	4:D:398:ALA:HB3	2.01	0.43	
1:A:770:ARG:HH12	3:B:154:LYS:NZ	2.17	0.42	
1:A:955:ILE:O	1:A:959:GLN:HG3	2.18	0.42	
1:A:1228:LEU:O	1:A:1232:TYR:HB2	2.19	0.42	
1:A:1299:ASN:ND2	1:A:1299:ASN:H	2.17	0.42	
1:A:1009:ARG:HH12	1:A:1071:ARG:HB3	1.84	0.42	
1:A:1300:MET:HG2	1:A:1317:ILE:HG13	2.01	0.42	
4:D:220:ILE:HB	4:D:356:ILE:HD11	2.01	0.42	
3:B:19:ARG:HB2	3:B:140:ASP:HB2	2.01	0.42	
1:A:770:ARG:HG2	1:A:774:CYS:HB2	2.01	0.42	
1:A:1076:LYS:HA	1:A:1079:ARG:HH12	1.84	0.42	
1:A:1151:TRP:HE3	1:A:1249:LEU:HD11	1.85	0.42	
3:B:83:ILE:HA	3:B:83:ILE:HD13	1.49	0.42	
4:D:293:LEU:HD21	4:D:326:TYR:CE2	2.54	0.42	
4:D:338:LEU:O	4:D:342:ILE:HG22	2.19	0.42	
2:F:367:GLY:HA3	2:F:371:GLN:HE21	1.84	0.42	
2:F:564:ARG:O	2:F:568:GLN:HG2	2.19	0.42	
1:A:1078:LYS:HE2	1:A:1078:LYS:HB2	1.92	0.42	
2:E:187:TRP:HE3	2:E:187:TRP:H	1.60	0.42	
2:E:440:CYS:HB2	2:E:466:CYS:SG	2.60	0.42	
3:B:88:ARG:CG	3:B:88:ARG:NH1	2.72	0.42	



	i i i i i i i i i i i i i i i i i i i	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
4:C:243:LYS:O	4:C:390:THR:OG1	2.37	0.42	
4:D:224:ILE:HB	4:D:229:LYS:HE3	2.01	0.42	
2:F:552:PHE:HA	2:F:555:ILE:HG22	2.01	0.42	
1:A:826:ARG:O	1:A:829:GLN:HG2	2.20	0.42	
1:A:904:GLU:CD	2:E:116:ASN:CB	2.88	0.42	
2:E:177:GLU:OE1	3:B:62:GLU:OE2	2.38	0.42	
3:B:29:VAL:HG12	3:B:122:ILE:HG21	2.00	0.42	
1:A:798:HIS:HD2	1:A:800:LYS:NZ	2.17	0.42	
1:A:1136:PHE:CD1	1:A:1273:ARG:HD2	2.55	0.42	
4:D:270:GLU:HB3	2:F:556:TYR:HE1	1.85	0.42	
1:A:690:ASN:HA	1:A:693:SER:OG	2.20	0.42	
1:A:862:ILE:O	1:A:866:VAL:HG13	2.19	0.42	
1:A:975:LEU:HB2	1:A:1314:ILE:HB	2.02	0.42	
1:A:996:ILE:HG22	1:A:1007:LYS:HG3	2.01	0.42	
4:D:253:THR:OG1	4:D:254:VAL:N	2.52	0.42	
4:D:297:LEU:HD12	4:D:297:LEU:HA	1.86	0.42	
4:D:348:ASP:CG	4:D:351:SER:HG	2.21	0.42	
1:A:871:TYR:O	1:A:876:GLY:N	2.52	0.42	
1:A:1233:ASN:OD1	1:A:1235:LYS:HE2	2.20	0.42	
1:A:1003:SER:O	1:A:1007:LYS:N	2.47	0.41	
1:A:1014:LEU:O	1:A:1018:ILE:HG12	2.19	0.41	
2:E:107:LYS:NZ	2:E:107:LYS:HB2	2.35	0.41	
2:E:574:ILE:O	2:E:578:VAL:HG22	2.19	0.41	
3:B:141:VAL:HA	3:B:305:MET:O	2.20	0.41	
2:E:351:PHE:CE1	4:C:333:ARG:HD3	2.54	0.41	
4:D:254:VAL:HG12	4:D:323:ILE:HG13	2.02	0.41	
1:A:918:GLU:OE2	2:E:128:LEU:CD1	2.55	0.41	
2:E:113:LEU:HD12	2:E:113:LEU:H	1.82	0.41	
2:F:355:ASN:HA	2:F:358:LYS:HZ3	1.85	0.41	
2:E:372:TYR:HB3	4:C:241:LYS:HD2	2.02	0.41	
3:B:34:TYR:HD2	3:B:41:LYS:HA	1.86	0.41	
3:B:40:MET:SD	3:B:313:TYR:CE1	3.13	0.41	
2:F:365:LYS:HA	2:F:365:LYS:HD3	1.77	0.41	
2:E:409:SER:OG	2:E:410:ASN:N	2.53	0.41	
2:E:493:LYS:HA	2:E:493:LYS:HD2	1.73	0.41	
3:B:8:PHE:CD2	3:B:248:ARG:HD2	2.54	0.41	
2:F:362:PRO:O	2:F:365:LYS:NZ	2.46	0.41	
1:A:684:GLU:O	1:A:688:ILE:HG13	2.21	0.41	
1:A:910:ARG:HG3	1:A:911:GLU:N	2.36	0.41	
1:A:1028:LYS:O	1:A:1031:GLU:HG2	2.21	0.41	
1:A:1078:LYS:HA	1:A:1081:ASN:HD21	1.85	0.41	



Atom-1	Atom-2	Interatomic	Clash
	1100111 2	distance (Å)	overlap (Å)
1:A:1165:ASN:OD1	1:A:1204:TYR:N	2.51	0.41
3:B:251:PHE:CZ	3:B:255:ILE:HG13	2.55	0.41
3:B:86:LEU:HA	3:B:86:LEU:HD23	1.76	0.41
4:D:236:TRP:CD2	2:F:372:TYR:CD2	2.97	0.41
2:E:442:TYR:CE2	2:E:465:LYS:HB2	2.56	0.41
1:A:808:PHE:O	1:A:811:GLU:HG3	2.21	0.41
1:A:842:THR:O	1:A:846:LYS:HG3	2.21	0.41
1:A:1149:ARG:HA	1:A:1149:ARG:HD2	1.87	0.41
1:A:1223:TRP:HA	1:A:1226:GLU:HG3	2.02	0.41
2:E:305:GLU:HB2	2:E:347:ASN:HD21	1.85	0.41
2:E:402:ASN:N	2:E:403:PRO:HD3	2.36	0.41
3:B:40:MET:HG3	3:B:44:ARG:HH21	1.86	0.41
4:D:235:ASP:O	4:D:239:VAL:HG12	2.20	0.41
1:A:1009:ARG:HG2	1:A:1074:TYR:CZ	2.56	0.41
1:A:1228:LEU:HD13	1:A:1232:TYR:CD2	2.56	0.41
2:E:126:GLU:O	2:E:126:GLU:CG	2.69	0.41
2:E:184:THR:OG1	3:B:73:GLU:CG	2.69	0.41
2:E:450:ASP:OD2	3:B:365:THR:OG1	2.36	0.41
2:E:177:GLU:H	2:E:177:GLU:HG2	1.52	0.40
2:E:316:MET:SD	2:E:316:MET:N	2.94	0.40
2:E:515:GLN:HG3	2:E:516:ASN:N	2.25	0.40
3:B:113:PHE:CE2	3:B:116:LEU:HA	2.57	0.40
4:C:258:LEU:HD23	4:C:258:LEU:HA	1.93	0.40
4:C:341:LEU:O	4:C:344:SER:OG	2.32	0.40
2:F:320:LYS:HA	2:F:323:GLU:HG3	2.03	0.40
2:E:578:VAL:HG11	2:F:575:ASP:CG	2.40	0.40
3:B:174:LEU:HD11	3:B:203:VAL:CG2	2.51	0.40
1:A:959:GLN:OE1	1:A:974:GLN:NE2	2.54	0.40
2:E:184:THR:OG1	3:B:73:GLU:HG2	2.21	0.40
2:E:306:CYS:O	2:E:310:ILE:HG12	2.22	0.40
2:E:375:GLU:OE1	2:E:376:ASN:ND2	2.54	0.40
1:A:767:CYS:SG	1:A:770:ARG:HB2	2.61	0.40
1:A:823:SER:O	1:A:827:THR:HG23	2.21	0.40
2:E:339:LEU:HB3	4:C:288:TYR:OH	2.20	0.40
3:B:317:ASN:O	3:B:321:THR:OG1	2.28	0.40
1:A:1005:PRO:O	1:A:1009:ARG:HG3	2.21	0.40
2:E:336:PHE:HD2	4:C:284:GLY:HA3	1.86	0.40
2:E:387:PHE:O	2:E:390:SER:HB2	2.21	0.40
4:C:338:LEU:O	4:C:342:ILE:HG13	2.21	0.40
4:D:248:LEU:HD21	4:D:326:TYR:CZ	2.56	0.40
4:D:262:GLU:HB2	4:D:282:CYS:SG	2.61	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	$\mathbf{n}$ tiles
1	А	598/1536~(39%)	573~(96%)	24~(4%)	1 (0%)	47	81
2	Е	343/684~(50%)	293~(85%)	41 (12%)	9~(3%)	5	35
2	F	152/684~(22%)	150 (99%)	2(1%)	0	100	100
3	В	383/433~(88%)	362~(94%)	18 (5%)	3~(1%)	19	60
4	С	181/401~(45%)	171 (94%)	9~(5%)	1 (1%)	25	65
4	D	183/401~(46%)	179~(98%)	4 (2%)	0	100	100
4	G	63/401~(16%)	62~(98%)	1 (2%)	0	100	100
5	a	95/136~(70%)	95 (100%)	0	0	100	100
5	е	97/136~(71%)	96~(99%)	1 (1%)	0	100	100
6	b	77/103~(75%)	72 (94%)	5~(6%)	0	100	100
6	f	80/103~(78%)	77~(96%)	3~(4%)	0	100	100
7	с	105/130~(81%)	101 (96%)	4 (4%)	0	100	100
7	g	105/130~(81%)	103~(98%)	2(2%)	0	100	100
8	d	92/126~(73%)	89~(97%)	3 (3%)	0	100	100
8	h	92/126~(73%)	88 (96%)	4 (4%)	0	100	100
All	All	2646/5530 (48%)	2511 (95%)	121 (5%)	14 (0%)	32	68

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Е	171	LEU
2	Е	174	ASN
2	Е	470	SER
3	В	114	ASP
3	В	115	GLY



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$\mathbf{Mol}$	Chain	$\operatorname{Res}$	Type
1	А	873	LYS
2	Е	125	ARG
2	Е	392	GLY
2	Е	517	ASN
4	С	241	LYS
2	Е	378	LYS
2	Е	471	PRO
2	Е	393	GLN
3	В	110	CYS

#### 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	Perce	entiles
1	А	560/1391~(40%)	532~(95%)	28~(5%)	24	51
2	Е	332/653~(51%)	293~(88%)	39 (12%)	5	23
2	F	148/653~(23%)	143 (97%)	5(3%)	37	61
3	В	326/367~(89%)	299~(92%)	27 (8%)	11	37
4	С	172/359~(48%)	159 (92%)	13 (8%)	13	40
4	D	174/359~(48%)	170 (98%)	4 (2%)	50	70
4	G	56/359~(16%)	56 (100%)	0	100	100
5	a	85/111 (77%)	77 (91%)	8 (9%)	8	30
5	е	86/111 (78%)	79~(92%)	7 (8%)	11	37
6	b	64/79~(81%)	61 (95%)	3(5%)	26	53
6	f	67/79~(85%)	64 (96%)	3 (4%)	27	54
7	с	83/100 (83%)	80 (96%)	3 (4%)	35	60
7	g	83/100 (83%)	78 (94%)	5 (6%)	19	46
8	d	80/105~(76%)	74 (92%)	6 (8%)	13	40
8	h	80/105 (76%)	76 (95%)	4 (5%)	24	51
All	All	2396/4931 (49%)	2241 (94%)	155 (6%)	21	44



$\mathbf{Mol}$	Chain	Res	Type
1	А	690	ASN
1	А	697	LEU
1	А	707	ASP
1	А	751	PHE
1	А	778	LEU
1	А	781	GLU
1	А	799	ARG
1	А	811	GLU
1	А	815	HIS
1	А	816	GLU
1	А	850	LYS
1	А	903	GLU
1	А	929	ASP
1	А	936	LYS
1	А	939	ASP
1	А	1012	ASP
1	А	1021	PHE
1	А	1065	LEU
1	А	1150	HIS
1	А	1153	THR
1	А	1191	LEU
1	А	1228	LEU
1	А	1249	LEU
1	А	1278	THR
1	А	1299	ASN
1	А	1316	TYR
1	А	1335	LYS
1	А	1341	TYR
2	Е	105	ASP
2	Ε	107	LYS
2	E	110	VAL
2	Е	111	THR
2	Е	113	LEU
2	Е	114	PRO
2	Е	123	ILE
2	Е	125	ARG
2	Е	126	GLU
2	Е	177	GLU
2	Ε	178	GLU
2	Е	179	SER
2	Е	180	ASN
2	Е	185	ILE

All (155) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
2	Е	187	TRP
2	Е	272	PHE
2	Е	295	ASN
2	Е	320	LYS
2	Е	375	GLU
2	Е	379	ILE
2	Е	384	ARG
2	Е	386	LEU
2	Е	387	PHE
2	Е	388	ASN
2	Е	402	ASN
2	Е	404	ASP
2	Е	420	CYS
2	Е	443	CYS
2	Ε	450	ASP
2	Е	454	ARG
2	Е	491	VAL
2	Е	496	ARG
2	Е	504	LEU
2	Е	514	TYR
2	Е	540	THR
2	Е	543	ASP
2	Е	545	ASN
2	Е	546	SER
2	Е	575	ASP
3	В	11	ILE
3	В	14	LYS
3	В	31	ASN
3	В	32	TYR
3	В	38	HIS
3	В	40	MET
3	В	41	LYS
3	В	72	GLN
3	В	83	ILE
3	В	84	ASP
3	В	86	LEU
3	В	87	SER
3	В	88	ARG
3	В	89	VAL
3	B	90	THR
3	В	108	ASP
3	В	111	PRO



Mol	Chain	Res	Type
3	В	113	PHE
3	В	114	ASP
3	В	136	ARG
3	В	150	HIS
3	В	201	ASP
3	В	240	ASP
3	В	274	ASP
3	В	280	ARG
3	В	281	LEU
3	В	350	ASP
4	С	222	LEU
4	С	235	ASP
4	С	241	LYS
4	С	242	ASP
4	С	281	TYR
4	С	285	LEU
4	С	288	TYR
4	С	292	CYS
4	С	293	LEU
4	С	307	ASP
4	С	376	ASP
4	С	390	THR
4	С	393	GLN
4	D	266	SER
4	D	288	TYR
4	D	315	LYS
4	D	348	ASP
2	F	272	PHE
2	F	276	ASP
2	F	369	ARG
2	F	560	MET
2	F	570	GLN
5	a	80	THR
5	a	81	ASP
5	a	86	SER
5	a	87	SER
5	a	89	VAL
5	a	90	MET
5	a	133	GLU
5	a	134	ARG
6	b	30	THR
6	b	92	ARG



Mol	Chain	Res	Type
6	b	96	THR
7	с	31	HIS
7	с	76	THR
7	с	118	LYS
8	d	31	ARG
8	d	33	ARG
8	d	34	LYS
8	d	51	ASP
8	d	112	SER
8	d	113	GLU
5	е	80	THR
5	е	81	ASP
5	е	86	SER
5	е	87	SER
5	е	89	VAL
5	е	90	MET
5	е	134	ARG
6	f	30	THR
6	f	82	THR
6	f	92	ARG
7	g	15	LYS
7	g	16	THR
7	g	31	HIS
7	g	50	TYR
7	g	76	THR
8	h	31	ARG
8	h	32	SER
8	h	33	ARG
8	h	106	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	779	ASN
1	А	798	HIS
1	А	829	GLN
1	А	930	HIS
1	А	1081	ASN
1	А	1283	GLN
1	А	1299	ASN
2	Ε	314	ASN
2	Ē	325	ASN



$\mathbf{Mol}$	Chain	Res	Type
2	Е	347	ASN
2	Е	350	GLN
2	Е	352	GLN
2	Е	376	ASN
2	Е	388	ASN
2	Е	516	ASN
2	Е	521	GLN
2	Е	541	GLN
2	Е	580	ASN
3	В	31	ASN
3	В	38	HIS
3	В	76	GLN
3	В	150	HIS
3	В	177	HIS
3	В	188	HIS
3	В	270	GLN
4	С	305	GLN
4	С	380	ASN
4	С	393	GLN
4	D	317	GLN
4	D	375	ASN
4	D	380	ASN
2	F	259	ASN
2	F	355	ASN
5	a	125	GLN
6	b	27	GLN
6	b	93	GLN
8	d	49	HIS
5	е	125	GLN
8	h	49	HIS
8	h	95	GLN
4	G	18	HIS

#### 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)

Of 7 ligands modelled in this entry, 7 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-37367. 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: 140



Y Index: 140



Z Index: 140

#### 6.2.2 Raw map



X Index: 140

Y Index: 140

Z Index: 140

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: 154



Y Index: 168



Z Index: 121

#### 6.3.2 Raw map



X Index: 154

Y Index: 134

Z Index: 121

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 0.012. 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.

#### 6.6 Mask visualisation (i)

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



# 7 Map analysis (i)

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

## 7.1 Map-value distribution (i)



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



## 7.2 Volume estimate (i)



The volume at the recommended contour level is 279  $\rm nm^3;$  this corresponds to an approximate mass of 252 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 0.227  ${\rm \AA^{-1}}$ 



## 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 0.227  ${\rm \AA^{-1}}$ 



### 8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.35	7.03	4.59
Unmasked-calculated*	6.41	9.30	6.86

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.41 differs from the reported value 4.4 by more than 10 %



# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-37367 and PDB model 8W9F. Per-residue inclusion information can be found in section 3 on page 7.

## 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.012 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 (0.012).



### 9.4 Atom inclusion (i)



At the recommended contour level, 61% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5710	0.1560
А	0.3860	0.0520
В	0.6130	0.0480
С	0.4590	0.0390
D	0.1660	0.0200
Е	0.2740	0.0410
F	0.0950	0.0210
G	0.0290	0.0430
a	0.7360	0.3290
b	0.7980	0.3710
с	0.8160	0.3750
d	0.8030	0.3820
e	0.8340	0.3790
f	0.8600	0.4020
g	0.7880	0.3750
h	0.8230	0.3800
i	0.8890	0.2500
j	0.9020	0.2260

