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PDB ID	:	7T3C
EMDB ID	:	EMD-25654
Title	:	GATOR1-RAG-RAGULATOR - Dual Complex
Authors	:	Egri, S.B.; Shen, K.
Deposited on	:	2021-12-07
Resolution	:	4.00 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 43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.00 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	Quality of chain	Quality of chain								
1	В	380	68%	26%	5%							
2	А	1603	45% 17%	38%	_							
3	Н	124	7% 71%	26%	••							
3	0	124	73%	23%	•							
4	G	125	• 59%	40%	-							
4	Ν	125	57%	41%	••							
5	J	91	77%	23%								
5	Q	91	5%	22%								



Mol	Chain	Length	Quality of	of chain			
6	Ι	99	30%		20%	14%	
6	Р	99	27%	27% •			
7	F	161	57%	31%	2		
7	М	161	52%	19%	29%		
8	С	569	5 6%	15%	29%		
9	D	313	59%		34%	• 5%	
9	Κ	313	61%		34%	• •	
10	Е	399	6% 51%	25%	•	23%	
11	L	399	49%	26%	•	23%	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	AF3	Κ	502	-	-	Х	-



2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 32452 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 GATOR complex protein NPRL2.

Mol	Chain	Residues		At	AltConf	Trace			
1	В	362	Total 2918	C 1868	N 486	0 546	S 18	0	0

• Molecule 2 is a protein called GATOR complex protein DEPDC5.

Mol	Chain	Residues		Α	AltConf	Trace			
2	Λ	000	Total	С	Ν	Ο	\mathbf{S}	0	0
2	А	990	8120	5243	1347	1485	45	0	0

• Molecule 3 is a protein called Ragulator complex protein LAMTOR3.

Mol	Chain	Residues		At	oms		AltConf	Trace	
3 H	101	Total	С	Ν	Ο	S	0	0	
	11	121	939	604	158	176	1	0	0
2	3 O	190	Total	С	Ν	Ο	\mathbf{S}	0	0
3		120	934	601	157	175	1	0	0

• Molecule 4 is a protein called Ragulator complex protein LAMTOR2.

Mol	Chain	Residues		At	oms		AltConf	Trace
4 G	195	Total	С	Ν	Ο	\mathbf{S}	0	0
	G	120	944	593	162	182	7	0
4 N	194	Total	С	Ν	Ο	S	0	0
	IN	124	936	588	161	181	6	0

• Molecule 5 is a protein called Ragulator complex protein LAMTOR5.

Mol	Chain	Residues		At	oms		AltConf	Trace	
5	5 I	01	Total	С	Ν	Ο	\mathbf{S}	1	0
0 0	J	91	672	409	116	139	8		0
5	Q	01	Total	С	Ν	0	S	0	0
0		31	666	406	115	138	7		



• Molecule 6 is a protein called Ragulator complex protein LAMTOR4.

Mol	Chain	Residues		At	oms	AltConf	Trace		
6	T	85	Total	С	Ν	0	\mathbf{S}	0	0
0	T	00	647	407	116	123	1	0	
6	D	07	Total	С	Ν	Ο	\mathbf{S}	0	0
0	Г	91	738	460	135	140	3		

• Molecule 7 is a protein called Ragulator complex protein LAMTOR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	111	Total 861	С 541	N 148	0 170	$\frac{S}{2}$	0	0
7	М	115	Total 892	C 560	N 155	0 175	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 8 is a protein called GATOR complex protein NPRL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	С	406	Total 3242	C 2087	N 568	O 568	S 19	0	0

• Molecule 9 is a protein called Ras-related GTP-binding protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
Q	р	296	Total	С	Ν	Ο	\mathbf{S}	0	0
	D		2429	1543	423	446	17		
0	K	200	Total	С	Ν	0	\mathbf{S}	0	0
9	Λ	500	2459	1561	428	452	18	U	0

• Molecule 10 is a protein called Ras-related GTP-binding protein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Е	306	Total 2471	C 1590	N 398	0 469	S 14	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Е	92	ALA	PHE	engineered mutation	UNP Q9HB90

• Molecule 11 is a protein called Ras-related GTP-binding protein C.



Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	307	Total 2488	C 1603	N 401	O 470	S 14	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	75	ASN	SER	engineered mutation	UNP Q9HB90

• Molecule 12 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		Ate	oms			AltConf
19	Л	1	Total	С	Ν	Ο	Р	0
	D	1	28	10	5	11	2	0
19	F	1	Total	С	Ν	Ο	Р	0
	Ľ	1	28	10	5	11	2	0
19	K	1	Total	С	Ν	0	Р	0
	Γ	1	28	10	5	11	2	0

• Molecule 13 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF₃) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	AltConf
13	D	1	Total Al F 4 1 3	0
13	Е	1	TotalAlF413	0
13	K	1	TotalAlF413	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: GATOR complex protein NPRL2











• Molecule 6: Rag	gulator complex prot	ein LAMTOR4		
Chain I:	30% 66%	2	20% 14%	
MET THR A.B. A.B. A.C. C.C. C.C. B.1.0 M.1.1 M.1.1 L12	P13 D14 D14 D16 V20 V20 V20 V20 V20 V20 V20 V20 V20 V20	G31 B32 L33 B34 B36 B37 G38 A40 A40	843 843 450 450 450 61 155 155 155 155 155 155 155 155 155	MET MET V61 V61 V63 F63 K64 K65 K65 K65 F71 F72 F72
V77 880 880 883 888 888 8930 930 8930 8930	ALY ARG GLU PRO ASP VAL			
• Molecule 6: Rag	gulator complex prote	ein LAMTOR4		
Chain P:	71%		27%	
M1 12 83 84 14 16 16 10 17 19 10 10 10 11 11	112 113 114 014 015 119 119 119 121 121 121 127 127 127 127	G31 G31 L33 L33 E37 G38 G38 M54 M50 M60	V61 P62 F63 R64 R65 R65 R65 L66 S67 V68 V68 V68 V68 V63 T74	L75 L76 V77 V77 V79 880 880 881 881 881 883 883 883 883 883
V86 V87 K88 K88 K88 R93 R93 R93 R94 F95 F95 F95 F95 F95 F95 F95 F95 F95 F95	ASP VAL			
• Molecule 7: Rag	gulator complex prote	ein LAMTOR1		
Chain F:	57%	12%	31%	-
MET CYS CYS CYS CYS SER SER SER ASP GLU GLU ASP SER	GLM ASP ASP ASP GLU GLU CLU LEU LEU LEU LEU LEU SER SER SER SER	TRU LYR LYR LYR LLEU ALA GLY GLY ALA ALA PRU PRU TYR TYR SER	PR0 SER ALA ARG TARG L53 C154	L58 A59 K60 S63
D83	K104 L105 L115 L111 T112 S113 Q114 Q117 Q117 Q117 Q117 Q117 Q117 Q117	8121 8122 8122 8126 8126 8126 8134 8134 8147 V148 8147 V148	E153 L154 V155 G159 G159 TLE PR0	
• Molecule 7: Rag	gulator complex prote	ein LAMTOR1		
Chain M:	52%	19%	29%	-
MET OLY CYS CYS CYS SER SER SER SER ASN OLU ASP SER SER	GLN ASP ASP ASP ASP GLU GLU CLU CLU LEU LEU LEU LEU SER SER SER SER SER	THRO THRO THRO THRO LVB ASN ASN ASN ASN TYR HIS SER	PR0 SER A46 D49 M64 I66 I66	087 V68 Q74 Q74
H79 E80 884 788 788 788 788 790 192 192	V94 195 195 195 199 1100 1100 1100 1100 110	P107 L108 S110 S110 L111 T112 P115 Q117 V118 V118 V118 C119	8121 8121 8123 1124 1124 1143 1146	A150 K151 E152 E153 L154 V156 V156 P100 PR0
• Molecule 8: GA	TOR complex protei	n NPRL3		
Chain C:	56%	15%	29%	-









L300 GLU ARG VAL ASP GLY PRO CLYS HIS SER HIS SER LEU LEU MET MET

• Molecule 10: Ras-related GTP-binding protein C





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56117	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	52.6	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.763	Depositor
Minimum map value	-0.291	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	381.8, 381.8, 381.8	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: AF3, GDP

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).

Mal	Chain	Bond	lengths	B	ond angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	В	0.39	0/2977	0.76	5/4034~(0.1%)
2	А	0.46	0/8337	0.76	16/11305~(0.1%)
3	Н	0.36	0/956	0.67	2/1297~(0.2%)
3	0	0.33	0/951	0.63	0/1290
4	G	0.38	0/955	0.82	2/1293~(0.2%)
4	N	0.36	0/947	0.81	1/1283~(0.1%)
5	J	0.32	0/678	0.77	2/919~(0.2%)
5	Q	0.31	0/672	0.68	2/911~(0.2%)
6	Ι	0.34	0/654	0.67	0/883
6	Р	0.30	0/747	0.64	0/1008
7	F	0.30	0/877	0.55	0/1192
7	М	0.28	0/908	0.54	0/1234
8	С	0.33	0/3306	0.66	2/4483~(0.0%)
9	D	0.41	0/2474	0.78	2/3331~(0.1%)
9	Κ	0.42	0/2505	0.78	4/3374~(0.1%)
10	Е	0.41	0/2523	0.80	4/3407~(0.1%)
11	L	0.39	0/2541	0.84	5/3431~(0.1%)
All	All	0.39	0/33008	0.74	$47/\overline{44675~(0.1\%)}$

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	В	0	7
2	А	0	6
4	Ν	0	2
5	J	0	1
7	М	0	1
8	С	0	1



	J J J J J J J J J J J J J J J J J J J					
Mol	Chain	#Chirality outliers	#Planarity outliers			
9	D	0	3			
9	Κ	0	3			
10	Ε	0	5			
11	L	0	7			
All	All	0	36			

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
9	Κ	53	LEU	CA-CB-CG	9.56	137.29	115.30
4	Ν	49	ILE	CG1-CB-CG2	-8.28	93.19	111.40
2	А	1214	LEU	CA-CB-CG	8.27	134.32	115.30
10	Ε	353	ASP	CB-CG-OD1	7.90	125.41	118.30
10	Ε	69	LEU	CA-CB-CG	7.30	132.09	115.30
11	L	278	ASP	CB-CG-OD1	7.11	124.70	118.30
1	В	319	MET	CA-CB-CG	7.03	125.25	113.30
8	С	543	LEU	CA-CB-CG	6.81	130.97	115.30
9	D	169	LEU	CA-CB-CG	6.80	130.94	115.30
5	J	67	LEU	CA-CB-CG	6.69	130.69	115.30
2	А	369	MET	CB-CG-SD	6.68	132.45	112.40
11	L	236	LEU	CA-CB-CG	6.58	130.44	115.30
1	В	54	LEU	CA-CB-CG	6.41	130.03	115.30
2	А	1214	LEU	CB-CG-CD1	-6.24	100.39	111.00
2	А	114	MET	CB-CG-SD	6.24	131.11	112.40
11	L	311	ASP	CB-CG-OD1	6.20	123.88	118.30
2	А	266	GLU	CA-CB-CG	6.16	126.95	113.40
1	В	78	ARG	NE-CZ-NH2	-6.14	117.23	120.30
2	А	414	LEU	CA-CB-CG	6.07	129.25	115.30
3	Н	117	LEU	CA-CB-CG	6.00	129.09	115.30
5	Q	59	PRO	N-CD-CG	-5.97	94.24	103.20
2	А	425	LEU	CA-CB-CG	5.97	129.03	115.30
9	D	252	MET	CA-CB-CG	5.87	123.29	113.30
2	А	366	LEU	CA-CB-CG	5.85	128.75	115.30
11	L	246	LEU	CA-CB-CG	5.83	128.70	115.30
5	J	11	ASP	CB-CG-OD1	5.81	123.53	118.30
2	А	181	MET	CG-SD-CE	5.71	109.34	100.20
2	А	413	GLN	C-N-CA	5.65	135.82	121.70
2	А	51	LEU	CA-CB-CG	5.42	127.77	115.30
9	Κ	12	LEU	CA-CB-CG	5.41	127.75	115.30
1	В	260	LEU	CA-CB-CG	5.37	127.66	115.30
2	А	377	VAL	CG1-CB-CG2	-5.35	102.33	110.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
10	Е	270	ILE	CG1-CB-CG2	-5.35	99.63	111.40
10	Е	157	LEU	CA-CB-CG	5.32	127.53	115.30
3	Н	117	LEU	CB-CG-CD2	-5.31	101.97	111.00
9	Κ	252	MET	CA-CB-CG	5.30	122.31	113.30
5	Q	59	PRO	CA-N-CD	-5.26	104.14	111.50
11	L	240	LEU	CA-CB-CG	5.23	127.34	115.30
1	В	319	MET	CB-CG-SD	5.18	127.94	112.40
2	А	312	LEU	CB-CG-CD1	-5.17	102.21	111.00
9	Κ	252	MET	CB-CG-SD	5.10	127.71	112.40
2	А	1402	VAL	CG1-CB-CG2	-5.10	102.74	110.90
2	А	1460	PHE	C-N-CA	5.07	134.38	121.70
2	А	177	MET	CA-CB-CG	5.07	121.92	113.30
8	С	543	LEU	CB-CG-CD1	-5.05	102.41	111.00
4	G	1	MET	CB-CG-SD	5.03	127.48	112.40
4	G	74	MET	CB-CG-SD	5.03	127.48	112.40

There are no chirality outliers.

Mol	Chain	Res	Type	Group
2	А	258	VAL	Peptide
2	А	264	ARG	Peptide
2	А	297	ASP	Peptide
2	А	377	VAL	Peptide
2	А	381	LYS	Peptide
2	А	740	VAL	Peptide
1	В	23	ILE	Peptide
1	В	235	LEU	Peptide
1	В	267	TYR	Peptide
1	В	27	VAL	Peptide
1	В	28	PRO	Peptide
1	В	78	ARG	Peptide
1	В	79	ASN	Peptide
8	С	329	CYS	Peptide
9	D	129	MET	Peptide
9	D	272	VAL	Peptide
9	D	50	VAL	Peptide
10	Е	171	MET	Peptide
10	Ε	269	TYR	Peptide
10	Е	330	GLU	Peptide
10	Е	331	VAL	Peptide
10	Е	342	ARG	Peptide

All (36) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
5	J	2	GLU	Peptide
9	Κ	223	ARG	Peptide
9	Κ	249	PHE	Peptide
9	Κ	258	ASN	Peptide
11	L	117	PHE	Peptide
11	L	169	PRO	Peptide
11	L	170	ASP	Peptide
11	L	226	PHE	Peptide
11	L	264	VAL	Peptide
11	L	320	LEU	Peptide
11	L	333	LYS	Peptide
7	М	151	LYS	Peptide
4	N	86	ARG	Peptide
4	Ν	87	VAL	Peptide

Continued from previous page...

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	В	2918	0	2945	73	0
2	А	8120	0	7898	156	0
3	Н	939	0	963	23	0
3	0	934	0	958	21	0
4	G	944	0	955	37	0
4	Ν	936	0	943	41	0
5	J	672	0	670	14	0
5	Q	666	0	666	17	0
6	Ι	647	0	657	19	0
6	Р	738	0	753	23	0
7	F	861	0	858	20	0
7	М	892	0	894	22	0
8	С	3242	0	3342	57	0
9	D	2429	0	2423	89	0
9	K	2459	0	2458	77	0
10	Е	2471	0	2444	76	0
11	L	2488	0	2461	76	0
12	D	28	0	10	3	0
12	Е	28	0	12	1	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	K	28	0	12	3	0
13	D	4	0	0	0	0
13	Е	4	0	0	0	0
13	K	4	0	0	2	0
All	All	32452	0	32322	755	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (755) 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:A:9:LEU:O	2:A:82:TYR:HA	1.10	1.25
2:A:9:LEU:O	2:A:82:TYR:CA	2.07	1.02
11:L:152:GLU:O	11:L:156:ARG:HB2	1.62	0.99
9:K:255:ARG:O	11:L:314:SER:HA	1.63	0.98
2:A:1508:THR:O	2:A:1551:ASN:HB2	1.66	0.95
2:A:1204:CYS:HA	2:A:1258:TYR:O	1.67	0.93
2:A:942:TRP:HB2	2:A:1390:TRP:O	1.71	0.90
10:E:66:LEU:HA	10:E:141:ILE:O	1.73	0.89
2:A:866:LYS:O	2:A:869:MET:HB2	1.75	0.85
11:L:102:ASP:O	11:L:106:ASN:HB2	1.77	0.85
11:L:164:ALA:O	11:L:168:ASN:HB2	1.77	0.84
4:N:113:VAL:O	4:N:117:GLU:HB2	1.79	0.83
8:C:84:PHE:HB3	8:C:95:GLY:O	1.80	0.81
8:C:539:GLN:O	8:C:543:LEU:HB2	1.81	0.81
2:A:1483:VAL:O	2:A:1502:TYR:HA	1.82	0.79
10:E:212:HIS:HE2	10:E:214:SER:HG	1.28	0.78
10:E:356:PHE:O	10:E:360:ARG:HB2	1.84	0.78
8:C:408:THR:HA	8:C:554:THR:O	1.85	0.77
5:Q:64:VAL:HA	5:Q:76:ILE:O	1.86	0.75
10:E:141:ILE:HA	10:E:174:GLU:O	1.88	0.73
2:A:343:PHE:O	2:A:380:PHE:HA	1.89	0.73
10:E:176:PHE:HA	10:E:216:TYR:O	1.89	0.72
9:D:69:PHE:O	9:D:73:TYR:HB2	1.89	0.72
7:M:92:LEU:O	7:M:96:SER:HB3	1.89	0.71
2:A:41:ILE:HA	2:A:86:TYR:O	1.91	0.70
3:H:24:VAL:HA	3:H:89:VAL:O	1.92	0.70
5:Q:74:ILE:HA	5:Q:86:VAL:O	1.92	0.70
2:A:1373:TYR:HB2	2:A:1387:LYS:O	1.91	0.69
2:A:215:GLU:HG3	2:A:328:ARG:HE	1.57	0.69



	the page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:A:1572:LEU:O	2:A:1576:PHE:HB2	1.92	0.68
9:K:283:SER:O	9:K:287:LEU:HB2	1.95	0.67
2:A:1439:LEU:O	2:A:1548:TRP:HB3	1.94	0.66
3:O:99:ASN:HB3	3:O:102:LEU:HB2	1.77	0.66
2:A:1565:ASP:H	2:A:1568:PHE:HB3	1.59	0.66
4:G:25:LEU:HD13	4:G:50:SER:HB2	1.76	0.66
11:L:258:LYS:HB2	11:L:340:ILE:HG12	1.78	0.66
9:D:247:ALA:HA	10:E:321:ASN:HB2	1.78	0.66
10:E:355:ASN:O	10:E:359:PHE:HB3	1.96	0.66
4:N:81:ARG:HH12	4:N:102:PHE:HA	1.60	0.66
8:C:252:LEU:N	8:C:318:TYR:HH	1.95	0.65
11:L:316:ALA:HB3	11:L:328:LEU:HB3	1.78	0.65
9:D:230:LYS:HD2	10:E:298:ILE:HD13	1.79	0.65
4:N:49:ILE:HA	11:L:350:GLY:HA3	1.79	0.64
9:K:205:LEU:HA	9:K:271:TYR:O	1.97	0.64
8:C:87:LYS:HB2	8:C:92:ARG:HG3	1.79	0.64
9:K:252:MET:HB2	9:K:263:ILE:HB	1.80	0.64
9:K:83:ARG:HD2	9:K:84:ASN:HB2	1.78	0.64
1:B:227:LEU:O	1:B:231:GLY:N	2.32	0.63
4:G:6:ALA:HB1	7:F:154:LEU:HD22	1.81	0.63
2:A:1390:TRP:HB2	2:A:1393:VAL:HG21	1.79	0.63
9:D:254:VAL:HG11	10:E:295:VAL:HG11	1.79	0.63
10:E:175:VAL:O	10:E:215:PHE:HA	1.98	0.63
4:N:22:SER:HB3	4:N:95:TYR:HB2	1.80	0.62
9:K:256:ASN:HB3	9:K:259:PHE:HB3	1.79	0.62
1:B:51:GLN:HA	1:B:68:PRO:HG2	1.81	0.62
9:D:251:SER:HB2	10:E:319:LYS:HB2	1.82	0.62
2:A:24:VAL:HB	2:A:68:SER:HB3	1.82	0.62
10:E:180:VAL:HG11	10:E:217:LEU:HB2	1.80	0.62
2:A:860:PHE:HB2	2:A:875:TYR:HB2	1.82	0.62
10:E:349:LYS:HA	10:E:352:ILE:HB	1.82	0.61
9:D:203:VAL:HG22	9:D:274:VAL:HG12	1.82	0.61
9:D:206:PHE:O	9:D:270:THR:OG1	2.17	0.61
11:L:320:LEU:O	11:L:323:THR:N	2.34	0.61
2:A:770:TYR:HA	2:A:876:LEU:O	2.01	0.61
3:H:24:VAL:HG11	3:H:117:LEU:HD21	1.82	0.61
8:C:275:PRO:HG2	8:C:278:CYS:HB2	1.83	0.61
8:C:543:LEU:HA	8:C:546:LYS:HD2	1.81	0.61
11:L:247:LEU:HD12	11:L:363:ILE:HG21	1.82	0.61
3:H:102:LEU:HD22	5:J:47:VAL:HG21	1.83	0.60
2:A:303:GLN:O	2:A:305:ASN:ND2	2.35	0.60



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:N:17:THR:O	4:N:108:LYS:NZ	2.34	0.60
2:A:775:TYR:HB2	2:A:872:VAL:HB	1.83	0.60
2:A:107:GLN:NE2	2:A:138:ARG:O	2.34	0.60
8:C:195:LEU:HD22	8:C:205:LYS:HD2	1.83	0.60
2:A:945:ARG:NH2	2:A:1501:GLN:OE1	2.34	0.60
8:C:501:VAL:HG12	8:C:503:ALA:H	1.64	0.60
3:H:21:ALA:HB3	3:H:93:ILE:HB	1.82	0.60
11:L:259:ALA:HA	11:L:339:CYS:HA	1.83	0.60
9:D:87:VAL:HG12	9:D:121:LYS:HG3	1.82	0.60
11:L:274:SER:HA	11:L:277:VAL:HB	1.84	0.60
4:N:51:SER:OG	11:L:349:LYS:N	2.34	0.60
5:Q:64:VAL:HB	6:P:69:VAL:HB	1.84	0.60
9:D:270:THR:OG1	9:D:271:TYR:N	2.35	0.59
9:K:27:ILE:HD11	9:K:212:LEU:HD21	1.83	0.59
4:N:118:GLU:HG2	4:N:119:PRO:HD3	1.84	0.59
11:L:289:ILE:HA	11:L:292:VAL:HG12	1.83	0.59
2:A:260:GLN:NE2	2:A:1435:LEU:O	2.36	0.59
8:C:329:CYS:SG	8:C:537:ARG:NH1	2.75	0.59
2:A:406:SER:HB2	2:A:742:VAL:HA	1.84	0.59
2:A:106:ASP:OD1	2:A:328:ARG:NH1	2.36	0.59
4:N:16:ASN:ND2	4:N:36:SER:O	2.35	0.59
9:D:266:PHE:HB2	9:D:272:VAL:HG22	1.85	0.58
2:A:885:GLN:HA	2:A:908:PHE:O	2.02	0.58
9:D:245:LEU:O	10:E:322:ASN:ND2	2.36	0.58
9:K:248:SER:H	11:L:321:ASN:HB3	1.68	0.58
4:G:13:GLN:O	5:J:1:MET:N	2.36	0.58
9:D:49:HIS:HA	9:D:58:LEU:O	2.04	0.58
9:D:291:ARG:O	9:D:295:LYS:NZ	2.37	0.58
9:K:129:MET:HB3	9:K:137:ARG:HG2	1.84	0.58
8:C:515:ARG:O	8:C:518:HIS:NE2	2.37	0.58
4:N:102:PHE:HB2	5:Q:30:ASN:H	1.68	0.58
11:L:228:ALA:HA	11:L:231:LYS:HD2	1.86	0.57
9:D:32:ILE:HG21	9:D:34:ARG:HH21	1.70	0.57
9:K:223:ARG:HD3	9:K:227:ARG:HE	1.69	0.57
11:L:318:ILE:HB	11:L:326:LEU:HB2	1.85	0.57
10:E:84:LYS:HG3	10:E:264:VAL:HG12	1.86	0.57
3:O:72:ILE:HG23	3:O:81:VAL:HG22	1.87	0.57
4:N:73:ILE:HD12	4:N:84:ILE:HB	1.85	0.57
2:A:772:GLU:OE2	9:K:38:ARG:NH1	2.38	0.57
1:B:174:VAL:HB	1:B:235:LEU:O	2.05	0.57
10:E:141:ILE:HG12	10:E:174:GLU:HB3	1.86	0.57



	t i c	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:A:44:PRO:HD3	2:A:85:VAL:HG12	1.86	0.57
10:E:185:ASP:HA	10:E:188:LYS:HD2	1.87	0.57
6:P:77:VAL:HG13	6:P:86:VAL:HG22	1.87	0.57
2:A:41:ILE:HG12	2:A:87:VAL:HG22	1.87	0.57
9:D:276:MET:HG3	9:D:279:PRO:HD2	1.87	0.57
1:B:121:MET:O	1:B:125:LYS:NZ	2.38	0.56
2:A:1583:ARG:NH1	2:A:1584:ASP:OD2	2.37	0.56
9:D:266:PHE:H	9:D:271:TYR:HA	1.70	0.56
3:O:75:TYR:HA	4:N:70:LEU:HA	1.86	0.56
11:L:258:LYS:HE3	11:L:274:SER:HB2	1.87	0.56
1:B:379:TRP:HB2	8:C:369:SER:HB2	1.86	0.56
2:A:356:ARG:NH1	2:A:909:SER:O	2.39	0.56
11:L:352:ILE:O	11:L:356:PHE:HB2	2.05	0.56
1:B:235:LEU:HB2	1:B:318:LEU:HD13	1.87	0.56
2:A:308:GLU:O	2:A:312:LEU:HB2	2.05	0.56
2:A:319:LYS:NZ	2:A:1427:PRO:O	2.38	0.56
6:I:76:LEU:HB2	6:I:89:ARG:HH21	1.71	0.56
8:C:560:VAL:O	8:C:564:PHE:HB2	2.04	0.56
9:D:258:ASN:ND2	10:E:299:TYR:O	2.39	0.56
6:P:89:ARG:NH1	7:M:119:LEU:O	2.37	0.56
9:D:252:MET:HG3	9:D:263:ILE:HD13	1.87	0.56
2:A:170:MET:HG2	2:A:215:GLU:HB2	1.88	0.56
2:A:782:ASP:HB3	2:A:786:ARG:HH12	1.70	0.56
10:E:254:SER:OG	10:E:355:ASN:ND2	2.33	0.56
8:C:483:THR:HG23	8:C:510:LEU:HD22	1.87	0.56
9:K:121:LYS:NZ	9:K:179:GLN:O	2.34	0.56
3:O:96:SER:O	5:Q:27:GLN:NE2	2.39	0.56
1:B:6:ARG:N	1:B:140:ASN:OD1	2.39	0.56
11:L:247:LEU:HG	11:L:359:PHE:HE2	1.71	0.56
1:B:263:ALA:O	1:B:267:TYR:HB3	2.05	0.55
4:G:80:ARG:NH1	4:G:99:VAL:O	2.39	0.55
1:B:278:LEU:O	1:B:282:PHE:HB2	2.06	0.55
2:A:317:PHE:O	2:A:320:HIS:ND1	2.40	0.55
4:G:43:ARG:HH22	9:D:280:SER:HB2	1.70	0.55
9:K:49:HIS:HA	9:K:60:LEU:H	1.72	0.55
9:K:44:ASP:O	9:K:73:TYR:OH	2.23	0.55
9:D:265:ILE:O	9:D:294:ARG:NH2	2.40	0.55
6:P:19:LEU:HB2	6:P:33:LEU:HB3	1.87	0.55
1:B:46:THR:OG1	1:B:47:LYS:N	2.38	0.55
3:H:73:CYS:O	3:H:79:GLN:HA	2.06	0.55
6:I:36:ASP:O	6:I:40:ALA:HB2	2.07	0.55



	A targe D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (\AA)
2:A:8:LYS:HB2	2:A:66:THR:HG22	1.87	0.55
9:D:8:LYS:NZ	9:D:180:LEU:O	2.40	0.55
5:Q:66:CYS:HA	5:Q:74:ILE:O	2.05	0.55
9:K:148:LEU:O	9:K:152:SER:HB3	2.06	0.55
2:A:786:ARG:HE	2:A:928:ALA:HB3	1.70	0.55
7:F:116:HIS:HA	7:F:119:LEU:HB2	1.87	0.55
10:E:331:VAL:HB	10:E:360:ARG:HE	1.71	0.55
9:K:17:GLY:N	12:K:501:GDP:O3B	2.40	0.55
9:K:149:ARG:NH2	9:K:159:CYS:SG	2.80	0.55
1:B:21:PRO:HG2	1:B:41:GLN:HG3	1.87	0.55
2:A:991:GLU:HB2	2:A:996:ILE:HB	1.89	0.55
9:D:166:ASP:HB2	9:D:168:THR:H	1.72	0.55
6:P:65:ARG:NH1	7:M:121:SER:OG	2.40	0.55
2:A:219:VAL:HA	2:A:257:VAL:HA	1.88	0.55
10:E:328:LEU:HA	10:E:337:LEU:O	2.07	0.55
11:L:229:PHE:HA	11:L:232:VAL:HG22	1.89	0.55
2:A:1420:LEU:HB3	2:A:1423:PRO:HB3	1.89	0.54
8:C:408:THR:HG23	8:C:553:VAL:HG13	1.90	0.54
9:D:208:ARG:NH1	9:D:268:SER:O	2.41	0.54
10:E:97:ASN:HA	10:E:118:PRO:HG3	1.90	0.54
11:L:64:ILE:HB	11:L:112:PHE:HE1	1.73	0.54
2:A:27:PRO:HB3	2:A:58:LEU:HD13	1.90	0.54
9:K:48:SER:OG	9:K:49:HIS:N	2.41	0.54
2:A:249:ARG:NH2	2:A:302:ALA:O	2.40	0.54
3:O:17:GLU:OE2	5:Q:51:GLN:NE2	2.40	0.54
2:A:42:ALA:HB3	2:A:86:TYR:HB2	1.89	0.54
2:A:949:LEU:O	2:A:1415:LEU:N	2.39	0.54
9:D:63:CYS:HG	9:D:73:TYR:HH	1.55	0.54
9:K:166:ASP:OD2	9:K:168:THR:OG1	2.25	0.54
5:J:68:GLU:O	6:I:64:LYS:N	2.40	0.54
8:C:290:SER:HB3	8:C:293:LYS:HB2	1.90	0.54
9:D:24:ARG:HH21	9:D:42:THR:HG21	1.72	0.54
9:D:53:LEU:HD12	9:D:181:ILE:HG12	1.89	0.54
8:C:526:LEU:HD11	8:C:540:LEU:HD22	1.90	0.54
9:K:2:PRO:O	9:K:55:ASN:ND2	2.40	0.54
4:G:31:LEU:HD23	9:D:282:PRO:HG3	1.90	0.54
6:I:65:ARG:HH12	7:F:121:SER:HB2	1.73	0.54
9:D:166:ASP:OD1	9:D:166:ASP:N	2.36	0.53
9:D:171:LYS:HE3	9:D:225:VAL:HG11	1.90	0.53
7:M:60:LYS:NZ	7:M:64:ASN:OD1	2.41	0.53
9:K:189:MET:HA	9:K:192:ARG:HB3	1.90	0.53



	la pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:A:97:LEU:HD21	2:A:100:VAL:HB	1.89	0.53
8:C:374:LEU:HD11	8:C:394:VAL:HG21	1.90	0.53
6:P:70:PHE:O	6:P:91:ASN:ND2	2.41	0.53
9:K:283:SER:O	9:K:287:LEU:CB	2.57	0.53
2:A:175:ILE:HD13	2:A:336:ILE:HG13	1.90	0.53
2:A:920:TYR:HE1	2:A:932:ASP:HB2	1.73	0.53
4:N:27:ASN:ND2	4:N:29:GLU:OE1	2.41	0.53
5:Q:55:LEU:HD22	6:P:75:LEU:HD12	1.90	0.53
9:K:121:LYS:HD3	9:K:179:GLN:HG3	1.90	0.53
9:K:208:ARG:HG3	9:K:269:ASN:HA	1.89	0.53
1:B:190:ASP:HB2	2:A:421:PRO:HD2	1.89	0.53
1:B:199:TYR:O	1:B:204:ARG:NH1	2.42	0.53
2:A:1510:PHE:HB2	2:A:1549:ALA:HB3	1.90	0.53
9:D:19:GLY:HA2	12:D:501:GDP:H5"	1.89	0.53
9:D:69:PHE:O	9:D:73:TYR:CB	2.56	0.53
9:K:134:GLU:HA	9:K:137:ARG:HD2	1.91	0.53
10:E:234:GLN:HG3	10:E:268:ILE:HD11	1.90	0.53
2:A:11:ILE:HG12	2:A:74:THR:HG21	1.90	0.53
2:A:1209:GLU:O	2:A:1213:TRP:HB2	2.09	0.53
4:N:33:LEU:HA	9:K:284:ALA:HB3	1.90	0.53
7:M:150:ALA:HB1	7:M:153:GLU:HG2	1.91	0.53
9:K:187:LEU:HD22	9:K:300:LEU:HD23	1.91	0.53
11:L:329:LYS:O	11:L:337:LEU:HB3	2.08	0.53
10:E:298:ILE:HG23	10:E:299:TYR:HD1	1.72	0.53
3:O:72:ILE:HB	4:N:74:LEU:HB2	1.90	0.53
1:B:380:LYS:HE2	8:C:342:VAL:H	1.74	0.52
9:D:162:THR:HG23	9:D:169:LEU:HB3	1.91	0.52
3:O:13:LEU:HA	3:O:19:LEU:HD23	1.91	0.52
6:P:65:ARG:NH2	7:M:122:GLU:O	2.42	0.52
9:K:130:ASP:OD1	9:K:130:ASP:N	2.38	0.52
2:A:36:GLY:N	2:A:55:VAL:O	2.40	0.52
2:A:299:SER:O	2:A:301:SER:N	2.42	0.52
10:E:268:ILE:HG12	10:E:270:ILE:HG13	1.90	0.52
2:A:1556:LYS:NZ	2:A:1566:GLU:OE1	2.43	0.52
9:D:148:LEU:O	9:D:152:SER:HB3	2.10	0.52
10:E:316:ALA:HB3	10:E:328:LEU:HG	1.92	0.52
9:D:188:GLU:O	9:D:192:ARG:HB3	2.10	0.52
10:E:63:ARG:HB2	10:E:114:ILE:HG23	1.91	0.52
7:M:78:GLN:NE2	7:M:80:GLU:OE2	2.43	0.52
1:B:43:TYR:OH	8:C:72:ILE:O	2.25	0.52
5:J:22:LEU:HB3	5:J:85:ALA:HB3	1.92	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
9:D:48:SER:OG	9:D:49:HIS:N	2.41	0.52
11:L:88:ASN:ND2	11:L:265:VAL:O	2.42	0.52
2:A:1554:LEU:O	2:A:1559:ARG:NH1	2.43	0.52
10:E:131:GLU:HA	10:E:134:PHE:HB2	1.92	0.52
2:A:384:ASN:OD1	2:A:384:ASN:N	2.41	0.51
2:A:858:ARG:NH2	2:A:879:TYR:O	2.42	0.51
4:G:51:ASN:OD1	10:E:348:ARG:NH1	2.42	0.51
8:C:412:LEU:HB3	8:C:521:ARG:HH21	1.75	0.51
4:G:56:TYR:HB3	4:G:69:LEU:HD11	1.93	0.51
9:D:12:LEU:HD11	9:D:60:LEU:HD12	1.92	0.51
10:E:318:ILE:O	10:E:325:VAL:HA	2.10	0.51
6:P:14:ASP:OD1	6:P:89:ARG:NE	2.43	0.51
2:A:12:HIS:NE2	2:A:21:ASP:O	2.36	0.51
2:A:1422:GLY:HA3	2:A:1431:TYR:HB3	1.92	0.51
2:A:1512:GLN:HB3	2:A:1547:ASN:HB2	1.92	0.51
10:E:273:ASP:OD1	10:E:273:ASP:N	2.44	0.51
3:O:19:LEU:HD11	3:O:92:PHE:HB3	1.92	0.51
2:A:284:LEU:HD12	2:A:285:VAL:HG23	1.92	0.51
9:D:163:SER:HB3	9:D:166:ASP:HB3	1.92	0.51
9:D:166:ASP:OD2	9:D:168:THR:OG1	2.23	0.51
10:E:208:LEU:HD13	10:E:211:LEU:HD13	1.92	0.51
4:N:119:PRO:HG2	7:M:154:LEU:HD22	1.92	0.51
5:Q:69:SER:HB3	6:P:63:PHE:HA	1.91	0.51
1:B:144:ARG:NH2	1:B:159:VAL:O	2.44	0.51
2:A:937:GLU:HA	2:A:941:PHE:HE1	1.76	0.51
2:A:1240:ILE:HA	2:A:1259:LYS:O	2.10	0.51
1:B:327:GLN:HE22	1:B:351:TYR:HB2	1.74	0.51
1:B:327:GLN:NE2	1:B:328:LYS:O	2.39	0.51
2:A:1349:PRO:HD2	2:A:1352:ARG:HH21	1.75	0.51
8:C:8:ILE:N	8:C:129:ALA:O	2.44	0.51
11:L:230:SER:OG	11:L:269:TYR:O	2.28	0.51
1:B:283:GLN:HA	1:B:286:CYS:HB2	1.92	0.51
2:A:322:ILE:HG23	2:A:943:ARG:HH21	1.75	0.51
2:A:769:ASP:OD1	2:A:878:LYS:NZ	2.44	0.51
4:G:1:MET:N	9:D:197:ILE:O	2.44	0.51
4:N:55:ALA:HB3	11:L:348:ARG:HE	1.76	0.51
9:K:123:PHE:HD1	9:K:158:ALA:HB3	1.76	0.51
2:A:927:SER:O	2:A:930:SER:OG	2.29	0.51
9:K:148:LEU:O	9:K:152:SER:CB	2.59	0.51
1:B:59:ALA:HB3	1:B:62:LYS:H	1.76	0.51
2:A:1311:PHE:HB3	2:A:1471:LEU:HB2	1.93	0.51



	the page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
9:D:129:MET:SD	9:D:129:MET:N	2.84	0.51
10:E:234:GLN:HG2	10:E:270:ILE:HG23	1.92	0.51
7:M:74:GLN:NE2	7:M:80:GLU:OE2	2.43	0.51
11:L:142:TYR:HB2	11:L:175:VAL:HA	1.92	0.51
1:B:273:HIS:O	1:B:275:ARG:NH1	2.44	0.51
2:A:263:ARG:NH2	2:A:327:ASP:OD2	2.44	0.51
2:A:997:ARG:NH1	10:E:205:ASP:OD1	2.43	0.51
3:H:26:ASP:OD1	3:H:26:ASP:N	2.44	0.51
4:N:16:ASN:HA	4:N:20:VAL:HB	1.92	0.51
7:M:115:PRO:HA	7:M:118:VAL:HG12	1.92	0.51
9:K:42:THR:N	12:K:501:GDP:O1B	2.41	0.51
9:K:256:ASN:HD21	11:L:312:LYS:HD2	1.76	0.51
3:H:85:ARG:NE	3:H:107:GLU:OE2	2.44	0.50
4:G:114:TYR:OH	7:F:152:GLU:O	2.30	0.50
2:A:372:GLN:NE2	2:A:739:THR:O	2.45	0.50
9:D:36:THR:HA	9:D:39:LEU:HD23	1.93	0.50
9:K:263:ILE:HG23	9:K:273:MET:HB3	1.91	0.50
2:A:281:TYR:HA	2:A:284:LEU:HG	1.92	0.50
1:B:171:GLU:HA	1:B:206:ILE:HD13	1.93	0.50
9:D:181:ILE:HD12	9:D:182:PRO:HD2	1.93	0.50
7:M:143:LEU:HA	7:M:146:ILE:HG13	1.93	0.50
3:H:85:ARG:HH11	3:H:118:ARG:HH22	1.59	0.50
4:G:72:ILE:O	4:G:82:ALA:HA	2.11	0.50
8:C:407:HIS:O	8:C:555:THR:HA	2.12	0.50
4:G:26:ASN:OD1	4:G:30:SER:N	2.45	0.50
6:I:51:CYS:O	6:I:54:ARG:NH2	2.44	0.50
7:F:116:HIS:O	7:F:120:ALA:HB2	2.12	0.50
1:B:54:LEU:HD11	1:B:99:GLU:HB3	1.94	0.50
2:A:1393:VAL:HG11	2:A:1398:LEU:HD22	1.94	0.50
10:E:329:LYS:O	10:E:360:ARG:NH2	2.45	0.50
11:L:258:LYS:HD3	11:L:340:ILE:HD11	1.93	0.50
2:A:132:VAL:N	2:A:139:ALA:O	2.45	0.50
2:A:174:PHE:O	2:A:335:VAL:HA	2.12	0.50
3:H:4:ASP:OD1	3:H:4:ASP:N	2.43	0.50
8:C:162:TYR:HD1	8:C:165:ARG:HD2	1.76	0.50
2:A:179:CYS:HB3	2:A:297:ASP:HB2	1.94	0.49
2:A:934:SER:OG	2:A:935:LEU:N	2.43	0.49
2:A:959:ILE:HA	2:A:963:GLU:H	1.77	0.49
3:H:102:LEU:HD12	5:J:44:VAL:HG22	1.93	0.49
8:C:397:MET:O	8:C:402:LEU:N	2.43	0.49
10:E:233:VAL:HG23	10:E:236:LEU:HD12	1.92	0.49



	t i c	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:A:221:PHE:HA	2:A:254:PHE:O	2.12	0.49
2:A:254:PHE:HD2	2:A:285:VAL:HG22	1.77	0.49
9:D:207:GLU:OE1	9:D:210:THR:N	2.45	0.49
11:L:74:LYS:NZ	11:L:145:ASP:OD1	2.45	0.49
1:B:71:ILE:HD11	1:B:83:PHE:HE1	1.78	0.49
1:B:255:VAL:HG22	1:B:278:LEU:HD21	1.93	0.49
2:A:1449:LEU:HA	2:A:1456:LEU:HD13	1.93	0.49
4:G:32:LEU:HA	9:D:284:ALA:HB3	1.94	0.49
6:I:36:ASP:O	6:I:40:ALA:CB	2.60	0.49
9:K:61:TRP:HZ3	9:K:81:ILE:HG22	1.77	0.49
7:F:54:LEU:HA	7:F:57:ILE:HD12	1.94	0.49
4:N:83:ALA:HB3	4:N:94:MET:HB2	1.94	0.49
9:D:202:GLU:HB3	9:D:275:VAL:HB	1.93	0.49
10:E:82:PHE:HA	10:E:265:VAL:HG13	1.94	0.49
11:L:96:THR:OG1	11:L:97:ASN:N	2.46	0.49
5:J:61:ASP:OD1	6:I:71:GLY:N	2.44	0.49
2:A:948:LEU:HB3	2:A:1384:PHE:HB3	1.93	0.49
8:C:278:CYS:SG	8:C:279:SER:N	2.83	0.49
9:D:58:LEU:HD11	9:D:180:LEU:HD21	1.94	0.49
10:E:104:ILE:HG21	10:E:265:VAL:HG21	1.95	0.49
11:L:240:LEU:HB2	11:L:243:LEU:HB3	1.94	0.49
9:K:10:VAL:HG11	9:K:58:LEU:HD23	1.95	0.49
9:K:23:MET:HB2	9:K:169:LEU:HD11	1.95	0.49
1:B:123:GLU:O	1:B:127:LYS:NZ	2.44	0.49
1:B:173:ASP:HA	1:B:236:VAL:HA	1.95	0.49
2:A:35:LEU:HD22	2:A:57:SER:HA	1.94	0.49
2:A:61:ASP:OD1	2:A:61:ASP:N	2.46	0.49
9:D:94:VAL:HG22	9:D:128:LYS:HB2	1.93	0.49
2:A:920:TYR:O	2:A:924:TYR:HB2	2.13	0.49
7:F:49:ASP:OD1	7:F:49:ASP:N	2.45	0.49
9:D:143:GLU:OE1	9:D:144:ARG:NE	2.44	0.49
9:K:205:LEU:HD11	9:K:270:THR:HB	1.94	0.49
11:L:331:VAL:HG11	11:L:364:HIS:HB2	1.95	0.49
9:D:26:ILE:O	9:D:236:LYS:NZ	2.42	0.48
2:A:26:ASN:HB2	2:A:62:LEU:HD12	1.95	0.48
4:G:68:ASN:OD1	4:G:70:LYS:NZ	2.47	0.48
6:I:76:LEU:HD13	6:I:89:ARG:HE	1.78	0.48
2:A:23:LEU:HD21	2:A:67:ILE:HD11	1.95	0.48
9:D:275:VAL:HG12	9:D:277:SER:HB3	1.95	0.48
2:A:1350:GLU:O	2:A:1376:GLY:N	2.47	0.48
4:N:54:TRP:O	4:N:58:ASP:N	2.46	0.48



	tion and the second sec	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:346:THR:OG1	1:B:347:GLY:N	2.46	0.48
8:C:264:LEU:HD11	8:C:323:ILE:HG12	1.95	0.48
9:D:119:ASP:OD1	9:D:119:ASP:N	2.45	0.48
2:A:1228:ILE:HA	2:A:1231:MET:HG2	1.96	0.48
9:K:107:GLN:OE1	9:K:153:ARG:NH2	2.46	0.48
2:A:104:PHE:HB3	2:A:329:THR:HG21	1.94	0.48
4:G:86:VAL:HG23	4:G:89:LEU:HB2	1.95	0.48
7:F:116:HIS:O	7:F:120:ALA:CB	2.62	0.48
9:D:167:GLU:HG3	9:D:226:HIS:HB3	1.94	0.48
12:K:501:GDP:O2B	13:K:502:AF3:F3	2.22	0.48
11:L:360:ARG:HA	11:L:363:ILE:HG12	1.96	0.48
2:A:217:THR:O	2:A:217:THR:OG1	2.31	0.48
10:E:85:MET:SD	10:E:85:MET:N	2.87	0.48
2:A:1448:LEU:HD21	2:A:1587:LEU:HG	1.95	0.48
9:K:223:ARG:HB3	9:K:227:ARG:HG2	1.96	0.48
11:L:216:TYR:CG	11:L:225:ILE:HG23	2.49	0.48
3:H:115:GLU:OE2	3:H:118:ARG:NH2	2.47	0.47
4:G:119:LEU:HA	4:G:122:VAL:HG12	1.96	0.47
9:D:129:MET:HA	9:D:132:VAL:HG22	1.95	0.47
7:M:92:LEU:O	7:M:96:SER:CB	2.61	0.47
9:D:173:TRP:HA	9:D:176:ILE:HB	1.96	0.47
5:Q:41:HIS:NE2	6:P:54:ARG:O	2.43	0.47
6:P:79:VAL:H	7:M:111:LEU:HB2	1.78	0.47
9:K:119:ASP:OD1	9:K:119:ASP:N	2.47	0.47
2:A:863:VAL:HA	2:A:871:THR:O	2.14	0.47
2:A:978:ASP:O	2:A:982:LEU:HB2	2.14	0.47
4:N:106:LYS:HD2	5:Q:29:LEU:HD12	1.96	0.47
11:L:314:SER:OG	11:L:330:GLU:OE2	2.32	0.47
1:B:166:PRO:HB3	1:B:228:LEU:HD22	1.96	0.47
1:B:287:SER:O	1:B:300:ARG:NH1	2.46	0.47
2:A:103:THR:O	2:A:105:LYS:NZ	2.42	0.47
2:A:376:ALA:HB3	2:A:379:LEU:HD23	1.96	0.47
2:A:1445:ILE:HD12	2:A:1448:LEU:HD12	1.96	0.47
2:A:337:THR:OG1	2:A:366:LEU:O	2.30	0.47
4:G:33:ALA:HB1	9:D:281:ILE:HD12	1.97	0.47
5:J:74:ILE:HA	5:J:86:VAL:O	2.14	0.47
11:L:184:SER:OG	11:L:185:ASP:N	2.47	0.47
11:L:325:VAL:O	11:L:341:LEU:N	2.47	0.47
1:B:263:ALA:O	1:B:267:TYR:CB	2.63	0.47
2:A:1436:ARG:HA	2:A:1436:ARG:HD2	1.71	0.47
3:H:31:PRO:HB3	3:H:34:LYS:HE3	1.96	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:G:106:ALA:O	7:F:147:ARG:NH1	2.47	0.47
8:C:258:TYR:HB2	8:C:326:TYR:HE1	1.79	0.47
9:D:79:ASP:N	9:D:79:ASP:OD1	2.47	0.47
9:D:279:PRO:HG2	9:D:281:ILE:HG12	1.96	0.47
3:O:66:SER:OG	3:O:67:LYS:N	2.47	0.47
9:K:110:LEU:HA	9:K:113:ILE:HG22	1.96	0.47
1:B:105:LEU:HD13	1:B:157:LEU:HD21	1.97	0.47
1:B:191:LEU:HA	1:B:194:GLN:HB2	1.96	0.47
1:B:317:GLY:HA2	1:B:322:LEU:HD12	1.97	0.47
2:A:189:ASP:OD1	2:A:189:ASP:N	2.48	0.47
2:A:215:GLU:OE2	2:A:263:ARG:NH2	2.48	0.47
10:E:142:TYR:HB2	10:E:175:VAL:HG22	1.96	0.47
10:E:244:GLU:O	10:E:248:ASN:ND2	2.47	0.47
5:Q:66:CYS:HB2	6:P:67:SER:HB2	1.96	0.47
9:K:34:ARG:O	9:K:37:ARG:NH1	2.48	0.47
2:A:196:VAL:HA	2:A:200:LEU:HB2	1.96	0.47
10:E:243:LEU:HD12	10:E:246:LEU:HD22	1.97	0.47
4:N:32:LEU:HB3	9:K:282:PRO:HG2	1.97	0.47
6:P:16:LEU:HB2	6:P:88:LYS:HB3	1.96	0.47
1:B:208:LYS:O	1:B:212:GLU:CB	2.62	0.47
2:A:1575:ASP:OD1	2:A:1586:ARG:NH1	2.48	0.47
6:I:16:LEU:HB2	6:I:88:LYS:HB2	1.95	0.47
3:O:23:VAL:HG22	3:O:34:LYS:HG3	1.96	0.47
9:K:9:LYS:NZ	9:K:81:ILE:O	2.48	0.47
2:A:223:ARG:HH22	2:A:302:ALA:HB3	1.80	0.47
7:F:60:LYS:HA	7:F:63:SER:HB3	1.96	0.47
10:E:337:LEU:HB2	10:E:360:ARG:HH12	1.80	0.47
9:K:132:VAL:HG23	9:K:137:ARG:HG3	1.97	0.47
10:E:272:THR:OG1	10:E:273:ASP:N	2.48	0.46
9:K:123:PHE:CG	9:K:176:ILE:HG12	2.50	0.46
1:B:32:ILE:HD12	1:B:37:PHE:HE2	1.80	0.46
2:A:36:GLY:HA2	2:A:54:GLN:HE21	1.80	0.46
2:A:1351:GLN:HE22	2:A:1387:LYS:HD2	1.81	0.46
4:G:102:GLY:N	5:J:30:ASN:O	2.47	0.46
9:D:92:PHE:HE1	9:D:102:ASP:HB3	1.80	0.46
4:N:3:LEU:HD21	4:N:119:PRO:HB3	1.95	0.46
4:N:52:ASN:HD21	7:M:66:ILE:HG21	1.80	0.46
11:L:65:LEU:HD11	11:L:113:GLN:HG2	1.97	0.46
11:L:137:THR:O	11:L:168:ASN:ND2	2.40	0.46
1:B:15:PHE:HB2	1:B:45:ILE:HG21	1.97	0.46
1:B:101:ILE:HG23	1:B:157:LEU:HD12	1.97	0.46



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:249:PRO:HD2	1:B:324:ARG:HH12	1.79	0.46
2:A:1232:GLN:OE1	2:A:1251:PHE:N	2.40	0.46
4:G:44:VAL:HG21	10:E:357:HIS:CG	2.51	0.46
4:G:116:GLU:O	4:G:120:THR:N	2.41	0.46
1:B:255:VAL:O	1:B:258:LYS:NZ	2.47	0.46
2:A:1543:ARG:NH1	2:A:1544:VAL:O	2.48	0.46
6:I:65:ARG:HD3	7:F:118:VAL:HB	1.97	0.46
9:K:162:THR:OG1	9:K:163:SER:O	2.25	0.46
11:L:353:ASP:OD1	11:L:353:ASP:N	2.47	0.46
1:B:37:PHE:HA	1:B:40:VAL:HG12	1.97	0.46
1:B:78:ARG:NH2	12:D:501:GDP:O3A	2.47	0.46
10:E:140:LEU:HB3	10:E:173:PHE:HD1	1.79	0.46
11:L:100:TYR:HE1	11:L:367:PHE:HB3	1.81	0.46
10:E:331:VAL:H	10:E:360:ARG:HH21	1.64	0.46
5:Q:56:THR:OG1	5:Q:57:SER:N	2.49	0.46
1:B:121:MET:O	1:B:124:SER:OG	2.34	0.46
1:B:207:GLN:HA	1:B:210:SER:HB3	1.97	0.46
2:A:1191:VAL:HG21	2:A:1210:VAL:HG22	1.98	0.46
6:I:89:ARG:NH1	7:F:119:LEU:O	2.49	0.46
11:L:62:PRO:HG3	11:L:233:VAL:HG22	1.98	0.46
11:L:276:PRO:HA	11:L:280:GLN:HE22	1.81	0.46
2:A:97:LEU:HA	2:A:146:VAL:HG13	1.98	0.46
8:C:264:LEU:HG	8:C:322:ALA:HA	1.98	0.46
9:K:10:VAL:HG12	9:K:87:VAL:HB	1.97	0.46
9:K:253:GLU:OE2	9:K:283:SER:OG	2.29	0.46
1:B:186:ASN:OD1	1:B:194:GLN:NE2	2.41	0.46
2:A:314:PHE:HA	2:A:317:PHE:HB2	1.97	0.46
2:A:1379:SER:HB3	2:A:1382:ALA:HB3	1.97	0.46
9:K:24:ARG:HA	9:K:27:ILE:HG22	1.98	0.46
9:K:201:ASP:N	9:K:275:VAL:O	2.49	0.46
9:D:207:GLU:HB3	9:D:212:LEU:H	1.82	0.45
3:O:16:VAL:HB	3:O:19:LEU:HD22	1.96	0.45
2:A:40:GLU:HB2	2:A:50:PRO:HB3	1.96	0.45
9:D:129:MET:HB2	9:D:137:ARG:HG2	1.97	0.45
3:O:32:VAL:HA	7:M:88:TYR:HB3	1.98	0.45
2:A:300:THR:HG21	2:A:339:GLY:HA3	1.98	0.45
2:A:1444:ASN:OD1	2:A:1447:CYS:N	2.50	0.45
8:C:514:ALA:HA	8:C:517:LEU:HB2	1.98	0.45
5:J:69:SER:OG	5:J:71:ASN:OD1	2.29	0.45
8:C:365:LEU:O	8:C:369:SER:N	2.50	0.45
9:D:249:PHE:CZ	9:D:252:MET:HB2	2.51	0.45



	la pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
9:K:63:CYS:O	13:K:502:AF3:F1	2.25	0.45
11:L:248:ASN:HD21	11:L:272:THR:HB	1.82	0.45
2:A:105:LYS:HB2	2:A:105:LYS:HE2	1.78	0.45
2:A:329:THR:OG1	2:A:330:GLY:N	2.49	0.45
4:G:24:LEU:HD11	4:G:115:LEU:HD22	1.99	0.45
7:F:60:LYS:NZ	10:E:365:GLU:OE2	2.44	0.45
9:D:170:TYR:HB2	9:D:229:GLU:HB3	1.99	0.45
9:D:208:ARG:NH1	9:D:269:ASN:O	2.49	0.45
4:N:4:ARG:HH21	7:M:156:VAL:HG23	1.81	0.45
6:P:80:SER:O	6:P:83:ARG:HB2	2.16	0.45
7:M:110:SER:OG	7:M:112:THR:O	2.35	0.45
6:I:9:LEU:HD23	6:I:12:ILE:HD13	1.99	0.45
8:C:288:THR:O	8:C:293:LYS:NZ	2.40	0.45
10:E:333:LYS:HB3	10:E:333:LYS:HE3	1.77	0.45
4:N:81:ARG:NH2	4:N:100:VAL:O	2.49	0.45
6:P:11:ARG:O	6:P:11:ARG:NH1	2.49	0.45
9:K:15:LYS:HA	9:K:15:LYS:HD3	1.80	0.45
11:L:146:ALA:HB2	11:L:180:VAL:HA	1.97	0.45
2:A:967:ASP:OD1	2:A:967:ASP:N	2.43	0.45
7:F:114:GLN:HG3	7:F:117:GLN:H	1.81	0.45
9:D:193:ASN:OD1	9:D:196:GLN:NE2	2.50	0.45
10:E:99:ILE:HG23	10:E:117:PHE:HE1	1.82	0.45
10:E:161:VAL:HG21	10:E:213:LEU:HD21	1.98	0.45
3:O:113:LEU:HA	3:O:116:GLU:HG2	1.99	0.45
11:L:116:ASP:OD1	11:L:116:ASP:N	2.46	0.45
4:G:79:GLY:HA2	4:G:96:LYS:HA	1.99	0.45
5:J:22:LEU:HD11	5:J:42:ALA:HB2	1.99	0.45
10:E:62:PRO:HG2	10:E:109:PHE:HD1	1.82	0.45
10:E:73:GLY:N	12:E:501:GDP:O3B	2.49	0.45
3:0:12:LYS:0	3:O:15:SER:OG	2.33	0.45
4:G:122:VAL:HA	4:G:125:SER:HB3	1.99	0.45
8:C:17:SER:OG	9:D:80:ASN:O	2.35	0.45
8:C:21:LYS:HD2	8:C:171:LEU:HD13	1.99	0.45
9:D:79:ASP:O	9:D:83:ARG:HB2	2.17	0.45
10:E:262:PHE:HB3	10:E:268:ILE:O	2.17	0.45
5:Q:12:THR:HG22	5:Q:18:ILE:HG21	1.99	0.45
11:L:136:GLY:HA2	11:L:169:PRO:HG2	1.98	0.45
2:A:1368:GLU:OE2	2:A:1394:THR:N	2.44	0.44
4:N:33:LEU:HG	9:K:285:ALA:HB2	1.99	0.44
6:P:6:THR:HA	6:P:9:LEU:HB2	1.99	0.44
8:C:17:SER:OG	9:D:80:ASN:OD1	2.35	0.44



	tus page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
10:E:100:TYR:HB3	10:E:116:ASP:HB3	2.00	0.44
10:E:131:GLU:O	10:E:135:ARG:NH1	2.50	0.44
4:N:113:VAL:O	4:N:117:GLU:CB	2.56	0.44
11:L:269:TYR:O	11:L:282:TYR:OH	2.35	0.44
1:B:16:HIS:CE1	1:B:19:LEU:HB2	2.52	0.44
7:F:134:ARG:HA	7:F:134:ARG:HD2	1.86	0.44
7:F:156:VAL:HG21	9:D:197:ILE:HB	1.98	0.44
8:C:262:LEU:HD11	8:C:395:VAL:HG13	1.99	0.44
9:D:224:ASP:OD2	9:D:226:HIS:ND1	2.47	0.44
4:N:90:LEU:HD12	4:N:120:LEU:HD23	1.98	0.44
11:L:243:LEU:HA	11:L:246:LEU:HG	1.97	0.44
1:B:254:LEU:O	1:B:261:GLN:NE2	2.42	0.44
2:A:1502:TYR:HB2	2:A:1511:LEU:HB3	2.00	0.44
3:H:81:VAL:HB	3:H:92:PHE:HB2	1.99	0.44
1:B:325:ARG:NH2	1:B:327:GLN:OE1	2.47	0.44
2:A:990:VAL:HG13	2:A:993:LEU:HD12	2.00	0.44
9:D:20:LYS:N	12:D:501:GDP:O2A	2.50	0.44
10:E:254:SER:HG	10:E:355:ASN:HD22	1.60	0.44
10:E:316:ALA:O	10:E:327:TYR:HA	2.18	0.44
4:N:125:ALA:HA	9:K:291:ARG:HD2	2.00	0.44
9:K:246:ALA:O	11:L:321:ASN:ND2	2.50	0.44
11:L:189:ILE:HG23	11:L:193:ARG:HH11	1.82	0.44
1:B:101:ILE:HG13	1:B:159:VAL:HG22	1.99	0.44
2:A:21:ASP:OD2	2:A:57:SER:OG	2.32	0.44
2:A:930:SER:OG	2:A:932:ASP:OD1	2.31	0.44
5:J:49:ALA:HB1	5:J:78:LYS:HB3	1.99	0.44
6:I:55:LEU:HD13	6:I:62:PRO:HA	2.00	0.44
10:E:64:ILE:HB	10:E:140:LEU:HA	2.00	0.44
9:K:140:ILE:HA	9:K:143:GLU:HB3	2.00	0.44
3:H:114:PHE:HB3	3:H:118:ARG:HH21	1.81	0.44
9:D:59:ASN:HB3	9:D:61:TRP:HE1	1.83	0.44
4:N:41:THR:HG22	4:N:47:ALA:HB2	1.99	0.44
11:L:121:MET:SD	11:L:121:MET:N	2.91	0.44
11:L:131:GLU:HG2	11:L:167:VAL:HG11	1.98	0.44
2:A:25:VAL:HG21	2:A:33:ILE:HG21	2.00	0.44
9:K:171:LYS:HB2	9:K:229:GLU:HG2	1.99	0.44
2:A:96:THR:HG23	2:A:157:SER:HB3	2.00	0.43
2:A:798:VAL:HA	2:A:801:GLU:HG3	2.00	0.43
3:H:9:LEU:HB3	3:H:35:VAL:HG21	1.99	0.43
4:G:26:ASN:HA	4:G:89:LEU:HD22	2.00	0.43
4:G:44:VAL:HG11	10:E:357:HIS:HB2	2.00	0.43



	h h	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
10:E:355:ASN:O	10:E:359:PHE:CB	2.65	0.43
4:N:15:ALA:HB2	4:N:112:LEU:HD11	2.00	0.43
1:B:216:GLU:HB2	1:B:219:LEU:HD23	2.00	0.43
2:A:123:SER:O	2:A:123:SER:OG	2.32	0.43
9:D:130:ASP:OD1	9:D:130:ASP:N	2.43	0.43
9:K:163:SER:OG	9:K:164:ILE:N	2.51	0.43
1:B:37:PHE:O	1:B:41:GLN:NE2	2.51	0.43
1:B:189:TRP:CD1	2:A:423:ILE:HD11	2.53	0.43
1:B:208:LYS:O	1:B:212:GLU:HB3	2.18	0.43
8:C:336:LEU:HD11	8:C:365:LEU:HD13	2.00	0.43
10:E:143:VAL:HA	10:E:176:PHE:O	2.19	0.43
10:E:256:ILE:HG13	10:E:341:LEU:HB3	2.00	0.43
4:N:22:SER:HA	4:N:37:GLY:HA3	1.99	0.43
11:L:62:PRO:HD2	11:L:236:LEU:HB2	2.00	0.43
11:L:186:ASP:OD1	11:L:186:ASP:N	2.51	0.43
4:G:59:ASN:O	4:G:63:ALA:N	2.52	0.43
6:I:82:GLN:HG3	6:I:83:ARG:HG3	2.00	0.43
9:D:259:PHE:HE2	10:E:300:GLY:HA2	1.82	0.43
3:0:12:LYS:HD2	3:O:12:LYS:HA	1.83	0.43
4:N:107:ALA:O	4:N:111:ALA:HB2	2.18	0.43
2:A:1504:HIS:ND1	2:A:1506:THR:OG1	2.37	0.43
5:J:4:THR:HA	5:J:7:GLN:HB2	1.99	0.43
9:D:266:PHE:O	9:D:294:ARG:NE	2.33	0.43
2:A:116:ARG:NH2	2:A:804:CYS:SG	2.77	0.43
3:H:117:LEU:HD12	3:H:120:VAL:HG21	2.00	0.43
8:C:13:VAL:HG22	8:C:22:LEU:HG	2.01	0.43
8:C:89:ASP:OD1	8:C:89:ASP:N	2.49	0.43
9:D:20:LYS:HG3	9:D:24:ARG:HH22	1.83	0.43
9:D:148:LEU:O	9:D:152:SER:CB	2.65	0.43
10:E:154:LEU:HD23	10:E:157:LEU:HD21	2.01	0.43
4:N:85:THR:OG1	4:N:86:ARG:N	2.52	0.43
1:B:9:CYS:SG	1:B:10:ILE:N	2.91	0.43
2:A:936:ILE:H	2:A:939:LEU:HD12	1.83	0.43
3:H:57:THR:HA	3:H:68:ASN:HD22	1.84	0.43
3:H:100:THR:N	5:J:27:GLN:O	2.51	0.43
10:E:63:ARG:HH22	10:E:232:VAL:HG12	1.84	0.43
9:K:251:SER:HB2	11:L:319:LYS:HB2	2.00	0.43
2:A:39:VAL:O	2:A:52:LEU:HA	2.19	0.43
4:G:117:GLU:HG2	4:G:118:PRO:HD3	2.01	0.43
5:Q:67:LEU:HD12	5:Q:74:ILE:HD12	2.01	0.43
11:L:301:LEU:HD13	11:L:312:LYS:HE2	2.00	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
11:L:319:LYS:HD3	11:L:323:THR:HB	2.01	0.43
11:L:325:VAL:HG13	11:L:341:LEU:HB3	2.01	0.43
1:B:103:LYS:HA	1:B:103:LYS:HD2	1.84	0.43
1:B:124:SER:HA	1:B:127:LYS:HE2	2.00	0.43
2:A:947:LEU:HD23	2:A:1419:VAL:HG21	2.01	0.43
4:G:33:ALA:HA	9:D:281:ILE:HG23	2.01	0.43
6:I:54:ARG:HA	6:I:62:PRO:HG3	2.00	0.43
8:C:263:LEU:HD23	8:C:322:ALA:HB2	2.01	0.43
4:N:102:PHE:HB3	5:Q:29:LEU:HD22	2.00	0.43
6:P:54:ARG:HH22	6:P:61:VAL:HA	1.84	0.43
6:P:68:VAL:O	6:P:74:THR:HA	2.19	0.43
9:K:92:PHE:O	9:K:127:HIS:ND1	2.50	0.43
1:B:118:PHE:O	1:B:124:SER:OG	2.35	0.42
2:A:37:ASP:O	2:A:54:GLN:HA	2.19	0.42
2:A:893:CYS:SG	2:A:897:SER:OG	2.77	0.42
2:A:950:PRO:HA	2:A:1414:PHE:HA	2.00	0.42
3:H:70:SER:O	4:G:75:ASP:HB3	2.18	0.42
7:F:57:ILE:HA	7:F:60:LYS:HZ2	1.84	0.42
8:C:333:VAL:O	8:C:405:GLN:HA	2.19	0.42
8:C:252:LEU:HG	8:C:314:ALA:HB1	2.01	0.42
8:C:258:TYR:HB3	8:C:531:TYR:CG	2.54	0.42
9:K:239:LYS:HA	9:K:239:LYS:HD2	1.78	0.42
4:G:22:THR:HG21	4:G:111:LEU:HD13	2.01	0.42
4:G:28:GLU:HG2	10:E:347:GLU:HG3	2.01	0.42
8:C:482:MET:HA	8:C:485:ASN:HB2	2.00	0.42
9:D:9:LYS:HE2	9:D:85:VAL:HG22	2.00	0.42
9:D:267:THR:OG1	9:D:270:THR:N	2.43	0.42
3:O:115:GLU:HA	3:O:118:ARG:HG2	2.00	0.42
11:L:65:LEU:HD12	11:L:65:LEU:HA	1.92	0.42
2:A:1560:SER:N	2:A:1563:THR:OG1	2.53	0.42
11:L:100:TYR:HD2	11:L:102:ASP:H	1.66	0.42
2:A:797:GLN:HA	2:A:800:GLU:HB2	2.00	0.42
7:F:58:LEU:HD11	10:E:242:THR:HA	2.01	0.42
7:M:84:ARG:HA	7:M:87:GLN:HG2	2.02	0.42
11:L:90:THR:HA	11:L:110:VAL:HG22	2.01	0.42
2:A:344:GLU:HB2	2:A:381:LYS:HE3	2.02	0.42
2:A:953:VAL:HG22	2:A:1562:ALA:HB2	2.02	0.42
2:A:967:ASP:HB2	2:A:1479:ARG:NE	2.34	0.42
4:G:85:ARG:HA	4:G:89:LEU:O	2.20	0.42
6:I:75:LEU:HG	6:I:88:LYS:HD3	2.02	0.42
9:D:163:SER:OG	9:D:164:ILE:N	2.53	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
11:L:254:SER:HB2	11:L:356:PHE:HZ	1.84	0.42
11:L:325:VAL:N	11:L:341:LEU:O	2.53	0.42
1:B:82:LEU:HD12	1:B:82:LEU:HA	1.89	0.42
2:A:1195:SER:OG	2:A:1196:GLU:N	2.52	0.42
10:E:163:LYS:HE3	10:E:163:LYS:HB3	1.88	0.42
10:E:272:THR:OG1	10:E:273:ASP:OD1	2.37	0.42
7:M:103:LYS:HG3	7:M:104:LYS:HG3	2.01	0.42
9:K:114:LEU:HD21	9:K:155:LEU:HD22	2.02	0.42
1:B:74:LYS:HE3	9:D:38:ARG:HG2	2.02	0.42
6:I:43:ILE:HG23	6:I:77:VAL:HG21	2.02	0.42
8:C:148:ARG:HB3	8:C:224:TRP:HH2	1.84	0.42
6:P:66:LEU:HD12	6:P:66:LEU:HA	1.93	0.42
9:K:127:HIS:CD2	9:K:128:LYS:HB2	2.55	0.42
9:K:132:VAL:O	9:K:137:ARG:NE	2.53	0.42
9:K:227:ARG:HA	9:K:230:LYS:HD2	2.02	0.42
4:G:53:TRP:CG	4:G:90:LEU:HD11	2.55	0.42
8:C:8:ILE:O	8:C:208:TYR:OH	2.35	0.42
3:O:23:VAL:HB	3:O:91:SER:O	2.20	0.42
11:L:355:ASN:HA	11:L:358:CYS:HB2	2.02	0.42
2:A:786:ARG:NH2	2:A:926:CYS:O	2.52	0.41
6:I:65:ARG:HA	7:F:111:LEU:HD23	2.01	0.41
8:C:527:GLU:O	8:C:531:TYR:HB2	2.20	0.41
9:D:85:VAL:HG11	9:D:113:ILE:HD11	2.01	0.41
9:K:130:ASP:OD2	9:K:165:TRP:NE1	2.49	0.41
2:A:109:ILE:HD13	2:A:137:ILE:HG23	2.02	0.41
3:H:71:ILE:HB	3:H:82:GLN:HB2	2.03	0.41
4:G:110:ALA:HB1	7:F:148:VAL:HG23	2.03	0.41
8:C:540:LEU:HD23	8:C:543:LEU:HD23	2.02	0.41
3:O:5:LEU:HD13	3:O:113:LEU:HD21	2.00	0.41
9:K:167:GLU:HB3	9:K:233:ASN:HB2	2.02	0.41
9:K:173:TRP:HA	9:K:176:ILE:HD12	2.02	0.41
9:K:195:ALA:O	9:K:200:ALA:N	2.53	0.41
11:L:102:ASP:O	11:L:106:ASN:CB	2.60	0.41
1:B:187:SER:OG	1:B:188:GLN:OE1	2.37	0.41
1:B:265:LEU:HD12	1:B:265:LEU:HA	1.92	0.41
2:A:945:ARG:HD3	2:A:1421:GLU:HA	2.03	0.41
3:H:60:GLY:HA2	3:H:63:LEU:HD12	2.02	0.41
6:I:54:ARG:HA	6:I:54:ARG:HD3	1.85	0.41
8:C:519:TYR:CG	8:C:529:ILE:HG12	2.55	0.41
9:D:50:VAL:HG22	9:D:58:LEU:HB2	2.02	0.41
3:O:63:LEU:HD13	4:N:82:VAL:HG21	2.01	0.41



	t i c	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
6:P:16:LEU:HD12	6:P:88:LYS:HG2	2.02	0.41
6:P:69:VAL:HG11	7:M:124:ILE:HD13	2.01	0.41
8:C:288:THR:HG22	8:C:293:LYS:HZ3	1.86	0.41
8:C:394:VAL:HA	8:C:403:LEU:HD12	2.02	0.41
10:E:181:ASP:OD1	10:E:181:ASP:N	2.51	0.41
1:B:108:TYR:CD2	1:B:155:ILE:HD13	2.55	0.41
3:H:19:LEU:HB2	3:H:103:ILE:HD11	2.02	0.41
9:D:263:ILE:HG23	9:D:273:MET:HB3	2.02	0.41
1:B:28:PRO:HG2	1:B:31:PHE:HZ	1.85	0.41
1:B:114:LEU:HD12	1:B:114:LEU:HA	1.91	0.41
1:B:255:VAL:HA	1:B:278:LEU:HD11	2.02	0.41
2:A:923:GLN:O	2:A:927:SER:OG	2.39	0.41
4:N:12:LEU:HB2	4:N:36:SER:HB3	2.02	0.41
4:N:34:ALA:HB2	9:K:281:ILE:HG23	2.02	0.41
10:E:135:ARG:HA	10:E:135:ARG:HD3	1.89	0.41
11:L:140:LEU:HB3	11:L:142:TYR:CZ	2.56	0.41
11:L:152:GLU:HA	11:L:155:THR:HG22	2.02	0.41
1:B:254:LEU:HD11	1:B:322:LEU:HD13	2.02	0.41
1:B:325:ARG:NH2	1:B:352:ASP:OD2	2.54	0.41
5:J:78:LYS:HB2	5:J:78:LYS:HE3	1.82	0.41
8:C:144:ASN:HA	8:C:147:ARG:HG2	2.03	0.41
10:E:79:LYS:HB3	10:E:85:MET:HE1	2.01	0.41
4:N:26:LEU:HD22	11:L:349:LYS:HD3	2.03	0.41
9:K:174:SER:HB2	9:K:213:VAL:H	1.86	0.41
11:L:142:TYR:O	11:L:176:PHE:N	2.52	0.41
2:A:372:GLN:HE22	2:A:740:VAL:HG22	1.86	0.41
2:A:917:LYS:HB3	2:A:917:LYS:HE3	1.84	0.41
2:A:1394:THR:HB	2:A:1397:VAL:HG22	2.03	0.41
3:H:79:GLN:HG3	3:H:94:ALA:HB3	2.02	0.41
8:C:271:LEU:HD23	8:C:274:LEU:HD12	2.03	0.41
9:D:135:ASP:OD1	9:D:135:ASP:N	2.53	0.41
10:E:139:ALA:HB2	10:E:236:LEU:HD21	2.03	0.41
3:O:21:ALA:HB3	3:O:93:ILE:HD12	2.02	0.41
5:Q:72:GLY:HA2	5:Q:88:LYS:O	2.21	0.41
9:K:174:SER:OG	9:K:213:VAL:O	2.34	0.41
11:L:243:LEU:HD12	11:L:246:LEU:HD11	2.02	0.41
1:B:54:LEU:HD22	8:C:89:ASP:HA	2.03	0.41
1:B:318:LEU:HD23	1:B:318:LEU:HA	1.92	0.41
8:C:282:LEU:HD13	8:C:312:LEU:HD22	2.02	0.41
9:K:267:THR:OG1	9:K:270:THR:OG1	2.31	0.41
2:A:1551:ASN:OD1	2:A:1553:MET:N	2.54	0.40



	the projection	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
8:C:490:LEU:HD21	8:C:517:LEU:HD21	2.03	0.40
10:E:263:ASP:H	10:E:266:SER:HG	1.66	0.40
9:K:282:PRO:HB2	9:K:283:SER:H	1.68	0.40
1:B:10:ILE:H	1:B:27:VAL:HG12	1.85	0.40
9:D:249:PHE:HZ	9:D:252:MET:HB2	1.85	0.40
10:E:218:THR:OG1	10:E:219:SER:N	2.54	0.40
3:O:46:ARG:HG3	3:O:48:GLY:H	1.86	0.40
4:N:46:THR:HA	11:L:354:TYR:HE1	1.86	0.40
1:B:190:ASP:O	1:B:193:THR:OG1	2.34	0.40
4:G:25:LEU:HD11	4:G:46:ALA:HB1	2.03	0.40
9:D:208:ARG:HG3	9:D:271:TYR:HE2	1.87	0.40
7:M:140:TYR:HA	7:M:143:LEU:HD12	2.04	0.40
9:K:64:GLY:N	9:K:73:TYR:OH	2.45	0.40
1:B:79:ASN:ND2	9:D:40:GLY:HA3	2.37	0.40
2:A:988:ARG:O	2:A:1408:LYS:NZ	2.40	0.40
2:A:1197:GLN:HE21	2:A:1200:LEU:HB2	1.86	0.40
2:A:1311:PHE:O	2:A:1468:ARG:NH1	2.55	0.40
4:N:92:LEU:HD21	4:N:112:LEU:HB2	2.04	0.40
6:P:16:LEU:HD11	6:P:90:GLN:HG2	2.02	0.40
7:M:68:VAL:HG12	11:L:351:LEU:HD21	2.03	0.40
9:K:20:LYS:HB2	9:K:20:LYS:HE3	1.80	0.40
11:L:200:ASN:O	11:L:204:ALA:N	2.55	0.40
1:B:38:ASP:O	8:C:76:LYS:NZ	2.37	0.40
2:A:97:LEU:HG	2:A:146:VAL:HG22	2.02	0.40
2:A:206:LYS:HD3	2:A:206:LYS:HA	1.93	0.40
4:G:109:GLN:HA	4:G:112:VAL:HG22	2.02	0.40
9:D:52:PHE:HE2	9:D:181:ILE:HB	1.87	0.40
11:L:238:PRO:HB2	11:L:241:PRO:HD3	2.04	0.40
11:L:264:VAL:O	11:L:266:SER:OG	2.33	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	В	358/380~(94%)	303~(85%)	55 (15%)	0	100	100
2	А	974/1603~(61%)	876 (90%)	97~(10%)	1 (0%)	51	84
3	Н	119/124~(96%)	108 (91%)	11 (9%)	0	100	100
3	Ο	118/124~(95%)	107 (91%)	11 (9%)	0	100	100
4	G	123/125~(98%)	107 (87%)	16 (13%)	0	100	100
4	Ν	122/125~(98%)	107 (88%)	15 (12%)	0	100	100
5	J	90/91~(99%)	84 (93%)	6 (7%)	0	100	100
5	Q	89/91~(98%)	80 (90%)	9 (10%)	0	100	100
6	Ι	81/99~(82%)	68 (84%)	13 (16%)	0	100	100
6	Р	95/99~(96%)	90~(95%)	5 (5%)	0	100	100
7	F	109/161~(68%)	100 (92%)	9(8%)	0	100	100
7	М	113/161~(70%)	105 (93%)	8 (7%)	0	100	100
8	С	394/569~(69%)	367~(93%)	27 (7%)	0	100	100
9	D	294/313~(94%)	260 (88%)	34 (12%)	0	100	100
9	K	298/313~(95%)	264 (89%)	32 (11%)	2 (1%)	22	61
10	Е	304/399~(76%)	263~(86%)	41 (14%)	0	100	100
11	L	305/399~(76%)	253 (83%)	52 (17%)	0	100	100
All	All	3986/5176~(77%)	3542 (89%)	441 (11%)	3 (0%)	54	84

All (3) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
2	А	300	THR
9	Κ	77	GLN
9	Κ	282	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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed Rotameric Outliers		Percentiles		
1	В	334/351~(95%)	334 (100%)	0	100 100	



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
2	А	891/1412~(63%)	888 (100%)	3~(0%)	92	95
3	Н	105/108~(97%)	105 (100%)	0	100	100
3	Ο	105/108~(97%)	105 (100%)	0	100	100
4	G	98/98~(100%)	98 (100%)	0	100	100
4	Ν	97/98~(99%)	96~(99%)	1 (1%)	76	86
5	J	78/77~(101%)	78 (100%)	0	100	100
5	Q	77/77~(100%)	77~(100%)	0	100	100
6	Ι	71/83~(86%)	71 (100%)	0	100	100
6	Р	81/83~(98%)	81 (100%)	0	100	100
7	F	96/141~(68%)	96 (100%)	0	100	100
7	М	99/141~(70%)	99~(100%)	0	100	100
8	С	363/504~(72%)	363~(100%)	0	100	100
9	D	271/287~(94%)	270 (100%)	1 (0%)	91	94
9	Κ	275/287~(96%)	275 (100%)	0	100	100
10	Е	279/339~(82%)	277 (99%)	2 (1%)	84	90
11	L	281/340~(83%)	281 (100%)	0	100	100
All	All	$360\overline{1/4534}$ (79%)	3594 (100%)	7 (0%)	93	96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
2	А	78	ARG
2	А	381	LYS
2	А	1407	ARG
9	D	153	ARG
10	Е	193	ARG
10	Е	333	LYS
4	Ν	44	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	41	GLN
2	А	107	GLN
9	D	196	GLN



Continued from previous page...

Mol	Chain	Res	Type
10	Е	355	ASN
11	L	248	ASN

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)

6 ligands are modelled in this entry.

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

Mal	Turne	Chain F	Dec	Tink	Bo	ond leng	ths	В	ond ang	gles	
			Ullalli	res	a	Les Link	Counts	RMSZ	# Z > 2	Counts	RMSZ
13	AF3	D	502	-	0,3,3	-	-	-			
13	AF3	K	502	-	0,3,3	-	-	-			
12	GDP	Е	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.48	5(16%)	
12	GDP	K	501	9	24,30,30	1.05	1 (4%)	30,47,47	1.48	5 (16%)	
12	GDP	D	501	9,1	24,30,30	1.18	2 (8%)	30,47,47	1.34	5 (16%)	
13	AF3	Е	502	-	0,3,3	-	-	-			

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	GDP	К	501	9	-	4/12/32/32	0/3/3/3
12	GDP	Е	501	-	-	3/12/32/32	0/3/3/3
12	GDP	D	501	9,1	-	4/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	501	GDP	C6-N1	-3.73	1.32	1.37
12	Κ	501	GDP	C6-N1	-3.15	1.33	1.37
12	Е	501	GDP	C6-N1	-2.59	1.34	1.37
12	D	501	GDP	O4'-C1'	2.07	1.44	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
12	Е	501	GDP	PA-O3A-PB	-4.40	117.73	132.83
12	D	501	GDP	PA-O3A-PB	-4.38	117.80	132.83
12	Κ	501	GDP	PA-O3A-PB	-4.20	118.40	132.83
12	Е	501	GDP	C3'-C2'-C1'	3.69	106.53	100.98
12	Κ	501	GDP	C3'-C2'-C1'	3.28	105.92	100.98
12	Κ	501	GDP	C8-N7-C5	2.76	108.25	102.99
12	D	501	GDP	C5-C6-N1	2.74	118.80	113.95
12	Κ	501	GDP	C5-C6-N1	2.47	118.31	113.95
12	Е	501	GDP	C5-C6-N1	2.27	117.97	113.95
12	Ε	501	GDP	C8-N7-C5	2.25	107.27	102.99
12	D	501	GDP	C8-N7-C5	2.17	107.13	102.99
12	Е	501	GDP	O5'-C5'-C4'	2.14	116.34	108.99
12	K	501	GDP	C2'-C3'-C4'	2.12	106.75	102.64
12	D	501	GDP	C2'-C3'-C4'	2.12	106.75	102.64
12	D	501	GDP	C2-N1-C6	-2.05	121.32	125.10

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	D	501	GDP	C5'-O5'-PA-O1A
12	D	501	GDP	C3'-C4'-C5'-O5'
12	D	501	GDP	O4'-C4'-C5'-O5'
12	Κ	501	GDP	O4'-C4'-C5'-O5'
12	D	501	GDP	C5'-O5'-PA-O3A
12	Κ	501	GDP	C3'-C4'-C5'-O5'



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Mol	Chain	Res	Type	Atoms		
12	Κ	501	GDP	C5'-O5'-PA-O3A		
12	Е	501	GDP	PB-O3A-PA-O1A		
12	Е	501	GDP	PB-O3A-PA-O2A		
12	Κ	501	GDP	PB-O3A-PA-O2A		
12	Е	501	GDP	O4'-C4'-C5'-O5'		

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	Κ	502	AF3	2	0
12	Е	501	GDP	1	0
12	Κ	501	GDP	3	0
12	D	501	GDP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





















5.7 Other polymers (i)

There are no such residues in this entry.



5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-25654. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

6.1.1 Primary map



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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 230



Y Index: 230



Z Index: 230 $\,$



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: 239

Y Index: 211

Z Index: 208

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



6.5 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 680 nm^3 ; this corresponds to an approximate mass of 614 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 0.250 \AA^{-1}



8 Fourier-Shell correlation (i)

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



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-25654 and PDB model 7T3C. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.1 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 (0.1).



9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 92% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9225	0.2420
А	0.9480	0.3030
В	0.9801	0.3120
C	0.9641	0.2540
D	0.9788	0.2660
Е	0.8842	0.2160
F	0.7565	0.2170
G	0.9817	0.1600
Н	0.8605	0.1410
I	0.5946	0.1580
J	0.8313	0.1600
K	0.9762	0.2480
L	0.9503	0.1820
М	0.7794	0.1560
N	0.9902	0.1740
0	0.9120	0.1770
Р	0.5798	0.1820
Q	0.9081	0.1610

