

Nov 7, 2022 – 01:14 AM EST

PDB ID	:	6NK6
EMDB ID	:	EMD-9394
Title	:	Electron Cryo-Microscopy Of Chikungunya VLP in complex with mouse Mxra8
		receptor
Authors	:	Basore, K.; Kim, A.S.; Nelson, C.A.; Fremont, D.H.; Center for Structural
		Genomics of Infectious Diseases (CSGID)
Deposited on	:	2019-01-04
Resolution	:	4.06 Å(reported)
Based on initial models	:	3J0C, 3N42, 6NK3, 5H23

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.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
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 4.06 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.



Matria	Whole archive	EM structures
INTEGLIC	$(\# { m Entries})$	$(\# { m Entries})$
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%

Mol	Chain	Length	Quality of chain	
1	М	269	75%	25%
1	N	269	69%	27% ••
1	0	269	71%	29% •
1	Р	269	74%	25% •
2	А	439	84%	15% •
2	В	439	80%	20%
2	С	439	80%	20% •
2	D	439	78%	22%
3	Е	419	71%	28% •



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Mol	Chain	Length	Quality of chain		
3	F	419	68%	32%	•
3	G	419	76%	23%	•
3	Н	419	75%	25%	
4	Ι	151	81%	16%	•
4	J	151	79%	21%	
4	K	151	81%	17%	•
4	L	151	83%	17%	_



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 39805 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	М	260	Total	С	Ν	0	S	0	0
1	111	209	2169	1344	416	400	9	0	0
1	N	961	Total	С	Ν	0	S	0	0
1	IN	201	2111	1306	408	388	9	0	0
1	0	O 269	Total	С	Ν	0	S	0	0
1	1 0		2168	1344	416	399	9	0	0
1 P	260	Total	С	Ν	0	S	0	0	
	Ľ	209	2169	1344	416	400	9	0	U

• Molecule 1 is a protein called Matrix remodeling-associated protein 8.

• Molecule 2 is a protein called E1 glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Λ	430	Total	С	Ν	0	S	0	0
	Л	439	3318	2102	558	633	25	0	0
9	В	430	Total	С	Ν	0	S	0	0
	D	439	3318	2102	558	633	25	0	0
0	С	420	Total	С	Ν	0	S	0	0
	U	439	3318	2102	558	633	25	0	0
0	Л	420	Total	С	Ν	0	S	0	0
	D	439	3318	2102	558	633	25	0	0

• Molecule 3 is a protein called E2 glycoprotein.

Mol	Chain	Residues	Atoms				AltConf	Trace	
3	F	410	Total	С	Ν	0	S	0	0
5	Ľ	419	3280	2055	587	611	27	0	0
3	F	410	Total	С	Ν	0	S	0	0
J	Г	419	3280	2055	587	611	27	0	0
2	C	410	Total	С	Ν	0	S	0	0
J	G	419	3280	2055	587	611	27	0	0
9	2 II	410	Total	С	Ν	0	S	0	0
3	п	419	3280	2055	587	611	27	0	0

• Molecule 4 is a protein called Capsid protein.

Mol	Chain	Residues		At	oms			AltConf	Trace
4	Т	151	Total	С	Ν	0	\mathbf{S}	0	0
4	1	101	1157	731	204	216	6	0	0
4	т	151	Total	С	Ν	0	S	0	0
4	J	101	1157	731	204	216	6	0	0
4	K	151	Total	С	Ν	0	S	0	0
4	Т	101	1157	731	204	216	6	0	0
4	т	151	Total	С	Ν	0	S	0	0
4	Ľ	101	1157	731	204	216	6		

• Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
F	М	1	Total C N O	0
0	1/1	1	14 8 1 5	0
5	N	1	Total C N O	0
0	IN	1	14 8 1 5	0
5	0	1	Total C N O	0
0	0	1	14 8 1 5	0
5	P	1	Total C N O	0
0	1	1	14 8 1 5	0
5	Λ	1	Total C N O	0
0	Л	1	14 8 1 5	0
5	F	1	Total C N O	0
	Ľ	Ţ	14 8 1 5	0
5	В	1	Total C N O	0
0	D	1	14 8 1 5	0



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Mol	Chain	Residues	Atoms	AltConf
5	F	1	Total C N O	0
0	Г	1	14 8 1 5	0
5	С	1	Total C N O	0
0	U	1	14 8 1 5	0
5	С	1	Total C N O	0
0	G	1	14 8 1 5	0
5	Л	1	Total C N O	0
0	D	1	14 8 1 5	0
5	Ц	1	Total C N O	0
5	11	1	14 8 1 5	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. 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. 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.



 \bullet Molecule 1: Matrix remodeling-associated protein 8

• Molecule 1: Matrix remodeling-associated protein 8



• Molecule 2: E1 glycoprotein



- L432 F436 S437 R438 R438 H439
- Molecule 2: E1 glycoprotein



1321 1321 1339 1339 1339 1354 1354 1355 1355 1355 1355 1355 1355 1355 1355 1355 1355 1355 1355 1355 1357 1358

• Molecule 2: E1 glycoprotein









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	22486	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 $(e^-/\text{\AA}^2)$	50.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	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: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol Chain		Bond lengths		Bond angles		
WIOI	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	М	0.36	0/2224	0.76	7/3020~(0.2%)	
1	Ν	0.34	0/2162	0.70	2/2932~(0.1%)	
1	0	0.36	0/2223	0.78	3/3018~(0.1%)	
1	Р	0.36	0/2224	0.78	3/3020~(0.1%)	
2	А	0.39	0/3400	0.67	2/4643~(0.0%)	
2	В	0.39	0/3400	0.67	0/4643	
2	С	0.40	0/3400	0.71	4/4643~(0.1%)	
2	D	0.41	0/3400	0.70	2/4643~(0.0%)	
3	Е	0.39	0/3367	0.71	3/4592~(0.1%)	
3	F	0.34	0/3367	0.68	3/4592~(0.1%)	
3	G	0.37	0/3367	0.67	1/4592~(0.0%)	
3	Н	0.37	0/3367	0.68	2/4592~(0.0%)	
4	Ι	0.38	0/1185	0.73	3/1599~(0.2%)	
4	J	0.35	0/1185	0.74	1/1599~(0.1%)	
4	K	0.45	1/1185~(0.1%)	0.83	5/1599~(0.3%)	
4	L	0.37	0/1185	0.69	0/1599	
All	All	0.38	1/40641~(0.0%)	0.71	41/55326~(0.1%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Κ	233	ASN	CA-C	6.60	1.70	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	Е	362	LEU	CA-CB-CG	8.11	133.96	115.30
2	С	96	CYS	CA-CB-SG	7.75	127.95	114.00
2	D	370	CYS	CA-CB-SG	-7.68	100.17	114.00
4	K	233	ASN	O-C-N	-7.50	110.70	122.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	Е	225	CYS	CA-CB-SG	7.09	126.76	114.00
2	D	63	CYS	CA-CB-SG	6.89	126.41	114.00
1	Р	122	LEU	CA-CB-CG	6.80	130.94	115.30
2	А	219	LEU	CA-CB-CG	6.78	130.89	115.30
4	J	129	LEU	CA-CB-CG	6.74	130.79	115.30
1	Р	197	LEU	CA-CB-CG	6.66	130.61	115.30
1	М	138	LEU	CA-CB-CG	6.63	130.54	115.30
1	Р	167	ASP	CB-CG-OD1	6.62	124.26	118.30
4	K	233	ASN	CA-C-N	6.62	131.76	117.20
4	Ι	229	LEU	CA-CB-CG	6.57	130.40	115.30
2	С	44	LEU	CA-CB-CG	6.57	130.40	115.30
1	0	65	LEU	CA-CB-CG	6.55	130.37	115.30
1	0	76	LEU	CA-CB-CG	6.43	130.08	115.30
4	Ι	129	LEU	CA-CB-CG	6.41	130.04	115.30
1	М	65	LEU	CA-CB-CG	6.31	129.81	115.30
2	С	428	LEU	CA-CB-CG	6.14	129.43	115.30
1	М	173	LEU	CA-CB-CG	6.06	129.23	115.30
3	F	402	LEU	CA-CB-CG	6.03	129.17	115.30
4	K	232	ALA	C-N-CA	6.00	136.69	121.70
4	K	129	LEU	CA-CB-CG	5.92	128.93	115.30
3	F	415	LEU	CA-CB-CG	5.87	128.81	115.30
4	Ι	152	LEU	CA-CB-CG	5.80	128.65	115.30
1	М	161	LEU	CA-CB-CG	5.79	128.61	115.30
3	F	414	LEU	CA-CB-CG	5.73	128.49	115.30
1	0	161	LEU	CA-CB-CG	5.69	128.39	115.30
1	М	122	LEU	CA-CB-CG	5.61	128.19	115.30
2	С	244	LEU	CA-CB-CG	5.43	127.80	115.30
3	Н	402	LEU	CB-CG-CD2	-5.34	101.92	111.00
1	N	109	LEU	CA-CB-CG	5.34	127.57	115.30
2	А	311	ASP	CB-CG-OD1	5.30	123.08	118.30
4	K	219	ASP	CB-CG-OD1	5.28	123.05	118.30
3	Е	295	LEU	CA-CB-CG	5.27	127.43	115.30
1	N	161	LEU	CA-CB-CG	5.21	127.29	115.30
1	М	145	LEU	CA-CB-CG	5.20	127.26	115.30
3	G	378	LEU	CA-CB-CG	5.19	127.23	115.30
3	Н	343	SER	N-CA-C	5.05	124.64	111.00
1	М	201	GLN	CA-C-N	5.02	128.24	117.20

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There are no chirality outliers.

There are no planarity outliers.



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	М	2169	0	2062	40	0
1	Ν	2111	0	2011	45	0
1	0	2168	0	2062	52	0
1	Р	2169	0	2062	44	0
2	А	3318	0	3246	47	0
2	В	3318	0	3246	56	0
2	С	3318	0	3246	57	0
2	D	3318	0	3246	62	0
3	Е	3280	0	3210	85	0
3	F	3280	0	3210	89	0
3	G	3280	0	3210	64	0
3	Н	3280	0	3210	73	0
4	Ι	1157	0	1137	17	0
4	J	1157	0	1137	20	0
4	К	1157	0	1137	15	0
4	L	1157	0	1137	17	0
5	А	14	0	13	0	0
5	В	14	0	13	0	0
5	С	14	0	13	0	0
5	D	14	0	13	0	0
5	Е	14	0	13	0	0
5	F	14	0	13	0	0
5	G	14	0	13	0	0
5	Н	14	0	13	1	0
5	М	14	0	13	0	0
5	Ν	14	0	13	0	0
5	0	14	0	13	0	0
5	Р	14	0	13	0	0
All	All	39805	0	38725	721	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 9.

All (721) 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)
3:F:169:VAL:O	3:F:253:GLY:HA3	1.59	1.02
3:E:355:ILE:O	3:E:358:TYR:HB2	1.72	0.90
3:F:356:ILE:O	3:F:359:TYR:HB3	1.72	0.90
3:H:148:GLY:HA3	3:H:268:VAL:O	1.74	0.87
2:C:299:MET:HA	2:C:319:LYS:O	1.79	0.83
3:H:187:ASN:HA	3:H:217:ILE:O	1.81	0.80
4:I:154:PHE:HA	4:I:164:CYS:O	1.82	0.80
1:N:44:ALA:HA	1:N:291:THR:O	1.82	0.79
2:A:432:LEU:O	2:A:436:PHE:HB2	1.86	0.76
3:F:169:VAL:O	3:F:253:GLY:CA	2.35	0.75
3:H:14:PRO:HD3	3:H:68:ARG:HH21	1.54	0.72
1:O:204:VAL:HA	1:0:272:HIS:O	1.89	0.72
2:A:49:CYS:SG	2:A:50:GLU:N	2.63	0.72
1:N:64:ARG:HH12	1:N:200:ALA:HB2	1.55	0.71
3:F:83:LEU:HA	3:F:114:GLY:O	1.90	0.71
2:D:360:LEU:HD11	2:D:402:ILE:H	1.55	0.70
1:M:64:ARG:HE	3:F:26:HIS:HB3	1.57	0.68
2:D:428:LEU:HD11	3:H:392:ALA:HA	1.75	0.68
2:A:30:GLU:HB3	2:A:136:LEU:HB3	1.76	0.68
2:B:262:ALA:O	2:B:266:VAL:HA	1.95	0.67
4:K:229:LEU:HD11	4:K:243:VAL:HG23	1.77	0.67
2:A:196:ARG:HH12	2:A:199:GLN:HE21	1.43	0.66
1:N:143:CYS:SG	1:N:275:HIS:NE2	2.68	0.66
1:O:84:ARG:HH22	3:E:193:ASN:H	1.43	0.66
2:B:340:ARG:HH12	2:B:357:SER:HB2	1.61	0.66
3:H:183:GLN:HE21	3:H:222:ILE:H	1.42	0.66
1:P:196:HIS:NE2	1:P:198:GLU:O	2.29	0.65
3:E:272:ARG:NH1	3:E:273:ASN:OD1	2.29	0.65
1:O:151:VAL:HA	1:0:171:GLU:0	1.96	0.65
1:M:123:ILE:O	1:M:180:PRO:HA	1.96	0.65
2:B:183:ASP:OD2	2:B:247:ARG:NH2	2.29	0.65
4:I:133:LYS:NZ	4:I:134:VAL:O	2.29	0.64
1:N:96:GLN:HG2	1:N:109:LEU:HB3	1.78	0.64
1:P:151:VAL:HG11	1:P:183:MET:HG2	1.80	0.64
2:B:90:GLY:HA3	3:F:177:ASP:HA	1.79	0.64
2:B:196:ARG:HH21	2:B:199:GLN:HE21	1.46	0.64
1:P:123:ILE:O	1:P:180:PRO:HA	1.97	0.63
4:I:228:VAL:HA	4:I:242:VAL:HG22	1.80	0.63
1:0:223:ASP:0	1:O:230:ARG:HA	1.99	0.63
1:N:202:GLN:HB2	1:N:226:ALA:HB2	1.80	0.63
3:F:421:THR:HB	2:D:438:ARG:HB3	1.81	0.63
1:P:106:ARG:NH2	1:P:130:ASP:OD2	2.32	0.63



	o wo pwyc	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:H:138:ARG:NH1	3:H:331:GLY:O	2.32	0.63
3:H:271:ALA:HB2	3:H:331:GLY:HA3	1.80	0.62
3:H:269:PRO:O	3:H:332:ASN:ND2	2.33	0.62
1:M:230:ARG:HH12	1:M:244:VAL:H	1.46	0.62
1:O:151:VAL:HG22	1:O:171:GLU:HB2	1.81	0.62
3:E:144:ARG:NH1	3:F:25:GLY:O	2.33	0.62
2:C:160:LYS:HB2	2:C:281:ASP:HB3	1.82	0.62
2:A:59:TYR:HB3	2:A:103:LEU:HB3	1.82	0.61
2:C:30:GLU:HB3	2:C:136:LEU:HB2	1.81	0.61
2:D:340:ARG:NH2	2:D:357:SER:OG	2.33	0.61
2:C:428:LEU:HD22	3:G:395:ARG:HG2	1.83	0.61
1:M:209:GLN:HB2	1:M:268:ILE:HB	1.82	0.60
3:H:184:GLN:HB2	3:H:187:ASN:HB2	1.82	0.60
4:K:181:GLU:HG3	4:K:183:PRO:HD3	1.83	0.60
2:D:403:SER:HG	2:D:406:ALA:H	1.49	0.60
3:H:190:ILE:O	3:H:214:ASP:HA	2.02	0.60
3:H:370:ILE:HA	3:H:373:VAL:HG12	1.82	0.60
2:A:57:SER:HB3	3:E:244:ARG:HG3	1.84	0.60
1:0:51:LEU:O	1:O:255:SER:HA	2.01	0.60
2:B:229:VAL:HG21	3:F:243:PRO:HD3	1.83	0.60
1:M:112:SER:O	1:M:115:HIS:ND1	2.30	0.60
1:O:209:GLN:HB2	1:O:268:ILE:HB	1.83	0.60
1:P:262:GLU:HG3	1:P:264:ALA:H	1.66	0.60
2:A:90:GLY:HA3	3:E:177:ASP:HA	1.83	0.60
3:H:14:PRO:HG3	3:H:68:ARG:HB3	1.82	0.60
1:P:50:VAL:HG22	1:P:257:ARG:HG2	1.85	0.59
2:C:130:SER:HA	2:C:148:ALA:H	1.67	0.59
3:G:401:GLU:HG2	3:G:402:LEU:H	1.67	0.59
1:N:245:ASN:HB3	1:N:257:ARG:HH22	1.68	0.59
3:F:274:PRO:HB3	3:F:287:LEU:HD12	1.84	0.59
2:D:97:ASP:O	2:D:100:ASN:ND2	2.35	0.59
3:F:248:LEU:HD11	3:F:251:ARG:HH11	1.68	0.59
1:P:225:TYR:HE1	1:P:231:ARG:HH12	1.50	0.59
4:J:195:GLN:NE2	4:J:197:SER:OG	2.36	0.59
3:E:296:SER:HG	3:E:329:THR:HG1	1.49	0.59
1:N:34:SER:HB2	1:N:281:HIS:O	2.02	0.58
2:A:297:THR:O	2:A:321:THR:OG1	2.22	0.58
4:K:159:LYS:O	4:K:252:LYS:NZ	2.35	0.58
1:M:64:ARG:NH2	3:F:24:GLU:O	2.37	0.58
4:J:166:GLN:NE2	4:J:167:ILE:O	2.36	0.58
2:C:13:VAL:HG11	2:C:393:SER:HB3	1.84	0.58



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:A:404:THR:OG1	2:A:405:THR:N	2.37	0.58
3:F:322:PRO:HG2	3:F:325:GLY:H	1.68	0.58
3:G:173:PRO:HB3	3:G:245:ASN:HA	1.84	0.58
3:G:214:ASP:OD1	3:G:214:ASP:N	2.36	0.58
3:E:201:CYS:HB3	3:E:225:CYS:HA	1.84	0.58
1:M:67:ASP:HB3	1:M:199:GLU:HG2	1.86	0.58
3:G:412:LEU:HD22	3:G:420:THR:HG22	1.86	0.58
3:H:48:ILE:HB	3:H:101:ILE:HB	1.86	0.58
1:N:75:ASP:OD2	1:N:84:ARG:NH1	2.37	0.58
3:F:167:ILE:HG13	3:F:255:ILE:HG23	1.86	0.57
3:E:13:ARG:HH22	3:E:172:PRO:HG3	1.70	0.57
2:A:134:ARG:NH1	2:A:141:ASN:OD1	2.35	0.57
2:C:339:ILE:HD11	2:C:354:ILE:HB	1.86	0.57
3:H:355:ILE:O	3:H:359:TYR:N	2.38	0.57
1:P:151:VAL:HA	1:P:171:GLU:O	2.04	0.57
3:F:178:ARG:NH1	3:F:225:CYS:O	2.38	0.57
1:M:96:GLN:NE2	1:M:109:LEU:O	2.38	0.57
1:O:208:ARG:NH1	1:O:264:ALA:O	2.38	0.57
3:F:272:ARG:HG2	3:F:288:TYR:HB2	1.85	0.57
1:M:106:ARG:NH2	1:M:130:ASP:OD2	2.38	0.57
1:P:199:GLU:HG2	1:P:201:GLN:HG3	1.87	0.57
2:A:350:SER:OG	2:A:351:GLN:N	2.38	0.57
3:H:412:LEU:HD22	3:H:420:THR:HG22	1.87	0.57
2:A:57:SER:OG	3:E:242:VAL:O	2.22	0.57
3:E:176:PRO:HA	3:E:228:ALA:HA	1.87	0.56
1:N:64:ARG:HG2	1:N:67:ASP:HB2	1.88	0.56
1:N:271:CYS:O	1:N:283:ARG:HA	2.05	0.56
3:E:272:ARG:HD3	2:B:235:GLN:HE21	1.71	0.56
3:E:355:ILE:HG23	3:E:356:ILE:HD12	1.87	0.56
2:B:207:THR:HG22	2:B:210:SER:HB3	1.88	0.56
3:G:138:ARG:NH1	3:G:331:GLY:O	2.38	0.56
4:L:114:ILE:HG22	4:L:216:PRO:HD2	1.88	0.56
1:M:222:LEU:HD11	1:M:230:ARG:HB3	1.87	0.56
1:0:116:ASP:O	1:O:188:ARG:NH1	2.39	0.56
2:B:134:ARG:NH1	2:B:141:ASN:OD1	2.38	0.56
2:B:148:ALA:HA	2:B:163:VAL:HG23	1.87	0.56
2:D:59:TYR:HB3	2:D:103:LEU:HB3	1.86	0.56
4:L:203:ILE:HG23	4:L:240:LEU:HD11	1.86	0.56
1:N:60:TRP:NE1	1:N:67:ASP:OD2	2.38	0.56
1:N:34:SER:O	1:N:282:GLU:HA	2.04	0.56
3:E:272:ARG:NH1	3:E:273:ASN:O	2.39	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:F:69:TYR:OH	3:F:119:ARG:NH2	2.32	0.56
3:G:171:MET:SD	3:G:245:ASN:ND2	2.79	0.56
1:P:112:SER:O	1:P:115:HIS:ND1	2.36	0.56
3:E:86:ARG:HG2	3:E:90:PRO:HA	1.88	0.56
1:N:66:HIS:HB3	1:N:69:GLN:HB2	1.88	0.56
3:F:201:CYS:HA	3:F:225:CYS:HA	1.88	0.56
2:C:387:ILE:HD11	3:G:338:TYR:HB3	1.87	0.56
3:E:139:GLU:OE1	3:E:332:ASN:ND2	2.39	0.56
2:A:299:MET:HA	2:A:319:LYS:O	2.07	0.55
2:C:239:GLY:O	2:C:243:TRP:HB2	2.07	0.55
3:H:169:VAL:O	3:H:253:GLY:HA3	2.05	0.55
2:B:166:MET:SD	2:B:166:MET:N	2.77	0.55
3:G:148:GLY:HA2	3:G:270:LYS:HG2	1.87	0.55
1:O:86:ARG:NH1	1:0:89:ASP:OD2	2.39	0.55
1:0:112:SER:O	1:O:115:HIS:ND1	2.34	0.55
3:E:367:THR:HG23	3:E:370:ILE:HD12	1.87	0.55
4:I:144:ILE:HG12	4:I:149:LEU:HD12	1.89	0.55
3:F:296:SER:HB2	3:F:308:GLU:HG3	1.88	0.55
4:J:139:HIS:NE2	4:J:261:TRP:OXT	2.40	0.55
2:B:174:ASP:HB2	2:B:186:ASN:HD21	1.70	0.55
2:C:9:ASN:ND2	2:C:271:CYS:O	2.40	0.55
3:E:198:ARG:HB2	3:E:210:LEU:HD12	1.87	0.55
3:F:46:LEU:HB3	3:F:48:ILE:HD11	1.89	0.55
1:N:204:VAL:HG13	1:N:224:LEU:HB3	1.88	0.55
1:O:76:LEU:HD23	1:O:87:LEU:HD22	1.89	0.55
2:D:410:VAL:HA	2:D:413:ILE:HG22	1.87	0.55
1:N:223:ASP:HB2	1:N:231:ARG:HB2	1.88	0.55
2:B:155:THR:HA	2:B:159:ALA:O	2.07	0.55
3:F:66:LYS:NZ	3:F:79:GLU:OE1	2.37	0.55
2:D:57:SER:HB3	3:H:244:ARG:HG3	1.89	0.55
3:E:85:VAL:HG23	3:E:91:CYS:HB2	1.89	0.55
2:D:183:ASP:OD2	2:D:247:ARG:NH1	2.40	0.55
1:O:264:ALA:HA	2:D:211:LYS:HD3	1.89	0.54
1:O:139:HIS:ND1	1:O:145:LEU:O	2.40	0.54
3:G:404:PRO:HD3	4:K:133:LYS:HE3	1.89	0.54
2:A:427:ILE:HA	2:A:430:VAL:HG22	1.90	0.54
2:B:112:GLU:OE1	2:B:115:LYS:NZ	2.41	0.54
3:G:202:ASN:O	3:G:224:GLN:NE2	2.40	0.54
1:N:77:SER:HB3	1:N:84:ARG:HB3	1.90	0.54
1:O:70:ARG:NH2	1:0:194:ASP:OD1	2.39	0.54
3:G:144:ARG:HH21	3:G:267:ARG:HE	1.54	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:K:182:LYS:NZ	4:K:245:TRP:O	2.39	0.54
3:H:182:THR:OG1	3:H:184:GLN:NE2	2.38	0.54
2:B:183:ASP:N	2:B:183:ASP:OD1	2.35	0.54
2:B:130:SER:HA	2:B:147:TYR:HA	1.89	0.54
3:G:157:VAL:HG13	3:G:159:SER:H	1.73	0.54
1:N:32:SER:OG	1:N:33:SER:N	2.40	0.54
4:I:195:GLN:O	4:I:201:PHE:HA	2.08	0.54
1:O:206:TRP:HB2	1:O:222:LEU:HB3	1.90	0.53
2:C:105:GLU:OE1	3:G:244:ARG:NH1	2.42	0.53
4:I:152:LEU:HD11	4:I:168:PRO:HG3	1.89	0.53
3:H:13:ARG:HH11	3:H:234:ASN:HB3	1.73	0.53
3:H:178:ARG:HH12	3:H:226:HIS:HA	1.74	0.53
3:F:153:CYS:O	3:F:263:ASN:HA	2.08	0.53
2:C:51:TYR:HB3	2:C:203:ILE:HD13	1.90	0.53
1:O:42:SER:HG	1:O:291:THR:HG1	1.56	0.53
1:O:115:HIS:HA	1:O:194:ASP:HB2	1.89	0.53
3:E:412:LEU:HA	3:E:415:LEU:HB2	1.89	0.53
2:C:263:THR:O	2:C:267:ARG:NH2	2.41	0.53
3:G:95:GLY:H	3:G:102:LEU:HB2	1.74	0.53
3:H:188:VAL:O	3:H:216:VAL:HA	2.08	0.53
1:M:66:HIS:HB3	1:M:69:GLN:HB2	1.89	0.53
2:B:40:PRO:HA	2:B:127:ALA:HA	1.90	0.53
3:F:183:GLN:HE21	3:F:222:ILE:HG12	1.74	0.53
3:H:170:HIS:HB2	3:H:251:ARG:HB3	1.90	0.53
1:N:72:VAL:HG12	1:N:138:LEU:HD23	1.91	0.53
3:E:169:VAL:O	3:E:252:LYS:O	2.26	0.53
3:F:183:GLN:HE22	3:F:221:LYS:HB3	1.73	0.53
3:E:17:ALA:HB3	3:E:33:ALA:HB3	1.90	0.53
1:0:142:TYR:OH	1:O:202:GLN:NE2	2.41	0.53
1:M:62:GLN:HG2	1:M:249:PHE:HZ	1.74	0.52
1:P:209:GLN:HB2	1:P:268:ILE:HB	1.91	0.52
3:F:118:SER:OG	3:F:119:ARG:NH1	2.42	0.52
3:F:43:ASP:OD1	3:F:43:ASP:N	2.41	0.52
2:D:407:MET:SD	2:D:407:MET:N	2.80	0.52
1:M:72:VAL:HA	1:M:137:ASN:O	2.09	0.52
3:E:354:GLU:O	3:E:358:TYR:N	2.42	0.52
2:B:66:ALA:H	2:B:101:THR:HG21	1.73	0.52
3:F:201:CYS:O	3:F:207:ASN:ND2	2.42	0.52
3:G:32:ILE:HD12	3:G:113:VAL:HG23	1.91	0.52
2:C:239:GLY:O	2:C:243:TRP:CB	2.58	0.52
3:G:184:GLN:O	3:G:187:ASN:ND2	2.42	0.52



	louis page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:G:27:SER:OG	3:G:28:CYS:N	2.43	0.52
2:D:95:PHE:HZ	3:H:202:ASN:HB2	1.74	0.52
1:N:163:ARG:H	1:N:174:VAL:HB	1.75	0.52
3:H:13:ARG:HH22	3:H:172:PRO:HG3	1.74	0.52
1:N:72:VAL:HA	1:N:137:ASN:O	2.10	0.52
3:E:24:GLU:OE2	3:E:26:HIS:NE2	2.42	0.52
3:F:412:LEU:HA	3:F:415:LEU:HG	1.91	0.52
3:H:180:LEU:HD12	3:H:227:ALA:HB1	1.92	0.52
2:A:282:ILE:HD12	2:A:283:PRO:HD2	1.92	0.52
4:I:133:LYS:HZ1	4:I:164:CYS:HA	1.74	0.52
3:F:163:THR:OG1	3:F:164:ALA:N	2.43	0.52
4:J:172:LYS:HB2	4:L:234:GLU:HB2	1.92	0.52
2:D:129:ALA:O	2:D:148:ALA:N	2.43	0.52
3:H:262:ALA:HA	5:H:501:NAG:H82	1.91	0.52
2:A:310:SER:H	3:E:341:GLN:HE21	1.58	0.52
4:J:134:VAL:O	4:J:164:CYS:HA	2.10	0.52
4:L:219:ASP:OD1	4:L:223:ARG:N	2.43	0.52
3:G:146:GLN:O	3:G:267:ARG:NH1	2.43	0.51
2:D:265:PRO:O	2:D:267:ARG:NH1	2.41	0.51
4:L:194:VAL:HG12	4:L:203:ILE:HG22	1.92	0.51
1:N:136:CYS:O	1:N:148:SER:HA	2.10	0.51
2:C:191:PRO:HG2	2:C:194:ALA:HB3	1.93	0.51
2:C:433:CYS:HA	2:C:436:PHE:HB3	1.93	0.51
3:G:148:GLY:HA3	3:G:268:VAL:O	2.10	0.51
1:O:247:ASN:HB2	1:O:251:ARG:HH11	1.75	0.51
4:J:200:ARG:NH2	4:J:240:LEU:O	2.44	0.51
2:D:51:TYR:OH	2:D:236:ALA:O	2.29	0.51
1:P:266:GLU:O	2:C:211:LYS:NZ	2.37	0.51
3:F:42:THR:HG1	3:F:154:SER:H	1.55	0.51
1:P:85:ARG:HH22	1:P:100:GLU:HB2	1.75	0.51
1:P:202:GLN:HB3	1:P:226:ALA:HB2	1.93	0.51
2:C:34:GLN:HB2	2:C:132:LYS:HB3	1.91	0.51
2:C:107:HIS:NE2	2:C:109:GLU:OE2	2.43	0.51
3:G:347:THR:OG1	3:G:354:GLU:O	2.28	0.51
2:D:316:ALA:HB3	2:D:354:ILE:HG22	1.91	0.51
3:E:349:HIS:HD1	3:E:358:TYR:HH	1.39	0.51
2:B:265:PRO:O	2:B:267:ARG:NH1	2.43	0.51
3:F:169:VAL:HA	3:F:237:TYR:HA	1.92	0.51
3:G:17:ALA:HB3	3:G:33:ALA:HB3	1.93	0.51
1:O:207:ASP:O	1:O:269:TYR:HA	2.11	0.51
1:P:245:ASN:HB3	1:P:257:ARG:HH11	1.76	0.51



	bus puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:418:GLY:HA2	2:C:421:VAL:HG12	1.93	0.51
3:H:186:GLY:O	3:H:220:CYS:N	2.40	0.51
1:N:49:ALA:HB3	1:N:258:ILE:HB	1.93	0.51
1:O:163:ARG:H	1:0:174:VAL:HB	1.76	0.51
4:K:139:HIS:NE2	4:K:260:GLU:OE2	2.44	0.51
2:D:337:VAL:HG23	2:D:358:THR:HB	1.92	0.51
2:D:394:HIS:HD2	2:D:395:THR:HG23	1.76	0.51
1:N:68:ARG:HE	1:N:197:LEU:HG	1.76	0.51
3:F:102:LEU:HD21	3:F:156:TYR:HB2	1.93	0.51
1:N:84:ARG:NH2	3:G:191:THR:OG1	2.45	0.50
2:A:410:VAL:HA	2:A:413:ILE:HG12	1.93	0.50
2:A:432:LEU:O	2:A:436:PHE:CB	2.57	0.50
3:E:359:TYR:HA	3:E:362:LEU:HG	1.93	0.50
3:F:16:LEU:HD21	3:F:71:ASP:HA	1.92	0.50
2:C:77:SER:O	2:C:105:GLU:HA	2.10	0.50
3:G:400:TYR:HE1	3:G:408:VAL:HG22	1.76	0.50
3:E:360:TYR:HA	3:E:364:PRO:HB3	1.92	0.50
3:G:355:ILE:O	3:G:358:TYR:HB2	2.10	0.50
4:K:136:LYS:O	4:K:163:GLU:HB2	2.11	0.50
3:H:188:VAL:HG22	3:H:217:ILE:HB	1.93	0.50
2:B:388:VAL:HG21	3:F:341:GLN:HE21	1.77	0.50
3:G:154:SER:HB2	3:G:261:LEU:HD21	1.93	0.50
3:E:271:ALA:HB2	3:E:331:GLY:HA3	1.94	0.50
2:B:184:VAL:HG12	2:B:251:LEU:HD12	1.93	0.50
3:F:201:CYS:HB2	3:F:207:ASN:HB2	1.92	0.50
2:C:191:PRO:HB3	2:D:151:ASP:HB2	1.94	0.50
3:F:193:ASN:O	3:F:195:GLN:NE2	2.45	0.50
2:C:88:MET:HG2	3:G:176:PRO:HD2	1.93	0.50
3:H:139:GLU:HG3	3:H:293:THR:HG23	1.93	0.50
4:J:195:GLN:OE1	4:J:202:THR:OG1	2.23	0.49
2:D:155:THR:HB	2:D:160:LYS:HG2	1.94	0.49
3:H:412:LEU:HD13	3:H:420:THR:HA	1.94	0.49
1:P:199:GLU:OE2	1:P:201:GLN:NE2	2.42	0.49
3:F:139:GLU:HG3	3:F:293:THR:HG23	1.95	0.49
2:C:111:SER:HG	2:C:113:SER:HG	1.58	0.49
2:C:160:LYS:NZ	2:D:193:GLY:O	2.40	0.49
3:G:356:ILE:O	3:G:360:TYR:N	2.41	0.49
3:G:370:ILE:HA	3:G:373:VAL:HG12	1.94	0.49
1:O:190:HIS:HB3	1:O:195:ARG:HH21	1.77	0.49
2:B:284:ASP:HA	2:B:287:PHE:HD2	1.77	0.49
4:J:177:LYS:HB2	4:J:223:ARG:HG2	1.94	0.49



	loue page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:325:LYS:HA	2:C:346:VAL:O	2.12	0.49
1:O:215:HIS:CD2	1:O:216:ASP:H	2.30	0.49
1:O:275:HIS:HB3	1:O:280:LEU:HB2	1.93	0.49
2:C:102:GLN:HE22	2:C:104:SER:HB3	1.77	0.49
3:H:12:THR:O	3:H:68:ARG:NH2	2.45	0.49
1:O:49:ALA:HB2	1:O:261:LEU:HD11	1.94	0.49
4:I:167:ILE:O	4:I:172:LYS:NZ	2.38	0.49
4:I:180:HIS:CE1	4:I:248:ASP:H	2.29	0.49
2:B:282:ILE:HD12	2:B:283:PRO:HD2	1.95	0.49
3:G:13:ARG:HH21	3:G:234:ASN:HB2	1.77	0.49
2:D:171:THR:HG22	2:D:173:PHE:H	1.76	0.49
1:N:199:GLU:HG2	1:N:201:GLN:HB2	1.94	0.49
3:F:39:ASN:OD1	3:F:39:ASN:N	2.44	0.49
2:A:184:VAL:HG23	2:A:251:LEU:HD12	1.93	0.49
1:M:60:TRP:NE1	1:M:67:ASP:OD2	2.45	0.49
2:B:38:LEU:HB2	2:B:268:ALA:HB3	1.93	0.49
1:0:112:SER:HG	1:O:115:HIS:HD1	1.61	0.49
3:E:198:ARG:HA	3:E:210:LEU:HA	1.95	0.49
2:B:358:THR:HG22	2:B:360:LEU:H	1.78	0.49
2:C:134:ARG:NH1	2:C:141:ASN:OD1	2.38	0.49
2:A:410:VAL:HG23	2:A:413:ILE:HD11	1.95	0.48
2:D:158:ASP:HB3	2:D:283:PRO:HG3	1.94	0.48
2:D:418:GLY:HA2	2:D:421:VAL:HG22	1.95	0.48
1:O:50:VAL:HG12	1:O:257:ARG:HG2	1.94	0.48
2:C:347:GLU:OE2	2:C:350:SER:OG	2.29	0.48
2:C:406:ALA:HA	2:C:409:TRP:HB2	1.95	0.48
3:G:110:THR:OG1	3:G:111:LEU:N	2.45	0.48
2:A:217:THR:O	2:A:235:GLN:NE2	2.46	0.48
4:J:134:VAL:HB	4:J:165:ALA:HB3	1.95	0.48
2:D:256:PRO:HG3	3:H:304:PRO:HD3	1.96	0.48
1:M:60:TRP:HD1	1:M:142:TYR:HE1	1.60	0.48
1:O:195:ARG:H	1:O:197:LEU:HD13	1.78	0.48
2:A:78:CYS:HA	2:A:104:SER:O	2.12	0.48
1:N:156:THR:OG1	1:N:158:ASP:OD1	2.29	0.48
1:0:120:SER:HB2	1:O:184:THR:HA	1.94	0.48
2:A:16:LYS:HE3	2:A:339:ILE:O	2.13	0.48
3:E:77:ASP:O	3:E:118:SER:OG	2.30	0.48
2:D:432:LEU:O	2:D:436:PHE:HB2	2.14	0.48
3:H:22:CYS:SG	3:H:28:CYS:N	2.86	0.48
4:J:233:ASN:N	4:J:233:ASN:OD1	2.47	0.48
2:D:57:SER:OG	3:H:242:VAL:O	2.28	0.48



	lous page	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:P:205:HIS:HB2	1:P:272:HIS:HB2	1.96	0.48
3:E:107:LYS:HE2	3:E:132:GLU:HG3	1.94	0.48
3:F:148:GLY:HA2	3:F:270:LYS:HG3	1.95	0.48
3:F:355:ILE:HA	3:F:358:TYR:HB2	1.96	0.48
3:G:19:CYS:O	3:G:27:SER:OG	2.28	0.48
1:M:195:ARG:HE	3:E:64:TRP:HZ2	1.60	0.48
1:0:136:CYS:O	1:O:148:SER:HA	2.13	0.48
1:O:236:PRO:HA	1:O:239:ARG:HG2	1.96	0.48
3:E:347:THR:HG21	3:E:358:TYR:HA	1.95	0.48
2:C:59:TYR:HB3	2:C:103:LEU:HB3	1.94	0.48
2:D:43:SER:HB2	2:D:123:ARG:HB2	1.95	0.48
2:D:384:LYS:O	3:H:344:THR:OG1	2.32	0.48
2:A:21:ARG:NH2	2:A:284:ASP:OD1	2.46	0.48
3:F:14:PRO:O	3:F:236:GLN:NE2	2.47	0.48
3:F:154:SER:HA	3:F:262:ALA:O	2.14	0.48
2:A:186:ASN:HB2	2:A:251:LEU:HD21	1.96	0.47
2:B:57:SER:N	3:F:238:ASN:OD1	2.46	0.47
3:H:277:THR:HG1	3:H:284:THR:HG1	1.58	0.47
2:B:178:VAL:HG13	2:B:185:TYR:HB2	1.97	0.47
2:B:407:MET:HA	2:B:410:VAL:HG22	1.95	0.47
3:F:412:LEU:HD23	3:F:415:LEU:HD11	1.95	0.47
3:H:19:CYS:HA	3:H:20:PRO:HD3	1.76	0.47
3:E:32:ILE:HD12	3:E:113:VAL:HG13	1.95	0.47
4:J:117:VAL:HG23	4:J:144:ILE:HA	1.96	0.47
2:C:21:ARG:NH1	2:C:284:ASP:OD1	2.48	0.47
1:M:135:THR:HA	1:M:149:LEU:O	2.15	0.47
1:P:224:LEU:HD21	1:P:244:VAL:HG11	1.97	0.47
2:C:53:THR:HG21	2:C:235:GLN:HE22	1.79	0.47
2:D:426:LEU:HA	2:D:429:ILE:HG22	1.96	0.47
2:A:369:VAL:O	2:A:372:THR:HB	2.15	0.47
3:E:145:PRO:HG3	3:E:269:PRO:HB3	1.96	0.47
4:J:122:LYS:HB3	4:J:122:LYS:HE3	1.73	0.47
2:D:125:HIS:ND1	2:D:126:THR:OG1	2.43	0.47
4:L:196:TYR:HA	4:L:200:ARG:O	2.14	0.47
1:N:131:GLU:HG2	1:N:154:GLU:HA	1.95	0.47
2:A:262:ALA:O	2:A:266:VAL:HA	2.15	0.47
1:M:68:ARG:HE	1:M:197:LEU:HB2	1.78	0.47
3:F:12:THR:HB	3:F:53:GLN:HE22	1.78	0.47
3:F:114:GLY:HA2	3:F:123:HIS:O	2.15	0.47
3:G:347:THR:HB	3:G:357:LEU:HB2	1.96	0.47
2:D:38:LEU:HB2	2:D:268:ALA:HB3	1.96	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:79:LYS:HA	2:D:79:LYS:HD3	1.69	0.47
3:H:201:CYS:HB2	3:H:207:ASN:HA	1.97	0.47
1:O:205:HIS:HB3	1:O:220:ARG:NH2	2.30	0.47
3:E:155:THR:OG1	3:E:156:TYR:N	2.48	0.47
3:G:17:ALA:O	3:G:29:HIS:HA	2.15	0.47
3:G:169:VAL:HA	3:G:236:GLN:O	2.15	0.47
3:H:71:ASP:O	3:H:74:THR:OG1	2.31	0.47
2:A:239:GLY:O	2:A:243:TRP:HB2	2.15	0.47
3:E:109:GLU:OE2	3:E:130:HIS:ND1	2.40	0.47
2:B:161:PHE:HB3	2:B:280:ILE:HG23	1.97	0.47
3:G:85:VAL:HG23	3:G:91:CYS:HB2	1.97	0.47
3:H:273:ASN:OD1	3:H:273:ASN:N	2.48	0.47
3:F:36:ARG:HH12	3:F:38:ARG:HB3	1.80	0.47
3:F:202:ASN:HB3	3:F:224:GLN:HG2	1.97	0.47
3:F:290:ASP:OD2	3:F:291:HIS:ND1	2.47	0.47
3:E:408:VAL:HG12	3:E:411:LEU:HB3	1.97	0.46
2:D:191:PRO:HG2	2:D:194:ALA:HB3	1.97	0.46
4:L:195:GLN:O	4:L:201:PHE:HA	2.14	0.46
1:N:204:VAL:HA	1:N:272:HIS:O	2.15	0.46
1:P:210:LEU:HD23	2:C:211:LYS:HD2	1.97	0.46
1:0:158:ASP:OD1	1:O:158:ASP:N	2.40	0.46
3:E:403:THR:HG22	4:I:250:VAL:HG13	1.98	0.46
2:C:310:SER:HB2	3:G:341:GLN:HE22	1.80	0.46
3:H:13:ARG:HB2	3:H:234:ASN:HD22	1.80	0.46
3:H:97:MET:O	3:H:100:PHE:HB2	2.15	0.46
1:N:275:HIS:HB3	1:N:280:LEU:HB2	1.96	0.46
2:A:188:ASP:OD1	2:A:188:ASP:N	2.42	0.46
3:E:273:ASN:OD1	3:E:273:ASN:N	2.41	0.46
2:B:57:SER:OG	3:F:239:SER:O	2.33	0.46
4:J:229:LEU:HD22	4:J:243:VAL:HG13	1.98	0.46
2:C:282:ILE:HD12	2:C:283:PRO:HD2	1.96	0.46
2:C:366:ARG:HA	2:C:374:VAL:O	2.16	0.46
3:H:290:ASP:OD1	3:H:290:ASP:N	2.46	0.46
3:H:355:ILE:O	3:H:358:TYR:HB3	2.15	0.46
1:O:63:ASP:HB3	1:O:65:LEU:HD22	1.96	0.46
3:E:287:LEU:HD11	3:E:330:TRP:CE2	2.51	0.46
2:B:207:THR:HG23	2:B:209:GLU:H	1.79	0.46
2:C:369:VAL:O	2:C:372:THR:OG1	2.24	0.46
2:C:382:PRO:O	3:G:345:ASN:ND2	2.47	0.46
3:H:206:SER:O	3:H:206:SER:OG	2.31	0.46
1:O:96:GLN:HE22	1:O:109:LEU:H	1.62	0.46



	lo de page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:178:VAL:HG23	2:C:185:TYR:HB2	1.97	0.46
3:G:189:LYS:HG3	3:G:216:VAL:HG22	1.98	0.46
3:G:344:THR:OG1	3:G:345:ASN:N	2.49	0.46
2:D:303:VAL:HG11	2:D:378:ALA:HA	1.97	0.46
1:M:140:HIS:CE1	1:M:142:TYR:HB3	2.49	0.46
2:D:28:VAL:HG22	2:D:329:ALA:HB1	1.98	0.46
1:N:74:TRP:HA	1:N:135:THR:O	2.15	0.46
1:P:237:PHE:HE2	2:D:152:HIS:HE1	1.64	0.46
2:C:327:LYS:HD3	2:C:327:LYS:HA	1.65	0.46
3:E:280:LYS:HZ3	3:E:343:SER:HG	1.59	0.46
3:G:144:ARG:HH21	3:G:267:ARG:NE	2.14	0.46
3:H:71:ASP:N	3:H:71:ASP:OD1	2.48	0.46
1:M:247:ASN:HD22	2:B:226:ALA:HB1	1.80	0.46
1:P:34:SER:H	1:P:282:GLU:HA	1.81	0.46
1:P:139:HIS:ND1	1:P:146:ASP:OD1	2.49	0.46
3:E:196:THR:OG1	3:E:230:THR:O	2.32	0.46
3:F:15:TYR:HB2	3:F:51:SER:HB2	1.97	0.46
3:G:139:GLU:OE2	3:G:332:ASN:N	2.46	0.46
3:G:187:ASN:HA	3:G:218:ASN:HA	1.98	0.46
3:H:238:ASN:OD1	3:H:238:ASN:N	2.48	0.46
1:M:84:ARG:HH12	3:F:193:ASN:ND2	2.14	0.45
3:E:292:PRO:HA	3:E:311:VAL:O	2.15	0.45
3:G:107:LYS:HE3	3:G:132:GLU:HG3	1.98	0.45
2:D:125:HIS:HD1	2:D:126:THR:HG1	1.64	0.45
4:L:154:PHE:HA	4:L:164:CYS:O	2.16	0.45
4:L:228:VAL:HA	4:L:242:VAL:HG22	1.97	0.45
1:M:190:HIS:O	1:M:277:TYR:OH	2.34	0.45
1:P:76:LEU:HB2	1:P:87:LEU:HD21	1.98	0.45
1:P:208:ARG:HD3	1:P:221:LEU:HD11	1.98	0.45
3:E:251:ARG:HD2	3:E:252:LYS:H	1.81	0.45
3:G:38:ARG:HB2	3:G:47:LYS:HB3	1.98	0.45
3:H:148:GLY:HA2	3:H:270:LYS:HG2	1.98	0.45
3:E:71:ASP:O	3:E:74:THR:OG1	2.33	0.45
2:B:212:ASP:OD1	2:B:212:ASP:N	2.46	0.45
2:B:327:LYS:HD2	2:B:327:LYS:HA	1.79	0.45
3:G:42:THR:OG1	3:G:154:SER:N	2.50	0.45
3:G:140:ARG:HB2	3:G:292:PRO:HB2	1.98	0.45
1:M:57:ARG:NH2	1:M:143:CYS:SG	2.83	0.45
3:E:114:GLY:HA2	3:E:123:HIS:O	2.15	0.45
3:F:166:GLU:OE2	3:F:255:ILE:N	2.49	0.45
3:F:196:THR:HB	3:F:210:LEU:HD11	1.97	0.45



	lo uo puge	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	(Å)
$3 \cdot E \cdot 263 \cdot ASN \cdot OD1$	3·E·263·ASN·N	2.49	0.45
4:K:117:VAL:HG11	4·K·136·LYS·HE2	1.97	0.45
1·M·64·ABG·HB2	3·F·26·HIS·CG	2.52	0.45
$2 \cdot B \cdot 59 \cdot TYB \cdot HE1$	$2 \cdot B \cdot 61 \cdot LYS \cdot HE3$	1.81	0.45
3·H·17·ALA·HB3	3·H·33·ALA·HB3	1.91	0.45
3·E·321·VAL·HG12	3·E·326·LEU·HD13	1.00	0.45
2:C:38:LEU:HB2	2:C:268:ALA:HB3	1.98	0.45
2:C:51:TYB:OH	2:C:236:ALA:O	2.35	0.45
2:D:371:SER:O	2:D:371:SER:OG	2.29	0.45
1:P:135:THR:HA	1:P:149:LEU:O	2.16	0.45
2:B:142:ILE:HD12	2:B:142:ILE:HA	1.87	0.45
2:C:184:VAL:HG23	2:C:251:LEU:HD12	1.99	0.45
2:D:84:VAL:HG11	2:D:102:GLN:HB2	1.98	0.45
3:H:50:VAL:O	3:H:99:HIS:ND1	2.44	0.45
2:A:335:ASN:N	2:A:335:ASN:OD1	2.48	0.45
3:F:370:ILE:HA	3:F:373:VAL:HG12	1.99	0.45
3:H:38:ARG:HB2	3:H:47:LYS:HB3	1.99	0.45
3:H:418:VAL:HG22	3:H:419:ABG:HG3	1.98	0.45
2:B:305:ALA:HB1	2:D:23:GLY:HA2	1.99	0.45
3:G:32:ILE:HG22	3:G:52:LEU:HD22	1.99	0.45
3:G:196:THR:O	3:G:230:THR:N	2.48	0.45
2:D:68:CYS:HB3	2:D:103:LEU:HD11	1.99	0.45
1:M:154:GLU:O	1:M:174:VAL:HA	2.16	0.44
1:P:68:ARG:NH1	1:P:196:HIS:O	2.50	0.44
3:F:71:ASP:OD1	3:F:74:THR:OG1	2.36	0.44
2:C:319:LYS:HD2	2:C:351:GLN:HB3	1.98	0.44
3:G:36:ARG:HB3	3:G:49:GLN:HG2	2.00	0.44
1:N:205:HIS:ND1	1:N:223:ASP:OD1	2.48	0.44
3:E:272:ARG:NH2	2:B:235:GLN:O	2.51	0.44
4:I:229:LEU:HD23	4:I:243:VAL:HG13	2.00	0.44
2:B:371:SER:O	2:B:371:SER:OG	2.33	0.44
2:C:265:PRO:O	2:C:267:ARG:NE	2.46	0.44
2:A:299:MET:HB2	2:A:374:VAL:HG11	2.00	0.44
2:A:396:THR:O	2:A:396:THR:OG1	2.33	0.44
2:A:429:ILE:HD12	2:A:432:LEU:HB2	1.99	0.44
3:E:17:ALA:HB1	3:E:241:LEU:HD22	1.99	0.44
3:E:144:ARG:NH1	3:F:21:ASP:OD1	2.51	0.44
2:B:241:LYS:NZ	3:F:39:ASN:O	2.45	0.44
2:B:383:PRO:HD2	3:F:342:MET:HB2	2.00	0.44
2:C:284:ASP:HA	2:C:287:PHE:HD2	1.83	0.44
3:G:71:ASP:OD1	3:G:71:ASP:N	2.50	0.44



	bus puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3·H·399·PRO·HB2	4·L·249·ILE·HD11	1.99	0.44
1:M:204:VAL:HG13	1:M:224:LEU:HB3	2.00	0.44
1:0:112:SEB:OG	1:0:115:HIS:ND1	2.50	0.44
1:P:65:LEU:O	1:P:66:HIS:ND1	2.51	0.44
3:E:175:THR:HB	3:E:229:VAL:HB	2.00	0.44
2:B:255:ALA:O	3:F:298:ARG:NH1	2.51	0.44
3:G:72:SER:O	3:G:72:SER:OG	2.33	0.44
4:K:122:LYS:HB2	4:K:122:LYS:HE3	1.80	0.44
1:M:195:ARG:HA	1:M:195:ARG:HD3	1.83	0.44
1:N:76:LEU:HB2	1:N:87:LEU:HD11	1.99	0.44
1:P:85:ARG:NH2	1:P:100:GLU:HB2	2.33	0.44
3:E:296:SER:OG	3:E:329:THR:OG1	2.25	0.44
2:B:184:VAL:HB	2:B:261:ILE:HD12	2.00	0.44
2:C:63:CYS:HA	2:C:99:GLU:HB3	1.99	0.44
3:H:169:VAL:HG22	3:H:235:TRP:HB3	2.00	0.44
3:F:269:PRO:O	3:F:332:ASN:ND2	2.49	0.44
3:F:272:ARG:O	3:F:330:TRP:NE1	2.48	0.44
1:N:152:ARG:HB3	1:N:172:VAL:HG22	1.99	0.44
2:A:166:MET:SD	2:A:166:MET:N	2.88	0.44
3:E:349:HIS:ND1	3:E:358:TYR:OH	2.31	0.44
4:I:151:LYS:HB3	4:I:151:LYS:HE3	1.80	0.44
3:F:63:ASP:OD2	3:F:66:LYS:N	2.48	0.44
2:C:205:SER:OG	2:C:210:SER:OG	2.35	0.44
2:D:85:TYR:HE1	2:D:97:ASP:HB2	1.83	0.44
4:K:129:LEU:HD12	4:K:175:ALA:HA	2.00	0.43
2:D:251:LEU:HA	2:D:254:THR:HG22	1.98	0.43
2:D:427:ILE:HA	2:D:430:VAL:HG22	1.99	0.43
1:M:275:HIS:ND1	1:M:278:CYS:SG	2.92	0.43
2:A:148:ALA:HA	2:A:163:VAL:HG23	2.00	0.43
2:A:239:GLY:O	2:A:243:TRP:CB	2.67	0.43
3:F:314:LYS:HE2	3:F:314:LYS:HB3	1.72	0.43
1:N:65:LEU:HG	3:G:28:CYS:HA	2.00	0.43
1:0:234:GLY:0	1:O:239:ARG:NH2	2.37	0.43
1:P:49:ALA:HB2	1:P:261:LEU:HD11	2.00	0.43
3:E:58:THR:HA	3:E:68:ARG:HH11	1.83	0.43
3:F:40:GLU:OE1	3:F:156:TYR:OH	2.36	0.43
3:H:148:GLY:CA	3:H:268:VAL:O	2.57	0.43
1:N:75:ASP:O	1:N:134:TYR:HA	2.18	0.43
1:P:195:ARG:HH22	3:H:6:PHE:HB2	1.84	0.43
2:A:251:LEU:HA	2:A:254:THR:HG22	2.00	0.43
3:F:223:ASP:OD1	3:F:223:ASP:N	2.51	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
4:J:247:LYS:HD2	4:J:247:LYS:HA	1.70	0.43
1:0:106:ARG:NH2	1:0:130:ASP:OD2	2.51	0.43
1:P:164:ALA:HA	1:P:172:VAL:O	2.18	0.43
3:E:343:SEB:HB3	3:E:344:THB:H	1.64	0.43
3:F:252:LYS:HA	3:F:252:LYS:HD3	1.80	0.43
2:C:263:THR:OG1	2:C:264:ASN:N	2.52	0.43
1:P:189:ALA:HB3	1:P:192:TRP:HD1	1.84	0.43
2:A:129:ALA:O	2:A:148:ALA:N	2.50	0.43
3:F:11:ALA:O	3:F:235:TRP:N	2.48	0.43
2:D:386:HIS:CE1	3:H:344:THR:H	2.37	0.43
1:M:49:ALA:HB2	1:M:261:LEU:HD11	2.00	0.43
1:M:202:GLN:HG2	1:M:226:ALA:HB2	2.00	0.43
3:H:5:ASN:O	3:H:62:HIS:NE2	2.52	0.43
3:H:102:LEU:HD11	3:H:259:PHE:CG	2.53	0.43
1:M:152:ARG:HB3	1:M:172:VAL:HG22	1.99	0.43
1:0:231:ARG:HD2	1:O:231:ARG:HA	1.77	0.43
2:A:275:ASN:OD1	2:A:275:ASN:N	2.52	0.43
3:E:355:ILE:HA	3:E:358:TYR:CD2	2.54	0.43
2:B:432:LEU:O	2:B:436:PHE:HB2	2.19	0.43
3:G:39:ASN:N	3:G:39:ASN:OD1	2.49	0.43
3:G:297:TYR:CZ	3:G:307:HIS:HB2	2.53	0.43
3:H:323:THR:HA	3:H:340:PRO:HG3	2.00	0.43
1:M:103:ASP:OD1	1:M:106:ARG:NH1	2.51	0.43
3:E:139:GLU:HG3	3:E:293:THR:HG23	2.00	0.43
3:E:366:MET:SD	3:E:366:MET:N	2.91	0.43
3:F:364:PRO:C	3:F:366:MET:H	2.22	0.43
2:D:15:TYR:O	2:D:30:GLU:HA	2.19	0.43
3:H:163:THR:HG22	3:H:164:ALA:H	1.82	0.43
3:H:422:LYS:HD2	3:H:422:LYS:HA	1.79	0.43
1:P:126:VAL:HG11	1:P:175:VAL:HG13	2.00	0.43
1:N:51:LEU:HD21	1:N:288:LEU:HD21	2.00	0.42
1:N:116:ASP:HB2	1:N:188:ARG:HH12	1.84	0.42
3:E:250:ASP:OD1	3:E:250:ASP:N	2.52	0.42
2:D:196:ARG:HH12	2:D:199:GLN:HG3	1.83	0.42
3:H:183:GLN:HG3	3:H:222:ILE:HG13	2.00	0.42
2:A:219:LEU:HD12	2:A:235:GLN:HE22	1.84	0.42
3:E:286:LEU:HD13	3:E:316:GLU:HB3	2.00	0.42
3:F:152:PRO:HA	3:F:265:THR:HA	2.01	0.42
4:J:146:ASN:HD22	4:J:149:LEU:H	1.65	0.42
3:G:286:LEU:HD13	3:G:316:GLU:HB3	1.99	0.42
2:D:394:HIS:CD2	2:D:395:THR:HG23	2.54	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:L:177:LYS:HG3	4:L:223:ARG:HG2	2.00	0.42
1:M:72:VAL:HG12	1:M:138:LEU:HD13	2.00	0.42
1:P:74:TRP:CE2	1:P:121:LEU:HB2	2.54	0.42
3:E:52:LEU:O	3:E:99:HIS:ND1	2.53	0.42
3:E:130:HIS:CD2	3:G:290:ASP:HB2	2.55	0.42
3:E:201:CYS:HB2	3:E:202:ASN:H	1.74	0.42
2:B:9:ASN:ND2	2:B:271:CYS:O	2.52	0.42
2:C:111:SER:OG	2:C:113:SER:OG	2.34	0.42
1:0:32:SER:O	1:O:32:SER:OG	2.34	0.42
4:I:130:VAL:O	4:I:133:LYS:HB3	2.19	0.42
4:I:189:TRP:CE2	4:I:191:HIS:HB2	2.54	0.42
3:G:149:LYS:HE2	3:G:270:LYS:HE3	2.00	0.42
1:0:63:ASP:OD1	1:O:64:ARG:N	2.52	0.42
1:O:273:LEU:HG	1:O:282:GLU:HB2	2.01	0.42
1:P:76:LEU:HG	1:P:87:LEU:HD11	2.00	0.42
3:E:393:ARG:HE	3:E:417:CYS:HB3	1.85	0.42
2:B:239:GLY:HA2	2:B:242:TYR:CE1	2.54	0.42
3:F:10:LYS:HA	3:F:10:LYS:HD3	1.86	0.42
3:F:112:THR:HB	3:F:126:THR:HG22	2.00	0.42
3:F:287:LEU:HD23	3:F:311:VAL:HG21	2.01	0.42
2:C:136:LEU:HD23	2:C:136:LEU:HA	1.89	0.42
1:M:38:GLU:HG3	1:M:285:VAL:HB	2.01	0.42
1:P:291:THR:O	1:P:291:THR:OG1	2.32	0.42
2:A:20:ASN:OD1	2:A:20:ASN:N	2.52	0.42
3:E:379:LEU:HA	3:E:382:VAL:HG22	2.01	0.42
2:B:315:VAL:HG11	2:D:291:VAL:HG11	2.01	0.42
3:F:17:ALA:HB3	3:F:33:ALA:HB3	2.01	0.42
3:F:203:CYS:O	3:F:207:ASN:ND2	2.52	0.42
2:C:32:GLU:HB3	2:C:134:ARG:HB3	2.01	0.42
3:G:170:HIS:HB2	3:G:251:ARG:HD3	2.01	0.42
1:P:259:ASP:OD1	1:P:259:ASP:N	2.47	0.42
3:H:32:ILE:HD12	3:H:113:VAL:HG13	2.02	0.42
4:J:240:LEU:HD12	4:J:242:VAL:HB	2.02	0.42
3:G:151:LEU:HD23	3:G:268:VAL:HG11	2.02	0.42
3:H:50:VAL:HG13	3:H:52:LEU:H	1.85	0.42
1:O:97:ARG:HB2	3:E:119:ARG:HE	1.83	0.42
3:E:171:MET:HB2	3:E:245:ASN:HD21	1.85	0.42
4:I:211:GLY:N	4:I:261:TRP:O	2.46	0.42
2:C:250:SER:OG	2:C:251:LEU:N	2.53	0.42
1:M:44:ALA:HB2	1:M:293:PRO:HB3	2.02	0.42
1:O:89:ASP:OD1	1:O:90:MET:N	2.53	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:P:140:HIS:CE1	1:P:142:TYR:HB3	2.55	0.42
2:A:255:ALA:O	3:E:298:ARG:NH1	2.53	0.42
2:A:417:VAL:HG21	3:E:385:ALA:HB2	2.02	0.42
3:F:175:THR:HB	3:F:229:VAL:HG12	2.00	0.42
2:D:224:PRO:HA	2:D:232:PRO:HG3	2.02	0.42
3:H:367:THR:H	3:H:369:VAL:HG22	1.85	0.42
1:M:204:VAL:HA	1:M:272:HIS:O	2.20	0.41
1:0:241:ARG:NE	1:0:265:ASP:OD1	2.52	0.41
1:P:48:GLN:HE21	1:P:259:ASP:HB3	1.85	0.41
3:G:201:CYS:HB2	3:G:207:ASN:HA	2.01	0.41
4:K:194:VAL:HG22	4:K:203:ILE:HD11	2.02	0.41
2:D:30:GLU:OE2	2:D:134:ARG:NH1	2.53	0.41
1:M:103:ASP:HB3	1:M:107:LEU:HG	2.01	0.41
1:O:173:LEU:HG	1:O:175:VAL:HG13	2.02	0.41
2:A:406:ALA:HA	2:A:409:TRP:HB2	2.02	0.41
3:E:138:ARG:HG2	3:E:294:LEU:HD21	2.02	0.41
3:E:239:SER:HB3	3:E:242:VAL:HB	2.01	0.41
4:J:232:ALA:HB2	4:J:258:ALA:HA	2.02	0.41
3:G:8:VAL:HG12	3:G:255:ILE:HG22	2.01	0.41
1:N:106:ARG:HA	1:N:124:ARG:HG2	2.01	0.41
1:N:173:LEU:HG	1:N:175:VAL:HG13	2.02	0.41
3:E:79:GLU:HG3	3:E:81:ALA:H	1.85	0.41
3:E:169:VAL:HG22	3:E:235:TRP:HE3	1.85	0.41
3:H:276:VAL:HG12	3:H:285:MET:HG2	2.02	0.41
3:E:16:LEU:HD21	3:E:70:MET:HB3	2.02	0.41
3:E:188:VAL:HB	3:E:217:ILE:HB	2.02	0.41
4:L:202:THR:HA	4:L:238:THR:O	2.20	0.41
1:P:142:TYR:OH	1:P:202:GLN:OE1	2.38	0.41
2:D:206:ARG:HD2	2:D:206:ARG:HA	1.86	0.41
1:N:33:SER:HB2	1:N:283:ARG:HB3	2.01	0.41
1:O:96:GLN:NE2	1:O:109:LEU:H	2.18	0.41
3:F:22:CYS:HB3	3:F:28:CYS:HB2	1.85	0.41
3:F:363:TYR:HB3	3:F:366:MET:HB2	2.01	0.41
2:C:148:ALA:HA	2:C:163:VAL:HG23	2.01	0.41
2:A:181:LYS:HB3	2:A:182:GLY:H	1.77	0.41
3:E:15:TYR:CZ	3:E:236:GLN:HA	2.54	0.41
4:J:141:LYS:HB2	4:J:141:LYS:HE2	1.68	0.41
4:J:155:LYS:HB3	4:J:164:CYS:SG	2.61	0.41
4:L:162:LEU:HA	4:L:162:LEU:HD12	1.85	0.41
1:P:158:ASP:OD1	1:P:158:ASP:N	2.48	0.41
2:B:79:LYS:HD2	2:B:79:LYS:HA	1.67	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:F:147:HIS:HA	3:F:267:ARG:HH21	1.85	0.41
3:F:170:HIS:HB2	3:F:251:ARG:HG2	2.03	0.41
2:C:297:THR:HG23	2:C:321:THR:HB	2.03	0.41
2:D:403:SER:OG	2:D:405:THR:N	2.49	0.41
1:M:155:VAL:HA	1:M:175:VAL:O	2.21	0.41
1:N:195:ARG:HA	1:N:195:ARG:HD3	1.36	0.41
3:E:393:ARG:NE	3:E:417:CYS:HB3	2.36	0.41
3:E:404:PRO:HG2	4:I:245:TRP:CE2	2.55	0.41
3:F:280:LYS:HZ3	3:F:281:ASN:HB2	1.86	0.41
2:C:120:SER:HG	2:C:122:TYR:HE2	1.69	0.41
2:D:95:PHE:HB2	3:H:226:HIS:HB2	2.02	0.41
3:H:254:LYS:HE3	3:H:254:LYS:HB2	1.87	0.41
4:L:209:LYS:HE2	4:L:209:LYS:HB2	1.84	0.41
4:L:249:ILE:HD12	4:L:249:ILE:HA	1.86	0.41
1:P:173:LEU:HD11	1:P:183:MET:HB2	2.03	0.41
3:F:13:ARG:HD3	3:F:234:ASN:HB2	2.02	0.41
3:F:95:GLY:O	3:F:101:ILE:HA	2.21	0.41
3:F:192:VAL:HG13	3:F:194:GLY:H	1.86	0.41
4:J:231:GLY:HA2	4:J:240:LEU:HA	2.02	0.41
2:D:359:ALA:HB2	2:D:395:THR:HB	2.03	0.41
3:H:347:THR:HG23	3:H:357:LEU:HD23	2.03	0.41
1:M:271:CYS:O	1:M:283:ARG:HA	2.21	0.40
1:N:88:VAL:HG22	1:N:98:VAL:HA	2.03	0.40
1:N:235:PRO:HD2	1:N:238:LEU:HD12	2.02	0.40
1:O:84:ARG:NH2	3:E:192:VAL:H	2.19	0.40
1:P:75:ASP:O	1:P:134:TYR:HA	2.21	0.40
2:A:299:MET:HG2	2:A:320:TYR:HA	2.02	0.40
3:E:137:GLY:HA3	3:E:332:ASN:HD21	1.85	0.40
3:E:368:VAL:HA	3:E:371:VAL:HG22	2.02	0.40
4:I:202:THR:HG23	4:I:237:ARG:HH21	1.86	0.40
2:B:300:SER:O	2:B:318:ILE:HA	2.20	0.40
3:F:213:THR:OG1	3:F:214:ASP:N	2.54	0.40
1:N:206:TRP:CH2	1:N:271:CYS:HB2	2.56	0.40
1:N:209:GLN:HB3	1:N:268:ILE:HB	2.03	0.40
1:O:88:VAL:HG12	1:O:98:VAL:HA	2.03	0.40
1:P:189:ALA:HB3	1:P:192:TRP:CD1	2.56	0.40
2:B:366:ARG:HA	2:B:374:VAL:O	2.21	0.40
4:K:207:ALA:O	4:K:209:LYS:NZ	2.48	0.40
2:D:300:SER:O	2:D:318:ILE:HA	2.21	0.40
1:M:245:ASN:HB3	1:M:257:ARG:HH22	1.87	0.40
1:O:212:GLY:HA2	3:H:166:GLU:HG3	2.04	0.40



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Atom-1	Atom-2	Interatomic	Clash						
	Atom-2	distance (Å)	overlap (Å)						
3:F:409:PRO:O	3:F:413:SER:OG	2.28	0.40						
4:K:129:LEU:HA	4:K:133:LYS:O	2.22	0.40						
4:K:187:TYR:HD1	4:K:219:ASP:HA	1.86	0.40						
4:L:151:LYS:HE3	4:L:151:LYS:HB3	1.76	0.40						
4:L:187:TYR:HB2	4:L:194:VAL:HG23	2.03	0.40						
3:E:110:THR:OG1	3:E:127:HIS:O	2.33	0.40						
2:B:47:ILE:HD12	2:B:208:PRO:HG3	2.04	0.40						
2:B:72:SER:O	2:B:72:SER:OG	2.32	0.40						
2:B:421:VAL:HA	3:F:388:MET:HG3	2.03	0.40						
3:G:408:VAL:HG12	3:G:412:LEU:H	1.86	0.40						
4:K:202:THR:HA	4:K:238:THR:O	2.21	0.40						
2:D:34:GLN:HB2	2:D:132:LYS:HB3	2.03	0.40						
2:D:97:ASP:OD1	2:D:97:ASP:N	2.53	0.40						
1:O:222:LEU:HD11	1:O:230:ARG:HB2	2.04	0.40						
2:A:437:SER:OG	2:A:438:ARG:NH1	2.55	0.40						
2:B:93:TYR:HD1	3:F:176:PRO:HG3	1.87	0.40						
2:B:217:THR:HB	2:B:236:ALA:HB1	2.02	0.40						
2:B:251:LEU:HB2	2:B:261:ILE:HD13	2.02	0.40						
3:G:85:VAL:HG12	3:G:113:VAL:HG12	2.04	0.40						
2:D:297:THR:O	2:D:321:THR:OG1	2.39	0.40						
2:D:327:LYS:HD3	2:D:327:LYS:HA	1.92	0.40						
3:H:252:LYS:HD3	3:H:252:LYS:HA	1.88	0.40						
3:H:353:HIS:CG	3:H:354:GLU:H	2.39	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	entiles
1	М	267/269~(99%)	251 (94%)	16 (6%)	0	100	100
1	Ν	259/269~(96%)	242 (93%)	15 (6%)	2 (1%)	19	58



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	Ο	267/269~(99%)	250~(94%)	17~(6%)	0	100	100
1	Р	267/269~(99%)	250 (94%)	16 (6%)	1 (0%)	34	71
2	А	437/439~(100%)	413 (94%)	23~(5%)	1 (0%)	47	80
2	В	437/439~(100%)	413 (94%)	23 (5%)	1 (0%)	47	80
2	С	437/439~(100%)	410 (94%)	26 (6%)	1 (0%)	47	80
2	D	437/439~(100%)	417 (95%)	19 (4%)	1 (0%)	47	80
3	Е	417/419 (100%)	360 (86%)	56 (13%)	1 (0%)	47	80
3	F	417/419 (100%)	363 (87%)	51 (12%)	3 (1%)	22	61
3	G	417/419 (100%)	361 (87%)	54 (13%)	2(0%)	29	67
3	Н	417/419 (100%)	361 (87%)	55 (13%)	1 (0%)	47	80
4	Ι	149/151~(99%)	145 (97%)	4 (3%)	0	100	100
4	J	149/151~(99%)	146 (98%)	3 (2%)	0	100	100
4	K	149/151~(99%)	145 (97%)	4 (3%)	0	100	100
4	L	149/151~(99%)	147 (99%)	2 (1%)	0	100	100
All	All	5072/5112 (99%)	4674 (92%)	384 (8%)	14 (0%)	44	75

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	А	181	LYS
3	F	402	LEU
2	С	181	LYS
3	G	342	MET
3	G	344	THR
2	D	181	LYS
3	Н	343	SER
1	Ν	195	ARG
1	Р	197	LEU
2	В	405	THR
3	Е	343	SER
3	F	367	THR
1	Ν	197	LEU
3	F	173	PRO



5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	М	232/232~(100%)	232~(100%)	0	100	100
1	Ν	226/232~(97%)	223~(99%)	3 (1%)	69	82
1	Ο	232/232~(100%)	232~(100%)	0	100	100
1	Р	232/232~(100%)	230~(99%)	2(1%)	78	88
2	А	366/366~(100%)	363~(99%)	3~(1%)	81	89
2	В	366/366~(100%)	361~(99%)	5 (1%)	67	80
2	С	366/366~(100%)	364 (100%)	2~(0%)	88	93
2	D	366/366~(100%)	365~(100%)	1 (0%)	92	95
3	Ε	369/369~(100%)	366~(99%)	3(1%)	81	89
3	F	369/369~(100%)	367~(100%)	2(0%)	88	93
3	G	369/369~(100%)	361~(98%)	8 (2%)	52	71
3	Н	369/369~(100%)	369~(100%)	0	100	100
4	Ι	120/120~(100%)	117~(98%)	3~(2%)	47	68
4	J	120/120~(100%)	119~(99%)	1 (1%)	81	89
4	Κ	120/120~(100%)	118 (98%)	2(2%)	60	78
4	L	120/120~(100%)	119 (99%)	1 (1%)	81	89
All	All	4342/4348 (100%)	4306 (99%)	36 (1%)	82	89

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Ν	37	SER
1	Ν	195	ARG
1	Ν	197	LEU
1	Р	43	LEU
1	Р	201	GLN
2	А	242	TYR
2	А	303	VAL
2	А	369	VAL



Mol	Chain	Res	Type
3	Е	119	ARG
3	Е	342	MET
3	Е	343	SER
4	Ι	129	LEU
4	Ι	189	TRP
4	Ι	201	PHE
2	В	53	THR
2	В	158	ASP
2	В	371	SER
2	В	372	THR
2	В	396	THR
3	F	147	HIS
3	F	404	PRO
4	J	189	TRP
2	С	96	CYS
2	С	327	LYS
3	G	9	TYR
3	G	28	CYS
3	G	34	LEU
3	G	43	ASP
3	G	237	TYR
3	G	342	MET
3	G	395	ARG
3	G	396	CYS
4	K	189	TRP
4	K	229	LEU
2	D	301	CYS
4	L	189	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	М	48	GLN
1	М	276	HIS
1	М	281	HIS
1	Ν	247	ASN
1	0	202	GLN
1	0	209	GLN
1	0	215	HIS
1	0	281	HIS
1	Р	48	GLN
2	А	199	GLN



Mol	Chain	Res	Type
3	Е	73	HIS
3	Е	183	GLN
3	Е	195	GLN
3	Е	238	ASN
3	Е	281	ASN
3	Е	332	ASN
3	Е	341	GLN
4	Ι	170	HIS
2	В	20	ASN
2	В	199	GLN
2	В	216	ASN
2	В	235	GLN
2	В	252	GLN
3	F	29	HIS
3	F	146	GLN
3	F	147	HIS
3	F	219	ASN
3	F	234	ASN
3	F	236	GLN
3	F	341	GLN
4	J	146	ASN
2	С	20	ASN
2	С	102	GLN
2	С	138	GLN
2	С	230	HIS
3	G	53	GLN
3	G	142	HIS
3	G	158	GLN
3	G	202	ASN
2	D	100	ASN
2	D	230	HIS
2	D	252	GLN
2	D	260	GLN
2	D	270	ASN
2	D	353	GLN
2	D	439	HIS
3	Н	183	GLN
3	Н	184	GLN
3	H	226	HIS
3	Н	234	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)

12 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	Type	Chain	Dog	Tink	Bo	ond leng	ths	B	ond ang	gles
	туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	В	501	2	14,14,15	0.29	0	17,19,21	0.69	1 (5%)
5	NAG	C	501	2	14,14,15	0.27	0	17,19,21	0.68	1 (5%)
5	NAG	N	401	1	14,14,15	0.36	0	17,19,21	0.67	1 (5%)
5	NAG	А	501	2	14,14,15	0.29	0	17,19,21	0.71	1 (5%)
5	NAG	D	501	2	14,14,15	0.25	0	17,19,21	0.58	0
5	NAG	Н	501	3	14,14,15	0.22	0	17,19,21	0.66	1 (5%)
5	NAG	G	501	3	14,14,15	0.45	0	17,19,21	0.66	1 (5%)
5	NAG	F	501	3	14,14,15	0.52	0	17,19,21	0.60	0
5	NAG	М	501	1	14,14,15	0.47	0	17,19,21	0.49	0
5	NAG	0	501	1	14,14,15	0.34	0	17,19,21	0.59	1 (5%)
5	NAG	Е	501	3	14,14,15	0.37	0	17,19,21	0.55	0
5	NAG	Р	501	1	14,14,15	0.46	0	17,19,21	0.71	1 (5%)

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.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	В	501	2	-	2/6/23/26	0/1/1/1
5	NAG	С	501	2	-	1/6/23/26	0/1/1/1
5	NAG	N	401	1	-	1/6/23/26	0/1/1/1
5	NAG	А	501	2	-	0/6/23/26	0/1/1/1
5	NAG	D	501	2	-	2/6/23/26	0/1/1/1
5	NAG	Н	501	3	-	2/6/23/26	0/1/1/1
5	NAG	G	501	3	-	2/6/23/26	0/1/1/1
5	NAG	F	501	3	-	2/6/23/26	0/1/1/1
5	NAG	М	501	1	-	2/6/23/26	0/1/1/1
5	NAG	0	501	1	-	0/6/23/26	0/1/1/1
5	NAG	Е	501	3	-	0/6/23/26	0/1/1/1
5	NAG	Р	501	1	-	0/6/23/26	0/1/1/1

'-' means no outliers of that kind were identified.

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
5	А	501	NAG	C1-O5-C5	2.65	115.78	112.19
5	Р	501	NAG	C1-O5-C5	2.52	115.61	112.19
5	В	501	NAG	C1-O5-C5	2.43	115.49	112.19
5	Ν	401	NAG	C1-O5-C5	2.32	115.33	112.19
5	С	501	NAG	C1-O5-C5	2.25	115.24	112.19
5	G	501	NAG	C1-O5-C5	2.20	115.18	112.19
5	Н	501	NAG	C1-O5-C5	2.15	115.10	112.19
5	0	501	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Н	501	NAG	C4-C5-C6-O6
5	М	501	NAG	C4-C5-C6-O6
5	D	501	NAG	O5-C5-C6-O6
5	М	501	NAG	O5-C5-C6-O6
5	Н	501	NAG	O5-C5-C6-O6
5	F	501	NAG	O5-C5-C6-O6
5	G	501	NAG	O5-C5-C6-O6
5	D	501	NAG	C4-C5-C6-O6
5	F	501	NAG	C4-C5-C6-O6



Mol	Chain	Res	Type	Atoms
5	G	501	NAG	C4-C5-C6-O6
5	В	501	NAG	C4-C5-C6-O6
5	В	501	NAG	O5-C5-C6-O6
5	N	401	NAG	O5-C5-C6-O6
5	С	501	NAG	C4-C5-C6-O6

Continued from previous page...

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Н	501	NAG	1	0

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-9394. 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)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

6.4 Orthogonal surface views (i)

This section was not generated.

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)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.



8 Fourier-Shell correlation (i)

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



9 Map-model fit (i)

This section was not generated.

