

Mar 19, 2024 - 02:45 pm GMT

PDB ID	:	80ES
EMDB ID	:	EMD-16808
Title	:	MUC5B amino acids 26-1435 Three beads
Authors	:	Khmelnitsky, L.; Fass, D.
Deposited on	:	2023-03-12
Resolution	:	3.00 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 (i)) were used in the production of this report:

EMDB validation analysis	:	0.0.1. dev 92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 3.00 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${ m EM~structures}\ (\#{ m Entries})$
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 $\geq=3, 2, 1$ and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq=5\%$ The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain								
1	А	1227	•	63%			30%	• 5%			
1	В	1227	60%				6 0%			32%	• 5%
1	С	1227	5%	63%			30%	• 5%			
1	D	1227		63%			30%	• 5%			
1	Е	1227	22%		19%	•	42%				
1	F	1227	17%		19%	•	42%				
1	G	1227	9%	12% •			63%				
1	Н	1227	24%	12% •			63%				



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Mol	Chain	Length	Quality of chain					
2	Ι	100	62%	34%	•			
2	J	100	60%	38%				
2	K	100	43%	35%				
2	L	100	30% 62%	34%	•			
2	М	100	95% 62%	35%	- .			
2	Ν	100	94% 63%	34%	• •			

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 57846 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		A	toms			AltConf	Trace		
1	Δ	1169	Total	С	Ν	Ο	S	2	0		
	A	1108	8793	5438	1533	1700	122	Δ	0		
1	P	1169	Total	С	Ν	0	S	0	0		
	D	1108	8793	5438	1533	1700	122	2	0		
1	С	1168	Total	С	Ν	0	S	9	0		
		C	1108	8793	5438	1533	1700	122	2	0	
1	П	1168	Total	С	Ν	Ο	\mathbf{S}	2	0		
	D		D	1100	8793	5438	1533	1700	122	2	0
1	F	715	Total	С	Ν	Ο	\mathbf{S}	2	0		
		110	5383	3331	943	1041	68	2	0		
1	F	715	Total	С	Ν	Ο	\mathbf{S}	2	0		
	Ľ	110	5383	3331	943	1041	68	2	0		
1	C	453	Total	l C	Ν	Ο	\mathbf{S}	0	0		
	G	400	3410	2107	590	659	54	0	0		
1	1 U	453	Total	C	Ν	Ō	S	0			
	453	3410	2107	590	659	54	0				

• Molecule 1 is a protein called Mucin-5B.

• Molecule 2 is a protein called Mucin-5B.

Mol	Chain	Residues	Atoms					AltConf	Trace						
2	T	100	Total	С	Ν	Ο	\mathbf{S}	0	0						
2	T	100	781	482	137	149	13	0	0						
9	Т	100	Total	С	Ν	0	\mathbf{S}	0	0						
	J	100	781	482	137	149	13	0	0						
9	K	100	Total	С	Ν	0	S	0	0						
	IX	IX	IX		100	781	482	137	149	13	0	U			
0	т	100	Total	С	Ν	0	S	0	0						
		100	781	482	137	149	13	0							
0	м	м	м	М	М	М	м	100	Total	С	Ν	0	S	0	0
	100	781	482	137	149	13	0	0							
2 N	N	100	Total	С	Ν	0	S	0	0						
	1 N	100	781	482	137	149	13	0	U						

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).



Mol	Chain	Residues	Atoms	AltConf
3	А	3	Total Ca 3 3	0
3	В	3	Total Ca 3 3	0
3	С	3	Total Ca 3 3	0
3	D	3	Total Ca 3 3	0
3	Е	2	Total Ca 2 2	0
3	F	2	Total Ca 2 2	0
3	G	1	Total Ca 1 1	0
3	Н	1	Total Ca 1 1	0
3	Ι	1	Total Ca 1 1	0
3	J	1	Total Ca 1 1	0
3	K	1	Total Ca 1 1	0
3	L	1	Total Ca 1 1	0
3	М	1	Total Ca 1 1	0
3	Ν	1	Total Ca 1 1	0

• Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





Mol	Chain	Residues	A	Atoms			
1	Δ	1	Total	С	Ν	0	0
	Π	1	14	8	1	5	0
4	А	1	Total	С	Ν	Ο	0
		-	14	8	1	5	
4	А	1	Total	C	N	Õ	0
			14	8	1	5	
4	А	1	Total	C	N	O E	0
			14	8	1 	5	
4	А	1	Total	C	N 1	0	0
			14 Tetal	$\frac{8}{C}$	1 	0	
4	В	1		° °	IN 1	5	0
			Total	$\frac{\circ}{C}$		$\frac{0}{0}$	
4	В	1	10tai	8	1N 1	5	0
			Total	$\frac{0}{C}$	N	$\frac{0}{0}$	
4	В	1	14	8	1	5	0
			Total	C	N	0	
4	В	1	14	8	1	$\overline{5}$	0
	D	-	Total	С	Ν	0	
4	В	1	14	8	1	5	0
4	C	1	Total	С	Ν	Ο	0
4	C	1	14	8	1	5	0
4	C	1	Total	С	Ν	Ο	0
4		1	14	8	1	5	U
4	C	1	Total	С	N	0	0
		1	14	8	1	5	0
4	С	1	Total	С	Ν	Ο	0
1			14	8	1	5	



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Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	С	Ν	Ο	0
4	C	1	14	8	1	5	0
4	D	1	Total	С	Ν	Ο	0
4	D	L	14	8	1	5	0
4	р	1	Total	С	Ν	0	0
4	D	L	14	8	1	5	0
4	Л	1	Total	С	Ν	Ο	0
4	D	L	14	8	1	5	0
4	р	1	Total	С	Ν	Ο	0
4	D	T	14	8	1	5	0
4	F	1	Total	С	Ν	Ο	0
-1	Ľ	I	14	8	1	5	0
4	E	1	Total	С	Ν	Ο	0
Ŧ	Ľ	I	14	8	1	5	0
	E	1	Total	С	Ν	Ο	0
	Ľ	I	14	8	1	5	0
4	E	1	Total	С	Ν	Ο	0
Ŧ	Ľ	I	14	8	1	5	0
4	F	1	Total	С	Ν	Ο	0
T	T,	I	14	8	1	5	0
	F	1	Total	С	Ν	Ο	0
	1	T	14	8	1	5	0
	F	1	Total	С	Ν	Ο	0
	L	1	14	8	1	5	0
4	F	1	Total	С	Ν	Ο	0
- T	T	1	14	8	1	5	



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: Mucin-5B







• Molecule 1: Mucin-5B

Chain B:	60%	32% • 5%
6LN PRO PRO CLU CLU CLU CLU PRO CLU PRO CLY MRT ALA ALA ALA ALA	THR THR SER SER PPRO THR ARG ARG ARG VAL PHE PPRO PPRO PPRO PPRO PPRO PRO PRO PRO PR	ALEU ALEU ALEU A71 PRO 77 77 1779 083 180 083 183 788 783 783 783 783 783 783 783 783 7
C90 C97 C97 C98 C98 C98 C98 C198 C114 C114 C114 C114 C114 C115 C1118 C1119 C121 C122 C121	8125 8126 8126 7129 7130 9137 9158 9158 7162 8169 8169 8169 8169 8169 8169 8169 8169	I173 V174 V175 V176 R178 R178 R178 R178 R178 R178 R178 R178 L179 L192 F183 R186 R188 R188 R198 L198 L198 L198 L198 L198 L198 L193 L193 L193 L193 L194 L193
¥199 A200 N201 Q202 Q203 Q204 Q205 Q205 Q205 Q205 Q214 A215 Q216 Q217 Q216 Q216 Q217 Q218 Q216 Y220 Y220	q235 K236 L237 D238 D238 P247 P247 P247 P255 P255 C255 C255 C255 C255 C255 C255	F271 F271 C274 C274 C278 D279 S280 F283 F283 F283 F285 F285 C295 C295 F302 F302
N303 N303 E304 Y305 Y305 Y316 H311 H311 H311 H311 H312 H313 M3332 M3332 M334 M341 M341 M341	1343 1343 1344 1344 1345 1345 8347 8345 8347 8345 8345 8345 8347 8345 8347 8345 8347 8345 8347 8350 8351 8350 8352 8350 8357 8350 8356 8350 8356 8350 8356 8350 8356 8350 8356 8355 8356 8355 8356 8355 8356 8355 8356 8355 8356 8355 8356 8355 8357 8355 8356 8355 8356 8355 8357 8355 8356 8355 8357 8357 8357 8357 8357 8357 8357 <td>C379 1388 1388 1398 1398 1398 1398 1398 139</td>	C379 1388 1388 1398 1398 1398 1398 1398 139
P 422 C 425 C 425 S 426 V 427 V 427 V 427 D 442 C 445 S 448 V 450 V 450 V 455 C 445 C 454 C 455 C 455	L463 E466 E466 E466 E466 C469 C469 C469 C471 T472 L471 T472 T472 T470 C479 T485 T485 T486 T486 C479 C479 T486 C479 C493 C495	F501 F501 F502 F507 F510 F511 F511 F514 F524 F529 F529 F529
L536 L537 L537 L537 C538 R544 C538 C544 C548 C544 C559 C559 C559 C559 C559 C559 C559	1574 1574 1573 1574 1573 1583 1581 1583 1583 1583 1583 1583 158	8603 F604 F605 E605 B606 P607 C608 8611 V617 V617 V617 V617 V617 V617 V617 V
D627 8630 8631 1632 1632 1633 1636 1636 1649 1664 1661 0651 0655 1656 1655 1656 1655 1655	E665 1660 1660 1662 1662 1663 1669 1689 1689 1689 1689 1689 1689 1689 1689 1689 1689 1689 1689 1689 1689 1689 1689 1689 1689 1680	D706 0709 7711 7711 7711 7711 7713 7713 7721 7721
P735 D742 D742 C751 C752 C753 C754 P753 P763 C754 P763 C764 P766 V766 V766 V766 V766 C770	A772 V773 C774 C774 C776 C776 C776 C776 T777 C776 C776 C776	P197 P197 P197 P197 P198 P1800 P1800 P1800 P1800 P1800 P181
R817 818 818 818 7821 1821 1822 1822 1822	V841 V842 0845 0845 0847 0855 0855 0855 0855 0855 0855 0855 0873 0873 0873 0873 0873 0873	R880 N881 N882 N882 R882 R888 R888 C891 L899 C893 C893 C893 C893 C893 C893 C893 C
6908 8910 1920 1920 1920 1933 1933 1933 1933 1933 1933 1933 193	1945 1946 1946 1955 1955 1955 1965 1965 1965 1965 196	0000 0981 0982 0983 0984 0988 0988 0991 1991 1991 1992 1995 1995 1995 1995 1
A1001 81003 81003 81006 81006 81006 81006 81006 81006 81010 81013 81013 81013 81013 81013 81013 81013 81013 81013 81013 81013 81020	D1031 N1035 D1035 D1036 R1040 S1044 S1044 S1044 V1044 F1051 N1055 N1055 S1058 S1058 S1058 S1058 S1058 S1058 S1060 D1061 D1062 D1062 D1062	K1068 D1069 A1073 R1077 R1077 F1088 F1088 A1094 A1094 A1094 A1094 A1094 A1094







G1195 C1196 S109 Q109 F1207 N1208 E1209 Y1197 P1198 K1199 <mark>C1214</mark> V1215 A1216 THR ALA GLU ASN CYS GLN SER • Molecule 1: Mucin-5B Chain D: 63% 30% • 5% F216 N217 E218 F219 Y220 A221 H222 P251 A252 G253 N254 N254 C255 T256 D257 P269 A270 E273 A276 L277 V278 A285 C292 R293 C294 P295 P295 C297 C297 C299 C321 P322 E323 L324 L324 C325 C325 P326 R327 <mark>1315</mark> 2316 3317 2330 L331 1334 1335 3339 1332 1333 1338 351 F400 N401 T402 5405 5406 5406 7407 <mark>Q539</mark> L540 4544 4545 7546 7546 3549 1550 q529 T530 .536 <u>1670</u> 1671 3624 .625 N654 C655 E656 <mark>ж684</mark> D685 G686 G688 C688 T689 T689 M692 M692 Q693 N692 N693 7632 3633 T711 661 683 G785 ALA SER SER LEU GLN LYS SER SER THR S806 S807 A808 F7 39 L7 40 N7 41 D7 42 V767 H768 A813 E814 C819 C819 H820 T821 C835 V836 C837 C837 C837 C837 P838 P838 P839 P839 C840 C841 V842 S843 S843 1850 1851 1852 1852 1853 1854 1855 1042 1043 1044 1056 1057 1060 1061 1062







WORLDWIDE PROTEIN DATA BANK

													••														•••		
D68: W68:	R68 D68	C68	T689 K690	M690	N69v	C691 P696	8695 8695	1003	Y70: A70:		A70	C70	P710	C71: 571:	G7 14	L71(S71(E7 10 A7 18	D7 19	T72:	C72: S72:	V724 S729	P728	0730 0730	C73: T73:	C73 C73	A730 G73	T738 F73	L74(N74:	D/4: A74: G74: A74!
••	•••	•••		••	••			••	••		••	••	••		••	••	••		••	••	••	•							
C746 11747	V141 P748 A749	0750 8751	E/ 51 C752	P753 C754	Y755 A756	H757	G758 T759	V760 L761	A762 P763	G764	E765 V766	V767 H768	D769 5770	E771 G771	A772 V773	C774 S775	C776	1777 G778	<mark>G779</mark> K780	L781 S782	C783 L784	G785 ALA	SER LEU	LYS SER	THR GLY	CYS ALA ALA	PRO MET	VAL TYR LEU ASP	CYS SER ASN
SER SER	ALA GLY THR	PR0 GLY	ALA GLU	LEU ARG	SER CYS	HIS THR	LEU ASP	VAL GLY CVS	PHE SER	THR HIS	CYS VAL	SER GLY CVS	VAL	PRO PRO	GLY LEU	VAL SER ASP	GLY	GLY	CYS ILE	GLU GLU	ASP CYS	PRO CYS	VAL HIS ASN	GLU	THR TYR LYS				
PRO GLY	GLU THR ILE	ARG VAL	ASP CYS	THR	THR CYS	ARG ASN	ARG	GLU GLU	SER HIS	ARG LEU	CYS	GLY THR CVS	VAL	TYR GLY	ASP GLY	TLF	THR	ASP GLY	ASP ARG	TYK SER DHF	GLV	SER CYS	TYR	ALA	GLN ASP TYR				
CYS GLY	ASP ASN THR	THR HIS	GLY THR	FRE ARG ILE	VAL THR	GLU ASN	ILE PRO	CYS GLY THB	THR GLY	THR THR	CYS SER	LYS ALA TLE	LYS	PHE	GLU SER	I Y K GLU I FII	ILE I FU	GLU	GL Y THR	PHE LYS AT A	VAL	ARG GLY	GLY GLY	ASP PRO	PRO TYR LYS				
LE RG	YR ET LY	LE HE	EU AL	LU HR	LY	ET LA	AL ER	SP	AG YS HR	ER AL	HELE	EU EU TS	LN	YR	LY RG	AL YS TV	EU	NS.	HE SP	SN	LE	SP HE	HR RG	ER RG	ER AL AL				
Α	ΗΣO	нч	121	101	цто	MA	201	T. A. A.	ЧЦЪ	S >	дн.	ч Ц п	304	4 1	04:	>00	2 1 0	0.04	η 4.	4 4 4		A T .	4 L 4	0 4 0	~ ~ ~				
GLY ASP	ALA LEU GLU	PHE	ASN SER	LEU	SER PRO	SER CYS	PRO ASP	ALA LEU	PRO LYS	ASP PRO	CYS THR	ALA ASN PRO	PHE	LYS	TRP ALA	CL N CL N	CYS	LEU	GLY	THR	ALA	CYS ARG	GLN VAL	ASP SER	THR LYS TYR				
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TY	CYC	AS	AL	CY	SE	GL	GL	PH	AL	VA	AL	AL GL	CY	AS	EE GE	VA	TR	TH TH PR	AS TH	PR	PH	PH	AS AS PR	HI	C A C				
TRP HIS	TYR GLN PRO	CYS GLY	ALA PRO	LEU	THR CYS	ARG ASN	PRO SER	SIH SIH	LEU VAL	ASP LEU	PRO GLY	CLU GLU	CYS	PRO	CYS PRO	SER	PRO PHF	PHE	GLU ASP	MET	CYS VAL	GLN	CYS CYS	TYR ASP	LYS ASP GLY				
SN YR	YR SP AL	LY LA	RG AL	HR LA	LU	YS LN	ER YS	YS YS	RO ER	LY	LN YS																		
A T	ΤΨΝ	A G	A D C	u H M	A G	0 8	ຮັບ	4 U F	-iΩ;Ω	5 H	80																		
• 1	Mole	ecul	e 1	: N	luci	in-	5В																						
$\mathbf{C}\mathbf{h}$	ain	C٠	9	%	2.40/				1.20/								6.20	1/						I					
		u.			24%	5			12%	•							057	/0											
GLY	PRO VAL GLU	PRO SER	GLU	ALA GLY	HIS THR	MET ASP	GLY GLY	PR0 TUD	SER	PRO THR	ARG	VAL SER PHE	VAL	PRO	VAL	PRO	LEU	PRO	PRO	ALA HIS	GLY ARG	CYS	THR	GLY	PHE HIS TYR				
LYS THR	PHE ASP GLY	ASP VAL	PHE ARG	FRD GLY GLY	LEU CYS	ASN TYR	VAL PHE	SER GLU HIS	CYS CYS ARG	ALA ALA	TYR GLU	ASP PHE ASN	VAL GLN	LEU ARG	ARG GLY	VAL	SER ABG	PRO VAL	VAL THR	ARG VAL VAT	LYS	ALA GLN	LEU VAL	LEU GLU	ALA SER ASN				
	_																						_						
GLY SER	VAL LEU ILE	ASN GLY	GLN ARG	GLU GLU	PRO TYR	SER ARG	GLY	LEU LEU VAT	GLU GLU GLN	SER GLY	ASP TYR	LYS VAL	SER TI.F	ARG	VAL	PHE	TRP	GLU GLU	ASP SER	ALA LEU TEII	GLU	ASP PRO	TYR ALA	GLN	THR CYS GLY				
EU	LY SP HE	ILY ILY	EU RO	HE	HE	TR	SN SN	LA RG EII	HR RO	LU	HE	EU EU	YS	LY	RO HR	ILN ILN	RO SP	RO	RO EU	LA LA	SN SN	HR SP	ILV ILV	TLE YS	LLS RG HR				
IO	044	40	цц	4 H 4	O H	L	H I	4 4 1		цо	щ О.	4 1 0		40				4 14 14	цці	440				н 0 ,	4 4 6				
LEU LEU	GLY PRO ALA	PHE ALA	GLU CYS	ALA	VAL ASP	SER THR	ALA TYR	LEU ALA	CYS CYS ALA	GLN ASP	CYS	ARG CYS PRO	THR	PRO CYS	ALA THR	VAL	TYR	ARG	CYS ALA	ALA	GLN	PRO ARG	TRP	CYS PRO	GLU CYS				
چ چ	H S D	SN S			S X	H D	S H I	みておい	C E E	O N	RG			S S	김요	Y S H	4 S C		田工		5 H H	SE			X N S				
P) AF	E O F	L) A	WB	19 19	0 5	SI	O E	A II (AS AS	LI III	AI	330	D B	G H S	U AS	504		PI PI	T I	AS AS		H.	551	E D S	555				
PR0 CYS	THR HIS GLY	GL Y ARG	THR TYR	PRO GLY	THR	PHE ASN	THR	CYS SER SER	CYS THR	CYS SER	GLY	TRP	CYS CYS	ASP LEU	PRO CYS	GLY GLY	CYS	VAL GLN	GLY GLY	ALA HIS TIF	SER	TYR ASP	LEU	TYR ASP	LEU GLY				
S	L R	eu JR	<u>ເ</u> ເ	A d	R	H H	J D .	A.U.	n n n	'S Y	un R	NS II	N N	n s	A L	H D B		Y.	SP IR	र म र	N	LA SP	17.1	H D I	N H H				
ASCY	SE VA	SE	338	AL	SE	H H H	7 H H	GI AL	EV E	C I	日日:	AS AS	AS AS	5 8 2	AI VA		LE	5 5	AE H	A H Q	VA GL	AS	GI	H H	AS ES II				

















• Molecule 2: Mucin-5B





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88708	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 $(e^-/\text{\AA}^2)$	48	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.710	Depositor
Minimum map value	-0.488	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.056	Depositor
Map size (Å)	578.48, 578.48, 578.48	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8264, 0.8264, 0.8264	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, CA

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	Bo	ond lengths	Bond angles			
MOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5		
1	А	0.38	0/9014	0.58	1/12269~(0.0%)		
1	В	0.46	4/9014~(0.0%)	0.61	6/12269~(0.0%)		
1	С	0.38	0/9014	0.58	1/12269~(0.0%)		
1	D	0.38	0/9014	0.57	2/12269~(0.0%)		
1	Е	0.49	4/5514~(0.1%)	0.64	6/7511~(0.1%)		
1	F	0.49	4/5514~(0.1%)	0.64	6/7511~(0.1%)		
1	G	0.40	0/3500	0.55	1/4758~(0.0%)		
1	Н	0.40	0/3500	0.55	1/4758~(0.0%)		
2	Ι	0.28	0/800	0.62	0/1087		
2	J	0.30	0/800	0.60	1/1087~(0.1%)		
2	Κ	0.28	0/800	0.62	0/1087		
2	L	0.28	0/800	0.62	0/1087		
2	М	0.30	0/800	0.60	1/1087~(0.1%)		
2	N	0.30	0/800	0.60	1/1087~(0.1%)		
All	All	0.41	12/58884~(0.0%)	0.59	27/80136~(0.0%)		

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	Ε	295	PRO	CG-CD	-17.80	0.92	1.50
1	В	295	PRO	CG-CD	-17.79	0.92	1.50
1	F	295	PRO	CG-CD	-17.79	0.92	1.50
1	Ε	295	PRO	N-CD	10.94	1.63	1.47
1	F	295	PRO	N-CD	10.94	1.63	1.47
1	В	295	PRO	N-CD	10.93	1.63	1.47
1	F	295	PRO	CB-CG	7.96	1.89	1.50
1	В	295	PRO	CB-CG	7.95	1.89	1.50
1	Ε	295	PRO	CB-CG	7.95	1.89	1.50
1	В	295	PRO	N-CA	-5.65	1.37	1.47
1	Ε	295	PRO	N-CA	-5.65	1.37	1.47
1	F	295	PRO	N-CA	-5.64	1.37	1.47



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	Е	295	PRO	CA-N-CD	-13.67	92.36	111.50
1	В	295	PRO	CA-N-CD	-13.66	92.38	111.50
1	F	295	PRO	CA-N-CD	-13.65	92.38	111.50
1	F	295	PRO	N-CD-CG	-13.30	83.25	103.20
1	Е	295	PRO	N-CD-CG	-13.29	83.26	103.20
1	В	295	PRO	N-CD-CG	-13.29	83.27	103.20
1	С	295	PRO	CA-N-CD	-12.66	93.78	111.50
1	D	295	PRO	CA-N-CD	-12.64	93.80	111.50
1	А	295	PRO	CA-N-CD	-12.64	93.81	111.50
1	В	295	PRO	CA-CB-CG	-9.49	85.96	104.00
1	Е	295	PRO	CA-CB-CG	-9.49	85.96	104.00
1	F	295	PRO	CA-CB-CG	-9.49	85.97	104.00
1	D	1160	PRO	CA-N-CD	-6.86	101.89	111.50
1	Н	1160	PRO	CA-N-CD	-6.85	101.90	111.50
1	G	1160	PRO	CA-N-CD	-6.84	101.93	111.50
1	Е	179	LEU	CA-CB-CG	6.12	129.38	115.30
2	N	1389	PRO	CA-N-CD	-6.12	102.93	111.50
1	В	179	LEU	CA-CB-CG	6.12	129.37	115.30
1	F	179	LEU	CA-CB-CG	6.11	129.35	115.30
2	J	1389	PRO	CA-N-CD	-6.10	102.96	111.50
2	М	1389	PRO	CA-N-CD	-6.06	103.01	111.50
1	Е	722	CYS	CA-CB-SG	5.48	123.86	114.00
1	F	722	CYS	CA-CB-SG	5.46	123.84	114.00
1	В	722	CYS	CA-CB-SG	5.46	123.83	114.00
1	F	295	PRO	N-CA-CB	-5.18	96.91	102.60
1	В	295	PRO	N-CA-CB	-5.16	96.93	102.60
1	Е	295	PRO	N-CA-CB	-5.12	96.97	102.60

All (27) bond angle outliers are listed below:

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	А	8793	0	8176	277	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	В	8793	0	8176	297	0
1	С	8793	0	8176	281	0
1	D	8793	0	8177	289	0
1	Е	5383	0	5055	168	0
1	F	5383	0	5055	172	0
1	G	3410	0	3122	106	0
1	Н	3410	0	3122	108	0
2	Ι	781	0	712	30	0
2	J	781	0	712	47	0
2	К	781	0	712	34	0
2	L	781	0	712	33	0
2	М	781	0	712	32	0
2	Ν	781	0	712	30	0
3	А	3	0	0	0	0
3	В	3	0	0	0	0
3	С	3	0	0	0	0
3	D	3	0	0	0	0
3	Е	2	0	0	0	0
3	F	2	0	0	0	0
3	G	1	0	0	0	0
3	Н	1	0	0	0	0
3	Ι	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	М	1	0	0	0	0
3	N	1	0	0	0	0
4	А	70	0	65	0	0
4	В	70	0	65	1	0
4	С	70	0	65	0	0
4	D	56	0	52	0	0
4	Е	56	0	52	1	0
4	F	56	0	52	1	0
All	All	57846	0	53682	1760	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (1760) 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)
1:B:295:PRO:CB	1:B:295:PRO:CG	1.89	1.49
1:E:295:PRO:CG	1:E:295:PRO:CB	1.89	1.49
1:F:295:PRO:CB	1:F:295:PRO:CG	1.89	1.46
1:B:295:PRO:CG	1:B:295:PRO:N	1.77	1.44
1:F:295:PRO:CG	1:F:295:PRO:N	1.77	1.40
1:E:295:PRO:CG	1:E:295:PRO:N	1.77	1.40
1:D:763:PRO:HD2	2:J:1384:GLN:OE1	1.46	1.12
1:F:295:PRO:CG	1:F:295:PRO:HD3	1.60	1.11
1:D:763:PRO:HD2	2:J:1384:GLN:CD	1.70	1.11
1:B:295:PRO:CG	1:B:295:PRO:HD3	1.60	1.09
1:F:295:PRO:CG	1:F:295:PRO:HD2	1.60	1.09
1:A:713:ARG:NH2	1:C:501:PHE:HE2	1.49	1.08
1:B:295:PRO:CG	1:B:295:PRO:HD2	1.60	1.08
1:E:295:PRO:CG	1:E:295:PRO:HD3	1.60	1.07
1:B:295:PRO:CG	1:B:295:PRO:CA	2.33	1.07
1:E:295:PRO:CD	1:E:295:PRO:HG2	1.57	1.06
1:E:295:PRO:CG	1:E:295:PRO:CA	2.33	1.06
1:F:295:PRO:CD	1:F:295:PRO:HG3	1.57	1.06
1:B:295:PRO:CD	1:B:295:PRO:HG3	1.57	1.05
1:F:295:PRO:CD	1:F:295:PRO:HG2	1.57	1.05
1:F:295:PRO:CG	1:F:295:PRO:CA	2.33	1.05
1:E:295:PRO:CG	1:E:295:PRO:HD2	1.60	1.04
1:E:295:PRO:CD	1:E:295:PRO:HG3	1.57	1.04
1:B:295:PRO:CD	1:B:295:PRO:HG2	1.57	1.03
1:C:757:HIS:HE1	1:C:830:HIS:NE2	1.60	1.00
1:D:762:ALA:HB1	2:J:1384:GLN:OE1	1.61	0.99
1:A:501:PHE:HE2	1:C:713:ARG:HH22	1.00	0.95
1:B:713:ARG:HH22	1:D:501:PHE:HE2	1.15	0.95
1:C:757:HIS:CE1	1:C:830:HIS:NE2	2.34	0.95
1:A:770:GLU:OE2	1:C:597:CYS:SG	2.26	0.93
1:F:295:PRO:CG	1:F:295:PRO:CD	0.92	0.92
1:B:295:PRO:CG	1:B:295:PRO:CD	0.91	0.91
1:E:295:PRO:CG	1:E:295:PRO:CD	0.91	0.91
1:F:345:THR:HG22	1:F:371:LEU:HB3	1.54	0.89
1:D:757:HIS:HE1	1:D:830:HIS:NE2	1.70	0.89
1:B:345:THR:HG22	1:B:371:LEU:HB3	1.54	0.89
1:D:757:HIS:CE1	1:D:830:HIS:CD2	2.61	0.88
1:B:767:VAL:HG12	2:L:1416:LEU:HD13	1.56	0.87
1:D:763:PRO:CD	2:J:1384:GLN:OE1	2.22	0.87
1:E:345:THR:HG22	1:E:371:LEU:HB3	1.54	0.87
1:B:295:PRO:N	1:B:295:PRO:HG3	1.71	0.86
1:F:295:PRO:N	1:F:295:PRO:HG3	1.71	0.84



	juo pugeini	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:718:ALA:HB2	1:A:808:ALA:HB3	1.57	0.84
1:C:757:HIS:CE1	1:C:830:HIS:CD2	2.66	0.83
1:C:763:PRO:O	2:I:1384:GLN:NE2	2.11	0.83
1:A:501:PHE:HE2	1:C:713:ARG:NH2	1.76	0.82
1:D:757:HIS:CE1	1:D:830:HIS:NE2	2.47	0.82
1:H:987:ARG:NH1	1:H:1186:CYS:SG	2.53	0.81
1:D:762:ALA:HB1	2:J:1384:GLN:CD	2.00	0.81
1:G:987:ARG:NH1	1:G:1186:CYS:SG	2.54	0.81
1:D:987:ARG:NH1	1:D:1186:CYS:SG	2.53	0.81
1:H:871:ARG:HH11	1:H:1140:GLY:HA2	1.45	0.81
1:C:651:ASP:HB3	1:C:661:CYS:HB3	1.64	0.80
1:G:871:ARG:HH11	1:G:1140:GLY:HA2	1.45	0.80
1:D:871:ARG:HH11	1:D:1140:GLY:HA2	1.45	0.79
1:A:651:ASP:HB3	1:A:661:CYS:HB3	1.64	0.78
2:L:1381:ARG:NH1	2:L:1421:GLU:OE1	2.17	0.78
1:A:338:CYS:HA	1:A:359:CYS:HB3	1.66	0.77
1:D:651:ASP:HB3	1:D:661:CYS:HB3	1.64	0.77
1:D:763:PRO:O	2:J:1384:GLN:NE2	2.16	0.77
1:D:890:LEU:HB3	1:D:1016:GLN:HG3	1.66	0.77
1:G:890:LEU:HB3	1:G:1016:GLN:HG3	1.67	0.77
1:C:338:CYS:HA	1:C:359:CYS:HB3	1.66	0.77
1:D:338:CYS:HA	1:D:359:CYS:HB3	1.66	0.76
1:H:890:LEU:HB3	1:H:1016:GLN:HG3	1.66	0.76
2:I:1381:ARG:NH1	2:I:1421:GLU:OE1	2.17	0.76
1:C:178:ARG:HD2	1:C:179:LEU:HD23	1.68	0.76
2:K:1381:ARG:NH1	2:K:1421:GLU:OE1	2.17	0.76
2:M:1381:ARG:NH1	2:M:1382:ALA:O	2.20	0.75
1:B:890:LEU:HB3	1:B:1016:GLN:HG3	1.69	0.75
1:C:763:PRO:HD3	2:I:1385:LEU:HD21	1.69	0.75
2:N:1381:ARG:NH1	2:N:1382:ALA:O	2.20	0.75
1:A:178:ARG:HD2	1:A:179:LEU:HD23	1.68	0.75
1:C:890:LEU:HB3	1:C:1016:GLN:HG3	1.69	0.75
1:D:178:ARG:HD2	1:D:179:LEU:HD23	1.68	0.75
2:J:1381:ARG:NH1	2:J:1382:ALA:O	2.20	0.75
1:D:427:VAL:HG22	1:D:433:ILE:HG12	1.70	0.74
1:A:427:VAL:HG22	1:A:433:ILE:HG12	1.70	0.74
1:A:757:HIS:HE1	1:A:830:HIS:NE2	1.85	0.74
1:A:890:LEU:HB3	1:A:1016:GLN:HG3	1.69	0.73
1:E:295:PRO:N	1:E:295:PRO:HG3	1.71	0.73
1:C:760:VAL:HG11	2:I:1388:MET:SD	2.28	0.73
1:B:875:ASN:ND2	1:B:889:ARG:O	2.21	0.73



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:332:ASN:ND2	1:C:379:CYS:O	2.22	0.73
1:A:875:ASN:ND2	1:A:889:ARG:O	2.21	0.73
1:C:427:VAL:HG22	1:C:433:ILE:HG12	1.69	0.73
1:D:299:CYS:HA	1:D:302:PHE:HD2	1.54	0.72
1:D:332:ASN:ND2	1:D:379:CYS:O	2.22	0.72
1:A:332:ASN:ND2	1:A:379:CYS:O	2.22	0.72
1:C:243:GLN:OE1	1:C:243:GLN:N	2.23	0.72
1:A:299:CYS:HA	1:A:302:PHE:HD2	1.54	0.72
1:C:875:ASN:ND2	1:C:889:ARG:O	2.21	0.72
1:A:243:GLN:OE1	1:A:243:GLN:N	2.23	0.72
1:C:299:CYS:HA	1:C:302:PHE:HD2	1.54	0.72
1:E:651:ASP:HB3	1:E:661:CYS:HB3	1.72	0.71
1:F:651:ASP:HB3	1:F:661:CYS:HB3	1.72	0.71
1:D:243:GLN:OE1	1:D:243:GLN:N	2.23	0.71
1:E:299:CYS:HA	1:E:302:PHE:HD2	1.56	0.71
1:B:120:ARG:HB3	1:B:120:ARG:HH11	1.56	0.70
1:B:651:ASP:HB3	1:B:661:CYS:HB3	1.72	0.70
1:E:120:ARG:HB3	1:E:120:ARG:HH11	1.56	0.70
1:A:768:HIS:O	2:K:1414:PRO:HB3	1.90	0.70
1:B:299:CYS:HA	1:B:302:PHE:HD2	1.56	0.70
1:H:911:TYR:HH	1:H:1051:PHE:HE2	1.37	0.70
1:F:299:CYS:HA	1:F:302:PHE:HD2	1.56	0.70
1:A:1181:ASN:ND2	1:A:1185:HIS:O	2.23	0.70
1:C:1181:ASN:ND2	1:C:1185:HIS:O	2.23	0.70
1:B:1181:ASN:ND2	1:B:1185:HIS:O	2.23	0.70
1:G:875:ASN:ND2	1:G:889:ARG:O	2.23	0.70
1:F:655:CYS:HB3	1:F:658:SER:HA	1.75	0.69
2:K:1381:ARG:HH21	2:K:1386:PRO:HB3	1.57	0.69
1:A:904:ILE:HG12	1:A:910:ARG:HG2	1.74	0.69
1:B:718:ALA:HB2	1:B:808:ALA:HB3	1.74	0.69
1:C:904:ILE:HG12	1:C:910:ARG:HG2	1.74	0.69
1:D:875:ASN:ND2	1:D:889:ARG:O	2.23	0.69
1:H:875:ASN:ND2	1:H:889:ARG:O	2.23	0.69
1:F:120:ARG:HB3	1:F:120:ARG:HH11	1.56	0.69
1:A:245:PRO:HD3	2:J:1403:ARG:HH12	1.58	0.68
1:C:718:ALA:HB2	1:C:808:ALA:HB3	1.73	0.68
1:B:332:ASN:ND2	1:B:379:CYS:O	2.26	0.68
1:F:332:ASN:ND2	1:F:379:CYS:O	2.26	0.68
1:B:655:CYS:HB3	1:B:658:SER:HA	1.75	0.68
1:B:761:LEU:HD12	1:B:776:CYS:HB2	1.75	0.68
2:L:1381:ARG:HH21	2:L:1386:PRO:HB3	1.57	0.68



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:767:VAL:HG12	2:I:1416:LEU:HD22	1.74	0.68
1:E:332:ASN:ND2	1:E:379:CYS:O	2.26	0.68
1:B:904:ILE:HG12	1:B:910:ARG:HG2	1.74	0.68
1:D:656:GLU:OE2	1:D:656:GLU:N	2.18	0.68
1:G:904:ILE:HG12	1:G:910:ARG:HG2	1.76	0.68
1:H:904:ILE:HG12	1:H:910:ARG:HG2	1.76	0.68
1:E:761:LEU:HD12	1:E:776:CYS:HB2	1.75	0.68
1:E:655:CYS:HB3	1:E:658:SER:HA	1.75	0.68
1:D:346:CYS:HA	1:D:349:PRO:HB3	1.77	0.67
1:D:904:ILE:HG12	1:D:910:ARG:HG2	1.76	0.67
1:F:761:LEU:HD12	1:F:776:CYS:HB2	1.75	0.67
1:A:757:HIS:CE1	1:A:830:HIS:NE2	2.61	0.67
1:E:82:ASP:HA	1:E:127:PRO:HG3	1.76	0.67
1:E:333:MET:HE3	1:E:363:CYS:HB3	1.76	0.67
2:I:1376:ALA:O	2:I:1401:ARG:NH2	2.19	0.67
2:I:1381:ARG:HH21	2:I:1386:PRO:HB3	1.57	0.67
2:K:1376:ALA:O	2:K:1401:ARG:NH2	2.19	0.67
1:B:764:GLY:N	1:B:776:CYS:O	2.24	0.67
1:D:245:PRO:HD3	2:N:1403:ARG:HH12	1.58	0.67
1:F:333:MET:HE3	1:F:363:CYS:HB3	1.76	0.67
1:C:245:PRO:HD3	2:M:1403:ARG:HH12	1.58	0.67
1:B:82:ASP:HA	1:B:127:PRO:HG3	1.76	0.66
1:B:871:ARG:NH1	1:B:873:ASP:O	2.28	0.66
1:A:346:CYS:HA	1:A:349:PRO:HB3	1.77	0.66
1:A:745:ALA:HB3	2:K:1387:ASP:OD2	1.95	0.66
1:C:529:GLN:NE2	1:C:530:THR:O	2.28	0.66
1:C:871:ARG:NH1	1:C:873:ASP:O	2.28	0.66
1:A:871:ARG:NH1	1:A:873:ASP:O	2.28	0.66
1:C:346:CYS:HA	1:C:349:PRO:HB3	1.77	0.66
1:F:158:PRO:HG2	1:H:1062:PRO:HG3	1.77	0.66
1:D:529:GLN:NE2	1:D:530:THR:O	2.28	0.66
1:H:1123:GLU:OE2	1:H:1123:GLU:N	2.27	0.66
1:F:82:ASP:HA	1:F:127:PRO:HG3	1.76	0.66
1:F:338:CYS:HA	1:F:359:CYS:HB3	1.78	0.66
1:A:529:GLN:NE2	1:A:530:THR:O	2.28	0.66
1:B:158:PRO:HG2	1:D:1062:PRO:HG3	1.77	0.66
1:E:764:GLY:N	1:E:776:CYS:O	2.24	0.66
1:D:453:LYS:HE2	1:D:455:CYS:HA	1.78	0.66
1:F:764:GLY:N	1:F:776:CYS:O	2.24	0.66
1:A:453:LYS:HE2	1:A:455:CYS:HA	1.78	0.65
1:A:967:GLN:HG3	1:C:179:LEU:HD11	1.78	0.65



		Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:B:178:ARG:NE	1:D:940:GLU:OE2	2.30	0.65		
1:B:338:CYS:HA	1:B:359:CYS:HB3	1.78	0.65		
1:E:178:ARG:NE	1:G:940:GLU:OE2	2.29	0.65		
1:A:158:PRO:HG2	1:C:1062:PRO:HG3	1.79	0.65		
1:B:967:GLN:HG3	1:D:179:LEU:HD11	1.78	0.65		
1:E:280:SER:HA	1:E:283:TYR:HD2	1.61	0.65		
1:B:627:ASP:HB3	1:B:630:SER:HB3	1.79	0.65		
1:B:905:THR:OG1	1:B:906:PHE:N	2.29	0.65		
1:B:493:ARG:HH22	1:B:495:GLN:HE21	1.45	0.65		
1:A:179:LEU:HD11	1:C:967:GLN:HG3	1.78	0.65		
1:A:1062:PRO:HG3	1:C:158:PRO:HG2	1.79	0.65		
1:F:280:SER:HA	1:F:283:TYR:HD2	1.61	0.65		
1:B:1062:PRO:HG3	1:D:158:PRO:HG2	1.79	0.65		
1:F:178:ARG:NE	1:H:940:GLU:OE2	2.29	0.65		
1:F:605:GLU:OE2	1:F:605:GLU:N	2.26	0.65		
1:A:414:TRP:O	1:C:1042:ARG:NH2	2.30	0.65		
1:E:158:PRO:HG2	1:G:1062:PRO:HG3	1.77	0.65		
1:D:1222:ASP:OD1	1:D:1224:ASP:N	2.30	0.65		
1:E:338:CYS:HA	1:E:359:CYS:HB3	1.78	0.64		
1:E:493:ARG:HH22	1:E:495:GLN:HE21	1.45	0.64		
1:D:539:GLN:OE1	1:D:545:GLN:NE2	2.31	0.64		
1:G:1181:ASN:ND2	1:G:1185:HIS:O	2.30	0.64		
1:H:1181:ASN:ND2	1:H:1185:HIS:O	2.30	0.64		
1:B:280:SER:HA	1:B:283:TYR:HD2	1.61	0.64		
1:A:905:THR:OG1	1:A:906:PHE:N	2.29	0.64		
1:B:333:MET:HE3	1:B:363:CYS:HB3	1.77	0.64		
1:A:1042:ARG:NH2	1:C:414:TRP:O	2.30	0.64		
1:B:605:GLU:OE2	1:B:605:GLU:N	2.26	0.64		
1:D:1181:ASN:ND2	1:D:1185:HIS:O	2.30	0.64		
1:H:1222:ASP:OD1	1:H:1224:ASP:N	2.30	0.64		
1:B:1042:ARG:NH2	1:D:414:TRP:O	2.30	0.64		
1:C:453:LYS:HE2	1:C:455:CYS:HA	1.78	0.64		
1:F:627:ASP:HB3	1:F:630:SER:HB3	1.79	0.64		
1:A:767:VAL:HG12	2:K:1416:LEU:HD22	1.80	0.64		
1:F:350:GLN:N	1:F:350:GLN:OE1	2.31	0.64		
1:B:442:ASP:OD1	1:B:442:ASP:N	2.23	0.64		
1:A:689:THR:HA	1:A:692:MET:HG2	1.80	0.63		
1:C:539:GLN:OE1	1:C:545:GLN:NE2	2.31	0.63		
1:D:689:THR:HA	1:D:692:MET:HG2	1.80	0.63		
1:E:627:ASP:HB3	1:E:630:SER:HB3	1.79	0.63		
1:F:493:ARG:HH22	1:F:495:GLN:HE21	1.45	0.63		



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:539:GLN:OE1	1:A:545:GLN:NE2	2.31	0.63
1:D:1056:LYS:NZ	1:D:1063:ASP:OD1	2.24	0.63
1:A:115:ASN:OD1	1:A:117:GLN:NE2	2.30	0.63
1:E:605:GLU:OE2	1:E:605:GLU:N	2.26	0.63
1:C:656:GLU:OE2	1:C:656:GLU:N	2.18	0.63
1:D:115:ASN:OD1	1:D:117:GLN:NE2	2.30	0.63
1:F:179:LEU:HD11	1:H:967:GLN:HG3	1.81	0.63
1:B:1133:ALA:O	1:B:1137:HIS:ND1	2.24	0.62
1:C:182:THR:HB	1:C:194:GLU:HB2	1.82	0.62
1:H:992:PHE:HD2	1:H:1193:LEU:HD13	1.64	0.62
1:B:179:LEU:HD11	1:D:967:GLN:HG3	1.81	0.62
1:E:179:LEU:HD11	1:G:967:GLN:HG3	1.81	0.62
1:C:115:ASN:OD1	1:C:117:GLN:NE2	2.30	0.62
1:A:763:PRO:HD3	2:K:1385:LEU:HD21	1.82	0.62
1:D:992:PHE:HD2	1:D:1193:LEU:HD13	1.64	0.62
1:C:342:CYS:HB2	1:C:351:ARG:HG3	1.82	0.62
1:A:342:CYS:HB2	1:A:351:ARG:HG3	1.82	0.62
1:C:689:THR:HA	1:C:692:MET:HG2	1.80	0.62
1:D:1123:GLU:N	1:D:1123:GLU:OE2	2.27	0.62
1:B:762:ALA:HB1	2:L:1384:GLN:OE1	2.00	0.62
1:A:670:VAL:HG11	1:A:683:TRP:CH2	2.35	0.61
1:A:986:ILE:HG12	1:A:995:ILE:HG12	1.82	0.61
1:B:501:PHE:HE2	1:D:713:ARG:HH22	1.48	0.61
1:C:986:ILE:HG12	1:C:995:ILE:HG12	1.82	0.61
1:B:986:ILE:HG12	1:B:995:ILE:HG12	1.82	0.61
1:B:350:GLN:OE1	1:B:350:GLN:N	2.31	0.61
1:D:670:VAL:HG11	1:D:683:TRP:CH2	2.35	0.61
1:E:120:ARG:HB3	1:E:120:ARG:NH1	2.16	0.61
1:E:754:CYS:N	1:E:776:CYS:SG	2.72	0.61
1:D:342:CYS:HB2	1:D:351:ARG:HG3	1.82	0.61
1:G:1123:GLU:N	1:G:1123:GLU:OE2	2.27	0.61
1:D:718:ALA:HB2	1:D:808:ALA:HB3	1.82	0.61
1:A:182:THR:HB	1:A:194:GLU:HB2	1.82	0.61
1:A:713:ARG:NH1	1:A:742:ASP:OD2	2.34	0.61
1:C:713:ARG:NH1	1:C:742:ASP:OD2	2.34	0.61
1:F:691:TYR:HA	1:F:694:ASN:ND2	2.16	0.61
1:G:1222:ASP:OD1	1:G:1224:ASP:N	2.30	0.61
1:A:940:GLU:OE2	1:C:178:ARG:NE	2.34	0.61
1:B:713:ARG:NH2	1:D:501:PHE:HE2	1.92	0.61
1:C:1077:ARG:NH2	1:C:1121:ASP:OD2	2.28	0.61
1:F:182:THR:HB	1:F:194:GLU:HB2	1.83	0.61



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:905:THR:OG1	1:C:906:PHE:N	2.29	0.61
1:D:182:THR:HB	1:D:194:GLU:HB2	1.82	0.61
1:E:182:THR:HB	1:E:194:GLU:HB2	1.83	0.61
1:F:754:CYS:N	1:F:776:CYS:SG	2.72	0.61
1:G:1088:LEU:HD22	1:G:1132:TYR:HD2	1.66	0.61
1:H:923:GLN:HB3	1:H:936:ARG:HG2	1.82	0.61
1:D:713:ARG:NH1	1:D:742:ASP:OD2	2.34	0.60
1:G:1077:ARG:NH2	1:G:1121:ASP:OD2	2.32	0.60
1:B:345:THR:O	1:B:348:ASN:N	2.34	0.60
1:C:670:VAL:HG11	1:C:683:TRP:CH2	2.35	0.60
1:G:923:GLN:HB3	1:G:936:ARG:HG2	1.82	0.60
1:A:178:ARG:NE	1:C:940:GLU:OE2	2.34	0.60
1:C:691:TYR:HA	1:C:694:ASN:ND2	2.17	0.60
2:L:1376:ALA:O	2:L:1401:ARG:NH2	2.19	0.60
1:A:345:THR:O	1:A:348:ASN:N	2.35	0.60
1:B:278:VAL:HB	1:B:305:TYR:HE1	1.67	0.60
1:B:529:GLN:NE2	1:B:530:THR:O	2.35	0.60
1:F:278:VAL:HB	1:F:305:TYR:HE1	1.67	0.60
1:G:992:PHE:HD2	1:G:1193:LEU:HD13	1.64	0.60
1:C:1153:LEU:H	1:D:1154:PHE:HD2	1.50	0.60
1:D:691:TYR:HA	1:D:694:ASN:ND2	2.17	0.60
1:E:691:TYR:HA	1:E:694:ASN:ND2	2.16	0.60
1:B:453:LYS:HE2	1:B:455:CYS:HA	1.84	0.60
1:D:923:GLN:HB3	1:D:936:ARG:HG2	1.82	0.60
1:A:656:GLU:OE2	1:A:656:GLU:N	2.18	0.60
1:B:120:ARG:HB3	1:B:120:ARG:NH1	2.16	0.60
1:B:418:ASP:OD1	1:B:418:ASP:N	2.34	0.60
1:B:754:CYS:N	1:B:776:CYS:SG	2.72	0.60
1:A:691:TYR:HA	1:A:694:ASN:ND2	2.16	0.60
1:D:762:ALA:HB1	2:J:1384:GLN:NE2	2.17	0.60
1:E:278:VAL:HB	1:E:305:TYR:HE1	1.67	0.60
1:F:120:ARG:HB3	1:F:120:ARG:NH1	2.16	0.60
1:B:86:LYS:HE2	1:B:90:GLY:HA2	1.84	0.59
1:B:182:THR:HB	1:B:194:GLU:HB2	1.83	0.59
1:D:1088:LEU:HD22	1:D:1132:TYR:HD2	1.66	0.59
1:A:1077:ARG:NH2	1:A:1121:ASP:OD2	2.28	0.59
1:E:350:GLN:OE1	1:E:350:GLN:N	2.31	0.59
1:E:529:GLN:NE2	1:E:530:THR:O	2.35	0.59
1:B:1077:ARG:NH2	1:B:1121:ASP:OD2	2.28	0.59
1:D:345:THR:O	1:D:348:ASN:N	2.35	0.59
1:D:1077:ARG:NH2	1:D:1121:ASP:OD2	2.32	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:115:ASN:OD1	1:E:117:GLN:NE2	2.34	0.59
1:E:345:THR:O	1:E:348:ASN:N	2.34	0.59
1:F:529:GLN:NE2	1:F:530:THR:O	2.35	0.59
1:H:1077:ARG:NH2	1:H:1121:ASP:OD2	2.32	0.59
1:G:955:ILE:HB	1:G:966:LEU:HB2	1.84	0.59
1:H:955:ILE:HB	1:H:966:LEU:HB2	1.84	0.59
1:B:940:GLU:OE2	1:D:178:ARG:NE	2.34	0.59
1:D:1198:PRO:HB2	1:D:1214:CYS:SG	2.43	0.59
1:F:453:LYS:HE2	1:F:455:CYS:HA	1.84	0.59
2:K:1376:ALA:HB3	2:K:1425:LEU:HD23	1.84	0.59
1:B:690:LYS:HA	1:B:693:GLN:HG3	1.85	0.59
1:C:450:VAL:HA	1:C:463:LEU:HD23	1.84	0.59
1:E:453:LYS:HE2	1:E:455:CYS:HA	1.84	0.59
1:H:1198:PRO:HB2	1:H:1214:CYS:SG	2.43	0.59
1:G:991:ILE:HG21	1:G:1153:LEU:HD21	1.85	0.59
1:C:345:THR:O	1:C:348:ASN:N	2.35	0.59
1:D:450:VAL:HA	1:D:463:LEU:HD23	1.84	0.59
1:D:955:ILE:HB	1:D:966:LEU:HB2	1.84	0.59
1:E:418:ASP:OD1	1:E:418:ASP:N	2.34	0.59
1:B:691:TYR:HA	1:B:694:ASN:ND2	2.16	0.59
1:C:768:HIS:O	2:I:1414:PRO:HB3	2.03	0.59
1:D:960:GLU:OE2	1:D:960:GLU:N	2.36	0.59
1:G:994:VAL:HA	1:G:1002:VAL:O	2.03	0.59
1:B:115:ASN:OD1	1:B:117:GLN:NE2	2.34	0.59
1:B:768:HIS:O	2:L:1414:PRO:HB3	2.02	0.59
1:D:991:ILE:HG21	1:D:1153:LEU:HD21	1.85	0.59
1:D:994:VAL:HA	1:D:1002:VAL:O	2.03	0.59
1:F:86:LYS:HE2	1:F:90:GLY:HA2	1.84	0.59
1:F:690:LYS:HA	1:F:693:GLN:HG3	1.85	0.58
1:G:1198:PRO:HB2	1:G:1214:CYS:SG	2.43	0.58
1:D:763:PRO:CD	2:J:1384:GLN:CD	2.61	0.58
1:F:427:VAL:HG22	1:F:433:ILE:HG12	1.85	0.58
1:H:994:VAL:HA	1:H:1002:VAL:O	2.03	0.58
1:H:1088:LEU:HD22	1:H:1132:TYR:HD2	1.66	0.58
1:A:1002:VAL:HG22	1:A:1012:ILE:HG12	1.85	0.58
1:E:427:VAL:HG22	1:E:433:ILE:HG12	1.85	0.58
1:E:690:LYS:HA	1:E:693:GLN:HG3	1.85	0.58
1:F:414:TRP:CD1	1:H:1043:SER:HB3	2.38	0.58
1:H:960:GLU:N	1:H:960:GLU:OE2	2.36	0.58
1:A:1133:ALA:O	1:A:1137:HIS:ND1	2.24	0.58
1:B:162:THR:OG1	1:D:948:GLY:O	2.17	0.58



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:86:LYS:HE2	1:E:90:GLY:HA2	1.84	0.58
1:F:468:LYS:NZ	1:F:470:GLY:O	2.25	0.58
1:G:960:GLU:N	1:G:960:GLU:OE2	2.36	0.58
2:L:1376:ALA:HB3	2:L:1425:LEU:HD23	1.84	0.58
1:A:361:ASP:OD1	1:A:362:GLY:N	2.37	0.58
1:B:502:LEU:HD21	1:D:513:ALA:HB2	1.86	0.58
1:F:115:ASN:OD1	1:F:117:GLN:NE2	2.34	0.58
1:G:986:ILE:HG12	1:G:995:ILE:HG12	1.86	0.58
1:A:516:ILE:HG23	1:A:530:THR:HG22	1.86	0.58
1:B:126:ARG:HH21	1:B:297:CYS:HB3	1.68	0.58
1:C:361:ASP:OD1	1:C:362:GLY:N	2.37	0.58
1:E:414:TRP:CD1	1:G:1043:SER:HB3	2.38	0.58
2:I:1376:ALA:HB3	2:I:1425:LEU:HD23	1.84	0.58
2:L:1402:MET:N	2:L:1402:MET:SD	2.77	0.58
1:B:414:TRP:CD1	1:D:1043:SER:HB3	2.38	0.58
1:H:986:ILE:HG12	1:H:995:ILE:HG12	1.86	0.58
1:H:992:PHE:CD2	1:H:1193:LEU:HD13	2.39	0.58
2:I:1402:MET:N	2:I:1402:MET:SD	2.77	0.58
1:A:450:VAL:HA	1:A:463:LEU:HD23	1.84	0.58
1:A:414:TRP:CD1	1:C:1043:SER:HB3	2.39	0.58
1:D:205:GLY:HA2	1:D:235:GLN:HG2	1.86	0.58
1:D:427:VAL:HB	1:D:546:VAL:HG12	1.86	0.58
1:D:516:ILE:HG23	1:D:530:THR:HG22	1.86	0.58
1:F:126:ARG:HH21	1:F:297:CYS:HB3	1.68	0.58
2:K:1402:MET:N	2:K:1402:MET:SD	2.77	0.58
1:A:1043:SER:HB3	1:C:414:TRP:CD1	2.39	0.57
1:B:1153:LEU:H	1:H:1154:PHE:HD2	1.50	0.57
1:B:1043:SER:HB3	1:D:414:TRP:CD1	2.39	0.57
1:G:992:PHE:CD2	1:G:1193:LEU:HD13	2.39	0.57
1:H:991:ILE:HG21	1:H:1153:LEU:HD21	1.85	0.57
2:K:1381:ARG:HE	2:K:1386:PRO:HA	1.69	0.57
1:A:1153:LEU:H	1:G:1154:PHE:HD2	1.50	0.57
1:C:761:LEU:HD21	1:C:767:VAL:HG11	1.87	0.57
1:D:755:TYR:HE1	1:D:760:VAL:HG22	1.70	0.57
1:E:126:ARG:HH21	1:E:297:CYS:HB3	1.68	0.57
2:I:1381:ARG:HE	2:I:1386:PRO:HA	1.70	0.57
1:C:516:ILE:HG23	1:C:530:THR:HG22	1.86	0.57
1:C:1002:VAL:HG22	1:C:1012:ILE:HG12	1.85	0.57
1:B:992:PHE:CD2	1:B:1193:LEU:HD13	2.39	0.57
1:B:1002:VAL:HG22	1:B:1012:ILE:HG12	1.85	0.57
1:C:992:PHE:CD2	1:C:1193:LEU:HD13	2.40	0.57



	A i o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:992:PHE:HD2	1:C:1193:LEU:HD13	1.70	0.57
2:L:1398:ASP:OD1	2:L:1406:MET:HB3	2.05	0.57
1:B:923:GLN:HB3	1:B:936:ARG:HG2	1.87	0.57
1:C:991:ILE:HG21	1:C:1153:LEU:HD21	1.87	0.57
1:C:1179:CYS:HB2	1:C:1208:ASN:HA	1.87	0.57
1:D:361:ASP:OD1	1:D:362:GLY:N	2.37	0.57
1:A:295:PRO:HD2	1:A:296:THR:N	2.18	0.57
2:L:1381:ARG:HE	2:L:1386:PRO:HA	1.70	0.57
1:A:761:LEU:HD21	1:A:767:VAL:HG11	1.87	0.57
1:A:991:ILE:HG21	1:A:1153:LEU:HD21	1.87	0.57
1:A:1179:CYS:HB2	1:A:1208:ASN:HA	1.87	0.57
1:B:770:GLU:OE2	1:D:597:CYS:SG	2.62	0.57
1:B:955:ILE:HB	1:B:966:LEU:HB2	1.87	0.57
1:C:205:GLY:HA2	1:C:235:GLN:HG2	1.86	0.57
1:C:427:VAL:HB	1:C:546:VAL:HG12	1.86	0.57
1:C:755:TYR:HE1	1:C:760:VAL:HG22	1.70	0.57
1:C:955:ILE:HB	1:C:966:LEU:HB2	1.87	0.57
1:C:961:SER:HB3	1:C:977:GLY:HA3	1.87	0.57
1:E:573:PHE:HB2	1:E:580:VAL:HG13	1.87	0.57
1:G:816:LEU:HD23	1:G:836:VAL:HG13	1.87	0.57
2:K:1398:ASP:OD1	2:K:1406:MET:HB3	2.05	0.57
1:A:500:VAL:HG11	1:A:518:LEU:HD23	1.87	0.57
1:B:767:VAL:HG12	2:L:1416:LEU:HD22	1.86	0.57
1:C:923:GLN:HB3	1:C:936:ARG:HG2	1.87	0.57
1:F:780:LYS:H	1:F:780:LYS:HD2	1.70	0.57
1:G:1229:ASP:OD1	1:G:1230:VAL:N	2.38	0.57
2:K:1397:VAL:HG22	2:K:1407:CYS:HB2	1.87	0.57
1:D:624:ARG:NH1	1:D:685:ASP:O	2.26	0.57
1:F:538:VAL:HG22	1:F:546:VAL:HG23	1.87	0.57
1:A:713:ARG:NH2	1:C:501:PHE:CE2	2.40	0.56
1:C:500:VAL:HG11	1:C:518:LEU:HD23	1.87	0.56
1:D:761:LEU:HD21	1:D:767:VAL:HG11	1.87	0.56
2:L:1397:VAL:HG22	2:L:1407:CYS:HB2	1.87	0.56
2:N:1383:ALA:N	2:N:1419:ASP:O	2.35	0.56
1:B:991:ILE:HG21	1:B:1153:LEU:HD21	1.87	0.56
1:E:162:THR:OG1	1:G:948:GLY:O	2.17	0.56
1:H:1229:ASP:OD1	1:H:1230:VAL:N	2.38	0.56
1:A:896:VAL:HG22	1:A:1011:PHE:HD1	1.71	0.56
1:A:992:PHE:HD2	1:A:1193:LEU:HD13	1.70	0.56
1:B:137:GLN:HB3	1:D:946:THR:HA	1.86	0.56
1:B:178:ARG:HH22	1:D:956:LYS:HE3	1.71	0.56



	juo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:427:VAL:HG22	1:B:433:ILE:HG12	1.85	0.56
1:B:719:ASP:OD2	1:B:722:CYS:HB3	2.06	0.56
1:B:992:PHE:HD2	1:B:1193:LEU:HD13	1.70	0.56
1:C:691:TYR:HA	1:C:694:ASN:HD22	1.70	0.56
1:E:178:ARG:HH22	1:G:956:LYS:HE3	1.71	0.56
1:E:538:VAL:HG22	1:E:546:VAL:HG23	1.87	0.56
1:F:573:PHE:HB2	1:F:580:VAL:HG13	1.87	0.56
1:F:719:ASP:OD1	1:F:722:CYS:HB3	2.06	0.56
2:I:1397:VAL:HG22	2:I:1407:CYS:HB2	1.87	0.56
1:A:299:CYS:HA	1:A:302:PHE:CD2	2.40	0.56
1:B:564:ASN:ND2	1:B:571:ASP:OD2	2.32	0.56
1:D:992:PHE:CD2	1:D:1193:LEU:HD13	2.39	0.56
1:F:137:GLN:HB3	1:H:946:THR:HA	1.86	0.56
1:F:250:LEU:HD12	1:F:251:PRO:HD2	1.87	0.56
2:I:1398:ASP:OD2	2:I:1406:MET:HB3	2.05	0.56
2:M:1383:ALA:N	2:M:1419:ASP:O	2.35	0.56
1:A:427:VAL:HB	1:A:546:VAL:HG12	1.86	0.56
1:B:178:ARG:HD2	1:B:179:LEU:HD23	1.87	0.56
1:B:896:VAL:HG22	1:B:1011:PHE:HD1	1.71	0.56
1:B:1088:LEU:HD22	1:B:1132:TYR:HD2	1.70	0.56
1:C:295:PRO:HD2	1:C:296:THR:N	2.18	0.56
2:N:1362:GLU:N	2:N:1362:GLU:OE1	2.39	0.56
1:A:961:SER:HB3	1:A:977:GLY:HA3	1.87	0.56
1:B:538:VAL:HG22	1:B:546:VAL:HG23	1.87	0.56
1:B:871:ARG:HH21	1:B:1140:GLY:HA2	1.71	0.56
1:C:798:MET:HE2	1:C:798:MET:O	2.06	0.56
1:D:986:ILE:HG12	1:D:995:ILE:HG12	1.86	0.56
1:F:345:THR:O	1:F:348:ASN:N	2.34	0.56
2:M:1362:GLU:OE1	2:M:1362:GLU:N	2.39	0.56
1:A:691:TYR:HA	1:A:694:ASN:HD22	1.70	0.56
1:A:1198:PRO:HB2	1:A:1214:CYS:SG	2.46	0.56
1:D:108:ARG:HB3	1:D:202:GLN:HA	1.87	0.56
1:D:500:VAL:HG11	1:D:518:LEU:HD23	1.87	0.56
1:A:923:GLN:HB3	1:A:936:ARG:HG2	1.87	0.56
1:A:992:PHE:CD2	1:A:1193:LEU:HD13	2.39	0.56
1:B:974:VAL:O	1:B:976:ARG:HG2	2.06	0.56
1:E:564:ASN:ND2	1:E:571:ASP:OD2	2.32	0.56
1:E:780:LYS:H	1:E:780:LYS:HD2	1.70	0.56
1:A:205:GLY:HA2	1:A:235:GLN:HG2	1.86	0.56
1:A:798:MET:HE2	1:A:798:MET:O	2.06	0.56
1:B:961:SER:HB3	1:B:977:GLY:HA3	1.86	0.56



	A	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:345:THR:HB	1:C:371:LEU:HB3	1.88	0.56
1:F:632:PHE:HB3	1:F:669:TYR:HE2	1.71	0.56
2:J:1396:GLN:N	2:J:1412:GLN:OE1	2.33	0.56
1:A:700:ARG:HG2	1:A:735:PRO:HG3	1.88	0.56
1:B:108:ARG:HB3	1:B:202:GLN:HA	1.88	0.56
1:D:719:ASP:OD1	1:D:722:CYS:N	2.37	0.56
1:D:1229:ASP:OD1	1:D:1230:VAL:N	2.38	0.56
1:E:632:PHE:HB3	1:E:669:TYR:HE2	1.71	0.56
1:A:871:ARG:HH21	1:A:1140:GLY:HA2	1.71	0.55
1:A:955:ILE:HB	1:A:966:LEU:HB2	1.87	0.55
1:C:108:ARG:HB3	1:C:202:GLN:HA	1.88	0.55
1:C:299:CYS:HA	1:C:302:PHE:CD2	2.39	0.55
1:C:896:VAL:HG22	1:C:1011:PHE:HD1	1.71	0.55
1:E:137:GLN:HB3	1:G:946:THR:HA	1.86	0.55
1:E:719:ASP:OD1	1:E:722:CYS:HB3	2.06	0.55
1:B:780:LYS:H	1:B:780:LYS:HD2	1.70	0.55
1:B:1179:CYS:HB2	1:B:1208:ASN:HA	1.87	0.55
1:C:1088:LEU:HD22	1:C:1132:TYR:HD2	1.70	0.55
1:D:691:TYR:HA	1:D:694:ASN:HD22	1.71	0.55
1:D:753:PRO:HG3	2:J:1385:LEU:CD2	2.37	0.55
1:B:767:VAL:HG12	2:L:1416:LEU:CD1	2.32	0.55
1:D:401:ASN:HA	1:D:406:SER:HA	1.88	0.55
1:H:816:LEU:HD23	1:H:836:VAL:HG13	1.87	0.55
2:J:1362:GLU:OE1	2:J:1362:GLU:N	2.39	0.55
1:A:755:TYR:HE1	1:A:760:VAL:HG22	1.70	0.55
1:B:632:PHE:HB3	1:B:669:TYR:HE2	1.71	0.55
1:C:1043:SER:O	1:C:1043:SER:OG	2.25	0.55
1:D:345:THR:HB	1:D:371:LEU:HB3	1.88	0.55
1:D:816:LEU:HD23	1:D:836:VAL:HG13	1.87	0.55
1:F:500:VAL:HG11	1:F:518:LEU:HD23	1.89	0.55
1:A:236:LYS:NZ	1:A:238:ASP:OD1	2.30	0.55
1:A:974:VAL:O	1:A:976:ARG:HG2	2.06	0.55
1:B:573:PHE:HB2	1:B:580:VAL:HG13	1.87	0.55
1:B:798:MET:HE2	1:B:798:MET:O	2.05	0.55
1:C:763:PRO:CD	2:I:1385:LEU:HD21	2.36	0.55
1:D:911:TYR:HH	1:D:1051:PHE:HE2	1.55	0.55
1:E:108:ARG:HB3	1:E:202:GLN:HA	1.88	0.55
1:A:345:THR:HB	1:A:371:LEU:HB3	1.88	0.55
1:B:266:LEU:HD22	1:B:305:TYR:HD2	1.72	0.55
1:C:401:ASN:HA	1:C:406:SER:HA	1.88	0.55
1:A:1088:LEU:HD22	1:A:1132:TYR:HD2	1.71	0.55



	as pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:754:CYS:HB2	1:B:781:LEU:HD23	1.88	0.55
1:B:250:LEU:HD12	1:B:251:PRO:HD2	1.87	0.55
1:B:1198:PRO:HB2	1:B:1214:CYS:SG	2.46	0.55
1:B:1229:ASP:OD1	1:B:1230:VAL:N	2.40	0.55
1:C:1133:ALA:O	1:C:1137:HIS:ND1	2.24	0.55
1:C:1229:ASP:OD1	1:C:1230:VAL:N	2.40	0.55
1:D:700:ARG:HG2	1:D:735:PRO:HG3	1.88	0.55
1:E:178:ARG:HD2	1:E:179:LEU:HD23	1.87	0.55
1:G:961:SER:HB3	1:G:977:GLY:HA3	1.89	0.55
1:B:500:VAL:HG11	1:B:518:LEU:HD23	1.89	0.55
1:E:250:LEU:HD12	1:E:251:PRO:HD2	1.87	0.55
1:F:108:ARG:HB3	1:F:202:GLN:HA	1.88	0.55
1:F:178:ARG:HH22	1:H:956:LYS:HE3	1.71	0.55
1:F:564:ASN:ND2	1:F:571:ASP:OD2	2.32	0.55
1:F:754:CYS:HB2	1:F:781:LEU:HD23	1.88	0.55
1:A:401:ASN:HA	1:A:406:SER:HA	1.88	0.55
1:A:624:ARG:NH1	1:A:685:ASP:O	2.26	0.54
1:C:194:GLU:OE2	1:C:311:HIS:NE2	2.40	0.54
1:C:1198:PRO:HB2	1:C:1214:CYS:SG	2.46	0.54
1:D:961:SER:HB3	1:D:977:GLY:HA3	1.89	0.54
1:E:266:LEU:HD22	1:E:305:TYR:HD2	1.72	0.54
1:E:754:CYS:HB2	1:E:781:LEU:HD23	1.88	0.54
1:F:266:LEU:HD22	1:F:305:TYR:HD2	1.72	0.54
2:K:1401:ARG:HG2	2:K:1402:MET:SD	2.48	0.54
1:A:108:ARG:HB3	1:A:202:GLN:HA	1.88	0.54
1:A:760:VAL:HG11	2:K:1388:MET:SD	2.47	0.54
1:C:974:VAL:O	1:C:976:ARG:HG2	2.06	0.54
1:F:97:GLY:HA2	1:F:247:PRO:HG3	1.89	0.54
1:G:816:LEU:HD11	1:G:843:SER:HB3	1.90	0.54
1:H:816:LEU:HD11	1:H:843:SER:HB3	1.90	0.54
1:D:194:GLU:OE2	1:D:311:HIS:NE2	2.40	0.54
1:D:295:PRO:HD2	1:D:296:THR:N	2.18	0.54
1:D:937:ILE:HG12	1:D:957:LEU:HD23	1.88	0.54
1:F:442:ASP:OD1	1:F:442:ASP:N	2.23	0.54
2:L:1399:CYS:HA	2:L:1404:GLY:O	2.08	0.54
1:F:178:ARG:HD2	1:F:179:LEU:HD23	1.87	0.54
1:A:194:GLU:OE2	1:A:311:HIS:NE2	2.40	0.54
1:B:97:GLY:HA2	1:B:247:PRO:HG3	1.89	0.54
1:C:700:ARG:HG2	1:C:735:PRO:HG3	1.88	0.54
1:D:166:VAL:HG12	1:D:175:VAL:HG13	1.89	0.54
2:I:1399:CYS:HA	2:I:1404:GLY:O	2.08	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:I:1401:ARG:HG2	2:I:1402:MET:SD	2.48	0.54
2:L:1401:ARG:HG2	2:L:1402:MET:SD	2.48	0.54
1:A:659:GLU:HG2	1:A:690:LYS:HE2	1.90	0.54
1:D:659:GLU:HG2	1:D:690:LYS:HE2	1.90	0.54
1:E:500:VAL:HG11	1:E:518:LEU:HD23	1.89	0.54
1:H:937:ILE:HG12	1:H:957:LEU:HD23	1.88	0.54
2:K:1399:CYS:HA	2:K:1404:GLY:O	2.07	0.54
1:A:957:LEU:HD21	1:A:1002:VAL:HG21	1.89	0.54
1:C:871:ARG:HH21	1:C:1140:GLY:HA2	1.71	0.54
1:D:183:PHE:CZ	1:D:185:TRP:HB2	2.43	0.54
1:D:762:ALA:CB	2:J:1384:GLN:OE1	2.48	0.54
1:G:962:TYR:CE2	1:G:982:PRO:HA	2.43	0.54
1:H:962:TYR:CE2	1:H:982:PRO:HA	2.43	0.54
1:C:166:VAL:HG12	1:C:175:VAL:HG13	1.89	0.54
1:C:756:ALA:O	1:C:759:THR:OG1	2.20	0.54
1:D:763:PRO:HD2	2:J:1384:GLN:NE2	2.20	0.54
1:D:962:TYR:CE2	1:D:982:PRO:HA	2.43	0.54
1:F:361:ASP:OD1	1:F:362:GLY:N	2.41	0.54
1:G:1068:LYS:HE3	1:G:1073:ALA:HB2	1.90	0.54
1:H:1179:CYS:HB2	1:H:1208:ASN:HA	1.90	0.54
1:C:957:LEU:HD21	1:C:1002:VAL:HG21	1.89	0.53
1:E:361:ASP:OD1	1:E:362:GLY:N	2.41	0.53
1:H:1068:LYS:HE3	1:H:1073:ALA:HB2	1.90	0.53
1:A:936:ARG:HH21	1:A:958:PHE:HE2	1.57	0.53
1:A:1068:LYS:HD2	1:A:1073:ALA:HB2	1.91	0.53
1:A:1229:ASP:OD1	1:A:1230:VAL:N	2.40	0.53
1:B:468:LYS:NZ	1:B:470:GLY:O	2.25	0.53
1:C:1068:LYS:HD2	1:C:1073:ALA:HB2	1.91	0.53
1:G:937:ILE:HG12	1:G:957:LEU:HD23	1.88	0.53
2:N:1398:ASP:OD1	2:N:1398:ASP:N	2.42	0.53
1:C:183:PHE:CZ	1:C:185:TRP:HB2	2.43	0.53
2:J:1403:ARG:HD3	2:J:1406:MET:CE	2.38	0.53
2:N:1403:ARG:HD3	2:N:1406:MET:CE	2.38	0.53
1:A:763:PRO:CD	2:K:1385:LEU:HD21	2.38	0.53
1:B:796:ALA:HB3	1:B:798:MET:SD	2.49	0.53
1:B:957:LEU:HD21	1:B:1002:VAL:HG21	1.89	0.53
1:A:183:PHE:CZ	1:A:185:TRP:HB2	2.43	0.53
1:A:796:ALA:HB3	1:A:798:MET:SD	2.49	0.53
1:A:1056:LYS:NZ	1:A:1063:ASP:OD1	2.25	0.53
1:C:659:GLU:HG2	1:C:690:LYS:HE2	1.90	0.53
1:D:369:THR:O	1:D:369:THR:OG1	2.27	0.53


		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:361:ASP:OD1	1:B:362:GLY:N	2.41	0.53
1:C:86:LYS:HE2	1:C:90:GLY:HA2	1.91	0.53
1:E:254:ASN:O	1:E:256:THR:N	2.41	0.53
1:E:485:LEU:HB3	1:E:490:THR:HB	1.91	0.53
2:M:1398:ASP:OD1	2:M:1398:ASP:N	2.42	0.53
1:B:485:LEU:HB3	1:B:490:THR:HB	1.91	0.53
1:B:1043:SER:O	1:B:1043:SER:OG	2.25	0.53
1:C:79:THR:HG22	1:C:120:ARG:HH21	1.74	0.53
1:C:690:LYS:HA	1:C:693:GLN:HG3	1.91	0.53
1:D:299:CYS:HA	1:D:302:PHE:CD2	2.40	0.53
1:H:961:SER:HB3	1:H:977:GLY:HA3	1.89	0.53
1:A:166:VAL:HG12	1:A:175:VAL:HG13	1.89	0.53
1:A:627:ASP:HB3	1:A:630:SER:HB3	1.91	0.53
1:F:271:PHE:HB3	1:F:274:CYS:HB2	1.91	0.53
1:G:819:CYS:SG	1:G:856:PRO:HD2	2.49	0.53
1:A:79:THR:HG22	1:A:120:ARG:HH21	1.74	0.52
1:A:126:ARG:HD3	1:A:127:PRO:HD2	1.92	0.52
1:A:479:LYS:HZ1	2:I:1413:SER:HB3	1.74	0.52
1:B:1005:ASP:OD1	1:B:1007:LYS:N	2.35	0.52
1:D:753:PRO:HG3	2:J:1385:LEU:HD21	1.89	0.52
1:D:816:LEU:HD11	1:D:843:SER:HB3	1.89	0.52
1:E:97:GLY:HA2	1:E:247:PRO:HG3	1.89	0.52
1:A:89:ASP:HB2	1:A:214:PRO:HA	1.92	0.52
1:B:767:VAL:CG1	2:L:1416:LEU:HD13	2.33	0.52
1:C:796:ALA:HB3	1:C:798:MET:SD	2.49	0.52
1:D:1179:CYS:HB2	1:D:1208:ASN:HA	1.90	0.52
2:J:1383:ALA:N	2:J:1419:ASP:O	2.35	0.52
2:M:1403:ARG:HD3	2:M:1406:MET:CE	2.38	0.52
1:B:254:ASN:O	1:B:256:THR:N	2.41	0.52
1:C:621:TRP:HB2	1:C:662:LEU:HD11	1.92	0.52
1:C:627:ASP:HB3	1:C:630:SER:HB3	1.92	0.52
1:D:893:GLY:O	1:D:1013:ARG:HA	2.09	0.52
1:E:205:GLY:HA2	1:E:235:GLN:HG2	1.92	0.52
1:D:126:ARG:HD3	1:D:127:PRO:HD2	1.92	0.52
1:E:194:GLU:OE2	1:E:311:HIS:NE2	2.43	0.52
1:A:1043:SER:O	1:A:1043:SER:OG	2.25	0.52
1:B:271:PHE:HB3	1:B:274:CYS:HB2	1.91	0.52
1:B:450:VAL:HA	1:B:463:LEU:HD23	1.92	0.52
1:D:123:VAL:HG23	1:D:128:VAL:HG21	1.91	0.52
1:D:297:CYS:N	1:D:298:PRO:HD3	2.24	0.52
1:D:819:CYS:SG	1:D:856:PRO:HD2	2.49	0.52



	A t ama 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:896:VAL:HG22	1:D:1011:PHE:HD1	1.75	0.52
1:G:1179:CYS:HB2	1:G:1208:ASN:HA	1.90	0.52
1:A:621:TRP:HB2	1:A:662:LEU:HD11	1.92	0.52
1:D:82:ASP:HA	1:D:127:PRO:HG3	1.92	0.52
1:F:670:VAL:HG11	1:F:683:TRP:CH2	2.45	0.52
1:A:468:LYS:NZ	1:A:470:GLY:O	2.29	0.52
1:C:89:ASP:HB2	1:C:214:PRO:HA	1.92	0.52
1:C:371:LEU:HD12	1:C:372:ASP:H	1.75	0.52
1:D:941:ASN:OD1	1:D:953:LYS:NZ	2.43	0.52
1:F:126:ARG:HD3	1:F:127:PRO:HD2	1.92	0.52
1:F:479:LYS:NZ	2:N:1413:SER:HB2	2.25	0.52
1:A:82:ASP:HA	1:A:127:PRO:HG3	1.92	0.52
1:C:126:ARG:HD3	1:C:127:PRO:HD2	1.92	0.52
1:C:297:CYS:N	1:C:298:PRO:HD3	2.24	0.52
1:D:79:THR:HG22	1:D:120:ARG:HH21	1.74	0.52
1:D:86:LYS:HE2	1:D:90:GLY:HA2	1.91	0.52
1:G:893:GLY:O	1:G:1013:ARG:HA	2.09	0.52
1:A:1172:GLY:HA3	1:A:1197:TYR:CZ	2.45	0.52
1:B:670:VAL:HG11	1:B:683:TRP:CH2	2.45	0.52
1:B:962:TYR:OH	1:B:980:GLY:O	2.28	0.52
1:D:690:LYS:HA	1:D:693:GLN:HG3	1.91	0.52
1:D:1068:LYS:HE3	1:D:1073:ALA:HB2	1.90	0.52
1:E:450:VAL:HA	1:E:463:LEU:HD23	1.92	0.52
1:E:594:GLN:HE21	1:G:828:SER:HB2	1.75	0.52
1:G:896:VAL:HG22	1:G:1011:PHE:HD1	1.75	0.52
1:H:819:CYS:SG	1:H:856:PRO:HD2	2.49	0.52
1:H:893:GLY:O	1:H:1013:ARG:HA	2.09	0.52
2:J:1398:ASP:OD2	2:J:1398:ASP:N	2.42	0.52
1:B:1068:LYS:HD2	1:B:1073:ALA:HB2	1.91	0.51
1:D:902:HIS:CD2	1:D:1108:ALA:HB1	2.46	0.51
1:G:902:HIS:CD2	1:G:1108:ALA:HB1	2.45	0.51
1:A:297:CYS:N	1:A:298:PRO:HD3	2.25	0.51
1:A:690:LYS:HA	1:A:693:GLN:HG3	1.91	0.51
1:B:594:GLN:HE21	1:D:828:SER:HB2	1.75	0.51
1:B:936:ARG:HH21	1:B:958:PHE:HE2	1.57	0.51
1:C:123:VAL:HG23	1:C:128:VAL:HG21	1.91	0.51
1:D:621:TRP:HB2	1:D:662:LEU:HD11	1.92	0.51
1:E:442:ASP:OD1	1:E:442:ASP:N	2.23	0.51
1:F:485:LEU:HB3	1:F:490:THR:HB	1.91	0.51
1:F:509:LEU:HD22	1:F:518:LEU:HB3	1.93	0.51
1:B:194:GLU:OE2	1:B:311:HIS:NE2	2.43	0.51



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:936:ARG:HH21	1:C:958:PHE:HE2	1.57	0.51
1:C:962:TYR:OH	1:C:980:GLY:O	2.28	0.51
1:F:194:GLU:OE2	1:F:311:HIS:NE2	2.43	0.51
1:A:369:THR:O	1:A:369:THR:OG1	2.27	0.51
1:A:1222:ASP:OD1	1:A:1224:ASP:N	2.44	0.51
1:B:479:LYS:NZ	2:J:1413:SER:HB2	2.25	0.51
1:C:607:PRO:HG2	1:C:654:ASN:HB2	1.93	0.51
1:F:621:TRP:HB2	1:F:662:LEU:HD11	1.93	0.51
1:G:941:ASN:OD1	1:G:953:LYS:NZ	2.43	0.51
1:A:962:TYR:OH	1:A:980:GLY:O	2.28	0.51
1:D:556:GLY:N	1:D:565:PHE:O	2.32	0.51
1:E:126:ARG:HD3	1:E:127:PRO:HD2	1.92	0.51
1:E:670:VAL:HG11	1:E:683:TRP:CH2	2.45	0.51
1:G:911:TYR:OH	1:G:1051:PHE:HE2	1.94	0.51
1:B:205:GLY:HA2	1:B:235:GLN:HG2	1.92	0.51
1:B:1222:ASP:OD1	1:B:1224:ASP:N	2.44	0.51
1:C:719:ASP:OD1	1:C:722:CYS:N	2.37	0.51
1:A:123:VAL:HG23	1:A:128:VAL:HG21	1.91	0.51
1:B:621:TRP:HB2	1:B:662:LEU:HD11	1.93	0.51
1:D:627:ASP:HB3	1:D:630:SER:HB3	1.91	0.51
1:F:114:PHE:HE1	1:F:199:TYR:CD1	2.28	0.51
1:C:82:ASP:HA	1:C:127:PRO:HG3	1.92	0.51
1:D:89:ASP:HB2	1:D:214:PRO:HA	1.92	0.51
1:D:236:LYS:NZ	1:D:238:ASP:OD1	2.31	0.51
1:E:114:PHE:HE1	1:E:199:TYR:CD1	2.28	0.51
1:E:271:PHE:HB3	1:E:274:CYS:HB2	1.91	0.51
1:E:556:GLY:N	1:E:565:PHE:O	2.40	0.51
1:H:896:VAL:HG22	1:H:1011:PHE:HD1	1.75	0.51
1:A:86:LYS:HE2	1:A:90:GLY:HA2	1.91	0.51
1:A:607:PRO:HG2	1:A:654:ASN:HB2	1.93	0.51
1:C:556:GLY:N	1:C:565:PHE:O	2.32	0.51
1:D:763:PRO:N	2:J:1384:GLN:HE22	2.09	0.51
1:F:205:GLY:HA2	1:F:235:GLN:HG2	1.92	0.51
1:H:1043:SER:O	1:H:1043:SER:OG	2.29	0.51
1:A:719:ASP:OD2	1:A:722:CYS:N	2.37	0.51
1:E:344:ASP:OD1	1:E:352:ALA:N	2.38	0.51
1:E:479:LYS:NZ	2:M:1413:SER:HB2	2.25	0.51
1:E:766:VAL:HG22	1:E:775:SER:HB2	1.93	0.51
1:F:594:GLN:HE21	1:H:828:SER:HB2	1.75	0.51
1:H:902:HIS:CD2	1:H:1108:ALA:HB1	2.46	0.51
2:N:1378:ILE:HG12	2:N:1401:ARG:HA	1.93	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:N:1380:CYS:SG	2:N:1405:LEU:HD12	2.51	0.51
1:A:816:LEU:HD23	1:A:836:VAL:HG22	1.94	0.50
1:B:114:PHE:HE1	1:B:199:TYR:CD2	2.28	0.50
1:B:822:LEU:HD22	1:B:882:ARG:NH1	2.27	0.50
1:B:939:THR:HG22	1:B:955:ILE:HG13	1.94	0.50
1:D:422:PRO:HA	1:D:552:PRO:HD3	1.93	0.50
1:E:509:LEU:HD22	1:E:518:LEU:HB3	1.92	0.50
1:E:766:VAL:HA	1:E:774:CYS:O	2.11	0.50
1:F:450:VAL:HA	1:F:463:LEU:HD23	1.92	0.50
1:A:904:ILE:HD11	1:A:1105:TYR:HE1	1.77	0.50
1:B:509:LEU:HD22	1:B:518:LEU:HB3	1.92	0.50
1:B:1172:GLY:HA3	1:B:1197:TYR:CZ	2.45	0.50
1:C:1172:GLY:HA3	1:C:1197:TYR:CZ	2.45	0.50
1:D:855:CYS:HB2	1:D:882:ARG:HG2	1.94	0.50
1:E:346:CYS:HA	1:E:349:PRO:HB3	1.93	0.50
1:F:254:ASN:O	1:F:256:THR:N	2.41	0.50
1:F:346:CYS:HA	1:F:349:PRO:HB3	1.93	0.50
2:J:1378:ILE:HG12	2:J:1401:ARG:HA	1.93	0.50
2:J:1380:CYS:SG	2:J:1405:LEU:HD12	2.51	0.50
2:M:1396:GLN:N	2:M:1412:GLN:OE1	2.33	0.50
1:A:556:GLY:N	1:A:565:PHE:O	2.32	0.50
1:A:670:VAL:HG21	1:A:683:TRP:CE2	2.47	0.50
1:B:126:ARG:HD3	1:B:127:PRO:HD2	1.92	0.50
1:B:766:VAL:HG22	1:B:775:SER:HB2	1.93	0.50
1:H:1145:TRP:CD1	1:H:1145:TRP:N	2.77	0.50
1:B:766:VAL:HA	1:B:774:CYS:O	2.12	0.50
1:C:822:LEU:HD22	1:C:882:ARG:NH1	2.27	0.50
1:E:621:TRP:HB2	1:E:662:LEU:HD11	1.93	0.50
1:F:766:VAL:HG22	1:F:775:SER:HB2	1.93	0.50
2:J:1378:ILE:HG22	2:J:1424:VAL:HA	1.94	0.50
1:B:991:ILE:HG23	1:B:1195:GLY:HA2	1.94	0.50
1:C:1222:ASP:OD1	1:C:1224:ASP:N	2.44	0.50
1:D:756:ALA:O	1:D:759:THR:OG1	2.20	0.50
1:D:911:TYR:OH	1:D:1051:PHE:HE2	1.94	0.50
1:D:1133:ALA:O	1:D:1137:HIS:ND1	2.26	0.50
1:G:807:SER:O	1:G:810:THR:HG23	2.12	0.50
2:M:1380:CYS:SG	2:M:1405:LEU:HD12	2.51	0.50
2:N:1396:GLN:N	2:N:1412:GLN:OE1	2.33	0.50
1:A:371:LEU:HD12	1:A:372:ASP:H	1.75	0.50
1:A:991:ILE:HG23	1:A:1195:GLY:HA2	1.94	0.50
1:C:904:ILE:HD11	1:C:1105:TYR:HE1	1.77	0.50



	h i c	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:939:THR:HG22	1:C:955:ILE:HG13	1.94	0.50
1:D:805:ASN:OD1	1:D:806:SER:N	2.45	0.50
1:H:855:CYS:HB2	1:H:882:ARG:HG2	1.94	0.50
2:M:1378:ILE:HG12	2:M:1401:ARG:HA	1.93	0.50
1:A:422:PRO:HA	1:A:552:PRO:HD3	1.93	0.50
1:C:671:HIS:CD2	1:C:729:VAL:HG12	2.47	0.50
1:C:817:ARG:H	1:C:817:ARG:HD2	1.77	0.50
1:D:510:PRO:HA	1:D:518:LEU:O	2.12	0.50
1:D:671:HIS:CD2	1:D:729:VAL:HG12	2.47	0.50
1:F:766:VAL:HA	1:F:774:CYS:O	2.12	0.50
1:G:805:ASN:OD1	1:G:806:SER:N	2.45	0.50
1:G:957:LEU:HD21	1:G:1002:VAL:HG21	1.94	0.50
1:A:817:ARG:HD2	1:A:817:ARG:H	1.77	0.50
1:B:817:ARG:HH12	1:B:839:PRO:HA	1.77	0.50
1:B:904:ILE:HD11	1:B:910:ARG:HH11	1.77	0.50
1:B:958:PHE:CD1	1:B:963:GLU:HG2	2.47	0.50
1:C:816:LEU:HD23	1:C:836:VAL:HG22	1.94	0.50
1:C:991:ILE:HG23	1:C:1195:GLY:HA2	1.94	0.50
1:D:1145:TRP:CD1	1:D:1145:TRP:N	2.77	0.50
1:H:957:LEU:HD21	1:H:1002:VAL:HG21	1.94	0.50
1:A:671:HIS:CD2	1:A:729:VAL:HG12	2.47	0.50
1:B:447:CYS:SG	1:B:448:SER:N	2.85	0.50
1:B:479:LYS:HZ3	2:J:1413:SER:HB2	1.77	0.50
1:B:814:GLU:OE1	1:B:832:VAL:HG22	2.12	0.50
1:C:422:PRO:HA	1:C:552:PRO:HD3	1.93	0.50
1:C:624:ARG:NH1	1:C:685:ASP:O	2.26	0.50
1:D:607:PRO:HG2	1:D:654:ASN:HB2	1.93	0.50
1:H:805:ASN:OD1	1:H:806:SER:N	2.45	0.50
1:H:807:SER:O	1:H:810:THR:HG23	2.12	0.50
1:A:713:ARG:HD2	1:A:755:TYR:CE2	2.47	0.49
1:A:1005:ASP:OD1	1:A:1007:LYS:N	2.35	0.49
1:B:817:ARG:H	1:B:817:ARG:HD2	1.77	0.49
1:C:670:VAL:HG21	1:C:683:TRP:CE2	2.47	0.49
1:D:270:ALA:HA	1:D:317[B]:ARG:HB2	1.94	0.49
1:G:911:TYR:HH	1:G:1051:PHE:HE2	1.60	0.49
1:G:1058:SER:OG	1:G:1060:SER:OG	2.28	0.49
1:A:822:LEU:HD22	1:A:882:ARG:NH1	2.27	0.49
1:A:984:TYR:HA	1:A:996:GLU:O	2.12	0.49
1:B:427:VAL:HB	1:B:546:VAL:HG12	1.94	0.49
1:C:902:HIS:CD2	1:C:1108:ALA:HB1	2.47	0.49
1:C:904:ILE:HD11	1:C:910:ARG:HH11	1.77	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:371:LEU:HD12	1:D:372:ASP:H	1.75	0.49
1:D:713:ARG:HD2	1:D:755:TYR:CE2	2.47	0.49
1:F:447:CYS:SG	1:F:448:SER:N	2.85	0.49
1:G:855:CYS:HB2	1:G:882:ARG:HG2	1.94	0.49
1:H:798:MET:SD	1:H:835:CYS:HB3	2.53	0.49
1:H:1013:ARG:NH2	1:H:1138:ASP:OD2	2.46	0.49
1:A:904:ILE:HD11	1:A:910:ARG:HH11	1.77	0.49
1:A:958:PHE:CD1	1:A:963:GLU:HG2	2.47	0.49
1:B:984:TYR:HA	1:B:996:GLU:O	2.12	0.49
1:C:386:PRO:HA	1:C:396:PRO:HD3	1.94	0.49
1:C:817:ARG:HH12	1:C:839:PRO:HA	1.77	0.49
1:D:807:SER:O	1:D:810:THR:HG23	2.12	0.49
1:G:1043:SER:O	1:G:1043:SER:OG	2.29	0.49
1:G:1133:ALA:O	1:G:1137:HIS:ND1	2.26	0.49
1:A:817:ARG:HH12	1:A:839:PRO:HA	1.77	0.49
1:B:346:CYS:HA	1:B:349:PRO:HB3	1.93	0.49
1:B:904:ILE:HD11	1:B:1105:TYR:HE1	1.77	0.49
1:C:369:THR:O	1:C:369:THR:OG1	2.27	0.49
1:C:852:GLU:OE1	1:C:852:GLU:N	2.42	0.49
1:C:958:PHE:CD1	1:C:963:GLU:HG2	2.47	0.49
1:C:964:LEU:HD11	1:C:984:TYR:CE2	2.48	0.49
1:A:316:PRO:HG2	1:A:338:CYS:HB2	1.95	0.49
1:A:386:PRO:HA	1:A:396:PRO:HD3	1.94	0.49
1:A:814:GLU:OE1	1:A:832:VAL:HG22	2.12	0.49
1:B:700:ARG:NH1	1:B:735:PRO:HB3	2.28	0.49
1:B:816:LEU:HD23	1:B:836:VAL:HG22	1.94	0.49
1:D:1172:GLY:HA3	1:D:1197:TYR:CZ	2.48	0.49
1:E:700:ARG:NH1	1:E:735:PRO:HB3	2.28	0.49
2:M:1378:ILE:HG22	2:M:1424:VAL:HA	1.94	0.49
1:A:700:ARG:NH1	1:A:700:ARG:O	2.45	0.49
1:A:964:LEU:HD11	1:A:984:TYR:CE2	2.47	0.49
1:B:402:THR:N	1:B:405:SER:O	2.46	0.49
1:B:571:ASP:O	1:B:574:THR:OG1	2.23	0.49
1:C:920:ILE:HD13	1:C:923:GLN:OE1	2.13	0.49
1:C:984:TYR:HA	1:C:996:GLU:O	2.12	0.49
1:D:386:PRO:HA	1:D:396:PRO:HD3	1.93	0.49
1:F:446:ASP:OD1	1:F:467:ARG:NH1	2.36	0.49
1:G:1013:ARG:NH2	1:G:1138:ASP:OD2	2.46	0.49
1:H:941:ASN:OD1	1:H:953:LYS:NZ	2.43	0.49
1:H:1172:GLY:HA3	1:H:1197:TYR:CZ	2.48	0.49
2:I:1400:ASP:N	2:I:1400:ASP:OD1	2.46	0.49



	as pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:K:1405:LEU:HD11	2:K:1420:TYR:HB3	1.95	0.49
1:A:402:THR:N	1:A:405:SER:O	2.42	0.49
1:A:706:ASP:HB3	1:A:728:PRO:HB3	1.95	0.49
1:C:316:PRO:HG2	1:C:338:CYS:HB2	1.94	0.49
1:C:814:GLU:OE1	1:C:832:VAL:HG22	2.12	0.49
1:D:670:VAL:HG21	1:D:683:TRP:CE2	2.47	0.49
1:D:1058:SER:OG	1:D:1060:SER:OG	2.28	0.49
1:A:871:ARG:NH2	1:A:1138:ASP:O	2.44	0.49
1:A:939:THR:HG22	1:A:955:ILE:HG13	1.94	0.49
1:B:166:VAL:HG12	1:B:175:VAL:HG22	1.95	0.49
1:F:79:THR:O	1:F:190:SER:HA	2.13	0.49
1:F:625:LEU:O	1:F:636:HIS:NE2	2.45	0.49
1:F:656:GLU:OE1	1:F:656:GLU:N	2.31	0.49
1:G:798:MET:SD	1:G:835:CYS:HB3	2.53	0.49
1:A:1145:TRP:CD1	1:A:1145:TRP:N	2.79	0.49
1:D:632:PHE:HB3	1:D:669:TYR:HE2	1.78	0.49
1:F:166:VAL:HG12	1:F:175:VAL:HG22	1.95	0.49
1:F:342:CYS:HB2	1:F:351:ARG:HG3	1.95	0.49
1:F:418:ASP:OD1	1:F:418:ASP:N	2.34	0.49
2:M:1375:LEU:HD11	2:M:1401:ARG:O	2.13	0.49
2:N:1375:LEU:HD11	2:N:1401:ARG:O	2.13	0.49
1:A:902:HIS:CD2	1:A:1108:ALA:HB1	2.47	0.49
1:B:902:HIS:CD2	1:B:1108:ALA:HB1	2.47	0.49
1:B:1056:LYS:NZ	1:B:1063:ASP:OD1	2.25	0.49
1:C:632:PHE:HB3	1:C:669:TYR:HE2	1.78	0.49
1:C:706:ASP:HB3	1:C:728:PRO:HB3	1.95	0.49
1:C:871:ARG:NH2	1:C:1138:ASP:O	2.44	0.49
2:L:1405:LEU:HD11	2:L:1420:TYR:HB3	1.95	0.49
1:B:119:ARG:HG2	1:B:130:THR:OG1	2.13	0.48
1:B:342:CYS:HB2	1:B:351:ARG:HG3	1.95	0.48
1:C:1005:ASP:OD1	1:C:1007:LYS:N	2.35	0.48
1:D:700:ARG:NH1	1:D:700:ARG:O	2.45	0.48
1:E:79:THR:O	1:E:190:SER:HA	2.13	0.48
1:E:402:THR:N	1:E:405:SER:O	2.46	0.48
1:F:270:ALA:HA	1:F:317[A]:ARG:HB2	1.95	0.48
1:F:700:ARG:NH1	1:F:735:PRO:HB3	2.28	0.48
1:G:1172:GLY:HA3	1:G:1197:TYR:CZ	2.48	0.48
1:H:853:GLU:OE1	1:H:881:ASN:ND2	2.47	0.48
2:I:1405:LEU:HD11	2:I:1420:TYR:HB3	1.95	0.48
2:J:1375:LEU:HD11	2:J:1401:ARG:O	2.12	0.48
1:A:270:ALA:HA	1:A:317[B]:ARG:HB2	1.94	0.48



	A 4 a ma 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:79:THR:O	1:B:190:SER:HA	2.13	0.48
1:B:920:ILE:HD13	1:B:923:GLN:OE1	2.13	0.48
1:D:798:MET:SD	1:D:835:CYS:HB3	2.53	0.48
1:D:817:ARG:O	1:D:817:ARG:HG2	2.13	0.48
1:D:853:GLU:OE1	1:D:881:ASN:ND2	2.47	0.48
1:D:944:CYS:H	1:D:951:CYS:HB3	1.78	0.48
1:D:964:LEU:HD11	1:D:984:TYR:CE2	2.49	0.48
1:E:119:ARG:HG2	1:E:130:THR:OG1	2.13	0.48
1:E:342:CYS:HB2	1:E:351:ARG:HG3	1.95	0.48
2:N:1378:ILE:HG22	2:N:1424:VAL:HA	1.94	0.48
1:A:920:ILE:HD13	1:A:923:GLN:OE1	2.13	0.48
1:B:344:ASP:OD1	1:B:352:ALA:N	2.38	0.48
1:C:510:PRO:HA	1:C:518:LEU:O	2.12	0.48
1:D:706:ASP:HB3	1:D:728:PRO:HB3	1.95	0.48
1:D:957:LEU:HD21	1:D:1002:VAL:HG21	1.94	0.48
1:E:447:CYS:SG	1:E:448:SER:N	2.85	0.48
2:M:1414:PRO:O	2:M:1416:LEU:N	2.43	0.48
1:B:874:CYS:O	1:B:889:ARG:NH2	2.47	0.48
1:B:964:LEU:HD11	1:B:984:TYR:CE2	2.48	0.48
1:C:838:PRO:HG2	1:C:841:LEU:HD13	1.96	0.48
1:C:1215:VAL:HG22	1:C:1216:ALA:H	1.79	0.48
1:D:211:ASN:ND2	1:D:217:ASN:HD22	2.12	0.48
1:F:402:THR:N	1:F:405:SER:O	2.46	0.48
1:F:556:GLY:N	1:F:565:PHE:O	2.40	0.48
2:K:1396:GLN:HB2	2:K:1412:GLN:HE22	1.78	0.48
1:A:510:PRO:HA	1:A:518:LEU:O	2.12	0.48
1:A:757:HIS:CE1	1:A:830:HIS:CD2	3.01	0.48
1:A:989:MET:HB3	1:A:1193:LEU:HD11	1.96	0.48
1:B:1004:TRP:HD1	1:B:1010:VAL:HG22	1.78	0.48
1:C:700:ARG:NH1	1:C:700:ARG:O	2.45	0.48
1:C:713:ARG:HD2	1:C:755:TYR:CE2	2.47	0.48
1:C:874:CYS:O	1:C:889:ARG:NH2	2.47	0.48
1:C:1145:TRP:CD1	1:C:1145:TRP:N	2.79	0.48
1:F:517:THR:HG21	1:F:721:THR:HA	1.96	0.48
1:G:817:ARG:NH1	1:G:841:LEU:O	2.45	0.48
1:G:944:CYS:H	1:G:951:CYS:HB3	1.78	0.48
1:A:632:PHE:HB3	1:A:669:TYR:HE2	1.78	0.48
1:D:316:PRO:HG2	1:D:338:CYS:HB2	1.95	0.48
1:D:817:ARG:NH1	1:D:841:LEU:O	2.45	0.48
1:E:166:VAL:HG12	1:E:175:VAL:HG22	1.95	0.48
1:E:625:LEU:O	1:E:636:HIS:NE2	2.45	0.48



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:119:ARG:HG2	1:F:130:THR:OG1	2.13	0.48
1:G:817:ARG:O	1:G:817:ARG:HG2	2.13	0.48
1:G:920:ILE:HD13	1:G:923:GLN:OE1	2.13	0.48
1:H:911:TYR:OH	1:H:1051:PHE:HE2	1.94	0.48
1:H:920:ILE:HD13	1:H:923:GLN:OE1	2.13	0.48
1:B:806:SER:HB2	1:B:810:THR:HG21	1.96	0.48
1:B:989:MET:HB3	1:B:1193:LEU:HD11	1.96	0.48
1:C:745:ALA:HB3	2:I:1387:ASP:OD2	2.12	0.48
1:D:1013:ARG:NH2	1:D:1138:ASP:OD2	2.46	0.48
1:E:220:TYR:CE2	1:E:225:ARG:HB2	2.49	0.48
1:E:517:THR:HG21	1:E:721:THR:HA	1.96	0.48
1:A:1215:VAL:HG22	1:A:1216:ALA:H	1.79	0.48
1:B:99:CYS:HA	1:B:119:ARG:NH1	2.29	0.48
1:C:211:ASN:ND2	1:C:217:ASN:HD22	2.12	0.48
1:D:920:ILE:HD13	1:D:923:GLN:OE1	2.13	0.48
1:E:493:ARG:HH22	1:E:495:GLN:NE2	2.11	0.48
1:F:99:CYS:HA	1:F:119:ARG:NH1	2.29	0.48
1:G:853:GLU:OE1	1:G:881:ASN:ND2	2.47	0.48
1:H:964:LEU:HD11	1:H:984:TYR:CE2	2.49	0.48
2:L:1396:GLN:HB2	2:L:1412:GLN:HE22	1.78	0.48
1:A:874:CYS:O	1:A:889:ARG:NH2	2.47	0.48
1:A:1004:TRP:HD1	1:A:1010:VAL:HG22	1.78	0.48
1:B:346:CYS:HB3	1:B:370:VAL:HG21	1.95	0.48
1:B:1040:ARG:HG2	1:B:1055:TRP:CZ3	2.49	0.48
1:C:270:ALA:HA	1:C:317[B]:ARG:HB2	1.94	0.48
1:C:944:CYS:H	1:C:951:CYS:HB3	1.79	0.48
1:E:346:CYS:HB3	1:E:370:VAL:HG21	1.95	0.48
1:C:989:MET:HB3	1:C:1193:LEU:HD11	1.95	0.48
1:F:344:ASP:OD1	1:F:352:ALA:N	2.38	0.48
1:A:245:PRO:HD3	2:J:1403:ARG:NH1	2.29	0.47
1:B:656:GLU:OE1	1:B:656:GLU:N	2.31	0.47
1:E:178:ARG:HD2	1:E:179:LEU:CD2	2.44	0.47
1:E:427:VAL:HB	1:E:546:VAL:HG12	1.94	0.47
1:F:507:THR:HG21	1:F:511:LEU:HD13	1.96	0.47
1:G:955:ILE:HG21	1:G:966:LEU:HD22	1.96	0.47
1:G:964:LEU:HD11	1:G:984:TYR:CE2	2.49	0.47
1:H:817:ARG:HG2	1:H:817:ARG:O	2.13	0.47
1:H:944:CYS:H	1:H:951:CYS:HB3	1.78	0.47
1:H:1058:SER:OG	1:H:1060:SER:OG	2.28	0.47
1:B:1005:ASP:OD2	1:B:1009:SER:N	2.44	0.47
1:B:1215:VAL:HG22	1:B:1216:ALA:H	1.79	0.47



	A 4 arra 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:991:ILE:HG23	1:D:1195:GLY:HA2	1.97	0.47
1:D:1207:PHE:CZ	1:D:1209:GLU:HG3	2.49	0.47
2:I:1396:GLN:HB2	2:I:1412:GLN:HE22	1.78	0.47
1:A:171:ASP:OD1	1:A:171:ASP:N	2.47	0.47
1:A:687:VAL:HG22	1:A:688:CYS:SG	2.54	0.47
1:A:838:PRO:HG2	1:A:841:LEU:HD13	1.96	0.47
1:B:178:ARG:HD2	1:B:179:LEU:CD2	2.44	0.47
1:C:237:LEU:HD11	1:E:611:SER:HB2	1.97	0.47
1:D:671:HIS:HD2	1:D:729:VAL:HG12	1.79	0.47
1:E:270:ALA:HA	1:E:317[B]:ARG:HB2	1.97	0.47
1:E:468:LYS:NZ	1:E:470:GLY:O	2.25	0.47
1:F:401:ASN:HA	1:F:406:SER:HA	1.96	0.47
1:A:767:VAL:HG12	2:K:1416:LEU:HD13	1.96	0.47
1:B:871:ARG:NH2	1:B:1138:ASP:O	2.44	0.47
1:B:944:CYS:H	1:B:951:CYS:HB3	1.79	0.47
1:D:293:ARG:NH1	1:D:297:CYS:SG	2.88	0.47
1:B:549:ARG:HB2	1:B:549:ARG:CZ	2.44	0.47
1:B:706:ASP:HA	1:B:728:PRO:HB3	1.96	0.47
1:C:266:LEU:HD22	1:C:305:TYR:HD2	1.80	0.47
1:D:266:LEU:HD22	1:D:305:TYR:HD2	1.80	0.47
1:E:83:PHE:CE2	1:E:127:PRO:HB3	2.49	0.47
1:E:270:ALA:HA	1:E:317[A]:ARG:HB2	1.95	0.47
1:F:346:CYS:HB3	1:F:370:VAL:HG21	1.95	0.47
1:F:427:VAL:HB	1:F:546:VAL:HG12	1.94	0.47
1:A:996:GLU:OE1	1:A:1187:LEU:HB2	2.15	0.47
1:A:1040:ARG:HG2	1:A:1055:TRP:CZ3	2.49	0.47
1:B:777:THR:O	1:B:780:LYS:HD2	2.15	0.47
1:C:171:ASP:N	1:C:171:ASP:OD1	2.47	0.47
1:C:245:PRO:HD3	2:M:1403:ARG:NH1	2.29	0.47
1:C:817:ARG:O	1:C:817:ARG:HG2	2.15	0.47
1:D:402:THR:N	1:D:405:SER:O	2.42	0.47
1:D:852:GLU:OE1	1:D:852:GLU:N	2.47	0.47
1:H:1207:PHE:CZ	1:H:1209:GLU:HG3	2.49	0.47
2:N:1342:SER:OG	2:N:1343:TRP:N	2.48	0.47
1:A:237:LEU:HD11	1:B:611:SER:HB2	1.97	0.47
1:A:266:LEU:HD22	1:A:305:TYR:HD2	1.80	0.47
1:A:536:LEU:HD22	1:A:548:VAL:HG22	1.97	0.47
1:A:806:SER:HB2	1:A:810:THR:HG21	1.96	0.47
1:A:944:CYS:H	1:A:951:CYS:HB3	1.79	0.47
1:B:270:ALA:HA	1:B:317[A]:ARG:HB2	1.96	0.47
1:B:507:THR:HG21	1:B:511:LEU:HD13	1.96	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:B:517:THR:HG21	1:B:721:THR:HA	1.96	0.47
1:B:752:CYS:SG	1:B:753:PRO:HD2	2.55	0.47
1:B:960:GLU:HB3	1:B:961:SER:H	1.58	0.47
1:B:1091:PRO:HA	1:B:1094:ALA:HB2	1.97	0.47
1:C:671:HIS:HD2	1:C:729:VAL:HG12	1.79	0.47
1:C:687:VAL:HG22	1:C:688:CYS:SG	2.54	0.47
1:C:996:GLU:OE1	1:C:1187:LEU:HB2	2.15	0.47
1:E:752:CYS:SG	1:E:753:PRO:HD2	2.55	0.47
1:G:1207:PHE:CZ	1:G:1209:GLU:HG3	2.50	0.47
1:A:211:ASN:ND2	1:A:217:ASN:HD22	2.12	0.47
1:B:838:PRO:HG2	1:B:841:LEU:HD13	1.96	0.47
1:B:996:GLU:OE1	1:B:1187:LEU:HB2	2.15	0.47
1:C:806:SER:HB2	1:C:810:THR:HG21	1.96	0.47
1:E:99:CYS:HA	1:E:119:ARG:NH1	2.29	0.47
1:E:507:THR:HG21	1:E:511:LEU:HD13	1.96	0.47
1:F:83:PHE:CE2	1:F:127:PRO:HB3	2.49	0.47
1:A:293:ARG:NH1	1:A:297:CYS:SG	2.88	0.47
1:A:1102:SER:HB3	1:A:1132:TYR:CZ	2.50	0.47
1:A:1199:LYS:HE2	1:A:1199:LYS:HB2	1.75	0.47
1:B:220:TYR:CE2	1:B:225:ARG:HB2	2.49	0.47
1:B:401:ASN:HA	1:B:406:SER:HA	1.96	0.47
1:B:446:ASP:OD1	1:B:467:ARG:NH1	2.36	0.47
1:C:293:ARG:NH1	1:C:297:CYS:SG	2.88	0.47
1:C:1005:ASP:OD2	1:C:1009:SER:N	2.44	0.47
1:C:1040:ARG:HG2	1:C:1055:TRP:CZ3	2.49	0.47
1:D:237:LEU:HD11	1:F:611:SER:HB2	1.97	0.47
1:D:536:LEU:HD22	1:D:548:VAL:HG22	1.97	0.47
1:D:1043:SER:O	1:D:1043:SER:OG	2.29	0.47
1:E:106:HIS:NE2	1:E:202:GLN:OE1	2.40	0.47
1:F:270:ALA:HA	1:F:317[B]:ARG:HB2	1.97	0.47
1:H:991:ILE:HG23	1:H:1195:GLY:HA2	1.97	0.47
1:A:1005:ASP:OD2	1:A:1009:SER:N	2.44	0.47
1:B:270:ALA:HA	1:B:317[B]:ARG:HB2	1.97	0.47
1:B:297:CYS:N	1:B:298:PRO:HD3	2.30	0.47
1:C:1004:TRP:HD1	1:C:1010:VAL:HG22	1.78	0.47
1:E:297:CYS:N	1:E:298:PRO:HD3	2.30	0.47
1:E:571:ASP:O	1:E:574:THR:OG1	2.23	0.47
1:F:220:TYR:CE2	1:F:225:ARG:HB2	2.49	0.47
1:H:1068:LYS:HD3	1:H:1068:LYS:C	2.35	0.47
1:H:1199:LYS:HE2	1:H:1199:LYS:HB2	1.69	0.47
2:M:1342:SER:OG	2:M:1343:TRP:N	2.48	0.47



	A t arra 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:N:1414:PRO:O	2:N:1416:LEU:N	2.43	0.47
1:A:167:GLU:HG3	1:A:169:SER:HB3	1.97	0.46
1:A:414:TRP:HB2	1:C:1041:SER:O	2.15	0.46
1:A:468:LYS:HA	1:A:476:ASN:HD22	1.81	0.46
1:B:607:PRO:HG2	1:B:654:ASN:HB2	1.98	0.46
1:B:852:GLU:OE1	1:B:852:GLU:N	2.42	0.46
1:C:219:PHE:O	1:C:225:ARG:HA	2.15	0.46
1:C:633:SER:HA	1:C:636:HIS:ND1	2.30	0.46
1:F:178:ARG:HD2	1:F:179:LEU:CD2	2.44	0.46
1:F:595:ALA:HB2	1:H:821:THR:OG1	2.15	0.46
1:F:700:ARG:HH11	1:F:735:PRO:HB3	1.80	0.46
1:G:817:ARG:HG2	1:G:842:VAL:HA	1.97	0.46
1:G:991:ILE:HG23	1:G:1195:GLY:HA2	1.97	0.46
2:J:1342:SER:OG	2:J:1343:TRP:N	2.48	0.46
2:K:1400:ASP:N	2:K:1400:ASP:OD1	2.46	0.46
1:D:167:GLU:HG3	1:D:169:SER:HB3	1.97	0.46
1:D:171:ASP:OD1	1:D:171:ASP:N	2.47	0.46
1:D:633:SER:HA	1:D:636:HIS:ND1	2.30	0.46
1:D:687:VAL:HG22	1:D:688:CYS:SG	2.54	0.46
1:F:777:THR:O	1:F:780:LYS:HD2	2.15	0.46
1:H:955:ILE:HG21	1:H:966:LEU:HD22	1.96	0.46
1:B:83:PHE:CE2	1:B:127:PRO:HB3	2.49	0.46
1:B:595:ALA:HB2	1:D:821:THR:OG1	2.15	0.46
1:F:607:PRO:HG2	1:F:654:ASN:HB2	1.98	0.46
1:F:752:CYS:SG	1:F:753:PRO:HD2	2.55	0.46
1:H:817:ARG:NH1	1:H:841:LEU:O	2.45	0.46
2:L:1400:ASP:N	2:L:1400:ASP:OD1	2.46	0.46
1:A:157:LEU:HD12	1:A:167:GLU:HA	1.97	0.46
1:A:800:TYR:HE1	1:A:833:SER:HB3	1.81	0.46
1:A:819:CYS:SG	1:A:856:PRO:HD2	2.55	0.46
1:B:1102:SER:HB3	1:B:1132:TYR:CZ	2.50	0.46
1:C:564:ASN:ND2	1:C:571:ASP:OD2	2.44	0.46
1:D:219:PHE:O	1:D:225:ARG:HA	2.15	0.46
1:D:757:HIS:HE1	1:D:830:HIS:CD2	2.15	0.46
1:A:219:PHE:O	1:A:225:ARG:HA	2.15	0.46
1:C:76:VAL:O	1:C:88:PHE:HA	2.16	0.46
1:C:479:LYS:HZ1	2:K:1413:SER:HB3	1.80	0.46
1:D:270:ALA:HA	1:D:317[A]:ARG:HB2	1.97	0.46
1:E:549:ARG:HB2	1:E:549:ARG:CZ	2.44	0.46
1:E:607:PRO:HG2	1:E:654:ASN:HB2	1.98	0.46
1:A:76:VAL:O	1:A:88:PHE:HA	2.16	0.46



Atom_1	Atom_2	Interatomic	Clash
	Atom-2	distance (Å)	overlap (Å)
1:A:564:ASN:ND2	1:A:571:ASP:OD2	2.44	0.46
1:A:937:ILE:HG12	1:A:957:LEU:HD23	1.98	0.46
1:B:76:VAL:O	1:B:88:PHE:HA	2.16	0.46
1:B:510:PRO:HA	1:B:518:LEU:O	2.16	0.46
1:B:700:ARG:HH11	1:B:735:PRO:HB3	1.80	0.46
1:C:762:ALA:HB1	2:I:1384:GLN:OE1	2.15	0.46
1:E:76:VAL:O	1:E:88:PHE:HA	2.16	0.46
1:E:446:ASP:OD1	1:E:467:ARG:NH1	2.36	0.46
1:E:700:ARG:HH11	1:E:735:PRO:HB3	1.80	0.46
1:E:706:ASP:HA	1:E:728:PRO:HB3	1.97	0.46
1:F:510:PRO:HA	1:F:518:LEU:O	2.16	0.46
1:F:706:ASP:HA	1:F:728:PRO:HB3	1.97	0.46
1:G:1068:LYS:C	1:G:1068:LYS:HD3	2.35	0.46
2:J:1333:CYS:HB3	2:J:1432:CYS:HB2	1.68	0.46
2:L:1348:ARG:HG3	2:L:1348:ARG:HH11	1.81	0.46
2:M:1400:ASP:OD1	2:M:1400:ASP:N	2.49	0.46
1:B:1058:SER:OG	1:B:1060:SER:OG	2.33	0.46
1:B:1207:PHE:CZ	1:B:1209:GLU:HG3	2.51	0.46
1:C:167:GLU:HG3	1:C:169:SER:HB3	1.97	0.46
1:C:270:ALA:HA	1:C:317[A]:ARG:HB2	1.97	0.46
1:C:536:LEU:HD22	1:C:548:VAL:HG22	1.97	0.46
1:C:1058:SER:OG	1:C:1060:SER:OG	2.33	0.46
1:C:1098:SER:OG	1:C:1099:GLN:OE1	2.33	0.46
1:D:1068:LYS:C	1:D:1068:LYS:HD3	2.35	0.46
1:E:401:ASN:HA	1:E:406:SER:HA	1.96	0.46
1:E:777:THR:O	1:E:780:LYS:HD2	2.15	0.46
1:F:549:ARG:CZ	1:F:549:ARG:HB2	2.44	0.46
2:J:1343:TRP:CZ3	2:J:1423:ARG:HD2	2.51	0.46
2:J:1397:VAL:HG21	2:J:1420:TYR:CZ	2.51	0.46
2:N:1343:TRP:CZ3	2:N:1423:ARG:HD2	2.51	0.46
1:A:754:CYS:HB3	1:A:781:LEU:HB2	1.98	0.46
1:A:817:ARG:O	1:A:817:ARG:HG2	2.15	0.46
1:A:1091:PRO:HA	1:A:1094:ALA:HB2	1.97	0.46
1:A:1207:PHE:CZ	1:A:1209:GLU:HG3	2.51	0.46
1:B:556:GLY:N	1:B:565:PHE:O	2.40	0.46
1:B:800:TYR:HE1	1:B:833:SER:HB3	1.81	0.46
1:B:1041:SER:O	1:D:414:TRP:HB2	2.15	0.46
1:C:1102:SER:HB3	1:C:1132:TYR:CZ	2.50	0.46
1:D:955:ILE:HG21	1:D:966:LEU:HD22	1.96	0.46
1:F:76:VAL:O	1:F:88:PHE:HA	2.16	0.46
1:F:297:CYS:N	1:F:298:PRO:HD3	2.30	0.46



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
2:M:1397:VAL:HG21	2:M:1420:TYR:CZ	2.51	0.46
1:A:83:PHE:CE2	1:A:127:PRO:HB3	2.51	0.46
1:A:278:VAL:HB	1:A:305:TYR:HE1	1.81	0.46
1:A:509:LEU:HD22	1:A:518:LEU:HB3	1.98	0.46
1:A:796:ALA:HB1	1:A:797:PRO:HD2	1.98	0.46
1:C:83:PHE:CE2	1:C:127:PRO:HB3	2.51	0.46
1:C:468:LYS:HA	1:C:476:ASN:HD22	1.81	0.46
1:C:1091:PRO:HA	1:C:1094:ALA:HB2	1.97	0.46
1:D:760:VAL:O	2:J:1418:HIS:NE2	2.49	0.46
1:D:1220:CYS:HB2	1:D:1250:ILE:HG13	1.98	0.46
1:E:510:PRO:HA	1:E:518:LEU:O	2.16	0.46
1:E:595:ALA:HB2	1:G:821:THR:OG1	2.15	0.46
1:F:756:ALA:O	1:F:759:THR:OG1	2.25	0.46
1:H:1220:CYS:HB2	1:H:1250:ILE:HG13	1.98	0.46
2:N:1395:GLN:OE1	2:N:1420:TYR:OH	2.33	0.46
2:N:1397:VAL:HG21	2:N:1420:TYR:CZ	2.51	0.46
1:A:671:HIS:HD2	1:A:729:VAL:HG12	1.80	0.46
1:B:582:ALA:HB2	1:D:860:ASN:ND2	2.31	0.46
1:B:819:CYS:SG	1:B:856:PRO:HD2	2.56	0.46
1:B:1230:VAL:HA	1:B:1245:CYS:HB3	1.97	0.46
1:C:178:ARG:CD	1:C:179:LEU:HD23	2.43	0.46
1:D:157:LEU:HD12	1:D:167:GLU:HA	1.97	0.46
1:E:425:CYS:SG	1:E:426:SER:N	2.89	0.46
1:H:817:ARG:HG2	1:H:842:VAL:HA	1.97	0.46
2:I:1348:ARG:HG3	2:I:1348:ARG:HH11	1.81	0.46
2:J:1400:ASP:OD1	2:J:1400:ASP:N	2.49	0.46
2:M:1395:GLN:OE1	2:M:1420:TYR:OH	2.33	0.46
1:A:270:ALA:HA	1:A:317[A]:ARG:HB2	1.97	0.45
1:A:860:ASN:ND2	1:C:582:ALA:HB2	2.31	0.45
1:B:262:CYS:O	1:B:266:LEU:HB2	2.16	0.45
1:B:636:HIS:CD2	1:B:641:PRO:HG3	2.51	0.45
1:C:800:TYR:HE1	1:C:833:SER:HB3	1.81	0.45
1:D:278:VAL:HB	1:D:305:TYR:HE1	1.81	0.45
1:F:768:HIS:HE1	1:F:771:GLY:HA2	1.81	0.45
2:J:1395:GLN:OE1	2:J:1420:TYR:OH	2.33	0.45
1:B:796:ALA:HB1	1:B:797:PRO:HD2	1.98	0.45
1:E:768:HIS:HE1	1:E:771:GLY:HA2	1.81	0.45
1:F:262:CYS:O	1:F:266:LEU:HB2	2.16	0.45
1:G:909:ASP:OD1	1:G:910:ARG:N	2.49	0.45
1:H:1049:LEU:HD12	1:H:1049:LEU:HA	1.83	0.45
1:H:1133:ALA:O	1:H:1137:HIS:ND1	2.26	0.45



	A + a	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:M:1343:TRP:CZ3	2:M:1423:ARG:HD2	2.51	0.45
2:N:1400:ASP:N	2:N:1400:ASP:OD1	2.49	0.45
1:A:582:ALA:HB2	1:C:860:ASN:ND2	2.31	0.45
1:B:539:GLN:O	1:B:544:MET:HA	2.16	0.45
1:C:157:LEU:HD12	1:C:167:GLU:HA	1.97	0.45
1:C:341:PRO:HB3	1:C:360:VAL:HG21	1.98	0.45
1:C:509:LEU:HD22	1:C:518:LEU:HB3	1.98	0.45
1:C:819:CYS:SG	1:C:856:PRO:HD2	2.56	0.45
1:C:1035:ASN:HB2	1:C:1044:VAL:HG21	1.98	0.45
1:D:509:LEU:HD22	1:D:518:LEU:HB3	1.98	0.45
1:D:754:CYS:HB3	1:D:781:LEU:HB2	1.98	0.45
1:F:539:GLN:O	1:F:544:MET:HA	2.16	0.45
1:H:1078:LYS:HG2	1:H:1082:GLN:HE21	1.82	0.45
1:B:817:ARG:HG2	1:B:817:ARG:O	2.15	0.45
1:C:126:ARG:HE	1:C:293:ARG:HH12	1.65	0.45
1:D:1078:LYS:HG2	1:D:1082:GLN:HE21	1.81	0.45
1:E:266:LEU:HD22	1:E:305:TYR:CD2	2.52	0.45
1:F:493:ARG:HH22	1:F:495:GLN:NE2	2.11	0.45
1:F:582:ALA:HB2	1:H:860:ASN:ND2	2.31	0.45
1:F:604:PHE:N	1:F:605:GLU:OE2	2.48	0.45
1:G:1145:TRP:CD1	1:G:1145:TRP:N	2.77	0.45
2:M:1341:SER:OG	2:M:1344:TYR:OH	2.31	0.45
1:A:921:LEU:N	1:A:937:ILE:O	2.50	0.45
1:A:1041:SER:O	1:C:414:TRP:HB2	2.15	0.45
1:B:860:ASN:ND2	1:D:582:ALA:HB2	2.31	0.45
1:C:278:VAL:HB	1:C:305:TYR:HE1	1.81	0.45
1:F:425:CYS:SG	1:F:426:SER:N	2.89	0.45
1:G:817:ARG:HH12	1:G:839:PRO:HA	1.82	0.45
2:N:1341:SER:OG	2:N:1344:TYR:OH	2.31	0.45
1:B:768:HIS:HE1	1:B:771:GLY:HA2	1.81	0.45
1:B:937:ILE:HG12	1:B:957:LEU:HD23	1.98	0.45
1:E:582:ALA:HB2	1:G:860:ASN:ND2	2.31	0.45
1:F:636:HIS:CD2	1:F:641:PRO:HG3	2.51	0.45
1:G:907:ASP:OD1	1:G:1031:ASP:N	2.49	0.45
1:G:1220:CYS:HB2	1:G:1250:ILE:HG13	1.98	0.45
2:K:1348:ARG:HH11	2:K:1348:ARG:HG3	1.81	0.45
1:A:469:CYS:O	2:I:1411:GLN:HA	2.17	0.45
1:A:577:SER:HG	1:C:884:TRP:HD1	1.64	0.45
1:A:633:SER:HA	1:A:636:HIS:ND1	2.30	0.45
1:A:852:GLU:OE1	1:A:852:GLU:N	2.42	0.45
1:A:1230:VAL:HA	1:A:1245:CYS:HB3	1.97	0.45



	• • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:1230:VAL:HA	1:C:1245:CYS:HB3	1.98	0.45
1:D:245:PRO:HD3	2:N:1403:ARG:NH1	2.29	0.45
1:D:455:CYS:HB3	1:D:559:CYS:HB2	1.60	0.45
1:D:479:LYS:HZ1	2:L:1413:SER:HB3	1.81	0.45
1:E:539:GLN:O	1:E:544:MET:HA	2.16	0.45
1:E:636:HIS:CD2	1:E:641:PRO:HG3	2.51	0.45
2:I:1349:PRO:HG3	2:I:1418:HIS:O	2.17	0.45
1:A:126:ARG:HE	1:A:293:ARG:HH12	1.65	0.45
1:A:341:PRO:HB3	1:A:360:VAL:HG21	1.98	0.45
1:A:798:MET:HB3	1:A:837:CYS:HA	1.99	0.45
1:B:1199:LYS:HE2	1:B:1199:LYS:HB2	1.75	0.45
1:C:754:CYS:HB3	1:C:781:LEU:HB2	1.98	0.45
1:C:937:ILE:HG12	1:C:957:LEU:HD23	1.98	0.45
1:C:962:TYR:CE2	1:C:982:PRO:HA	2.51	0.45
1:E:262:CYS:O	1:E:266:LEU:HB2	2.16	0.45
1:E:592:LYS:NZ	1:E:599:ASN:OD1	2.48	0.45
1:H:852:GLU:OE1	1:H:852:GLU:N	2.47	0.45
1:H:1158:TYR:HB2	1:H:1166:TRP:CD1	2.52	0.45
1:B:493:ARG:HH22	1:B:495:GLN:NE2	2.11	0.45
1:B:625:LEU:O	1:B:636:HIS:NE2	2.45	0.45
1:B:962:TYR:CE2	1:B:982:PRO:HA	2.52	0.45
1:B:1035:ASN:HB2	1:B:1044:VAL:HG21	1.98	0.45
1:B:1156:ASP:HA	1:B:1159:ASN:HD22	1.82	0.45
1:D:76:VAL:O	1:D:88:PHE:HA	2.16	0.45
1:D:817:ARG:HG2	1:D:842:VAL:HA	1.97	0.45
1:D:1158:TYR:HB2	1:D:1166:TRP:CD1	2.52	0.45
1:G:1199:LYS:HB2	1:G:1199:LYS:HE2	1.69	0.45
1:A:1098:SER:OG	1:A:1099:GLN:OE1	2.33	0.45
1:B:106:HIS:NE2	1:B:202:GLN:OE1	2.40	0.45
1:B:425:CYS:SG	1:B:426:SER:N	2.89	0.45
1:B:798:MET:HB3	1:B:837:CYS:HA	1.99	0.45
1:C:159:TYR:HB3	1:C:166:VAL:HG22	1.99	0.45
1:C:447:CYS:SG	1:C:448:SER:N	2.90	0.45
1:C:853:GLU:OE1	1:C:881:ASN:ND2	2.50	0.45
1:C:1156:ASP:HA	1:C:1159:ASN:HD22	1.82	0.45
1:D:906:PHE:CZ	1:D:1014:LEU:HD12	2.52	0.45
1:E:371:LEU:HD12	1:E:372:ASP:H	1.82	0.45
1:G:1158:TYR:HB2	1:G:1166:TRP:CD1	2.52	0.45
2:I:1348:ARG:HG3	2:I:1348:ARG:NH1	2.32	0.45
1:A:740:LEU:HD12	1:A:740:LEU:O	2.17	0.44
1:A:853:GLU:OE1	1:A:881:ASN:ND2	2.51	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:962:TYR:CE2	1:A:982:PRO:HA	2.51	0.44
1:A:1058:SER:OG	1:A:1060:SER:OG	2.33	0.44
1:B:455:CYS:HB3	1:B:559:CYS:HB2	1.67	0.44
1:B:761:LEU:HD21	1:B:767:VAL:HG11	1.98	0.44
1:D:468:LYS:HA	1:D:476:ASN:HD22	1.81	0.44
1:D:909:ASP:OD1	1:D:910:ARG:N	2.49	0.44
1:H:1230:VAL:HA	1:H:1245:CYS:HB3	1.99	0.44
2:J:1414:PRO:O	2:J:1416:LEU:N	2.43	0.44
2:L:1349:PRO:HG3	2:L:1418:HIS:O	2.17	0.44
1:C:83:PHE:CZ	1:C:127:PRO:HB3	2.53	0.44
1:G:813:ALA:HB3	1:G:832:VAL:HG23	2.00	0.44
1:G:906:PHE:CZ	1:G:1014:LEU:HD12	2.52	0.44
2:K:1349:PRO:HG3	2:K:1418:HIS:O	2.17	0.44
2:M:1343:TRP:CE3	2:M:1423:ARG:HB3	2.53	0.44
1:A:625:LEU:HA	1:A:632:PHE:HD2	1.83	0.44
1:C:740:LEU:HD12	1:C:740:LEU:O	2.18	0.44
1:C:764:GLY:N	1:C:776:CYS:O	2.36	0.44
1:C:921:LEU:N	1:C:937:ILE:O	2.50	0.44
1:D:83:PHE:CZ	1:D:127:PRO:HB3	2.53	0.44
1:D:469:CYS:O	2:L:1411:GLN:HA	2.17	0.44
1:E:291:LEU:HD23	1:E:291:LEU:HA	1.84	0.44
1:F:295:PRO:CD	1:F:296:THR:N	2.80	0.44
1:H:1035:ASN:HB2	1:H:1044:VAL:HG21	2.00	0.44
2:M:1398:ASP:OD1	2:M:1406:MET:HB2	2.17	0.44
2:N:1398:ASP:OD1	2:N:1406:MET:HB2	2.17	0.44
1:A:1035:ASN:HB2	1:A:1044:VAL:HG21	1.98	0.44
1:B:295:PRO:CD	1:B:296:THR:N	2.80	0.44
1:D:447:CYS:SG	1:D:448:SER:N	2.90	0.44
1:E:263:HIS:O	1:E:267:LEU:HB2	2.18	0.44
1:F:651:ASP:O	1:F:655:CYS:N	2.47	0.44
2:N:1343:TRP:HA	2:N:1343:TRP:CE3	2.53	0.44
1:A:88:PHE:HE2	1:A:203:THR:HG21	1.82	0.44
1:A:763:PRO:O	2:K:1384:GLN:NE2	2.44	0.44
1:B:266:LEU:HD22	1:B:305:TYR:CD2	2.52	0.44
1:C:469:CYS:O	2:K:1411:GLN:HA	2.17	0.44
1:C:1207:PHE:CZ	1:C:1209:GLU:HG3	2.51	0.44
1:D:126:ARG:HE	1:D:293:ARG:HH12	1.65	0.44
1:D:341:PRO:HB3	1:D:360:VAL:HG21	1.98	0.44
1:D:740:LEU:HD12	1:D:740:LEU:O	2.17	0.44
1:G:1078:LYS:HG2	1:G:1082:GLN:HE21	1.81	0.44
2:J:1343:TRP:CE3	2:J:1423:ARG:HB3	2.53	0.44



	all page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:606:ASP:OD2	1:A:608:CYS:HB2	2.18	0.44
1:B:891:CYS:H	1:B:1016:GLN:HE21	1.65	0.44
1:B:921:LEU:N	1:B:937:ILE:O	2.50	0.44
1:C:1083:LYS:HE2	1:C:1083:LYS:HB2	1.80	0.44
1:D:83:PHE:CE2	1:D:127:PRO:HB3	2.51	0.44
1:E:761:LEU:HD21	1:E:767:VAL:HG11	1.98	0.44
1:A:1156:ASP:HA	1:A:1159:ASN:HD22	1.82	0.44
1:B:216:PHE:O	1:B:216:PHE:CD1	2.71	0.44
1:B:1137:HIS:HA	1:B:1141:LEU:O	2.18	0.44
1:D:159:TYR:HB3	1:D:166:VAL:HG22	1.99	0.44
1:D:817:ARG:HH12	1:D:839:PRO:HA	1.82	0.44
1:E:216:PHE:O	1:E:216:PHE:CD1	2.71	0.44
1:F:263:HIS:O	1:F:267:LEU:HB2	2.17	0.44
1:H:813:ALA:HB3	1:H:832:VAL:HG23	2.00	0.44
2:I:1341:SER:HG	2:I:1424:VAL:H	1.66	0.44
2:M:1333:CYS:HB3	2:M:1432:CYS:HB2	1.68	0.44
1:A:447:CYS:SG	1:A:448:SER:N	2.90	0.44
1:A:1137:HIS:HA	1:A:1141:LEU:O	2.18	0.44
1:B:83:PHE:CZ	1:B:127:PRO:HB3	2.53	0.44
1:B:800:TYR:CE1	1:B:833:SER:HB3	2.53	0.44
1:B:853:GLU:OE1	1:B:881:ASN:ND2	2.50	0.44
1:C:796:ALA:HB1	1:C:797:PRO:HD2	1.98	0.44
1:C:891:CYS:H	1:C:1016:GLN:HE21	1.65	0.44
1:D:1102:SER:HB3	1:D:1132:TYR:CZ	2.53	0.44
1:E:604:PHE:N	1:E:605:GLU:OE2	2.48	0.44
1:F:266:LEU:HD22	1:F:305:TYR:CD2	2.52	0.44
1:F:448:SER:HA	1:F:465:GLU:HA	2.00	0.44
1:H:1057:LEU:HD23	1:H:1057:LEU:HA	1.75	0.44
1:H:1102:SER:HB3	1:H:1132:TYR:CZ	2.53	0.44
2:N:1340:TRP:CE3	2:N:1423:ARG:HG3	2.53	0.44
1:B:604:PHE:N	1:B:605:GLU:OE2	2.48	0.44
1:B:1098:SER:OG	1:B:1099:GLN:OE1	2.33	0.44
1:C:625:LEU:HA	1:C:632:PHE:HD2	1.83	0.44
1:D:813:ALA:HB3	1:D:832:VAL:HG23	2.00	0.44
1:E:83:PHE:CZ	1:E:127:PRO:HB3	2.53	0.44
1:F:83:PHE:CZ	1:F:127:PRO:HB3	2.53	0.44
1:F:455:CYS:HB3	1:F:559:CYS:HB2	1.67	0.44
1:F:592:LYS:NZ	1:F:599:ASN:OD1	2.48	0.44
1:H:909:ASP:OD1	1:H:910:ARG:N	2.49	0.44
2:J:1398:ASP:OD2	2:J:1406:MET:HB2	2.17	0.44
1:B:560:GLY:HA2	1:B:591:TRP:CE2	2.53	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:422:PRO:HA	1:C:550:LEU:O	2.18	0.43
1:C:606:ASP:OD2	1:C:608:CYS:HB2	2.18	0.43
1:C:1137:HIS:HA	1:C:1141:LEU:O	2.18	0.43
1:D:763:PRO:N	2:J:1384:GLN:NE2	2.66	0.43
1:E:394:TYR:HB3	1:E:398:THR:OG1	2.18	0.43
1:E:560:GLY:HA2	1:E:591:TRP:CE2	2.53	0.43
1:F:761:LEU:HD21	1:F:767:VAL:HG11	1.98	0.43
1:H:1168:TYR:HA	1:H:1196:CYS:HB3	2.00	0.43
2:J:1340:TRP:CE3	2:J:1423:ARG:HG3	2.53	0.43
2:N:1343:TRP:CE3	2:N:1423:ARG:HB3	2.53	0.43
1:A:83:PHE:CZ	1:A:127:PRO:HB3	2.53	0.43
1:A:656:GLU:H	1:A:656:GLU:CD	2.15	0.43
1:B:394:TYR:HB3	1:B:398:THR:OG1	2.18	0.43
1:C:893:GLY:O	1:C:1013:ARG:HA	2.19	0.43
1:D:88:PHE:HE2	1:D:203:THR:HG21	1.82	0.43
1:D:1057:LEU:HD23	1:D:1057:LEU:HA	1.75	0.43
1:E:295:PRO:CD	1:E:296:THR:N	2.80	0.43
1:E:448:SER:HA	1:E:465:GLU:HA	2.00	0.43
1:E:656:GLU:OE1	1:E:656:GLU:N	2.31	0.43
1:E:756:ALA:O	1:E:759:THR:OG1	2.25	0.43
1:F:216:PHE:CD1	1:F:216:PHE:O	2.71	0.43
1:F:318:ASN:OD1	1:F:318:ASN:N	2.51	0.43
1:F:560:GLY:HA2	1:F:591:TRP:CE2	2.53	0.43
1:H:906:PHE:CZ	1:H:1014:LEU:HD12	2.52	0.43
2:K:1348:ARG:HG3	2:K:1348:ARG:NH1	2.32	0.43
1:A:651:ASP:O	1:A:655:CYS:N	2.48	0.43
1:A:800:TYR:CE1	1:A:833:SER:HB3	2.53	0.43
1:B:201:ASN:HD22	4:B:2006:NAG:C7	2.31	0.43
1:C:200:ALA:O	1:C:202:GLN:HG3	2.18	0.43
1:F:162:THR:OG1	1:H:948:GLY:O	2.17	0.43
1:F:633:SER:HA	1:F:636:HIS:CE1	2.54	0.43
2:J:1343:TRP:CE3	2:J:1343:TRP:HA	2.53	0.43
1:A:891:CYS:H	1:A:1016:GLN:HE21	1.65	0.43
1:B:220:TYR:OH	1:B:225:ARG:HD2	2.18	0.43
1:B:633:SER:HA	1:B:636:HIS:CE1	2.54	0.43
1:B:893:GLY:O	1:B:1013:ARG:HA	2.19	0.43
1:C:1057:LEU:HA	1:C:1057:LEU:HD23	1.77	0.43
1:D:850:ILE:HG22	1:D:851:ALA:O	2.19	0.43
1:E:608:CYS:SG	1:E:649:MET:HG3	2.59	0.43
1:E:617:TYR:CE1	1:E:621:TRP:CD1	3.07	0.43
1:F:220:TYR:OH	1:F:225:ARG:HD2	2.18	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:H:817:ARG:HH12	1:H:839:PRO:HA	1.82	0.43
1:B:318:ASN:N	1:B:318:ASN:OD1	2.51	0.43
1:B:891:CYS:O	1:B:1016:GLN:NE2	2.52	0.43
1:C:77:CYS:SG	1:C:193:LEU:HB2	2.59	0.43
1:C:867:GLY:H	1:C:880:ARG:HH21	1.67	0.43
1:D:77:CYS:SG	1:D:193:LEU:HB2	2.59	0.43
1:D:200:ALA:O	1:D:202:GLN:HG3	2.18	0.43
1:D:422:PRO:HA	1:D:550:LEU:O	2.18	0.43
1:F:371:LEU:HD12	1:F:372:ASP:H	1.82	0.43
1:H:850:ILE:HG22	1:H:851:ALA:O	2.19	0.43
1:B:608:CYS:SG	1:B:649:MET:HG3	2.59	0.43
1:B:852:GLU:OE2	1:B:853:GLU:HG2	2.19	0.43
1:C:798:MET:HB3	1:C:837:CYS:HA	1.99	0.43
1:D:651:ASP:O	1:D:655:CYS:N	2.48	0.43
1:G:1102:SER:HB3	1:G:1132:TYR:CZ	2.53	0.43
2:L:1333:CYS:SG	2:L:1334:VAL:N	2.92	0.43
2:M:1340:TRP:CE3	2:M:1423:ARG:HG3	2.53	0.43
1:A:422:PRO:HA	1:A:550:LEU:O	2.18	0.43
1:A:909:ASP:OD1	1:A:910:ARG:N	2.52	0.43
1:A:1057:LEU:HA	1:A:1057:LEU:HD23	1.77	0.43
1:B:448:SER:HA	1:B:465:GLU:HA	2.00	0.43
1:B:1168:TYR:HA	1:B:1196:CYS:HB3	2.00	0.43
1:E:220:TYR:OH	1:E:225:ARG:HD2	2.19	0.43
1:F:394:TYR:HB3	1:F:398:THR:OG1	2.18	0.43
1:F:447:CYS:HB2	1:F:597:CYS:HB3	1.97	0.43
1:F:617:TYR:CE1	1:F:621:TRP:CD1	3.07	0.43
1:G:1168:TYR:HA	1:G:1196:CYS:HB3	2.00	0.43
1:G:1180:ARG:O	1:G:1182:PRO:HD3	2.19	0.43
1:G:1230:VAL:HA	1:G:1245:CYS:HB3	1.99	0.43
1:G:1243:CYS:HA	1:G:1252:CYS:HB3	2.01	0.43
2:L:1348:ARG:HG3	2:L:1348:ARG:NH1	2.32	0.43
1:A:200:ALA:O	1:A:202:GLN:HG3	2.18	0.43
1:A:946:THR:HA	1:C:137:GLN:HB3	2.01	0.43
1:A:1168:TYR:HA	1:A:1196:CYS:HB3	2.00	0.43
1:B:592:LYS:NZ	1:B:599:ASN:OD1	2.48	0.43
1:B:909:ASP:OD1	1:B:910:ARG:N	2.52	0.43
1:B:1083:LYS:HE2	1:B:1083:LYS:HB2	1.80	0.43
1:C:455:CYS:HB3	1:C:559:CYS:HB2	1.60	0.43
1:C:800:TYR:CE1	1:C:833:SER:HB3	2.53	0.43
1:E:318:ASN:OD1	1:E:318:ASN:N	2.51	0.43
1:E:633:SER:HA	1:E:636:HIS:CE1	2.54	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:K:1333:CYS:SG	2:K:1334:VAL:N	2.92	0.43
1:B:236:LYS:NZ	1:B:238:ASP:OD1	2.36	0.43
1:B:907:ASP:OD1	1:B:1031:ASP:N	2.48	0.43
1:D:625:LEU:HA	1:D:632:PHE:HD2	1.83	0.43
1:D:1035:ASN:HB2	1:D:1044:VAL:HG21	2.00	0.43
2:M:1343:TRP:CE3	2:M:1343:TRP:HA	2.53	0.43
1:A:106:HIS:HB2	1:A:114:PHE:CE1	2.54	0.43
1:A:341:PRO:HB3	1:A:360:VAL:CG2	2.49	0.43
1:A:891:CYS:O	1:A:1016:GLN:NE2	2.52	0.43
1:A:1180:ARG:O	1:A:1182:PRO:HD3	2.19	0.43
1:B:263:HIS:O	1:B:267:LEU:HB2	2.18	0.43
1:C:88:PHE:HE2	1:C:203:THR:HG21	1.82	0.43
1:C:344:ASP:OD1	1:C:351:ARG:N	2.52	0.43
1:C:907:ASP:OD1	1:C:1031:ASP:N	2.49	0.43
1:D:341:PRO:HB3	1:D:360:VAL:CG2	2.49	0.43
1:D:907:ASP:OD1	1:D:1031:ASP:N	2.48	0.43
1:D:1243:CYS:HA	1:D:1252:CYS:HB3	2.01	0.43
2:L:1341:SER:HG	2:L:1424:VAL:H	1.67	0.43
1:A:77:CYS:SG	1:A:193:LEU:HB2	2.58	0.42
1:A:159:TYR:HB3	1:A:166:VAL:HG22	1.99	0.42
1:A:625:LEU:HD23	1:A:632:PHE:CD2	2.54	0.42
1:B:617:TYR:CE2	1:B:621:TRP:CD1	3.07	0.42
1:C:106:HIS:HB2	1:C:114:PHE:CE1	2.54	0.42
1:C:625:LEU:HD23	1:C:632:PHE:CD2	2.54	0.42
1:C:932:HIS:H	1:C:932:HIS:CD2	2.37	0.42
1:C:956:LYS:HB3	1:C:958:PHE:CE1	2.54	0.42
1:C:1168:TYR:HA	1:C:1196:CYS:HB3	2.00	0.42
1:G:1172:GLY:H	1:G:1193:LEU:H	1.67	0.42
1:G:1190:LEU:HD23	1:G:1190:LEU:HA	1.92	0.42
1:H:1154:PHE:CD1	1:H:1157:PHE:HB2	2.55	0.42
1:H:1243:CYS:HA	1:H:1252:CYS:HB3	2.01	0.42
1:B:89:ASP:O	1:B:214:PRO:HB3	2.19	0.42
1:C:852:GLU:OE2	1:C:853:GLU:HG2	2.19	0.42
1:D:606:ASP:OD2	1:D:608:CYS:HB2	2.18	0.42
1:D:1180:ARG:O	1:D:1182:PRO:HD3	2.19	0.42
1:G:850:ILE:HG22	1:G:851:ALA:O	2.19	0.42
1:H:907:ASP:OD1	1:H:1031:ASP:N	2.49	0.42
1:H:987:ARG:HD2	1:H:996:GLU:OE2	2.19	0.42
1:A:751:GLU:OE1	1:A:751:GLU:N	2.52	0.42
1:A:893:GLY:O	1:A:1013:ARG:HA	2.19	0.42
1:A:932:HIS:CD2	1:A:932:HIS:H	2.37	0.42



	At ama 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:211:ASN:ND2	1:B:217:ASN:HD22	2.18	0.42
1:B:660:ASP:OD1	1:B:691:TYR:OH	2.35	0.42
1:D:115:ASN:HB3	1:D:135:LYS:HB3	2.02	0.42
1:D:625:LEU:HD23	1:D:632:PHE:CD2	2.54	0.42
1:D:987:ARG:HD2	1:D:996:GLU:OE2	2.19	0.42
1:D:1160:PRO:O	1:D:1160:PRO:HD2	2.20	0.42
1:D:1168:TYR:HA	1:D:1196:CYS:HB3	2.00	0.42
1:E:500:VAL:HG21	1:E:509:LEU:HD11	2.01	0.42
1:F:605:GLU:H	1:F:605:GLU:CD	2.19	0.42
1:G:1049:LEU:HD12	1:G:1049:LEU:HA	1.83	0.42
2:I:1333:CYS:SG	2:I:1334:VAL:N	2.92	0.42
1:A:344:ASP:OD1	1:A:351:ARG:N	2.52	0.42
1:B:371:LEU:HD12	1:B:372:ASP:H	1.82	0.42
1:B:447:CYS:HB2	1:B:597:CYS:HB3	1.97	0.42
1:C:700:ARG:HH21	1:C:735:PRO:HA	1.84	0.42
1:D:344:ASP:OD1	1:D:351:ARG:N	2.52	0.42
1:D:1230:VAL:HA	1:D:1245:CYS:HB3	1.99	0.42
1:E:536:LEU:HD22	1:E:548:VAL:HG22	2.02	0.42
1:F:201:ASN:HD22	4:F:1305:NAG:C7	2.31	0.42
1:F:500:VAL:HG21	1:F:509:LEU:HD11	2.01	0.42
1:G:987:ARG:HD2	1:G:996:GLU:OE2	2.19	0.42
1:H:1088:LEU:HD22	1:H:1132:TYR:CD2	2.52	0.42
2:M:1403:ARG:HD3	2:M:1406:MET:HE1	2.01	0.42
1:A:956:LYS:HB3	1:A:958:PHE:CE1	2.54	0.42
1:B:651:ASP:O	1:B:655:CYS:N	2.47	0.42
1:B:767:VAL:CG1	2:L:1416:LEU:HD22	2.49	0.42
1:B:911:TYR:OH	1:B:1051:PHE:HE2	2.03	0.42
1:B:932:HIS:H	1:B:932:HIS:CD2	2.37	0.42
1:D:184:LEU:HD22	1:D:307:ARG:HH12	1.84	0.42
1:E:479:LYS:HZ3	2:M:1413:SER:HB2	1.82	0.42
2:N:1403:ARG:HD3	2:N:1406:MET:HE1	2.01	0.42
1:B:697:LYS:O	1:B:698:SER:OG	2.35	0.42
1:C:115:ASN:N	1:C:135:LYS:O	2.53	0.42
1:C:341:PRO:HB3	1:C:360:VAL:CG2	2.49	0.42
1:C:621:TRP:CB	1:C:662:LEU:HD11	2.49	0.42
1:C:909:ASP:OD1	1:C:910:ARG:N	2.52	0.42
1:C:1004:TRP:CE3	1:C:1006:ARG:HA	2.55	0.42
1:D:751:GLU:N	1:D:751:GLU:OE1	2.52	0.42
1:D:1244:ASN:O	1:D:1250:ILE:HA	2.20	0.42
1:E:89:ASP:O	1:E:214:PRO:HB3	2.19	0.42
1:G:1035:ASN:HB2	1:G:1044:VAL:HG21	2.00	0.42



	t i o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:1137:HIS:HA	1:G:1141:LEU:O	2.20	0.42
2:L:1333:CYS:HB3	2:L:1432:CYS:HB2	1.35	0.42
1:A:115:ASN:HB3	1:A:135:LYS:HB3	2.02	0.42
1:A:511:LEU:HD11	1:C:511:LEU:HD11	2.02	0.42
1:B:1004:TRP:CE3	1:B:1006:ARG:HA	2.55	0.42
1:C:960:GLU:HB3	1:C:961:SER:H	1.58	0.42
1:C:1180:ARG:O	1:C:1182:PRO:HD3	2.19	0.42
1:E:201:ASN:HD22	4:E:1305:NAG:C7	2.31	0.42
1:E:263:HIS:CE1	1:E:284:LEU:HD22	2.55	0.42
1:F:89:ASP:O	1:F:214:PRO:HB3	2.19	0.42
1:F:211:ASN:ND2	1:F:217:ASN:HD22	2.18	0.42
1:F:291:LEU:HD23	1:F:291:LEU:HA	1.84	0.42
1:F:536:LEU:HD22	1:F:548:VAL:HG22	2.02	0.42
1:G:1154:PHE:CD1	1:G:1157:PHE:HB2	2.54	0.42
1:B:615:GLU:OE1	1:B:615:GLU:HA	2.20	0.42
1:D:106:HIS:HB2	1:D:114:PHE:CE1	2.54	0.42
1:D:1172:GLY:H	1:D:1193:LEU:H	1.67	0.42
1:F:316:PRO:HG2	1:F:338:CYS:HB2	2.02	0.42
1:H:1137:HIS:HA	1:H:1141:LEU:O	2.20	0.42
1:H:1190:LEU:HD23	1:H:1190:LEU:HA	1.92	0.42
1:H:1244:ASN:O	1:H:1250:ILE:HA	2.20	0.42
2:K:1341:SER:HG	2:K:1424:VAL:H	1.65	0.42
1:A:137:GLN:HB3	1:C:946:THR:HA	2.01	0.42
1:A:424:THR:HA	1:A:548:VAL:O	2.20	0.42
1:B:235:GLN:OE1	1:B:235:GLN:N	2.53	0.42
1:C:891:CYS:O	1:C:1016:GLN:NE2	2.52	0.42
1:D:141:LEU:HD11	1:D:166:VAL:HG11	2.02	0.42
1:D:621:TRP:CB	1:D:662:LEU:HD11	2.49	0.42
1:D:921:LEU:N	1:D:937:ILE:O	2.53	0.42
1:D:1137:HIS:HA	1:D:1141:LEU:O	2.20	0.42
1:E:341:PRO:HG3	1:E:357:ASP:HB3	2.02	0.42
1:F:106:HIS:NE2	1:F:202:GLN:OE1	2.40	0.42
1:F:235:GLN:OE1	1:F:235:GLN:N	2.53	0.42
1:F:278:VAL:O	1:F:305:TYR:OH	2.22	0.42
1:F:532:LEU:HD13	1:F:532:LEU:HA	1.90	0.42
1:H:1180:ARG:O	1:H:1182:PRO:HD3	2.19	0.42
2:I:1378:ILE:C	2:I:1378:ILE:HD12	2.40	0.42
2:L:1340:TRP:CZ3	2:L:1425:LEU:HB2	2.55	0.42
1:A:189:ASP:N	1:A:189:ASP:OD1	2.53	0.42
1:B:867:GLY:H	1:B:880:ARG:HH21	1.67	0.42
1:B:956:LYS:HB3	1:B:958:PHE:CE1	2.54	0.42



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:424:THR:HA	1:C:548:VAL:O	2.20	0.42
1:E:422:PRO:HA	1:E:550:LEU:O	2.20	0.42
1:E:615:GLU:OE1	1:E:615:GLU:HA	2.20	0.42
1:F:608:CYS:SG	1:F:649:MET:HG3	2.59	0.42
1:F:615:GLU:OE1	1:F:615:GLU:HA	2.20	0.42
1:G:883:ARG:CZ	1:G:883:ARG:HB3	2.50	0.42
1:G:1153:LEU:HD12	1:G:1153:LEU:HA	1.93	0.42
1:H:921:LEU:N	1:H:937:ILE:O	2.53	0.42
1:H:1179:CYS:N	1:H:1207:PHE:O	2.52	0.42
2:I:1340:TRP:CZ3	2:I:1425:LEU:HB2	2.55	0.42
2:J:1343:TRP:CZ3	2:J:1423:ARG:HB3	2.55	0.42
2:K:1378:ILE:C	2:K:1378:ILE:HD12	2.40	0.42
2:M:1365:ARG:HE	2:M:1371:VAL:HB	1.85	0.42
2:N:1365:ARG:HE	2:N:1371:VAL:HB	1.85	0.42
1:A:700:ARG:HH21	1:A:735:PRO:HA	1.84	0.41
1:A:852:GLU:OE2	1:A:853:GLU:HG2	2.19	0.41
1:A:1034:ILE:H	1:A:1034:ILE:HG13	1.65	0.41
1:B:167:GLU:HG3	1:B:169:SER:HB3	2.02	0.41
1:B:278:VAL:O	1:B:305:TYR:OH	2.22	0.41
1:C:751:GLU:OE1	1:C:751:GLU:N	2.52	0.41
1:D:700:ARG:HH21	1:D:735:PRO:HA	1.85	0.41
1:D:1083:LYS:HE2	1:D:1083:LYS:HB2	1.87	0.41
1:H:816:LEU:HD22	1:H:817:ARG:N	2.35	0.41
2:J:1403:ARG:HD3	2:J:1406:MET:HE1	2.02	0.41
2:K:1333:CYS:HB3	2:K:1432:CYS:HB2	1.35	0.41
2:K:1414:PRO:O	2:K:1416:LEU:N	2.53	0.41
1:A:455:CYS:HB3	1:A:559:CYS:HB2	1.60	0.41
1:A:756:ALA:O	1:A:759:THR:OG1	2.20	0.41
1:A:1004:TRP:CE3	1:A:1006:ARG:HA	2.55	0.41
1:B:316:PRO:HG2	1:B:338:CYS:HB2	2.02	0.41
1:C:184:LEU:HD22	1:C:307:ARG:HH12	1.84	0.41
1:D:254:ASN:O	1:D:256:THR:N	2.53	0.41
1:D:454:LYS:HZ2	1:D:454:LYS:HG3	1.66	0.41
1:D:753:PRO:HG2	1:D:755:TYR:CZ	2.55	0.41
1:E:539:GLN:OE1	1:E:545:GLN:NE2	2.53	0.41
1:G:921:LEU:N	1:G:937:ILE:O	2.53	0.41
1:H:817:ARG:H	1:H:817:ARG:HD2	1.86	0.41
2:N:1343:TRP:CZ3	2:N:1423:ARG:HB3	2.55	0.41
1:A:184:LEU:HD22	1:A:307:ARG:HH12	1.84	0.41
1:B:1180:ARG:O	1:B:1182:PRO:HD3	2.19	0.41
1:C:141:LEU:HD11	1:C:166:VAL:HG11	2.02	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:148:VAL:O	1:C:154:ARG:HD2	2.21	0.41
1:C:1049:LEU:HD12	1:C:1049:LEU:HA	1.85	0.41
1:D:189:ASP:OD1	1:D:189:ASP:N	2.53	0.41
1:D:816:LEU:HD22	1:D:817:ARG:N	2.36	0.41
1:E:235:GLN:N	1:E:235:GLN:OE1	2.53	0.41
1:F:167:GLU:HG3	1:F:169:SER:HB3	2.02	0.41
1:G:1058:SER:HG	1:G:1060:SER:HG	1.63	0.41
1:A:148:VAL:O	1:A:154:ARG:HD2	2.21	0.41
1:A:254:ASN:O	1:A:256:THR:N	2.53	0.41
1:A:867:GLY:H	1:A:880:ARG:HH21	1.67	0.41
1:A:1109:CYS:HA	1:A:1128:ALA:HB1	2.02	0.41
1:C:526:ILE:HD11	1:C:540:LEU:HD11	2.03	0.41
1:C:802:ASP:OD2	1:C:804:SER:OG	2.26	0.41
1:D:1154:PHE:CD1	1:D:1157:PHE:HB2	2.55	0.41
1:E:77:CYS:SG	1:E:193:LEU:HB2	2.60	0.41
1:F:77:CYS:SG	1:F:193:LEU:HB2	2.60	0.41
1:F:183:PHE:HD1	1:F:193:LEU:CD2	2.33	0.41
1:G:1244:ASN:O	1:G:1250:ILE:HA	2.20	0.41
1:H:814:GLU:OE1	1:H:832:VAL:HG22	2.20	0.41
1:H:883:ARG:CZ	1:H:883:ARG:HB3	2.50	0.41
2:M:1343:TRP:CZ3	2:M:1423:ARG:HB3	2.55	0.41
1:A:400:PHE:CE1	1:A:407:CYS:HB2	2.56	0.41
1:B:183:PHE:HD1	1:B:193:LEU:CD2	2.34	0.41
1:B:263:HIS:CE1	1:B:284:LEU:HD22	2.55	0.41
1:B:594:GLN:HB2	1:B:597:CYS:SG	2.61	0.41
1:C:753:PRO:HG2	1:C:755:TYR:CZ	2.55	0.41
1:D:278:VAL:O	1:D:305:TYR:OH	2.28	0.41
1:D:656:GLU:H	1:D:656:GLU:CD	2.15	0.41
1:D:817:ARG:H	1:D:817:ARG:HD2	1.86	0.41
1:D:925:TYR:OH	1:D:934:THR:O	2.26	0.41
1:E:594:GLN:HB2	1:E:597:CYS:SG	2.61	0.41
1:G:1057:LEU:HA	1:G:1057:LEU:HD23	1.75	0.41
2:L:1378:ILE:C	2:L:1378:ILE:HD12	2.40	0.41
1:A:549:ARG:CZ	1:A:549:ARG:HB2	2.51	0.41
1:B:689:THR:HA	1:B:692:MET:HG2	2.02	0.41
1:B:946:THR:HA	1:D:137:GLN:HB3	2.01	0.41
1:C:115:ASN:HB3	1:C:135:LYS:HB3	2.02	0.41
1:C:1109:CYS:HA	1:C:1128:ALA:HB1	2.02	0.41
1:D:148:VAL:O	1:D:154:ARG:HD2	2.21	0.41
1:D:178:ARG:CD	1:D:179:LEU:HD23	2.43	0.41
1:D:400:PHE:CE1	1:D:407:CYS:HB2	2.56	0.41



	• • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:424:THR:HA	1:D:548:VAL:O	2.20	0.41
1:D:479:LYS:NZ	2:L:1413:SER:HB3	2.35	0.41
1:D:564:ASN:ND2	1:D:571:ASP:OD2	2.44	0.41
1:D:629:ASN:C	1:D:629:ASN:OD1	2.59	0.41
1:E:211:ASN:ND2	1:E:217:ASN:HD22	2.18	0.41
1:G:838:PRO:HG2	1:G:841:LEU:HD13	2.03	0.41
1:G:1160:PRO:O	1:G:1160:PRO:HD2	2.20	0.41
1:H:1208:ASN:O	1:H:1212:MET:N	2.53	0.41
1:B:77:CYS:SG	1:B:193:LEU:HB2	2.60	0.41
1:B:1109:CYS:HA	1:B:1128:ALA:HB1	2.02	0.41
1:C:911:TYR:OH	1:C:1051:PHE:HE2	2.03	0.41
1:E:581:GLU:HG3	1:E:587:PHE:HA	2.03	0.41
1:F:341:PRO:HG3	1:F:357:ASP:HB3	2.02	0.41
1:F:594:GLN:HB2	1:F:597:CYS:SG	2.61	0.41
1:G:1208:ASN:O	1:G:1212:MET:N	2.53	0.41
1:H:1146:ARG:NH1	1:H:1151:CYS:HB3	2.36	0.41
1:H:1160:PRO:O	1:H:1160:PRO:HD2	2.20	0.41
1:H:1172:GLY:H	1:H:1193:LEU:H	1.67	0.41
1:A:334:GLN:HG3	1:A:336:GLN:HG2	2.03	0.41
1:A:353:GLN:HE22	1:C:930:THR:HG23	1.86	0.41
1:A:621:TRP:CB	1:A:662:LEU:HD11	2.49	0.41
1:A:629:ASN:OD1	1:A:629:ASN:C	2.59	0.41
1:A:821:THR:OG1	1:C:595:ALA:HB2	2.21	0.41
1:C:324:LEU:HD23	1:C:324:LEU:HA	1.90	0.41
1:D:539:GLN:O	1:D:544:MET:HA	2.21	0.41
1:D:814:GLU:OE1	1:D:832:VAL:HG22	2.20	0.41
1:E:80:TRP:CE3	1:E:304:GLU:HG2	2.56	0.41
1:E:689:THR:HA	1:E:692:MET:HG2	2.02	0.41
1:F:118:LEU:HD23	1:F:129:VAL:HG11	2.03	0.41
1:G:816:LEU:HD22	1:G:817:ARG:N	2.36	0.41
1:G:852:GLU:OE1	1:G:852:GLU:N	2.47	0.41
1:H:900:ASP:O	1:H:914:GLU:HG3	2.21	0.41
2:J:1365:ARG:HE	2:J:1371:VAL:HB	1.85	0.41
2:K:1340:TRP:CZ3	2:K:1425:LEU:HB2	2.55	0.41
1:A:539:GLN:O	1:A:544:MET:HA	2.21	0.41
1:A:753:PRO:HG2	1:A:755:TYR:CZ	2.55	0.41
1:A:1020:GLY:N	1:A:1029:PHE:O	2.54	0.41
1:B:189:ASP:OD1	1:B:190:SER:N	2.54	0.41
1:B:500:VAL:HG21	1:B:509:LEU:HD11	2.01	0.41
1:B:536:LEU:HD22	1:B:548:VAL:HG22	2.02	0.41
1:B:539:GLN:OE1	1:B:545:GLN:NE2	2.53	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:656:GLU:HG3	2:J:1411:GLN:OE1	2.21	0.41
1:B:802:ASP:OD2	1:B:804:SER:OG	2.26	0.41
1:B:821:THR:OG1	1:D:595:ALA:HB2	2.21	0.41
1:B:828:SER:HB2	1:D:594:GLN:HE21	1.86	0.41
1:C:263:HIS:O	1:C:267:LEU:HB2	2.21	0.41
1:C:327:ARG:HB2	1:C:335:HIS:CD2	2.56	0.41
1:C:400:PHE:CE1	1:C:407:CYS:HB2	2.56	0.41
1:C:454:LYS:HZ2	1:C:454:LYS:HG3	1.67	0.41
1:C:651:ASP:O	1:C:655:CYS:N	2.48	0.41
1:C:690:LYS:O	1:C:693:GLN:NE2	2.54	0.41
1:C:1199:LYS:HE2	1:C:1199:LYS:HB2	1.75	0.41
1:D:549:ARG:CZ	1:D:549:ARG:HB2	2.51	0.41
1:D:670:VAL:HG21	1:D:683:TRP:CD2	2.56	0.41
1:D:1208:ASN:O	1:D:1212:MET:N	2.53	0.41
1:E:260:GLY:O	1:E:264:ARG:N	2.44	0.41
1:E:316:PRO:HG2	1:E:338:CYS:HB2	2.02	0.41
1:E:660:ASP:OD1	1:E:691:TYR:OH	2.35	0.41
1:F:263:HIS:CE1	1:F:284:LEU:HD22	2.55	0.41
1:F:324:LEU:HD23	1:F:324:LEU:HA	1.91	0.41
1:F:454:LYS:HZ2	1:F:454:LYS:HG3	1.69	0.41
1:F:539:GLN:OE1	1:F:545:GLN:NE2	2.53	0.41
2:L:1381:ARG:HG2	2:L:1421:GLU:OE1	2.21	0.41
1:A:278:VAL:O	1:A:305:TYR:OH	2.28	0.41
1:A:595:ALA:HB2	1:C:821:THR:OG1	2.21	0.41
1:A:911:TYR:OH	1:A:1051:PHE:HE2	2.03	0.41
1:B:174:LYS:HE3	1:B:182:THR:HG23	2.03	0.41
1:B:1057:LEU:HD23	1:B:1057:LEU:HA	1.77	0.41
1:B:1068:LYS:HZ2	1:B:1069:ASP:HB3	1.86	0.41
1:C:166:VAL:HG12	1:C:175:VAL:HG22	2.03	0.41
1:C:479:LYS:NZ	2:K:1413:SER:HB3	2.35	0.41
1:C:539:GLN:O	1:C:544:MET:HA	2.21	0.41
1:C:1020:GLY:N	1:C:1029:PHE:O	2.54	0.41
1:D:99:CYS:H	1:D:101:TYR:HE1	1.69	0.41
1:D:690:LYS:O	1:D:693:GLN:NE2	2.54	0.41
1:D:745:ALA:HB3	2:J:1387:ASP:OD2	2.21	0.41
1:D:763:PRO:CD	2:J:1384:GLN:NE2	2.81	0.41
1:D:838:PRO:HG2	1:D:841:LEU:HD13	2.03	0.41
1:D:852:GLU:OE2	1:D:853:GLU:HG2	2.21	0.41
1:E:414:TRP:HD1	1:G:1041:SER:HG	1.65	0.41
1:E:656:GLU:HG3	2:M:1411:GLN:OE1	2.21	0.41
1:F:422:PRO:HA	1:F:550:LEU:O	2.20	0.41



	juo pugem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:689:THR:HA	1:F:692:MET:HG2	2.02	0.41
1:G:874:CYS:O	1:G:889:ARG:NH2	2.54	0.41
1:G:900:ASP:O	1:G:914:GLU:HG3	2.21	0.41
1:A:166:VAL:HG12	1:A:175:VAL:HG22	2.03	0.40
1:B:80:TRP:CE3	1:B:304:GLU:HG2	2.56	0.40
1:C:216:PHE:CD1	1:C:216:PHE:O	2.74	0.40
1:D:216:PHE:O	1:D:216:PHE:CD1	2.74	0.40
1:D:764:GLY:N	1:D:776:CYS:O	2.36	0.40
1:D:1146:ARG:NH1	1:D:1151:CYS:HB3	2.36	0.40
1:E:524:PHE:CD2	1:E:731:GLY:HA2	2.56	0.40
1:F:189:ASP:OD1	1:F:190:SER:N	2.54	0.40
1:F:660:ASP:OD1	1:F:691:TYR:OH	2.35	0.40
2:K:1381:ARG:HG2	2:K:1421:GLU:OE1	2.21	0.40
1:A:289:GLN:O	1:A:292:CYS:HB2	2.22	0.40
1:A:560:GLY:HA2	1:A:591:TRP:CE2	2.57	0.40
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.91	0.40
1:B:581:GLU:HG3	1:B:587:PHE:HA	2.03	0.40
1:C:165:LEU:HG	1:C:167:GLU:OE1	2.21	0.40
1:C:752:CYS:O	1:C:763:PRO:HG3	2.21	0.40
1:D:324:LEU:HD23	1:D:324:LEU:HA	1.90	0.40
1:D:526:ILE:HD11	1:D:540:LEU:HD11	2.03	0.40
1:E:183:PHE:HD1	1:E:193:LEU:CD2	2.34	0.40
1:E:455:CYS:HB3	1:E:559:CYS:HB2	1.67	0.40
1:E:712:CYS:O	1:E:715:LEU:HG	2.22	0.40
1:F:751:GLU:OE1	1:F:751:GLU:N	2.54	0.40
1:G:814:GLU:OE1	1:G:832:VAL:HG22	2.20	0.40
1:H:802:ASP:HA	1:H:833:SER:OG	2.22	0.40
2:M:1381:ARG:CZ	2:M:1386:PRO:HB3	2.52	0.40
1:A:141:LEU:HD11	1:A:166:VAL:HG11	2.02	0.40
1:A:327:ARG:HB2	1:A:335:HIS:CD2	2.56	0.40
1:A:752:CYS:O	1:A:763:PRO:HG3	2.21	0.40
1:A:1068:LYS:HZ2	1:A:1069:ASP:HB3	1.86	0.40
1:B:118:LEU:HD23	1:B:129:VAL:HG11	2.03	0.40
1:B:422:PRO:HA	1:B:550:LEU:O	2.20	0.40
1:B:822:LEU:HD12	1:B:842:VAL:HG11	2.04	0.40
1:C:670:VAL:HG21	1:C:683:TRP:CD2	2.56	0.40
1:D:874:CYS:O	1:D:889:ARG:NH2	2.54	0.40
1:D:900:ASP:O	1:D:914:GLU:HG3	2.21	0.40
1:G:904:ILE:HA	1:G:909:ASP:O	2.22	0.40
2:L:1393:LEU:HB3	2:L:1395:GLN:HG2	2.04	0.40
1:A:88:PHE:CE1	1:A:195:LEU:HD23	2.57	0.40



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:A:958:PHE:CE1	1:A:963:GLU:HG2	2.57	0.40
1:B:341:PRO:HG3	1:B:357:ASP:HB3	2.02	0.40
1:B:524:PHE:CD2	1:B:731:GLY:HA2	2.56	0.40
1:B:751:GLU:N	1:B:751:GLU:OE1	2.54	0.40
1:C:183:PHE:HD1	1:C:193:LEU:CD2	2.34	0.40
1:C:245:PRO:HD3	2:M:1403:ARG:HH22	1.87	0.40
1:C:289:GLN:O	1:C:292:CYS:HB2	2.22	0.40
1:C:560:GLY:HA2	1:C:591:TRP:CE2	2.57	0.40
1:C:710:PRO:HB2	1:C:739:PHE:CD2	2.57	0.40
1:C:822:LEU:HD12	1:C:842:VAL:HG11	2.04	0.40
1:C:958:PHE:CE1	1:C:963:GLU:HG2	2.57	0.40
1:D:165:LEU:HG	1:D:167:GLU:OE1	2.21	0.40
1:D:327:ARG:HB2	1:D:335:HIS:CD2	2.56	0.40
1:D:710:PRO:HB2	1:D:739:PHE:CD2	2.57	0.40
1:D:1171:CYS:HB3	1:D:1192:GLY:HA3	2.03	0.40
1:E:751:GLU:N	1:E:751:GLU:OE1	2.54	0.40
1:F:80:TRP:CE3	1:F:304:GLU:HG2	2.56	0.40
1:F:581:GLU:HG3	1:F:587:PHE:HA	2.03	0.40
1:F:656:GLU:HG3	2:N:1411:GLN:OE1	2.21	0.40
1:H:1040:ARG:HG2	1:H:1055:TRP:CZ3	2.56	0.40
1:A:216:PHE:CD2	1:A:216:PHE:O	2.74	0.40
1:A:245:PRO:HD3	2:J:1403:ARG:HH22	1.86	0.40
1:A:700:ARG:HD2	1:A:701:TYR:O	2.22	0.40
1:B:1154:PHE:HB2	1:H:1152:PRO:CB	2.52	0.40
1:D:166:VAL:HG12	1:D:175:VAL:HG22	2.03	0.40
1:D:183:PHE:HD1	1:D:193:LEU:CD2	2.34	0.40
1:D:245:PRO:HD3	2:N:1403:ARG:HH22	1.87	0.40
1:D:747:VAL:HG23	1:D:748:PRO:O	2.22	0.40
1:D:904:ILE:HA	1:D:909:ASP:O	2.22	0.40
1:D:1040:ARG:HG2	1:D:1055:TRP:CZ3	2.56	0.40
1:D:1049:LEU:HA	1:D:1049:LEU:HD12	1.83	0.40
1:E:167:GLU:HG3	1:E:169:SER:HB3	2.02	0.40
1:F:524:PHE:CD2	1:F:731:GLY:HA2	2.56	0.40
1:G:1146:ARG:NH1	1:G:1151:CYS:HB3	2.36	0.40
1:H:874:CYS:O	1:H:889:ARG:NH2	2.54	0.40
1:H:904:ILE:HA	1:H:909:ASP:O	2.22	0.40
2:N:1381:ARG:CZ	2:N:1386:PRO:HB3	2.51	0.40

There are no symmetry-related clashes.



5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	1164/1227~(95%)	1067~(92%)	97~(8%)	0	100	100
1	В	1164/1227~(95%)	1072 (92%)	92~(8%)	0	100	100
1	С	1164/1227~(95%)	1068 (92%)	96 (8%)	0	100	100
1	D	1164/1227~(95%)	1067 (92%)	97~(8%)	0	100	100
1	Ε	715/1227~(58%)	667~(93%)	48 (7%)	0	100	100
1	F	715/1227~(58%)	668~(93%)	47 (7%)	0	100	100
1	G	449/1227~(37%)	405 (90%)	44 (10%)	0	100	100
1	Н	449/1227~(37%)	404 (90%)	45 (10%)	0	100	100
2	Ι	98/100~(98%)	96~(98%)	2(2%)	0	100	100
2	J	98/100~(98%)	94 (96%)	4 (4%)	0	100	100
2	K	98/100~(98%)	96~(98%)	2 (2%)	0	100	100
2	L	98/100~(98%)	96 (98%)	2 (2%)	0	100	100
2	М	98/100~(98%)	94 (96%)	4 (4%)	0	100	100
2	Ν	98/100~(98%)	94 (96%)	4 (4%)	0	100	100
All	All	7572/10416~(73%)	6988 (92%)	584 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	Perce	entiles
1	А	974/1023~(95%)	915~(94%)	59~(6%)	18	53
1	В	974/1023~(95%)	910~(93%)	64 (7%)	16	49
1	С	974/1023~(95%)	916 (94%)	58 (6%)	19	53
1	D	974/1023~(95%)	921~(95%)	53~(5%)	22	57
1	Ε	598/1023~(58%)	561 (94%)	37~(6%)	18	52
1	F	598/1023~(58%)	561 (94%)	37 (6%)	18	52
1	G	376/1023~(37%)	354 (94%)	22~(6%)	19	54
1	Н	376/1023~(37%)	354 (94%)	22 (6%)	19	54
2	Ι	86/88~(98%)	79~(92%)	7 (8%)	11	40
2	J	86/88~(98%)	81 (94%)	5 (6%)	20	55
2	K	86/88~(98%)	79~(92%)	7 (8%)	11	40
2	L	86/88~(98%)	79~(92%)	7 (8%)	11	40
2	М	86/88~(98%)	81 (94%)	5 (6%)	20	55
2	Ν	86/88~(98%)	80 (93%)	6 (7%)	15	47
All	All	6360/8712 (73%)	5971 (94%)	389 (6%)	22	53

All (389) residues with a non-rotameric side chain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	86	LYS
1	А	89	ASP
1	А	99	CYS
1	А	116	VAL
1	А	126	ARG
1	А	131	ARG
1	A	139	LEU
1	А	145	ASN
1	А	167	GLU
1	А	171	ASP
1	А	179	LEU
1	А	186	ASN
1	А	210	PHE
1	А	216	PHE
1	А	219	PHE
1	А	226	LEU
1	А	255	CYS
1	А	293	ARG
1	А	294	CYS



Mol	Chain	Res	Type
1	А	324	LEU
1	А	345	THR
1	А	361	ASP
1	А	479	LYS
1	А	511	LEU
1	А	571	ASP
1	А	604	PHE
1	А	611	SER
1	А	700	ARG
1	А	711	THR
1	А	741	ASN
1	А	752	CYS
1	А	768	HIS
1	А	794	CYS
1	А	798	MET
1	А	817	ARG
1	А	820	HIS
1	А	855	CYS
1	А	871	ARG
1	А	905	THR
1	А	932	HIS
1	А	940	GLU
1	А	1000	MET
1	А	1003	SER
1	А	1019	LYS
1	А	1021	ARG
1	А	1031	ASP
1	А	1035	ASN
1	А	1036	ASP
1	А	1042	ARG
1	A	1061	CYS
1	А	1083	LYS
1	А	1145	TRP
1	A	1156	ASP
1	A	1158	TYR
1	A	1164	CYS
1	А	1165	GLU
1	A	1179	CYS
1	А	1196	CYS
1	A	1220	CYS
1	В	87	THR
1	В	89	ASP



Mol	Chain	Res	Type
1	В	99	CYS
1	В	116	VAL
1	В	120	ARG
1	В	122	LEU
1	В	125	SER
1	В	145	ASN
1	В	171	ASP
1	В	172	TYR
1	В	186	ASN
1	В	210	PHE
1	В	216	PHE
1	В	219	PHE
1	В	318	ASN
1	В	340	SER
1	В	388	THR
1	В	418	ASP
1	В	426	SER
1	В	442	ASP
1	В	472	THR
1	В	479	LYS
1	В	571	ASP
1	В	583	THR
1	В	603	SER
1	В	604	PHE
1	В	611	SER
1	В	697	LYS
1	В	709	GLN
1	В	711	THR
1	В	719	ASP
1	В	720	VAL
1	В	742	ASP
1	В	768	HIS
1	В	773	VAL
1	В	780	LYS
1	В	781	LEU
1	В	794	CYS
1	В	798	MET
1	В	817	ARG
1	В	820	HIS
1	В	855	CYS
1	В	871	ARG
1	В	905	THR



Mol	Chain	Res	Type
1	В	932	HIS
1	В	940	GLU
1	В	1000	MET
1	В	1003	SER
1	В	1019	LYS
1	В	1021	ARG
1	В	1031	ASP
1	В	1035	ASN
1	В	1036	ASP
1	В	1042	ARG
1	В	1061	CYS
1	В	1083	LYS
1	В	1145	TRP
1	В	1156	ASP
1	В	1158	TYR
1	В	1164	CYS
1	В	1165	GLU
1	В	1179	CYS
1	В	1196	CYS
1	В	1220	CYS
1	С	86	LYS
1	С	89	ASP
1	С	99	CYS
1	С	116	VAL
1	С	126	ARG
1	С	131	ARG
1	С	139	LEU
1	С	145	ASN
1	С	167	GLU
1	С	171	ASP
1	С	179	LEU
1	С	186	ASN
1	С	210	PHE
1	С	219	PHE
1	С	226	LEU
1	С	255	CYS
1	С	293	ARG
1	С	294	CYS
1	С	324	LEU
1	С	345	THR
1	C	361	ASP
1	С	479	LYS



Mol	Chain	Res	Type
1	С	511	LEU
1	С	571	ASP
1	С	604	PHE
1	С	611	SER
1	С	700	ARG
1	С	711	THR
1	С	741	ASN
1	С	752	CYS
1	С	768	HIS
1	С	794	CYS
1	С	798	MET
1	С	817	ARG
1	С	820	HIS
1	С	855	CYS
1	С	871	ARG
1	С	905	THR
1	С	932	HIS
1	С	940	GLU
1	С	1000	MET
1	С	1003	SER
1	С	1019	LYS
1	С	1021	ARG
1	С	1031	ASP
1	С	1035	ASN
1	С	1036	ASP
1	С	1042	ARG
1	С	1061	CYS
1	С	1083	LYS
1	С	1145	TRP
1	С	1156	ASP
1	С	1158	TYR
1	С	1164	CYS
1	С	1165	GLU
1	C	1179	CYS
1	С	1196	CYS
1	С	1220	CYS
1	D	86	LYS
1	D	89	ASP
1	D	99	CYS
1	D	116	VAL
1	D	126	ARG
1	D	131	ARG



Mol	Chain	Res	Type
1	D	139	LEU
1	D	145	ASN
1	D	167	GLU
1	D	171	ASP
1	D	179	LEU
1	D	186	ASN
1	D	210	PHE
1	D	219	PHE
1	D	226	LEU
1	D	255	CYS
1	D	293	ARG
1	D	294	CYS
1	D	324	LEU
1	D	345	THR
1	D	361	ASP
1	D	479	LYS
1	D	511	LEU
1	D	571	ASP
1	D	604	PHE
1	D	611	SER
1	D	700	ARG
1	D	711	THR
1	D	741	ASN
1	D	752	CYS
1	D	768	HIS
1	D	798	MET
1	D	816	LEU
1	D	817	ARG
1	D	820	HIS
1	D	932	HIS
1	D	940	GLU
1	D	976	ARG
1	D	987	ARG
1	D	998	HIS
1	D	1000	MET
1	D	1003	SER
1	D	1019	LYS
1	D	1031	ASP
1	D	1042	ARG
1	D	1061	CYS
1	D	1077	ARG
1	D	1083	LYS


Mol	Chain	Res	Type
1	D	1145	TRP
1	D	1179	CYS
1	D	1210	ASP
1	D	1220	CYS
1	D	1222	ASP
1	Е	87	THR
1	Е	89	ASP
1	Е	99	CYS
1	Е	116	VAL
1	Е	120	ARG
1	Е	122	LEU
1	Е	125	SER
1	Е	145	ASN
1	Е	171	ASP
1	Е	172	TYR
1	Е	186	ASN
1	Е	210	PHE
1	Е	216	PHE
1	Е	219	PHE
1	Е	318	ASN
1	Е	340	SER
1	Е	388	THR
1	Е	418	ASP
1	Е	426	SER
1	Е	442	ASP
1	Е	472	THR
1	Е	479	LYS
1	Е	571	ASP
1	Е	583	THR
1	Е	603	SER
1	Е	604	PHE
1	Е	611	SER
1	Е	697	LYS
1	Е	709	GLN
1	Е	711	THR
1	Е	719	ASP
1	Е	720	VAL
1	Е	742	ASP
1	Е	768	HIS
1	Е	773	VAL
1	Е	780	LYS
1	Е	781	LEU



Mol	Chain	Res	Type
1	F	87	THR
1	F	89	ASP
1	F	99	CYS
1	F	116	VAL
1	F	120	ARG
1	F	122	LEU
1	F	125	SER
1	F	145	ASN
1	F	171	ASP
1	F	172	TYR
1	F	186	ASN
1	F	210	PHE
1	F	216	PHE
1	F	219	PHE
1	F	318	ASN
1	F	340	SER
1	F	388	THR
1	F	418	ASP
1	F	426	SER
1	F	442	ASP
1	F	472	THR
1	F	479	LYS
1	F	571	ASP
1	F	583	THR
1	F	603	SER
1	F	604	PHE
1	F	611	SER
1	F	697	LYS
1	F	709	GLN
1	F	711	THR
1	F	719	ASP
1	F	720	VAL
1	F	742	ASP
1	F	768	HIS
1	F	773	VAL
1	F	780	LYS
1	F	781	LEU
1	G	798	MET
1	G	816	LEU
1	G	817	ARG
1	G	820	HIS
1	G	932	HIS



Mol	Chain	Res	Type
1	G	940	GLU
1	G	976	ARG
1	G	987	ARG
1	G	998	HIS
1	G	1000	MET
1	G	1003	SER
1	G	1019	LYS
1	G	1031	ASP
1	G	1042	ARG
1	G	1061	CYS
1	G	1077	ARG
1	G	1083	LYS
1	G	1145	TRP
1	G	1179	CYS
1	G	1210	ASP
1	G	1220	CYS
1	G	1222	ASP
1	Н	798	MET
1	Н	816	LEU
1	Н	817	ARG
1	Н	820	HIS
1	Н	932	HIS
1	Н	940	GLU
1	Н	976	ARG
1	Н	987	ARG
1	Н	998	HIS
1	Н	1000	MET
1	Н	1003	SER
1	Н	1019	LYS
1	Н	1031	ASP
1	Н	1042	ARG
1	Н	1061	CYS
1	Н	1077	ARG
1	H	1083	LYS
1	Н	1145	TRP
1	H	1179	CYS
1	H	1210	ASP
1	Н	1220	CYS
1	H	1222	ASP
2	Ι	1363	ASN
2	Ι	1375	LEU
2	Ι	1399	CYS



Mol	Chain	Res	Type
2	Ι	1401	ARG
2	Ι	1406	MET
2	Ι	1421	GLU
2	Ι	1422	LEU
2	J	1336	GLU
2	J	1343	TRP
2	J	1388	MET
2	J	1406	MET
2	J	1422	LEU
2	K	1363	ASN
2	К	1375	LEU
2	K	1399	CYS
2	К	1401	ARG
2	K	1406	MET
2	К	1421	GLU
2	К	1422	LEU
2	L	1363	ASN
2	L	1375	LEU
2	L	1399	CYS
2	L	1401	ARG
2	L	1406	MET
2	L	1421	GLU
2	L	1422	LEU
2	М	1336	GLU
2	М	1343	TRP
2	М	1375	LEU
2	М	1406	MET
2	М	1422	LEU
2	N	1336	GLU
2	Ν	1343	TRP
2	N	1375	LEU
2	Ν	1388	MET
2	N	1406	MET
2	N	1422	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	168	GLN
1	А	217	ASN
1	А	332	ASN
1	А	476	ASN



Mol	Chain	Res	Type
1	А	545	GLN
1	А	569	GLN
1	А	654	ASN
1	А	694	ASN
1	А	757	HIS
1	А	881	ASN
1	А	998	HIS
1	В	217	ASN
1	В	476	ASN
1	В	495	GLN
1	В	545	GLN
1	В	569	GLN
1	В	594	GLN
1	В	616	ASN
1	В	654	ASN
1	В	881	ASN
1	С	168	GLN
1	С	217	ASN
1	С	332	ASN
1	С	476	ASN
1	С	545	GLN
1	С	569	GLN
1	С	654	ASN
1	С	694	ASN
1	С	757	HIS
1	С	881	ASN
1	С	998	HIS
1	D	168	GLN
1	D	217	ASN
1	D	332	ASN
1	D	476	ASN
1	D	545	GLN
1	D	569	GLN
1	D	594	GLN
1	D	654	ASN
1	D	694	ASN
1	D	757	HIS
1	D	881	ASN
1	D	929	ASN
1	Е	217	ASN
1	Е	476	ASN
1	Е	495	GLN



Mol	Chain	Res	Type
1	Е	545	GLN
1	Е	569	GLN
1	Е	594	GLN
1	Е	616	ASN
1	Е	654	ASN
1	F	217	ASN
1	F	476	ASN
1	F	495	GLN
1	F	545	GLN
1	F	569	GLN
1	F	594	GLN
1	F	616	ASN
1	F	654	ASN
1	G	881	ASN
1	G	929	ASN
1	Н	881	ASN
1	Н	929	ASN
2	Ι	1418	HIS
2	J	1363	ASN
2	К	1418	HIS
2	L	1418	HIS
2	М	1363	ASN
2	Ν	1363	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)

Of 51 ligands modelled in this entry, 24 are monoatomic - leaving 27 for Mogul analysis.



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	Dec	Tink	Bo	ond leng	$_{\rm sths}$	B	ond ang	les
	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	D	2007	1	14,14,15	0.35	0	17,19,21	0.59	0
4	NAG	С	2007	1	14,14,15	0.35	0	17,19,21	0.59	0
4	NAG	А	2006	1	14,14,15	0.29	0	17,19,21	0.47	0
4	NAG	В	2005	1	14,14,15	0.20	0	17,19,21	0.50	0
4	NAG	F	1304	1	14,14,15	0.20	0	17,19,21	0.50	0
4	NAG	С	2004	1	14,14,15	0.23	0	17,19,21	0.48	0
4	NAG	С	2005	1	14,14,15	0.28	0	17,19,21	0.52	0
4	NAG	D	2005	1	14,14,15	0.30	0	17,19,21	0.52	0
4	NAG	А	2008	1	14,14,15	0.30	0	17,19,21	0.40	0
4	NAG	В	2004	1	14,14,15	0.22	0	17,19,21	0.53	0
4	NAG	F	1305	1	14,14,15	0.33	0	17,19,21	0.57	0
4	NAG	А	2007	1	14,14,15	0.35	0	17,19,21	0.59	0
4	NAG	Е	1303	1	14,14,15	0.23	0	17,19,21	0.52	0
4	NAG	В	2008	1	14,14,15	0.30	0	17,19,21	0.41	0
4	NAG	В	2007	1	14,14,15	0.37	0	17,19,21	0.59	0
4	NAG	С	2006	1	14,14,15	0.29	0	17,19,21	0.47	0
4	NAG	D	2006	1	14,14,15	0.30	0	17,19,21	0.47	0
4	NAG	D	2004	1	14,14,15	0.23	0	17,19,21	0.48	0
4	NAG	Е	1304	1	14,14,15	0.20	0	17,19,21	0.49	0
4	NAG	Е	1305	1	14,14,15	0.34	0	17,19,21	0.57	0
4	NAG	F	1306	1	14,14,15	0.37	0	17,19,21	0.59	0
4	NAG	F	1303	1	14,14,15	0.22	0	17,19,21	0.52	0
4	NAG	Е	1306	1	14,14,15	0.38	0	17,19,21	0.59	0
4	NAG	А	2004	1	14,14,15	0.23	0	17,19,21	0.47	0
4	NAG	А	2005	1	14,14,15	0.29	0	17,19,21	0.52	0
4	NAG	В	2006	1	14,14,15	0.33	0	17,19,21	0.58	0
4	NAG	С	2008	1	14,14,15	0.30	0	17,19,21	0.41	0

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.

4 NAG D 2007 1 - 1/6/23/26 0/1/1	Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
	4	NAG	D	2007	1	-	1/6/23/26	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	С	2007	1	-	1/6/23/26	0/1/1/1
4	NAG	А	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	В	2005	1	-	2/6/23/26	0/1/1/1
4	NAG	F	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	С	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	С	2005	1	-	1/6/23/26	0/1/1/1
4	NAG	D	2005	1	-	1/6/23/26	0/1/1/1
4	NAG	A	2008	1	-	0/6/23/26	0/1/1/1
4	NAG	В	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	F	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	А	2007	1	-	1/6/23/26	0/1/1/1
4	NAG	E	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	В	2008	1	-	0/6/23/26	0/1/1/1
4	NAG	В	2007	1	-	3/6/23/26	0/1/1/1
4	NAG	С	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	D	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	D	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	Е	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	Е	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	F	1306	1	-	3/6/23/26	0/1/1/1
4	NAG	F	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	Е	1306	1	-	3/6/23/26	0/1/1/1
4	NAG	А	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	А	2005	1	-	1/6/23/26	0/1/1/1
4	NAG	В	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	С	2008	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	В	2006	NAG	C4-C5-C6-O6
4	Ε	1305	NAG	C4-C5-C6-O6
4	F	1305	NAG	C4-C5-C6-O6
4	В	2006	NAG	O5-C5-C6-O6



Mol	Chain	Res	Type	Atoms
4	F	1305	NAG	O5-C5-C6-O6
4	А	2006	NAG	C4-C5-C6-O6
4	С	2006	NAG	C4-C5-C6-O6
4	D	2006	NAG	C4-C5-C6-O6
4	Е	1305	NAG	O5-C5-C6-O6
4	А	2006	NAG	O5-C5-C6-O6
4	С	2006	NAG	O5-C5-C6-O6
4	D	2006	NAG	O5-C5-C6-O6
4	А	2004	NAG	C8-C7-N2-C2
4	А	2004	NAG	O7-C7-N2-C2
4	В	2004	NAG	C8-C7-N2-C2
4	В	2004	NAG	O7-C7-N2-C2
4	С	2004	NAG	C8-C7-N2-C2
4	С	2004	NAG	O7-C7-N2-C2
4	D	2004	NAG	C8-C7-N2-C2
4	D	2004	NAG	O7-C7-N2-C2
4	Е	1303	NAG	C8-C7-N2-C2
4	Е	1303	NAG	O7-C7-N2-C2
4	F	1303	NAG	C8-C7-N2-C2
4	F	1303	NAG	O7-C7-N2-C2
4	Ε	1306	NAG	C4-C5-C6-O6
4	В	2007	NAG	C4-C5-C6-O6
4	F	1306	NAG	C4-C5-C6-O6
4	А	2005	NAG	C3-C2-N2-C7
4	А	2007	NAG	C3-C2-N2-C7
4	С	2005	NAG	C3-C2-N2-C7
4	С	2007	NAG	C3-C2-N2-C7
4	D	2005	NAG	C3-C2-N2-C7
4	D	2007	NAG	C3-C2-N2-C7
4	В	2007	NAG	O5-C5-C6-O6
4	E	1306	NAG	O5-C5-C6-O6
4	F	1306	NAG	O5-C5-C6-O6
4	В	2005	NAG	C3-C2-N2-C7
4	В	2007	NAG	C3-C2-N2-C7
4	Е	1304	NAG	C3-C2-N2-C7
4	Е	1306	NAG	C3-C2-N2-C7
4	F	1304	NAG	C3-C2-N2-C7
4	F	1306	NAG	C3-C2-N2-C7
4	В	2005	NAG	C1-C2-N2-C7
4	E	1304	NAG	C1-C2-N2-C7
4	F	1304	NAG	C1-C2-N2-C7

Continued from previous page...

There are no ring outliers.



Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1305	NAG	1	0
4	Е	1305	NAG	1	0
4	В	2006	NAG	1	0

3 monomers are involved in 3 short contacts:

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-16808. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map



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



6.2 Central slices (i)

6.2.1 Primary map



X Index: 350



Y Index: 350



Z Index: 350

6.2.2 Raw map



X Index: 350

Y Index: 350



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: 328



Y Index: 353



Z Index: 343

6.3.2 Raw map



X Index: 0

Y Index: 0



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



6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.056. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

6.6 Mask visualisation (i)

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



7 Map analysis (i)

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

7.1 Map-value distribution (i)



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



7.2 Volume estimate (i)



The volume at the recommended contour level is 988 $\rm nm^3;$ this corresponds to an approximate mass of 892 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 0.333 \AA^{-1}



8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.333 $\mathrm{\AA^{-1}}$



8.2 Resolution estimates (i)

$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	Estimation criterion (FSC cut-off)			
Resolution estimate (A)	0.143	0.5	Half-bit	
Reported by author	3.00	-	-	
Author-provided FSC curve	-	-	-	
Unmasked-calculated*	6.71	9.90	7.41	

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.71 differs from the reported value 3.0 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-16808 and PDB model 80ES. 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 0.056 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 (0.056).



9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.056) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.7730	0.2290	
A	0.9100	0.3310	1 0
В	0.9320	0.3650	1.0
С	0.8640	0.2840	
D	0.8870	0.3150	
Е	0.5260	0.0330	
F	0.6140	0.0840	
G	0.6390	0.0310	
Н	0.6860	0.0570	
Ι	0.7350	0.3610	
J	0.7620	0.3840	0.0
K	0.4570	0.1090	 <0.0
L	0.5740	0.2130	
М	0.0930	0.0060	
N	0.0880	-0.0230	

