

# Full wwPDB X-ray Structure Validation Report (i)

#### Aug 15, 2023 – 06:04 PM EDT

PDB ID	:	1TWF
Title	:	RNA polymerase II complexed with UTP at 2.3 A resolution
Authors	:	Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.
Deposited on	:	2004-06-30
Resolution	:	2.30  Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.35
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.30 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.



Motric	Whole archive	Similar resolution
IVIEUTIC	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
R <sub>free</sub>	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575(2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality o	of chain	
1	А	1733	47%	31%	• 18%
2	В	1224	51%	36%	• 11%
3	С	318	44%	37%	• 16%
4	Е	215	66%		33% •
5	F	155	33% 21%	•	46%
6	Н	146	45%	40%	7% 9%
7	Ι	122	68%		29% •



Mol	Chain	Length		Quality of	chain			
8	J	70	44%		40%		9%	7%
9	K	120	54%			38%		• 5%
10	L	70	31%	26%	9%	34%	_	



#### $1 \mathrm{TWF}$

# 2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 28318 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called DNA-directed RNA polymerase II largest subunit.

Mol	Chain	Residues		A	toms		ZeroOcc	AltConf	Trace	
1	А	1419	Total 11154	C 7023	N 1952	0 2118	S 61	0	0	0

• Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
2	В	1094	Total 8711	C 5525	N 1519	0 1614	S 53	0	0	0

• Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
3	С	266	Total 2095	C 1317	N 348	0 417	S 13	0	0	0

• Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
4	Е	215	Total 1760	C 1116	N 310	0 322	S 12	0	0	0

• Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
5	F	84	Total 679	С 434	N 115	0 127	${ m S} { m 3}$	0	0	0

• Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
6	Н	133	Total 1068	C 673	N 180	O 211	$\frac{S}{4}$	0	0	0

• Molecule 7 is a protein called DNA-directed RNA polymerase II 14.2 kDa polypeptide.

Mol	Chain	Residues		A	toms		ZeroOcc	AltConf	Trace	
7	Ι	122	Total 997	C 613	N 182	O 191	S 11	0	0	0

• Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

Mol	Chain	Residues		Ato	$\mathbf{ms}$			ZeroOcc	AltConf	Trace
8	J	65	Total 532	C 339	N 93	0 94	S 6	0	0	0

• Molecule 9 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
9	K	114	Total 919	C 590	N 156	0 171	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0	0

• Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues		Atc	$\mathbf{ms}$			ZeroOcc	AltConf	Trace
10	L	46	Total 364	C 224	N 72	O 64	${S \atop 4}$	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	А	2	Total Zn 2 2	0	0
11	В	1	Total Zn 1 1	0	0
11	С	1	Total Zn 1 1	0	0
11	Ι	2	Total Zn 2 2	0	0
11	J	1	Total Zn 1 1	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	L	1	Total Zn 1 1	0	0

• Molecule 12 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	А	2	Total Mn 2 2	0	0

• Molecule 13 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula:  $C_9H_{15}N_2O_{15}P_3$ ).



Mol	Chain	Residues		At	oms	5		ZeroOcc	AltConf
12	В	1	Total	С	Ν	Ο	Р	0	0
10	D	1	29	9	2	15	3	0	0



# 3 Residue-property plots (i)

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



• Molecule 1: DNA-directed RNA polymerase II largest subunit



N1048 I1049	111050	V 1050 H1059	MIDER	V1064	G1065 V1066	L1067	A1068	11072	G1073	E1074	A1076	T1077	Q1078 M1079	T1080	L1081	THR	PHE	HIS PHE	ALA	GLY	ALA	SER	K1092	S1096	G1097	V1098 P1099	R1100	L1101 V1100	E1103	11104	N1106	M1111		P1114	S1115 11116	T1117	V1118 V1110	L1120	H1124	D11.07	17770
Q1128 E1129	Q1130	K1132	L1133 T1134	FOTT	E1139 H1140		K1144 C114E	V1146		S1150 E11E1	11152 11152		D1155	T1161	V1162	11163 P1164	E1165	D1166 E1167		Q1171	H1173		L1176	ASP	GLU	GLU AI.A	GLU	GLN	PHE	ASP	q1188	S1189 D1100	V1191	L1192	1105	E1196	L1197 D1198	R1199	A1200 A1201	M1202	•
K1205	T1208	Q1211	V1212	R1215	11216 K1217	<b>Q1218</b>	T1219 E1220	F1220 K1221	N1222	D1223	11227		I1238 R1239		V1243	PRO	LYS	SER LEII	ASP	ALA	THR	GLU	A1254	H1258	M1259	K1262	I1263	E1264 M126E	T1266	M1267 1 1268	E1269	N1270 11271		V1276	E1277 N1278	11279 11279	E1280 B1281		M1285 K1286	Y1287	
S1293 P1294	T1295	E1297	V1305	L1306	E1307 T1308	D1309	G1310 W1211	V1312 N1312		E1315	T1318	V1319	P1320 61321	11322	D1323	r1324 T1325	-	Y1328 T1329		11333	E1337	V1338	L1339	G1340 11341	E1342	R1345		L1348	E1351	V1352	V1355	N136A	Y1365	R1366	1 1370	L1371	V1372	V1374	M1375 T1376	T1377	
<mark>S1383</mark>	R1386	R1391	S1392 N1393		A1396 L1397	M1398	R1399	51401 S1401	F1402	E1403	L1409	F1410	<u>41414</u>		E1417	L1418 D1419	D1420	C1421	V1424	S1425 E1476	E1420 N1427	V1428	, <mark>10</mark>	G1431 01432	M1433	A1434 P1435	I1436	G1437 T1/20		F1441	D1446	E1447 E1448	51449	L1450	VAL	TYR	MET	GLU	GLN	ILE THR	VUT
GLU	GLU	GLY	GLN	GLY	GLY VAL	THR	PRO	I IK SER	ASN	GLU	GLY	LEU	VAL	ALA	ASP	ASP	VAL	LYS	GLU	LEU	PHE	SER	PRO	VAL	ASP	SER GLY	SER	ASN	ALA	MET	GLY	GLY	THR	ALA	TYR	GLY	ALA	TYR	GLU	ALA THR	1111 T
SER PRO	PHE	ALA	TYR	GLU	ALA PRO	THR	SER	GLY	PHE	GLY	SER	SER	PRO GLY	PHE	SER	THR	SER	PRO THR	TYR	SER	THR	SER	PRO	ALA TYR	SER	PRO THR	SER	PRO GED	TYR	SER	THR	SER	SER	TYR	SER	THR	SER	SER	SER	PRO THR	TILL
SER PRO	SER	SER	PR.O THR	SER	PRO SER	TYR	SER	THR	SER	PR0 ced	TYR	SER	PRO THR	SER	PRO	TYR	SER	PR.O THR	SER	PR0 GFD	TYR	SER	PRO	THR	PRO	SER TYR	SER	PRO TUD	SER	PRO SED	TYR	SER	THR	SER	PR0 SED	TYR	SER	THR	PRO	SER TVR	1111
SER PRO	THR	PRO	SER	SER	PR0 THR	SER	PR0 cen	TYR	SER	PR0 TUD	SER	PRO	ALA TYR	SER	PRO	SER	PRO	SER	SER	PR0 TUB	SER	PRO	SER	TYR	PRO	THR	PRO	SER	SER	PRO TUD	SER	PR0 SED	TYR	SER	PR0 TUD	SER	PRO	TYR	PRO	THR	1170
PRO SER	TYR	PRO	THR	PRO	GLY TYR	SER	PRO	SER	PRO	ALA TVB	SER	PRO	LYS	ASP	GLU	TAS	HIS	ASN	ASN	GLU	SER	ARG																			
• ]	Mo	ole	cu	le	2:	Ι	ON	N/	<b>\</b> -0	di	re	ct	ed	F	٢N	JA	ŀŀ	00	ly	me	era	as	e	II	1	40	k	D	a j	ро	ly	pe	ept	tic	le						
Cł	nai	n	B:	-								5	1%														3(	5%						·		119	6				
MET SER	ASP	ALA	ASN SFR	GLU	LYS TYR	TYR	ASP	ASP	PRO	TYR	F18	E19	D20 E21		125	E28	D29	<u>335</u>		F38	K41		Q46	053	F54	T58	L59	060 De1	162 162	I63	<b>S67</b>	T68 160	170 170	LEU	GLU	LEU	ALA	HIS	THK	GLU	11110
ASP ASN	ILE	ARG	LYS TVR	E89	190 S91		K94 TOF	96X	<b>V97</b>	T98 V00	eeu	V102	N103	V108	T109	L112	Y113	P114 0115		R118	N121	L122	T123	Y124 S125	S126	G127 1.128	F129	V130 D121		Y137	ALA	ILE	VAL	PRO	GLY	GLU	LEU	TYR	GLU LEU	ILE	WITH
GLU GLU	SER	ASP	ASP SFR	GLU	SER GLY	K164	V165 E166	r167 1167	G168	R169	P171	1172	M173 1.174	R175	0 1 7		L1 <mark>81</mark>	1.192	K193	E194	P196	F197		6200 6201	Y202	F203 T204	1205	N206		L212	q215	E216 B217	S218	A219	TOOD	7771	V225 F226	K227	A230	P231	
1234 S235	H236 11236	A238 A238	E239	S242	A243 L244		R249	r 250 I 251		0255 17756	K257	L258	Y259 G260	R261	E262	A266	R267	T268 1269	K270	1200	Y275	1276		1824	1284	1285 F286	R287	A288 1.700	G290	1291 1707	P293	D294	E296	1297	L298 5700	H300	1311	E312	M313 L314	K315 P316	1010
C317	D320	13 <mark>24</mark>	R307	E328	T329 A330	L331	D332 E222	1000	R336	R337	T339	A340	1343	K344	K345	E346 K347	R348	Y351		1355 1356	0357 0357	K358	E359	F360 L361		T365 0366	L367	E071	<b>S372</b>	R373	r of	N383 P384	L385	L386	L387	G402	RAOR		L420	L424 T425	0711







• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide



• Molecule 4: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide









• Molecule 9: DNA-directed RNA polymerase II 13.6 kDa polypeptide



• Molecule 10: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	123.00Å 223.00Å 374.00Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
$\mathbf{Posolution} \left( \overset{\circ}{\mathbf{A}} \right)$	40.00 - 2.30	Depositor
Resolution (A)	39.69 - 2.19	EDS
% Data completeness	(Not available) $(40.00-2.30)$	Depositor
(in resolution range)	90.5(39.69-2.19)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.95 (at 2.20 \text{\AA})$	Xtriage
Refinement program	CNS	Depositor
B B.	0.247 , $0.294$	Depositor
II, II, <i>free</i>	0.292 , $0.290$	DCC
$R_{free}$ test set	5166 reflections $(2.00\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	47.4	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33 , $46.7$	EDS
L-test for $twinning^2$	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	28318	wwPDB-VP
Average B, all atoms $(Å^2)$	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.09% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: MN, UTP, ZN

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

Mal	Chain	Bo	nd lengths	Bo	ond angles
WIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.43	1/11352~(0.0%)	0.66	2/15352~(0.0%)
2	В	0.41	0/8882	0.64	1/11976~(0.0%)
3	С	0.41	0/2133	0.60	0/2891
4	Е	0.41	0/1796	0.63	1/2416~(0.0%)
5	F	0.44	0/691	0.63	0/933
6	Н	0.30	0/1086	0.58	0/1470
7	Ι	0.40	0/1016	0.60	0/1365
8	J	0.41	0/541	0.65	0/727
9	K	0.39	0/937	0.56	0/1265
10	L	0.37	0/366	0.55	0/485
All	All	0.41	1/28800~(0.0%)	0.64	$4/38880 \ (0.0\%)$

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	764	CYS	CB-SG	-7.44	1.69	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	472	LEU	CA-CB-CG	-7.72	97.54	115.30
2	В	829	CYS	N-CA-C	-6.17	94.35	111.00
4	Е	200	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	А	779	PHE	N-CA-C	-5.00	97.50	111.00

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	11154	0	11224	555	0
2	В	8711	0	8738	427	0
3	С	2095	0	2051	139	0
4	Е	1760	0	1788	53	0
5	F	679	0	701	34	0
6	Н	1068	0	1040	57	0
7	Ι	997	0	953	40	0
8	J	532	0	542	53	0
9	Κ	919	0	929	62	0
10	L	364	0	389	33	0
11	А	2	0	0	0	0
11	В	1	0	0	0	0
11	С	1	0	0	0	0
11	Ι	2	0	0	0	0
11	J	1	0	0	0	0
11	L	1	0	0	0	0
12	A	2	0	0	0	0
13	В	29	0	11	1	0
All	All	28318	0	28366	1291	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 23.

All (1291) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom-2	Interatomic	$\mathbf{Clash}$
Atom-1		distance (Å)	overlap (Å)
1:A:855:THR:HG21	1:A:857:ARG:HE	1.09	1.14
6:H:130:ARG:HA	6:H:133:ASN:HD22	1.11	1.11
1:A:1364:ASN:ND2	1:A:1366:ARG:HH11	1.53	1.05
1:A:351:THR:HG22	1:A:352:VAL:H	1.20	1.05
1:A:1364:ASN:HD21	1:A:1366:ARG:NH1	1.58	0.99
1:A:901:LEU:H	1:A:926:GLN:NE2	1.60	0.98
2:B:680:THR:HG22	2:B:681:TRP:H	1.28	0.98
1:A:725:ALA:HA	1:A:728:LYS:HE3	1.48	0.95
9:K:65:HIS:HD2	9:K:67:PHE:H	1.01	0.94



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.32	0.93
2:B:118:ARG:NH1	2:B:204:ILE:HD11	1.83	0.93
1:A:1162:VAL:HG11	7:I:41:PRO:HG3	1.51	0.92
3:C:137:LYS:H	3:C:137:LYS:HD2	1.35	0.91
8:J:48:ARG:HH11	8:J:48:ARG:HG2	1.34	0.91
1:A:337:ARG:HG2	1:A:341:MET:HE2	1.51	0.91
1:A:901:LEU:H	1:A:926:GLN:HE21	1.19	0.90
1:A:187:LYS:HB2	1:A:194:ALA:HB1	1.53	0.90
1:A:1376:THR:HG22	4:E:212:ARG:HH22	1.37	0.89
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.55	0.89
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.03	0.88
1:A:446:ARG:HD3	1:A:480:ALA:HB2	1.52	0.88
5:F:81:THR:CG2	5:F:136:ARG:HH11	1.87	0.88
2:B:63:ILE:HB	2:B:95:ILE:HD11	1.55	0.87
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.09	0.87
3:C:242:GLN:HE21	3:C:246:ARG:HH21	1.23	0.87
1:A:1116:LEU:HD12	1:A:1329:THR:HB	1.57	0.86
1:A:55:ASP:H	1:A:56:PRO:HD2	1.40	0.86
1:A:313:GLN:HE21	1:A:322:VAL:HG12	1.40	0.86
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.57	0.86
1:A:351:THR:HG22	1:A:352:VAL:N	1.90	0.86
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.57	0.86
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.56	0.85
1:A:1376:THR:HG22	4:E:212:ARG:NH2	1.91	0.85
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.58	0.85
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	0.86	0.85
1:A:246:VAL:HG12	1:A:328:ARG:HH12	1.39	0.85
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.57	0.85
5:F:90:ARG:HD3	5:F:155:LEU:HD12	1.58	0.85
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.58	0.85
1:A:317:LYS:HD2	1:A:321:PRO:HG2	1.57	0.85
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.76	0.85
1:A:1208:THR:HB	1:A:1211:GLN:HG3	1.59	0.85
3:C:167:HIS:HD2	3:C:169:LYS:H	1.21	0.85
9:K:65:HIS:CD2	9:K:67:PHE:H	1.93	0.84
3:C:73:GLN:HE21	3:C:75:MET:H	1.25	0.84
6:H:101:ALA:HB1	6:H:103:LYS:HG3	1.58	0.84
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.58	0.84
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.58	0.84
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.60	0.83
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.43	0.83



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.59	0.83
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.08	0.83
2:B:526:GLU:HG2	2:B:538:ASN:ND2	1.93	0.83
3:C:56:THR:HG23	3:C:58:LEU:H	1.42	0.83
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.60	0.83
2:B:864:LYS:HB3	2:B:871:THR:HA	1.58	0.83
4:E:124:VAL:HG13	4:E:132:ILE:HB	1.59	0.83
5:F:81:THR:HG22	5:F:136:ARG:NH1	1.93	0.82
3:C:258:ILE:HD11	9:K:42:LEU:HD21	1.61	0.82
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.44	0.82
2:B:25:ILE:HD12	2:B:653:VAL:HG23	1.62	0.82
3:C:54:ASN:OD1	3:C:56:THR:HG22	1.80	0.82
1:A:356:ASP:HB3	1:A:359:LEU:HD12	1.62	0.81
1:A:869:GLY:O	4:E:204:THR:HG21	1.80	0.81
1:A:1398:MET:HG3	1:A:1426:GLU:HG2	1.62	0.81
7:I:98:VAL:HG21	7:I:113:ASP:HB2	1.63	0.81
1:A:666:ILE:HD12	2:B:1030:LEU:HD22	1.64	0.80
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.63	0.80
1:A:982:THR:O	1:A:985:ASP:HB2	1.82	0.80
1:A:855:THR:CG2	1:A:857:ARG:HE	1.91	0.80
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.64	0.79
2:B:871:THR:HG22	2:B:872:GLU:H	1.44	0.79
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.29	0.79
2:B:800:GLN:HB3	8:J:52:THR:CG2	2.13	0.79
1:A:1266:THR:HG23	1:A:1270:ASN:HD22	1.48	0.79
3:C:258:ILE:HD13	9:K:35:PHE:HE2	1.48	0.78
1:A:741:ASN:HD22	1:A:744:LYS:H	1.31	0.78
5:F:81:THR:HG22	5:F:136:ARG:HH11	1.49	0.78
1:A:1446:ASP:HB2	5:F:133:VAL:HG23	1.63	0.78
2:B:882:THR:HG21	2:B:935:ARG:HG2	1.67	0.77
1:A:1398:MET:HG2	1:A:1425:SER:HB2	1.65	0.77
2:B:193:LYS:HE2	8:J:65:PRO:HG3	1.66	0.77
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.30	0.77
2:B:1006:ILE:HD11	8:J:43:ARG:HB2	1.67	0.77
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.49	0.77
3:C:73:GLN:NE2	3:C:75:MET:HB2	2.00	0.77
6:H:26:ILE:HD12	6:H:42:ILE:HD12	1.65	0.76
1:A:472:LEU:HD13	2:B:835:GLN:NE2	1.98	0.76
1:A:672:ASP:H	1:A:736:ASN:ND2	1.84	0.76
1:A:709:THR:HB	1:A:712:GLU:HG3	1.66	0.76
2:B:801:LYS:O	8:J:52:THR:HG23	1.86	0.76



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:399:HIS:O	1:A:401:GLY:N	2.18	0.76
1:A:855:THR:HG21	1:A:857:ARG:NE	1.94	0.76
1:A:108:MET:H	1:A:171:GLN:NE2	1.83	0.75
1:A:840:ARG:HH11	1:A:1386:ARG:HB3	1.51	0.75
2:B:515:HIS:HD2	2:B:517:THR:H	1.33	0.75
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.52	0.74
2:B:901:PRO:HD3	10:L:58:LYS:HB3	1.69	0.74
2:B:918:ILE:HD12	2:B:935:ARG:HD2	1.68	0.74
3:C:124:LEU:O	3:C:127:ARG:HG2	1.87	0.74
1:A:55:ASP:N	1:A:56:PRO:HD2	2.02	0.74
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.69	0.74
2:B:809:MET:HG2	2:B:814:PHE:HB3	1.70	0.74
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.69	0.74
2:B:680:THR:HG22	2:B:681:TRP:N	2.02	0.74
1:A:179:LEU:HG	1:A:308:ILE:HG21	1.67	0.74
5:F:81:THR:CG2	5:F:136:ARG:NH1	2.50	0.74
1:A:946:VAL:HG22	4:E:201:LYS:HD2	1.69	0.74
1:A:1215:ARG:HA	1:A:1218:GLN:HE21	1.53	0.74
1:A:450:LEU:HD12	1:A:450:LEU:H	1.50	0.73
1:A:666:ILE:HD11	2:B:1030:LEU:HB2	1.69	0.73
2:B:324:ILE:HG12	2:B:329:THR:HG22	1.70	0.73
10:L:38:LEU:HG	10:L:39:SER:H	1.53	0.73
2:B:953:LEU:HD21	2:B:955:THR:HG23	1.68	0.73
2:B:914:LYS:HB3	2:B:937:ALA:O	1.87	0.73
3:C:51:VAL:HG22	3:C:155:LEU:HD22	1.71	0.73
1:A:907:THR:HG22	1:A:908:LEU:H	1.53	0.73
1:A:79:GLY:HA3	1:A:245:PRO:HG3	1.71	0.73
3:C:42:PRO:HB3	3:C:161:LYS:HE3	1.69	0.72
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.24	0.72
1:A:1151:GLU:HG2	7:I:45:ARG:HD2	1.71	0.72
2:B:46:GLN:HE22	2:B:496:ARG:HB3	1.54	0.72
1:A:567:LYS:HB3	6:H:96:VAL:N	2.05	0.72
3:C:57:VAL:HG11	8:J:60:PHE:HB3	1.72	0.72
1:A:571:LEU:HD22	6:H:46:LEU:HD11	1.71	0.72
9:K:43:GLY:O	9:K:47:ARG:HB2	1.89	0.72
1:A:1342:GLU:OE2	4:E:212:ARG:NH1	2.23	0.72
2:B:294:ASP:H	7:I:12:ASN:ND2	1.87	0.72
3:C:214:ASN:HB2	3:C:217:ASP:OD2	1.90	0.71
2:B:281:PRO:HG2	2:B:284:ILE:HD12	1.71	0.71
2:B:822:ASN:HD22	8:J:52:THR:HG21	1.54	0.71
1:A:103:CYS:SG	1:A:207:ILE:HD12	2.31	0.71



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:208:LEU:HD21	1:A:212:LYS:HE3	1.72	0.71
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.73	0.71
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.04	0.71
1:A:875:ALA:HB2	1:A:1366:ARG:CD	2.19	0.71
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.73	0.71
2:B:1222:ARG:H	2:B:1222:ARG:HD2	1.55	0.71
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.72	0.71
5:F:72:LYS:N	5:F:142:SER:HA	2.06	0.71
1:A:55:ASP:H	1:A:56:PRO:CD	2.04	0.71
1:A:567:LYS:HB3	6:H:96:VAL:H	1.55	0.71
1:A:1192:LEU:HD11	1:A:1239:ARG:HB2	1.73	0.70
1:A:1438:THR:HG22	2:B:1144:ALA:H	1.56	0.70
2:B:644:GLU:HB2	2:B:654:ARG:HH22	1.55	0.70
1:A:587:HIS:HA	1:A:607:ILE:O	1.91	0.70
2:B:806:THR:HG22	2:B:809:MET:H	1.57	0.70
1:A:567:LYS:HE2	6:H:95:TYR:CZ	2.27	0.70
1:A:246:VAL:HG12	1:A:328:ARG:NH1	2.06	0.70
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.72	0.70
2:B:705:MET:CE	2:B:745:PRO:HB3	2.21	0.70
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.72	0.70
1:A:754:SER:H	1:A:757:ASN:HD22	1.38	0.70
1:A:1364:ASN:ND2	1:A:1366:ARG:H	1.89	0.70
1:A:340:LEU:HD13	1:A:1399:ARG:HG2	1.74	0.70
1:A:574:GLY:O	1:A:577:ILE:HG13	1.92	0.70
2:B:864:LYS:HG2	2:B:871:THR:HG23	1.73	0.70
1:A:1059:HIS:HE1	5:F:155:LEU:HD22	1.56	0.70
1:A:1276:VAL:HB	1:A:1279:ILE:HD13	1.72	0.70
2:B:824:ILE:HD11	8:J:48:ARG:NH1	2.07	0.70
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.27	0.69
2:B:324:ILE:HD13	2:B:330:ALA:HA	1.73	0.69
1:A:134:ARG:HD2	1:A:221:SER:O	1.91	0.69
6:H:81:PRO:HB2	6:H:82:PRO:HD3	1.75	0.69
2:B:824:ILE:HD11	8:J:48:ARG:HH12	1.57	0.69
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.73	0.69
1:A:264:PHE:HD1	1:A:315:LEU:HB3	1.58	0.69
3:C:20:PHE:HE1	3:C:22:LEU:HG	1.58	0.69
2:B:755:ILE:HG22	2:B:755:ILE:O	1.91	0.69
2:B:957:ASN:ND2	2:B:958:GLN:H	1.91	0.69
3:C:56:THR:HG21	3:C:63:ILE:HD11	1.73	0.68
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.76	0.68
1:A:683:ILE:HD11	1:A:764:CYS:HB2	1.74	0.68



	<b>A</b>   <b>O</b>	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:381:THR:HG22	5:F:104:ASN:OD1	1.93	0.68
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.75	0.68
2:B:955:THR:HG22	10:L:55:ILE:HA	1.73	0.68
2:B:955:THR:HG22	10:L:54:ARG:O	1.94	0.68
1:A:533:LYS:NZ	1:A:660:ASN:HD21	1.92	0.68
2:B:67:SER:O	2:B:91:SER:HA	1.93	0.68
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.75	0.68
1:A:351:THR:CG2	1:A:352:VAL:H	2.01	0.68
1:A:914:GLU:HG3	1:A:979:SER:O	1.94	0.68
2:B:69:LEU:HD21	2:B:425:THR:HG23	1.73	0.68
1:A:567:LYS:HE2	6:H:95:TYR:CE1	2.29	0.68
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.29	0.68
1:A:53:LEU:HD23	1:A:54:ASN:H	1.58	0.67
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.76	0.67
1:A:598:LEU:HG	6:H:115:TYR:HE2	1.60	0.67
1:A:1277:GLU:O	1:A:1278:ASN:HB2	1.92	0.67
1:A:786:HIS:HE1	2:B:742:GLU:OE2	1.76	0.67
1:A:853:ASP:OD1	1:A:855:THR:HB	1.95	0.67
1:A:82:GLY:HA3	1:A:241:VAL:HB	1.76	0.67
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.77	0.67
2:B:879:ARG:HB3	2:B:883:LEU:HD23	1.77	0.67
3:C:73:GLN:HE21	3:C:75:MET:N	1.92	0.67
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.76	0.67
2:B:268:THR:HG21	2:B:270:LYS:HE3	1.76	0.67
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.77	0.67
1:A:901:LEU:HD22	1:A:919:ILE:CG2	2.25	0.67
1:A:907:THR:HG22	1:A:908:LEU:N	2.09	0.67
6:H:40:LEU:HD13	6:H:123:MET:HB2	1.76	0.66
1:A:1066:VAL:HG12	2:B:1140:ALA:HB2	1.77	0.66
2:B:950:ASP:HB2	2:B:969:ARG:HB2	1.77	0.66
5:F:109:VAL:HG11	5:F:123:LYS:HG2	1.77	0.66
6:H:79:TRP:CZ3	6:H:81:PRO:HG3	2.30	0.66
2:B:324:ILE:HD11	2:B:333:PHE:HB2	1.76	0.66
3:C:35:ARG:NH1	9:K:41:THR:N	2.43	0.66
1:A:203:SER:OG	1:A:206:GLU:HG3	1.95	0.66
2:B:876:LYS:HE3	2:B:893:LEU:O	1.96	0.66
3:C:166:GLU:HG2	10:L:70:ARG:NH1	2.09	0.66
1:A:472:LEU:O	1:A:475:THR:HB	1.96	0.66
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.77	0.66
6:H:103:LYS:HB3	6:H:105:GLU:OE2	1.96	0.66
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.76	0.66



A 4 1	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
6:H:130:ARG:HA	6:H:133:ASN:ND2	1.97	0.66
1:A:31:SER:HB2	1:A:83:HIS:HB2	1.78	0.65
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.77	0.65
1:A:1124:HIS:HB3	1:A:1130:GLN:HG3	1.77	0.65
1:A:1145:SER:HB2	1:A:1205:LYS:NZ	2.10	0.65
2:B:175:ARG:HH11	2:B:175:ARG:HB3	1.61	0.65
1:A:694:THR:O	1:A:698:GLN:HG3	1.96	0.65
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.12	0.65
2:B:841:MET:HE2	2:B:1010:LEU:HD11	1.79	0.65
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.93	0.65
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.78	0.65
2:B:1174:LYS:HD2	2:B:1179:GLN:HB2	1.77	0.65
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.77	0.65
1:A:130:ASP:HB3	1:A:133:LYS:HB2	1.78	0.65
1:A:834:THR:HG21	1:A:1077:THR:HA	1.79	0.65
2:B:864:LYS:CG	2:B:871:THR:HG23	2.27	0.65
3:C:57:VAL:HG11	8:J:60:PHE:CB	2.26	0.65
1:A:567:LYS:CB	1:A:568:PRO:CD	2.75	0.65
2:B:89:GLU:HB2	2:B:137:TYR:HB2	1.79	0.65
1:A:867:ILE:HD11	1:A:999:VAL:HG11	1.79	0.65
1:A:1279:ILE:HD11	1:A:1312:ASN:HB3	1.77	0.65
1:A:998:LEU:HD12	1:A:1001:ARG:NH1	2.10	0.64
1:A:1068:ALA:O	1:A:1072:ILE:HG13	1.97	0.64
5:F:87:LYS:HA	5:F:155:LEU:HD13	1.78	0.64
1:A:1263:ILE:O	1:A:1267:MET:HG3	1.96	0.64
2:B:276:ILE:HG23	2:B:337:ARG:HB2	1.80	0.64
8:J:36:LEU:HD11	8:J:51:LEU:HB2	1.80	0.64
1:A:347:PHE:H	2:B:1107:ALA:HA	1.63	0.64
1:A:673:GLY:N	1:A:674:PRO:HD2	2.12	0.64
5:F:81:THR:HG21	5:F:136:ARG:HH11	1.59	0.64
2:B:872:GLU:HB3	2:B:914:LYS:HD3	1.78	0.64
1:A:534:LEU:HD11	1:A:577:ILE:HD11	1.78	0.64
1:A:1449:SER:HB3	5:F:149:GLU:OE2	1.97	0.64
3:C:196:ASP:HB3	3:C:199:LYS:HB2	1.78	0.64
1:A:903:ASN:ND2	1:A:905:ASP:H	1.95	0.64
2:B:125:SER:HA	2:B:171:PRO:HA	1.80	0.64
2:B:25:ILE:HD13	2:B:658:ILE:HD11	1.80	0.63
2:B:577:ALA:HB1	2:B:589:VAL:HG22	1.80	0.63
1:A:1258:HIS:O	1:A:1262:LYS:HG3	1.98	0.63
2:B:205:ILE:HD11	2:B:461:LEU:HD23	1.80	0.63
3:C:248:ILE:HD13	9:K:101:LEU:HD13	1.80	0.63



A 4 1		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:754:SER:N	1:A:757:ASN:HD22	1.95	0.63
1:A:789:LYS:HE3	7:I:67:THR:OG1	1.98	0.63
1:A:986:ILE:HG21	1:A:1028:THR:HA	1.81	0.63
2:B:464:GLY:O	2:B:477:ALA:HB3	1.98	0.63
6:H:4:THR:HA	6:H:60:ALA:HA	1.79	0.63
1:A:864:ILE:HD13	1:A:1374:VAL:HG22	1.80	0.63
1:A:1151:GLU:CG	7:I:45:ARG:HD2	2.28	0.63
2:B:550:ASP:OD1	2:B:552:MET:HG3	1.98	0.63
2:B:195:CYS:SG	2:B:783:THR:HG23	2.38	0.63
2:B:839:MET:CE	2:B:1010:LEU:HG	2.28	0.63
1:A:443:LEU:HB3	1:A:490:HIS:HB2	1.80	0.63
1:A:567:LYS:HD3	6:H:96:VAL:H	1.64	0.63
1:A:672:ASP:H	1:A:736:ASN:HD21	1.47	0.63
3:C:22:LEU:HD12	3:C:230:MET:CE	2.29	0.63
2:B:130:VAL:HG12	2:B:131:ASP:H	1.63	0.63
4:E:43:LYS:O	4:E:47:CYS:HB2	1.98	0.63
4:E:64:PRO:HG2	4:E:75:MET:O	1.98	0.63
3:C:242:GLN:NE2	3:C:246:ARG:HH21	1.94	0.62
10:L:27:LEU:HD13	10:L:37:LYS:HE2	1.81	0.62
1:A:728:LYS:HA	1:A:731:ARG:HD2	1.80	0.62
2:B:58:THR:O	2:B:62:ILE:HG13	1.98	0.62
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.34	0.62
2:B:839:MET:HE1	2:B:1010:LEU:HG	1.82	0.62
1:A:873:MET:HE2	1:A:957:PRO:HG3	1.80	0.62
7:I:59:VAL:HG12	7:I:60:GLN:H	1.65	0.62
1:A:329:LEU:O	1:A:333:GLU:HG2	2.00	0.62
1:A:31:SER:CB	1:A:83:HIS:HB2	2.30	0.62
1:A:873:MET:CE	1:A:957:PRO:HG3	2.30	0.62
1:A:525:GLN:HB2	2:B:835:GLN:OE1	2.00	0.62
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.35	0.62
1:A:665:GLY:C	2:B:1026:LEU:HD13	2.20	0.62
3:C:92:CYS:SG	3:C:94:LYS:HB2	2.40	0.62
5:F:79:ARG:HH22	5:F:150:GLU:CD	2.03	0.62
1:A:901:LEU:N	1:A:926:GLN:NE2	2.43	0.62
1:A:1318:THR:HG21	4:E:11:ARG:HH12	1.65	0.62
1:A:1025:ARG:HD3	1:A:1030:ARG:HH21	1.64	0.62
2:B:477:ALA:HB1	2:B:479:VAL:HG23	1.82	0.62
1:A:867:ILE:HD11	1:A:999:VAL:CG1	2.30	0.61
1:A:1195:LEU:HD11	1:A:1267:MET:HE3	1.83	0.61
1:A:1164:PRO:O	1:A:1167:GLU:HG3	1.99	0.61
7:I:50:THR:HG22	7:I:52:ILE:HG22	1.81	0.61



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.81	0.61
3:C:148:ARG:NH1	8:J:64:ASN:HA	2.15	0.61
1:A:32:VAL:HG11	1:A:68:GLN:HE22	1.65	0.61
1:A:137:ALA:O	1:A:141:LEU:HD13	2.00	0.61
1:A:902:LEU:HD23	1:A:921:GLY:HA2	1.82	0.61
2:B:638:PHE:CE1	2:B:743:ILE:HA	2.36	0.61
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.41	0.61
1:A:579:SER:OG	1:A:612:ILE:HG22	2.01	0.61
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.30	0.61
1:A:1318:THR:CG2	4:E:11:ARG:HH12	2.13	0.61
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.81	0.61
1:A:857:ARG:HG2	1:A:863:VAL:HA	1.81	0.61
3:C:58:LEU:HD11	8:J:2:ILE:CD1	2.31	0.61
9:K:47:ARG:HH11	9:K:47:ARG:HB3	1.66	0.60
10:L:26:THR:HG22	10:L:27:LEU:H	1.65	0.60
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.82	0.60
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.66	0.60
7:I:59:VAL:HG12	7:I:60:GLN:N	2.16	0.60
1:A:187:LYS:HB2	1:A:194:ALA:CB	2.31	0.60
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.31	0.60
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.65	0.60
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.82	0.60
1:A:345:VAL:HG11	2:B:1129:ARG:HA	1.84	0.60
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.82	0.60
7:I:56:ALA:O	7:I:89:GLN:HG3	2.02	0.60
1:A:535:THR:CG2	1:A:575:LYS:HG2	2.31	0.60
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.82	0.60
1:A:1219:THR:HG21	1:A:1271:ILE:HG12	1.82	0.60
2:B:531:GLN:CD	2:B:531:GLN:H	2.05	0.60
2:B:983:ARG:HH11	2:B:1091:TYR:HB3	1.67	0.60
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.65	0.60
7:I:45:ARG:HG2	7:I:45:ARG:HH11	1.65	0.60
1:A:535:THR:O	1:A:575:LYS:HE2	2.02	0.60
1:A:1333:ILE:O	1:A:1337:GLU:HG3	2.02	0.60
2:B:515:HIS:H	2:B:518:HIS:CD2	2.19	0.60
3:C:166:GLU:HG2	10:L:70:ARG:HH12	1.67	0.60
2:B:60:GLN:HA	2:B:95:ILE:HD12	1.84	0.60
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.31	0.59
2:B:193:LYS:HD3	2:B:787:VAL:HG11	1.83	0.59
2:B:365:THR:HG22	2:B:367:LEU:H	1.65	0.59
1:A:1323:ASP:OD1	1:A:1325:THR:HB	2.03	0.59



	• • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.84	0.59
3:C:258:ILE:CD1	9:K:42:LEU:HD21	2.31	0.59
1:A:35:ILE:HD12	1:A:35:ILE:N	2.18	0.59
2:B:25:ILE:HD12	2:B:653:VAL:CG2	2.32	0.59
4:E:117:THR:HG22	4:E:119:SER:H	1.67	0.59
8:J:48:ARG:HG2	8:J:48:ARG:NH1	2.11	0.59
1:A:61:ILE:HG22	1:A:62:ASP:H	1.67	0.59
1:A:388:LEU:HD22	1:A:432:VAL:HB	1.85	0.59
1:A:903:ASN:HD22	1:A:904:THR:N	2.00	0.59
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.84	0.59
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.84	0.59
9:K:29:ASN:HD21	9:K:79:GLU:HA	1.67	0.59
1:A:80:HIS:O	1:A:243:PRO:HB3	2.02	0.59
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.83	0.59
2:B:1008:PRO:HB3	2:B:1087:PHE:CE1	2.32	0.59
1:A:903:ASN:HD22	1:A:903:ASN:C	2.06	0.59
2:B:885:MET:HA	2:B:936:ASP:HB2	1.85	0.59
10:L:27:LEU:HB3	10:L:37:LYS:HD3	1.84	0.59
1:A:523:ILE:HD12	1:A:523:ILE:N	2.17	0.59
2:B:755:ILE:O	2:B:755:ILE:CG2	2.50	0.59
1:A:883:LEU:O	1:A:886:ILE:HG22	2.03	0.58
3:C:71:PRO:O	3:C:72:LEU:HD23	2.03	0.58
6:H:6:PHE:O	6:H:58:THR:HG23	2.03	0.58
2:B:239:GLU:CD	2:B:255:GLN:HE21	2.07	0.58
2:B:651:LEU:CD2	2:B:710:LEU:HD11	2.33	0.58
2:B:874:PHE:O	2:B:875:GLU:HG3	2.04	0.58
1:A:587:HIS:CE1	1:A:609:ASP:H	2.21	0.58
1:A:1096:SER:O	1:A:1099:PRO:HG2	2.03	0.58
2:B:130:VAL:HG21	2:B:167:ILE:HD12	1.85	0.58
2:B:792:MET:SD	2:B:857:ARG:NH2	2.76	0.58
1:A:264:PHE:HB3	1:A:315:LEU:HD22	1.85	0.58
1:A:537:ARG:NH1	6:H:120:GLY:O	2.36	0.58
1:A:598:LEU:HG	6:H:115:TYR:CE2	2.38	0.58
1:A:858:ASN:C	1:A:858:ASN:HD22	2.06	0.58
2:B:953:LEU:HD21	2:B:955:THR:CG2	2.33	0.58
3:C:62:PHE:O	3:C:66:ARG:HG3	2.03	0.58
1:A:914:GLU:C	1:A:916:GLY:H	2.06	0.58
1:A:1064:VAL:HG12	1:A:1370:LEU:CD2	2.34	0.58
2:B:791:THR:HG22	2:B:792:MET:HG3	1.85	0.58
3:C:39:ALA:O	3:C:163:ILE:HG23	2.04	0.58
1:A:739:ASP:OD2	6:H:19:ARG:HD2	2.03	0.58



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:523:ILE:HB	1:A:622:VAL:CG1	2.33	0.58
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.85	0.58
1:A:317:LYS:CD	1:A:321:PRO:HG2	2.31	0.58
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.38	0.58
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.02	0.58
4:E:180:ARG:HH21	4:E:192:ARG:HB2	1.69	0.57
1:A:451:HIS:CG	1:A:1074:GLU:HG3	2.40	0.57
1:A:986:ILE:HD12	1:A:1028:THR:HG23	1.86	0.57
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.39	0.57
7:I:17:ARG:HG3	7:I:28:GLU:HG2	1.86	0.57
1:A:913:LEU:HD12	1:A:914:GLU:N	2.19	0.57
1:A:1066:VAL:CG1	2:B:1140:ALA:HB2	2.34	0.57
4:E:15:ALA:O	4:E:19:VAL:HG23	2.03	0.57
9:K:20:LYS:HB2	9:K:34:THR:HB	1.86	0.57
1:A:878:ILE:CG2	1:A:955:PRO:HB2	2.34	0.57
8:J:2:ILE:HG22	8:J:3:VAL:N	2.20	0.57
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.70	0.57
1:A:1220:PHE:O	1:A:1223:ASP:HB2	2.05	0.57
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	2.20	0.57
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.52	0.57
1:A:329:LEU:HB3	1:A:333:GLU:HB3	1.86	0.57
1:A:550:LEU:HD22	1:A:556:TRP:NE1	2.19	0.57
1:A:244:PRO:N	1:A:245:PRO:HD2	2.20	0.57
2:B:522:VAL:HG11	2:B:537:LYS:HD2	1.85	0.57
2:B:754:SER:HB3	2:B:812:LEU:HD11	1.87	0.57
2:B:785:TYR:CD2	2:B:795:ILE:HG12	2.40	0.57
2:B:824:ILE:CD1	8:J:48:ARG:HH12	2.18	0.57
2:B:834:ASN:HA	2:B:838:SER:OG	2.05	0.57
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.40	0.57
2:B:230:ALA:N	2:B:231:PRO:HD2	2.20	0.56
7:I:103:CYS:O	7:I:107:SER:HA	2.05	0.56
2:B:172:ILE:HD11	2:B:178:ASN:HD22	1.70	0.56
1:A:886:ILE:HD12	1:A:943:LEU:HB3	1.87	0.56
1:A:913:LEU:HD12	1:A:914:GLU:H	1.68	0.56
1:A:1364:ASN:HD22	1:A:1366:ARG:H	1.53	0.56
1:A:1366:ARG:HB3	1:A:1366:ARG:CZ	2.36	0.56
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.88	0.56
2:B:879:ARG:HD3	2:B:883:LEU:HD22	1.88	0.56
1:A:243:PRO:C	1:A:245:PRO:HD2	2.26	0.56
2:B:1065:GLN:O	2:B:1065:GLN:HG3	2.05	0.56
1:A:14:VAL:N	1:A:1432:GLN:HE22	2.00	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:679:ILE:HD13	1:A:763:ALA:HB2	1.88	0.56
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.86	0.56
1:A:858:ASN:ND2	1:A:862:ASN:H	2.03	0.56
2:B:175:ARG:HB3	2:B:175:ARG:NH1	2.21	0.56
2:B:215:GLN:HE22	2:B:499:ASN:ND2	2.03	0.56
1:A:489:LEU:C	1:A:489:LEU:HD23	2.26	0.56
1:A:849:MET:CE	1:A:1436:ILE:HA	2.35	0.56
1:A:1127:ASP:HB2	1:A:1130:GLN:HB2	1.87	0.56
2:B:1159:ARG:HH11	2:B:1159:ARG:HB3	1.71	0.56
4:E:19:VAL:HG22	4:E:140:LEU:HD13	1.87	0.56
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.40	0.56
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.36	0.56
3:C:6:PRO:HG2	9:K:101:LEU:HB2	1.87	0.56
1:A:587:HIS:NE2	1:A:969:GLN:HG2	2.21	0.56
2:B:809:MET:HG2	2:B:814:PHE:CB	2.36	0.56
2:B:751:VAL:HG13	2:B:812:LEU:HD22	1.87	0.55
1:A:1025:ARG:HD3	1:A:1030:ARG:NH2	2.20	0.55
2:B:871:THR:HG22	2:B:872:GLU:N	2.17	0.55
8:J:48:ARG:NE	8:J:49:MET:HE2	2.22	0.55
10:L:38:LEU:HG	10:L:39:SER:N	2.21	0.55
1:A:106:VAL:HG21	1:A:214:ILE:HG12	1.88	0.55
2:B:800:GLN:HB3	8:J:52:THR:HG21	1.88	0.55
3:C:56:THR:HG23	3:C:58:LEU:N	2.18	0.55
6:H:118:PHE:HB2	6:H:121:LEU:HB2	1.88	0.55
1:A:492:PRO:HB2	1:A:497:THR:HG22	1.87	0.55
2:B:680:THR:O	2:B:683:SER:HB2	2.07	0.55
2:B:822:ASN:ND2	8:J:52:THR:HG21	2.21	0.55
2:B:871:THR:O	2:B:917:PRO:HD2	2.07	0.55
3:C:22:LEU:HD21	9:K:101:LEU:HD21	1.89	0.55
9:K:24:ASP:HB3	9:K:30:ALA:HB3	1.89	0.55
1:A:503:GLN:HE21	5:F:90:ARG:HH21	1.55	0.55
2:B:193:LYS:CE	8:J:65:PRO:HG3	2.35	0.55
2:B:680:THR:CG2	2:B:681:TRP:H	2.09	0.55
2:B:800:GLN:CB	8:J:52:THR:HG22	2.37	0.55
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.39	0.55
3:C:248:ILE:HD13	9:K:101:LEU:CD1	2.37	0.55
5:F:93:ILE:CD1	5:F:134:ILE:HD11	2.35	0.55
6:H:113:ALA:HB1	6:H:124:ARG:HE	1.72	0.55
1:A:901:LEU:O	1:A:920:LEU:HD23	2.07	0.54
1:A:15:LYS:O	1:A:1421:CYS:HB2	2.07	0.54
1:A:273:ASN:O	1:A:277:GLU:HG3	2.07	0.54



	t i c	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:841:MET:HG3	2:B:1010:LEU:HD12	1.90	0.54
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.08	0.54
3:C:258:ILE:HD13	9:K:35:PHE:CE2	2.37	0.54
6:H:12:VAL:HA	6:H:28:ALA:HB2	1.88	0.54
7:I:55:THR:O	7:I:58:VAL:HG23	2.07	0.54
7:I:115:LYS:O	7:I:117:LYS:HG3	2.06	0.54
1:A:709:THR:HG22	1:A:710:LEU:N	2.22	0.54
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.89	0.54
2:B:971:THR:OG1	3:C:61:GLU:HG3	2.07	0.54
3:C:11:ARG:HD2	3:C:21:ILE:HD11	1.89	0.54
4:E:5:ASN:O	4:E:9:ILE:HG13	2.07	0.54
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.90	0.54
1:A:313:GLN:HB3	1:A:320:ARG:C	2.27	0.54
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.73	0.54
1:A:885:THR:HG22	1:A:893:PHE:HE1	1.73	0.54
2:B:1051:THR:O	2:B:1055:ILE:HG13	2.07	0.54
1:A:519:PRO:HD3	1:A:631:HIS:ND1	2.23	0.54
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.89	0.54
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.37	0.54
2:B:172:ILE:CD1	2:B:178:ASN:HD22	2.20	0.54
3:C:43:THR:HG22	3:C:44:LEU:N	2.23	0.54
8:J:48:ARG:NH1	8:J:48:ARG:CG	2.71	0.54
2:B:757:PRO:HD3	2:B:983:ARG:NH2	2.23	0.54
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.88	0.54
1:A:208:LEU:C	1:A:208:LEU:HD23	2.28	0.54
1:A:697:ALA:HB2	1:A:702:LEU:HD23	1.89	0.54
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.43	0.54
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.43	0.54
1:A:464:PRO:O	1:A:465:TYR:O	2.25	0.54
7:I:57:GLY:O	7:I:59:VAL:HG23	2.08	0.54
10:L:26:THR:HG22	10:L:27:LEU:N	2.23	0.54
1:A:689:LYS:O	1:A:693:VAL:HG23	2.08	0.54
1:A:929:LEU:HD11	1:A:983:ILE:HD13	1.90	0.54
2:B:41:LYS:HE2	2:B:544:CYS:SG	2.48	0.54
2:B:205:ILE:HG21	2:B:462:ALA:HB2	1.89	0.54
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.90	0.54
2:B:644:GLU:CD	2:B:646:LEU:HB2	2.29	0.54
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.90	0.54
4:E:96:PHE:CE2	4:E:110:PHE:HB2	2.43	0.54
9:K:56:VAL:HA	9:K:77:THR:HG22	1.89	0.54
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.08	0.53



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:666:ILE:CD1	2:B:1030:LEU:HD22	2.36	0.53
1:A:1102:LYS:HD3	1:A:1106:ASN:HD21	1.73	0.53
2:B:339:THR:HG23	2:B:343:ILE:HD12	1.89	0.53
5:F:77:ASP:O	5:F:78:GLN:HB2	2.07	0.53
1:A:69:THR:O	2:B:1174:LYS:HG2	2.08	0.53
1:A:500:GLU:OE2	2:B:1145:SER:HB2	2.09	0.53
2:B:281:PRO:HG2	2:B:284:ILE:CD1	2.38	0.53
7:I:50:THR:HB	7:I:92:ARG:HH22	1.73	0.53
1:A:523:ILE:HG23	1:A:527:THR:HB	1.90	0.53
2:B:1023:VAL:HG12	2:B:1027:ILE:HD11	1.90	0.53
3:C:25:VAL:HG23	3:C:228:PHE:HE1	1.73	0.53
5:F:107:VAL:HG11	5:F:111:LEU:HD11	1.90	0.53
8:J:48:ARG:HH11	8:J:48:ARG:CG	2.10	0.53
1:A:320:ARG:N	1:A:321:PRO:HD3	2.24	0.53
1:A:709:THR:HG22	1:A:711:ARG:H	1.74	0.53
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.71	0.53
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.91	0.53
4:E:114:ASN:OD1	4:E:115:ASN:N	2.42	0.53
1:A:434:ARG:HH21	1:A:437:MET:HG3	1.74	0.53
1:A:1111:MET:CE	1:A:1114:PRO:HA	2.38	0.53
2:B:515:HIS:H	2:B:518:HIS:HD2	1.56	0.53
2:B:845:SER:HB3	2:B:850:LEU:HD22	1.91	0.53
2:B:868:MET:O	2:B:870:ILE:HG13	2.08	0.53
2:B:954:VAL:O	10:L:55:ILE:O	2.26	0.53
1:A:1199:ARG:HA	1:A:1202:MET:HB2	1.91	0.53
3:C:258:ILE:HD11	9:K:42:LEU:CD2	2.38	0.53
4:E:161:LYS:HE2	4:E:165:LEU:HD11	1.91	0.53
8:J:25:LEU:O	8:J:29:GLU:HA	2.09	0.53
1:A:858:ASN:HD21	1:A:862:ASN:H	1.56	0.53
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.44	0.53
4:E:127:ILE:HD11	4:E:132:ILE:HD11	1.91	0.53
1:A:366:VAL:HG11	1:A:436:ILE:HD11	1.90	0.53
1:A:499:ALA:O	1:A:503:GLN:HB2	2.08	0.53
1:A:849:MET:HE3	1:A:1063:MET:SD	2.49	0.53
2:B:344:LYS:H	2:B:347:LYS:HE3	1.74	0.53
2:B:429:PHE:HA	2:B:432:MET:CE	2.39	0.53
3:C:58:LEU:HD11	8:J:2:ILE:HD12	1.91	0.53
1:A:55:ASP:N	1:A:56:PRO:CD	2.69	0.52
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.91	0.52
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.44	0.52
5:F:128:LYS:HD2	5:F:149:GLU:HA	1.91	0.52



<u> </u>		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:1264:GLU:OE1	7:I:44:TYR:HE2	1.93	0.52
1:A:1279:ILE:N	1:A:1279:ILE:HD12	2.24	0.52
2:B:636:PRO:HA	2:B:691:GLU:O	2.08	0.52
3:C:21:ILE:HG12	3:C:229:TYR:HD2	1.74	0.52
4:E:181:ALA:HA	4:E:186:LEU:HD21	1.91	0.52
5:F:107:VAL:HG12	5:F:109:VAL:H	1.74	0.52
7:I:50:THR:CB	7:I:92:ARG:HH22	2.22	0.52
1:A:528:LEU:HD23	1:A:751:SER:HB3	1.91	0.52
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.92	0.52
1:A:516:SER:O	1:A:518:LYS:HG2	2.10	0.52
1:A:533:LYS:NZ	1:A:660:ASN:ND2	2.56	0.52
1:A:901:LEU:HD23	1:A:907:THR:HG23	1.92	0.52
2:B:249:ARG:O	2:B:251:ILE:HG13	2.10	0.52
2:B:296:GLU:O	2:B:300:HIS:HD2	1.93	0.52
2:B:898:LEU:HD21	2:B:964:VAL:HG11	1.92	0.52
4:E:124:VAL:HB	4:E:125:PRO:HD3	1.90	0.52
6:H:81:PRO:HB2	6:H:82:PRO:CD	2.38	0.52
9:K:1:MET:HG3	9:K:2:ASN:N	2.25	0.52
2:B:759:PRO:HG2	2:B:1046:PRO:HB3	1.91	0.52
3:C:242:GLN:OE1	3:C:242:GLN:HA	2.10	0.52
1:A:817:ALA:HA	2:B:764:SER:OG	2.09	0.52
2:B:1002:THR:HG22	2:B:1006:ILE:N	2.24	0.52
4:E:124:VAL:HB	4:E:125:PRO:CD	2.40	0.52
1:A:492:PRO:CB	1:A:497:THR:HG22	2.40	0.52
1:A:868:TYR:HE1	1:A:1064:VAL:CG1	2.23	0.52
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.43	0.52
1:A:1162:VAL:CG1	7:I:41:PRO:HG3	2.34	0.52
2:B:552:MET:N	2:B:553:PRO:HD2	2.25	0.52
2:B:864:LYS:HB2	2:B:864:LYS:NZ	2.25	0.52
3:C:6:PRO:HB2	9:K:101:LEU:HD23	1.92	0.52
1:A:795:GLU:HG2	2:B:731:VAL:CG2	2.40	0.52
2:B:528:PRO:HG3	2:B:536:VAL:HB	1.92	0.52
2:B:846:ILE:HG12	2:B:974:PRO:HB2	1.92	0.52
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.92	0.52
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.92	0.52
1:A:575:LYS:HD3	1:A:612:ILE:CD1	2.40	0.51
2:B:292:ILE:N	2:B:293:PRO:HD2	2.26	0.51
5:F:109:VAL:HG21	5:F:124:GLU:HA	1.92	0.51
1:A:24:PRO:HG2	1:A:25:GLU:OE2	2.10	0.51
2:B:314:LEU:O	2:B:317:CYS:HB2	2.11	0.51
2:B:885:MET:HA	2:B:936:ASP:CB	2.40	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:C:145:CYS:SG	3:C:146:LYS:N	2.83	0.51
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.41	0.51
2:B:128:LEU:HB3	2:B:167:ILE:O	2.11	0.51
2:B:852:ARG:NH2	10:L:70:ARG:O	2.38	0.51
3:C:53:THR:O	3:C:153:LEU:HA	2.10	0.51
1:A:384:ASN:OD1	1:A:388:LEU:HD12	2.10	0.51
1:A:465:TYR:CE2	9:K:4:PRO:HD2	2.45	0.51
1:A:673:GLY:N	1:A:674:PRO:CD	2.73	0.51
1:A:1376:THR:HG22	1:A:1376:THR:O	2.09	0.51
1:A:1187:GLN:HG3	1:A:1188:GLN:H	1.75	0.51
4:E:23:VAL:HG12	4:E:28:TYR:HB2	1.93	0.51
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.25	0.51
2:B:574:SER:HB3	2:B:591:ARG:NH2	2.26	0.51
2:B:859:TYR:O	2:B:965:LYS:HA	2.11	0.51
2:B:1037:LEU:HD21	8:J:44:TYR:HD2	1.75	0.51
4:E:93:MET:O	4:E:97:VAL:HG23	2.10	0.51
1:A:32:VAL:HG23	1:A:33:ALA:N	2.24	0.51
1:A:523:ILE:CG2	1:A:527:THR:HB	2.41	0.51
1:A:705:LYS:H	1:A:705:LYS:HD2	1.75	0.51
1:A:840:ARG:NH1	1:A:1386:ARG:HB3	2.23	0.51
2:B:577:ALA:HB1	2:B:589:VAL:CG2	2.39	0.51
2:B:653:VAL:HG13	2:B:689:LEU:HB3	1.92	0.51
2:B:1198:TYR:CE1	2:B:1201:LYS:HD2	2.46	0.51
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.39	0.51
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.26	0.51
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.44	0.51
1:A:2:VAL:HG21	2:B:1157:ALA:O	2.11	0.51
1:A:216:VAL:HA	1:A:219:PHE:CZ	2.46	0.51
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.11	0.51
1:A:903:ASN:HD22	1:A:905:ASP:H	1.58	0.51
1:A:1348:LEU:HD21	1:A:1375:MET:CE	2.40	0.51
2:B:847:ASP:O	3:C:65:HIS:HE1	1.94	0.51
3:C:58:LEU:HD11	8:J:2:ILE:HD11	1.92	0.51
5:F:81:THR:HB	5:F:144:GLU:OE1	2.11	0.51
7:I:98:VAL:CG2	7:I:113:ASP:HB2	2.39	0.51
8:J:57:ILE:O	8:J:61:LEU:HG	2.10	0.51
1:A:95:PHE:CE2	1:A:1414:ALA:HB2	2.46	0.51
1:A:313:GLN:HB2	1:A:320:ARG:HB3	1.93	0.51
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.93	0.51
2:B:913:GLY:HA2	2:B:938:SER:CB	2.41	0.50
3:C:14:SER:HA	9:K:114:LEU:O	2.10	0.50



	i as pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
6:H:104:PHE:O	6:H:106:GLU:N	2.44	0.50
9:K:49:GLU:HG3	9:K:94:ILE:CG1	2.41	0.50
1:A:497:THR:HG23	2:B:1146:PHE:HD1	1.76	0.50
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.93	0.50
1:A:208:LEU:CD2	1:A:212:LYS:HE3	2.41	0.50
1:A:605:MET:HE2	1:A:606:LEU:H	1.75	0.50
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.59	0.50
2:B:914:LYS:HD2	2:B:937:ALA:HB3	1.92	0.50
10:L:30:ILE:HG13	10:L:59:ALA:HB2	1.93	0.50
1:A:38:PRO:HB3	1:A:270:LEU:HB3	1.92	0.50
1:A:1004:ASN:ND2	4:E:167:ARG:HD2	2.26	0.50
2:B:558:LEU:O	2:B:563:MET:HB2	2.12	0.50
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.92	0.50
1:A:849:MET:HE3	1:A:1436:ILE:HA	1.92	0.50
1:A:1391:ARG:NH2	1:A:1417:GLU:OE2	2.44	0.50
4:E:65:THR:O	4:E:69:ILE:HG13	2.12	0.50
8:J:64:ASN:N	8:J:65:PRO:HD2	2.26	0.50
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	2.12	0.50
1:A:1376:THR:O	1:A:1376:THR:CG2	2.59	0.50
3:C:73:GLN:NE2	3:C:75:MET:CB	2.74	0.50
2:B:38:PHE:HZ	2:B:541:LEU:HB3	1.77	0.50
2:B:168:GLY:H	2:B:450:ALA:HB1	1.77	0.50
1:A:53:LEU:CD2	1:A:54:ASN:H	2.23	0.50
1:A:147:VAL:HG22	1:A:170:THR:HG22	1.93	0.50
2:B:63:ILE:CB	2:B:95:ILE:HD11	2.34	0.50
2:B:169:ARG:O	2:B:457:LEU:HD12	2.11	0.50
1:A:1399:ARG:HH11	1:A:1401:SER:HA	1.75	0.49
2:B:314:LEU:HD21	2:B:386:LEU:HD11	1.92	0.49
2:B:1177:HIS:CB	2:B:1179:GLN:HE21	2.23	0.49
10:L:38:LEU:HD13	10:L:48:CYS:HA	1.94	0.49
1:A:338:GLY:HA2	1:A:343:LYS:HD2	1.94	0.49
1:A:1120:LEU:HG	1:A:1134:ILE:HD12	1.94	0.49
4:E:100:ILE:HD13	4:E:108:GLY:HA3	1.94	0.49
4:E:112:TYR:O	4:E:137:GLU:HG3	2.12	0.49
2:B:901:PRO:CD	10:L:58:LYS:HB3	2.40	0.49
3:C:50:GLU:HB2	3:C:156:THR:HB	1.93	0.49
1:A:219:PHE:O	1:A:224:PHE:HB2	2.13	0.49
1:A:786:HIS:CE1	2:B:742:GLU:OE2	2.62	0.49
2:B:492:LEU:O	2:B:496:ARG:HG2	2.12	0.49
1:A:19:PHE:HZ	1:A:1397:LEU:HG	1.78	0.49
2:B:870:ILE:HG23	2:B:917:PRO:O	2.13	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:C:46:ILE:HB	3:C:68:GLY:HA2	1.93	0.49
6:H:11:GLN:HE21	6:H:52:GLN:HA	1.77	0.49
1:A:463:ILE:HD11	1:A:469:ARG:HG3	1.94	0.49
1:A:1285:MET:HG3	1:A:1307:GLU:OE1	2.13	0.49
2:B:1051:THR:HG22	2:B:1052:VAL:N	2.28	0.49
1:A:17:VAL:HB	1:A:1419:ASP:HB2	1.94	0.49
1:A:71:GLN:HG2	2:B:1176:ASN:ND2	2.27	0.49
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.45	0.49
1:A:724:GLU:O	1:A:728:LYS:HG2	2.13	0.49
2:B:204:ILE:C	2:B:205:ILE:HD12	2.32	0.49
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.95	0.49
1:A:58:LEU:HD22	1:A:80:HIS:O	2.12	0.49
1:A:75:ASN:HB2	1:A:76:GLU:OE2	2.13	0.49
1:A:1139:GLU:HG3	1:A:1280:GLU:O	2.13	0.49
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.12	0.49
2:B:332:ASP:O	2:B:336:ARG:HG3	2.13	0.49
2:B:806:THR:CG2	2:B:808:ALA:H	2.26	0.49
3:C:73:GLN:NE2	3:C:75:MET:N	2.60	0.49
1:A:376:TYR:CZ	1:A:498:ARG:HD2	2.48	0.49
1:A:1438:THR:HG23	2:B:1144:ALA:HB3	1.95	0.49
2:B:219:ALA:HB3	2:B:222:ILE:HD12	1.94	0.49
2:B:650:GLU:HG3	2:B:651:LEU:N	2.28	0.49
3:C:137:LYS:H	3:C:137:LYS:CD	2.10	0.49
1:A:148:CYS:O	1:A:168:GLY:HA2	2.13	0.49
2:B:54:PHE:HA	2:B:58:THR:HB	1.95	0.49
2:B:234:ILE:HD13	2:B:257:LYS:HD3	1.95	0.49
2:B:913:GLY:HA2	2:B:938:SER:HB3	1.94	0.49
2:B:918:ILE:CD1	2:B:935:ARG:HD2	2.41	0.49
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.48	0.49
3:C:12:GLU:HB2	3:C:19:ASP:HB3	1.94	0.49
1:A:984:LYS:HB3	1:A:988:LEU:HD12	1.94	0.48
1:A:1215:ARG:HA	1:A:1218:GLN:HG2	1.95	0.48
1:A:1410:PHE:CD2	2:B:1212:ILE:HD11	2.39	0.48
2:B:1022:THR:HG23	2:B:1022:THR:O	2.13	0.48
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.48	0.48
1:A:1146:VAL:HG12	1:A:1197:LEU:HD22	1.95	0.48
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.95	0.48
2:B:591:ARG:O	2:B:592:ASN:HB2	2.13	0.48
2:B:843:GLN:HB2	2:B:993:THR:HB	1.94	0.48
9:K:47:ARG:C	9:K:47:ARG:HD2	2.32	0.48
1:A:1116:LEU:HD13	1:A:1311:VAL:HG13	1.94	0.48



	• • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1341:ILE:HD11	1:A:1376:THR:HG23	1.94	0.48
2:B:25:ILE:HG23	2:B:29:ASP:CB	2.43	0.48
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.95	0.48
2:B:545:ILE:HG12	2:B:633:VAL:HG22	1.94	0.48
3:C:163:ILE:HG23	3:C:165:LYS:H	1.78	0.48
6:H:95:TYR:CE2	6:H:97:MET:HG3	2.49	0.48
9:K:12:LEU:HD12	9:K:12:LEU:N	2.28	0.48
9:K:20:LYS:O	9:K:33:ILE:HA	2.13	0.48
1:A:597:LEU:HD12	1:A:597:LEU:H	1.78	0.48
2:B:1065:GLN:HE21	2:B:1067:ARG:N	2.11	0.48
1:A:38:PRO:HB3	1:A:270:LEU:HD23	1.95	0.48
1:A:338:GLY:CA	1:A:343:LYS:HD2	2.44	0.48
1:A:534:LEU:O	1:A:574:GLY:HA3	2.14	0.48
1:A:845:LEU:HD22	1:A:1374:VAL:HG21	1.94	0.48
2:B:122:LEU:CD2	2:B:958:GLN:HG2	2.43	0.48
10:L:42:ARG:C	10:L:44:ASP:H	2.17	0.48
10:L:48:CYS:SG	10:L:49:LYS:N	2.87	0.48
1:A:765:VAL:HG23	1:A:802:ASN:O	2.14	0.48
1:A:849:MET:CE	1:A:1063:MET:SD	3.01	0.48
1:A:1198:ASP:OD1	1:A:1200:ALA:HB3	2.13	0.48
2:B:298:LEU:HD22	2:B:314:LEU:HD13	1.93	0.48
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.13	0.48
2:B:864:LYS:HB2	2:B:864:LYS:HZ2	1.77	0.48
2:B:979:LYS:CE	2:B:987:LYS:HD2	2.44	0.48
2:B:979:LYS:HE3	2:B:987:LYS:HD2	1.95	0.48
6:H:26:ILE:HD13	6:H:49:VAL:HG11	1.95	0.48
9:K:61:TYR:HA	9:K:72:LYS:O	2.12	0.48
1:A:472:LEU:HD21	2:B:835:GLN:HB2	1.96	0.48
1:A:517:ASN:HB2	1:A:878:ILE:O	2.13	0.48
1:A:547:LEU:HD22	9:K:58:PHE:CD1	2.48	0.48
1:A:1102:LYS:HD3	1:A:1106:ASN:ND2	2.28	0.48
2:B:315:LYS:N	2:B:316:PRO:HD2	2.27	0.48
2:B:497:ARG:HH22	2:B:775:LYS:HE3	1.78	0.48
2:B:806:THR:HG23	2:B:808:ALA:H	1.79	0.48
1:A:1434:ALA:O	1:A:1436:ILE:N	2.41	0.48
1:A:1447:GLU:OE1	1:A:1447:GLU:HA	2.14	0.48
2:B:324:ILE:HD11	2:B:333:PHE:CB	2.43	0.48
2:B:429:PHE:HA	2:B:432:MET:HE3	1.95	0.48
3:C:134:ILE:HG21	3:C:139:GLY:HA2	1.96	0.48
9:K:30:ALA:HA	9:K:75:ILE:O	2.14	0.48
1:A:249:SER:HB2	1:A:258:GLY:O	2.13	0.48



	t i c	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:B:98:THR:HG22	2:B:99:LYS:N	2.28	0.48
2:B:953:LEU:C	2:B:953:LEU:HD23	2.34	0.48
6:H:125:LEU:C	6:H:130:ARG:HH12	2.17	0.48
8:J:1:MET:HG3	8:J:60:PHE:HE2	1.78	0.48
1:A:51:GLY:O	1:A:56:PRO:HB3	2.13	0.48
1:A:682:THR:HG21	1:A:728:LYS:HG3	1.96	0.48
1:A:857:ARG:HD3	1:A:861:GLY:O	2.14	0.48
2:B:564:GLU:HB2	2:B:589:VAL:HG12	1.96	0.48
3:C:209:TYR:CD1	3:C:209:TYR:N	2.82	0.48
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.96	0.48
1:A:740:LEU:HD12	1:A:740:LEU:N	2.29	0.47
2:B:294:ASP:H	7:I:12:ASN:HD22	1.57	0.47
2:B:776:GLN:HA	2:B:1096:ARG:NH1	2.29	0.47
3:C:108:GLU:OE1	3:C:149:LYS:HD3	2.14	0.47
3:C:121:VAL:HG12	3:C:121:VAL:O	2.14	0.47
7:I:50:THR:CB	7:I:92:ARG:HH12	2.27	0.47
1:A:1145:SER:HB2	1:A:1205:LYS:HZ3	1.78	0.47
2:B:285:ILE:O	2:B:289:LEU:HG	2.13	0.47
3:C:166:GLU:CG	10:L:70:ARG:HH12	2.27	0.47
4:E:99:HIS:O	4:E:103:LYS:HG2	2.15	0.47
1:A:602:ASP:O	1:A:615:GLY:HA2	2.14	0.47
1:A:1118:VAL:CG2	1:A:1306:LEU:HD12	2.44	0.47
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.44	0.47
3:C:22:LEU:HD12	3:C:230:MET:HE1	1.95	0.47
3:C:73:GLN:NE2	3:C:75:MET:H	2.05	0.47
1:A:144:THR:O	1:A:146:MET:HG3	2.14	0.47
1:A:483:ASP:OD1	13:B:3571:UTP:O1B	2.32	0.47
1:A:1279:ILE:HD11	1:A:1312:ASN:CB	2.43	0.47
1:A:1281:ARG:HB2	1:A:1309:ASP:HB2	1.97	0.47
2:B:108:VAL:HG12	2:B:109:THR:N	2.29	0.47
2:B:202:TYR:CD2	2:B:202:TYR:N	2.83	0.47
2:B:528:PRO:CG	2:B:536:VAL:HB	2.44	0.47
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.79	0.47
3:C:244:VAL:O	3:C:248:ILE:HG13	2.14	0.47
10:L:58:LYS:O	10:L:59:ALA:HB3	2.14	0.47
1:A:346:ASP:O	1:A:347:PHE:HB2	2.15	0.47
9:K:49:GLU:HG3	9:K:94:ILE:HG12	1.95	0.47
1:A:984:LYS:O	1:A:988:LEU:HB2	2.14	0.47
2:B:914:LYS:HG2	2:B:915:THR:N	2.28	0.47
2:B:955:THR:CG2	10:L:55:ILE:HA	2.43	0.47
2:B:1165:ILE:HG13	2:B:1187:ASN:ND2	2.29	0.47



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:C:169:LYS:HZ3	10:L:70:ARG:HG2	1.79	0.47
7:I:50:THR:CG2	7:I:52:ILE:HG22	2.45	0.47
7:I:95:THR:HG22	7:I:96:SER:O	2.14	0.47
1:A:44:THR:O	1:A:45:GLN:HB2	2.14	0.47
1:A:440:ASP:O	1:A:460:VAL:HG23	2.15	0.47
1:A:598:LEU:HD11	6:H:124:ARG:CB	2.44	0.47
1:A:842:VAL:HG11	2:B:1136:ASP:CG	2.35	0.47
1:A:1167:GLU:O	1:A:1171:GLN:HG3	2.14	0.47
1:A:1431:GLY:HA2	2:B:1152:MET:CE	2.45	0.47
3:C:167:HIS:CD2	3:C:169:LYS:H	2.13	0.47
5:F:81:THR:HG21	5:F:136:ARG:HD3	1.96	0.47
5:F:109:VAL:HG13	5:F:127:GLU:OE1	2.15	0.47
6:H:40:LEU:CD1	6:H:123:MET:HB2	2.42	0.47
6:H:100:THR:HG23	6:H:138:GLU:HG3	1.96	0.47
7:I:98:VAL:HG22	7:I:111:THR:HG22	1.97	0.47
8:J:2:ILE:HD11	8:J:57:ILE:CD1	2.45	0.47
2:B:1060:ARG:NH2	3:C:202:PRO:HG3	2.30	0.47
5:F:134:ILE:HD12	5:F:151:LEU:CD1	2.45	0.47
8:J:2:ILE:HD11	8:J:57:ILE:HD12	1.96	0.47
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.96	0.47
1:A:381:THR:HB	1:A:382:PRO:HD2	1.97	0.47
1:A:880:LYS:HA	1:A:955:PRO:HA	1.95	0.47
2:B:461:LEU:HD12	2:B:466:TRP:HH2	1.80	0.47
1:A:365:GLY:O	1:A:468:PHE:HA	2.14	0.47
1:A:516:SER:O	1:A:517:ASN:C	2.52	0.47
1:A:1146:VAL:HG11	1:A:1202:MET:SD	2.55	0.47
1:A:1351:GLU:O	1:A:1355:VAL:HG23	2.14	0.47
3:C:55:THR:HB	3:C:152:GLU:H	1.80	0.47
4:E:120:ALA:O	4:E:123:LEU:HB2	2.15	0.47
1:A:268:ASP:HB3	1:A:299:HIS:CD2	2.51	0.46
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.51	0.46
1:A:1064:VAL:HG12	1:A:1370:LEU:HD22	1.97	0.46
1:A:1124:HIS:CB	1:A:1130:GLN:HG3	2.45	0.46
2:B:683:SER:O	2:B:687:GLU:HG3	2.14	0.46
3:C:35:ARG:NH1	9:K:41:THR:H	2.12	0.46
6:H:96:VAL:HG13	6:H:143:LEU:CD2	2.45	0.46
6:H:125:LEU:HB3	6:H:130:ARG:NH1	2.31	0.46
10:L:51:CYS:HB3	10:L:53:HIS:CD2	2.50	0.46
1:A:115:LEU:CD1	1:A:141:LEU:HB3	2.44	0.46
1:A:1277:GLU:O	1:A:1278:ASN:CB	2.61	0.46
2:B:287:ARG:NH1	2:B:324:ILE:O	2.48	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.97	0.46
2:B:889:THR:HG22	2:B:891:ASP:H	1.80	0.46
7:I:95:THR:HG22	7:I:96:SER:N	2.31	0.46
1:A:418:SER:C	1:A:420:ARG:H	2.17	0.46
1:A:565:ILE:HG23	1:A:567:LYS:CG	2.44	0.46
1:A:907:THR:CG2	1:A:908:LEU:H	2.26	0.46
1:A:1129:GLU:O	1:A:1133:LEU:HG	2.15	0.46
2:B:60:GLN:O	2:B:63:ILE:HG22	2.16	0.46
2:B:97:VAL:HG12	2:B:178:ASN:HD21	1.80	0.46
2:B:98:THR:O	2:B:126:SER:HB3	2.15	0.46
2:B:420:LEU:HD13	2:B:453:ILE:HA	1.97	0.46
2:B:778:MET:SD	2:B:1094:ARG:HD3	2.56	0.46
3:C:44:LEU:HG	3:C:159:ALA:HB1	1.97	0.46
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.51	0.46
1:A:1293:SER:HB3	1:A:1297:GLU:O	2.15	0.46
2:B:642:ASP:HB3	2:B:649:LYS:HG2	1.98	0.46
2:B:651:LEU:HD23	2:B:710:LEU:HD11	1.96	0.46
1:A:345:VAL:CG1	2:B:1129:ARG:HA	2.46	0.46
1:A:401:GLY:H	1:A:435:HIS:HD1	1.64	0.46
1:A:704:ALA:HB2	1:A:710:LEU:HD12	1.98	0.46
8:J:30:LEU:HD11	8:J:38:ARG:NH2	2.31	0.46
2:B:103:ASN:HB2	2:B:169:ARG:NH1	2.31	0.46
2:B:859:TYR:CD1	2:B:859:TYR:N	2.83	0.46
2:B:884:ARG:O	2:B:936:ASP:HB2	2.16	0.46
6:H:12:VAL:HG13	6:H:26:ILE:HG23	1.98	0.46
6:H:130:ARG:HD3	6:H:134:ASN:HD21	1.81	0.46
1:A:912:LEU:HD22	1:A:1033:GLN:HA	1.97	0.46
1:A:1039:LYS:O	1:A:1043:ASP:OD1	2.34	0.46
3:C:11:ARG:HD2	3:C:21:ILE:CD1	2.46	0.46
1:A:226:GLU:HG3	1:A:227:VAL:HG23	1.98	0.46
1:A:1339:LEU:HD13	4:E:147:HIS:CD2	2.51	0.46
1:A:1396:ALA:HB2	1:A:1417:GLU:OE1	2.16	0.46
2:B:25:ILE:HG13	2:B:654:ARG:HA	1.97	0.46
2:B:174:LEU:O	2:B:200:GLY:O	2.33	0.46
2:B:616:ILE:HG13	2:B:697:GLU:HA	1.98	0.46
3:C:102:GLN:OE1	3:C:154:LYS:HE2	2.16	0.46
3:C:242:GLN:HE21	3:C:246:ARG:NH2	2.03	0.46
3:C:89:GLU:O	3:C:90:ASP:HB3	2.16	0.46
3:C:249:ASP:O	3:C:252:GLN:HB3	2.16	0.46
6:H:12:VAL:HA	6:H:28:ALA:CB	2.46	0.46
1:A:666:ILE:HG12	2:B:1026:LEU:HB3	1.98	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:1152:ILE:HB	7:I:44:TYR:HB3	1.97	0.46
1:A:1212:VAL:O	1:A:1216:ILE:HG13	2.16	0.46
2:B:493:SER:OG	2:B:497:ARG:NH2	2.49	0.46
4:E:16:PHE:CZ	4:E:20:LYS:HE2	2.50	0.46
1:A:35:ILE:HD13	1:A:83:HIS:H	1.81	0.45
1:A:752:LYS:HG2	2:B:1015:HIS:O	2.17	0.45
1:A:795:GLU:HG2	2:B:731:VAL:HG22	1.98	0.45
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.30	0.45
2:B:705:MET:HB3	2:B:706:GLN:NE2	2.31	0.45
10:L:49:LYS:O	10:L:50:ASP:HB2	2.16	0.45
2:B:227:LYS:NZ	2:B:236:HIS:HE1	2.15	0.45
2:B:1191:ILE:HG22	2:B:1192:TYR:N	2.30	0.45
3:C:42:PRO:HG3	3:C:163:ILE:HD11	1.97	0.45
3:C:55:THR:HG22	3:C:55:THR:O	2.16	0.45
4:E:180:ARG:HB2	4:E:215:MET:OXT	2.16	0.45
1:A:62:ASP:HB2	1:A:64:ASN:ND2	2.31	0.45
1:A:239:LEU:HD23	1:A:240:PRO:N	2.31	0.45
1:A:1259:MET:O	1:A:1263:ILE:HG13	2.15	0.45
2:B:118:ARG:HG3	2:B:204:ILE:HD13	1.97	0.45
2:B:1051:THR:HG22	2:B:1053:GLU:N	2.23	0.45
3:C:6:PRO:CB	9:K:101:LEU:HD23	2.46	0.45
3:C:100:THR:HG22	3:C:101:LEU:N	2.32	0.45
6:H:105:GLU:O	6:H:107:VAL:HG23	2.15	0.45
1:A:489:LEU:HD23	1:A:490:HIS:N	2.31	0.45
1:A:565:ILE:HG23	1:A:567:LYS:HE3	1.98	0.45
1:A:853:ASP:O	1:A:854:ASN:HB2	2.17	0.45
6:H:31:THR:HG22	6:H:32:THR:N	2.31	0.45
1:A:1295:THR:HB	1:A:1297:GLU:OE1	2.17	0.45
1:A:1386:ARG:O	1:A:1386:ARG:HG3	2.16	0.45
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.51	0.45
2:B:904:ARG:HH21	2:B:948:ILE:HD11	1.81	0.45
3:C:6:PRO:HA	3:C:25:VAL:HG13	1.98	0.45
3:C:57:VAL:HG12	3:C:57:VAL:O	2.17	0.45
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.98	0.45
6:H:56:THR:O	6:H:144:ILE:HA	2.17	0.45
9:K:33:ILE:HD13	9:K:87:LEU:HD22	1.97	0.45
10:L:41:SER:HB2	10:L:42:ARG:HH21	1.82	0.45
1:A:71:GLN:HG2	2:B:1176:ASN:HD22	1.82	0.45
1:A:84:ILE:HG23	1:A:84:ILE:O	2.17	0.45
1:A:464:PRO:HB2	9:K:4:PRO:HD3	1.98	0.45
1:A:765:VAL:HB	1:A:800:VAL:CG1	2.47	0.45



	the second se	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:822:GLU:HG3	2:B:513:GLN:HE22	1.81	0.45	
1:A:1322:ILE:HG13	1:A:1323:ASP:N	2.31	0.45	
2:B:276:ILE:CD1	2:B:355:ILE:HD13	2.47	0.45	
2:B:830:TYR:CE1	2:B:1000:PRO:HB3	2.51	0.45	
2:B:879:ARG:HG3	2:B:885:MET:HE1	1.97	0.45	
10:L:38:LEU:O	10:L:39:SER:HB2	2.17	0.45	
1:A:1364:ASN:ND2	1:A:1366:ARG:CG	2.79	0.45	
2:B:1084:GLN:NE2	3:C:192:TRP:N	2.65	0.45	
3:C:25:VAL:HG23	3:C:228:PHE:CE1	2.49	0.45	
9:K:12:LEU:HD12	9:K:12:LEU:H	1.82	0.45	
1:A:368:LYS:NZ	1:A:368:LYS:HB2	2.32	0.45	
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.98	0.45	
2:B:276:ILE:HD11	2:B:355:ILE:HD13	1.98	0.45	
2:B:638:PHE:HB2	2:B:741:CYS:O	2.17	0.45	
3:C:48:SER:HB3	3:C:158:VAL:HB	1.99	0.45	
8:J:48:ARG:NH2	8:J:49:MET:HE1	2.31	0.45	
1:A:329:LEU:HA	1:A:332:LYS:HB2	1.99	0.45	
1:A:805:LEU:CD1	2:B:1052:VAL:HG21	2.47	0.45	
2:B:28:GLU:OE1	2:B:807:ARG:NH2	2.50	0.45	
2:B:1023:VAL:O	2:B:1027:ILE:HG13	2.17	0.45	
2:B:1079:LYS:HB2	3:C:27:LEU:HD21	1.97	0.45	
4:E:88:VAL:HG13	4:E:92:THR:HB	1.99	0.45	
6:H:31:THR:HG22	6:H:32:THR:H	1.81	0.45	
8:J:14:VAL:HG23	8:J:41:LEU:HD21	1.99	0.45	
8:J:36:LEU:HD21	8:J:50:ILE:HB	1.99	0.45	
1:A:388:LEU:HD22	1:A:432:VAL:CB	2.46	0.45	
2:B:98:THR:HG22	2:B:99:LYS:H	1.82	0.45	
2:B:345:LYS:HA	2:B:348:ARG:NH1	2.32	0.45	
2:B:402:GLY:HA2	2:B:695:ALA:HB3	1.99	0.45	
9:K:21:ILE:HG12	9:K:33:ILE:HG12	1.97	0.45	
1:A:682:THR:HG23	1:A:728:LYS:NZ	2.32	0.44	
1:A:709:THR:HG21	7:I:93:LYS:O	2.17	0.44	
2:B:757:PRO:HD3	2:B:983:ARG:CZ	2.47	0.44	
3:C:71:PRO:C	3:C:72:LEU:HD23	2.38	0.44	
3:C:261:ALA:O	3:C:265:MET:HB2	2.17	0.44	
5:F:85:MET:O	5:F:155:LEU:HD21	2.17	0.44	
10:L:68:GLU:C	10:L:70:ARG:H	2.21	0.44	
1:A:849:MET:CE	1:A:1437:GLY:H	2.31	0.44	
1:A:1025:ARG:O	1:A:1035:TYR:HE1	2.00	0.44	
1:A:1348:LEU:HD21	1:A:1375:MET:HE2	1.99	0.44	
2:B:872:GLU:HG2	2:B:916:THR:OG1	2.17	0.44	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
3:C:35:ARG:HH12	9:K:41:THR:H	1.64	0.44	
3:C:239:PRO:O	3:C:242:GLN:HB2	2.16	0.44	
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.98	0.44	
1:A:35:ILE:HA	1:A:52:GLY:O	2.17	0.44	
1:A:208:LEU:HD23	1:A:208:LEU:O	2.17	0.44	
1:A:589:GLN:HB2	1:A:961:ARG:NH2	2.32	0.44	
1:A:704:ALA:HB2	1:A:710:LEU:HA	1.99	0.44	
1:A:1150:SER:HB3	1:A:1195:LEU:HD22	2.00	0.44	
1:A:1190:PRO:HG3	7:I:18:GLU:OE2	2.18	0.44	
1:A:54:ASN:HD21	1:A:259:GLU:HG2	1.83	0.44	
1:A:472:LEU:HD13	2:B:835:GLN:HE21	1.82	0.44	
1:A:854:ASN:O	1:A:867:ILE:HA	2.17	0.44	
1:A:1144:LYS:HB2	1:A:1268:LEU:O	2.18	0.44	
2:B:405:ARG:HA	2:B:631:GLY:O	2.17	0.44	
4:E:159:ASP:HA	4:E:162:ARG:NH1	2.32	0.44	
1:A:549:MET:HE1	1:A:577:ILE:HD13	1.99	0.44	
1:A:940:ARG:O	1:A:944:ARG:HG3	2.18	0.44	
1:A:1220:PHE:HE1	1:A:1267:MET:HG2	1.83	0.44	
2:B:654:ARG:N	2:B:657:HIS:HD2	2.16	0.44	
2:B:744:HIS:HD2	2:B:746:SER:H	1.66	0.44	
2:B:1159:ARG:CG	2:B:1193:GLN:HE21	2.31	0.44	
6:H:42:ILE:HG23	6:H:95:TYR:CE1	2.53	0.44	
8:J:45:CYS:O	8:J:48:ARG:HG3	2.18	0.44	
1:A:247:ARG:HD3	1:A:263:THR:OG1	2.17	0.44	
1:A:1079:MET:HE3	1:A:1098:VAL:HG22	1.99	0.44	
2:B:53:GLN:HB2	2:B:547:VAL:CG2	2.48	0.44	
2:B:238:ALA:HB3	2:B:256:VAL:HB	2.00	0.44	
2:B:849:GLY:HA2	2:B:852:ARG:HG3	1.99	0.44	
2:B:1177:HIS:HB2	2:B:1179:GLN:HE21	1.81	0.44	
3:C:66:ARG:NH2	8:J:3:VAL:O	2.51	0.44	
1:A:16:GLU:HG3	2:B:1220:ARG:HA	1.99	0.44	
1:A:57:ARG:O	1:A:68:GLN:HG3	2.16	0.44	
1:A:248:PRO:O	1:A:260:ASP:HB2	2.17	0.44	
1:A:672:ASP:HB2	1:A:736:ASN:OD1	2.17	0.44	
1:A:1295:THR:HG22	1:A:1295:THR:O	2.18	0.44	
1:A:1315:GLU:O	1:A:1318:THR:HG22	2.17	0.44	
1:A:1424:VAL:O	1:A:1428:VAL:HG23	2.17	0.44	
2:B:46:GLN:HE21	2:B:496:ARG:HH11	1.66	0.44	
2:B:1009:ASP:O	2:B:1010:LEU:HD12	2.18	0.44	
5:F:138:LEU:HD12	5:F:142:SER:OG	2.18	0.44	
10:L:61:THR:HB	10:L:63:ARG:HG2	1.99	0.44	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:A:185:TRP:O	1:A:186:LYS:HB2	2.18	0.44	
1:A:302:THR:HG21	1:A:312:PRO:CG	2.48	0.44	
2:B:299:GLU:HG2	2:B:571:PRO:HG2	1.98	0.44	
2:B:791:THR:O	2:B:857:ARG:HA	2.18	0.44	
6:H:81:PRO:HD2	6:H:82:PRO:HD2	1.99	0.44	
1:A:445:ASN:ND2	1:A:446:ARG:N	2.65	0.44	
5:F:81:THR:HG21	5:F:136:ARG:CD	2.48	0.44	
6:H:62:SER:O	6:H:63:LEU:C	2.56	0.44	
7:I:50:THR:HB	7:I:92:ARG:HH12	1.82	0.44	
1:A:647:GLY:O	1:A:651:LYS:HG3	2.18	0.43	
1:A:768:GLN:HG3	1:A:816:HIS:HA	2.00	0.43	
1:A:1364:ASN:HD22	1:A:1366:ARG:N	2.15	0.43	
2:B:491:THR:O	2:B:495:LEU:HD12	2.18	0.43	
2:B:979:LYS:NZ	2:B:987:LYS:HD2	2.33	0.43	
8:J:64:ASN:N	8:J:65:PRO:CD	2.81	0.43	
1:A:523:ILE:HD13	1:A:622:VAL:HG13	2.00	0.43	
2:B:235:SER:OG	2:B:236:HIS:HD2	2.01	0.43	
2:B:900:ALA:HB2	10:L:58:LYS:HD2	2.00	0.43	
3:C:62:PHE:CD2	3:C:66:ARG:HD2	2.53	0.43	
8:J:64:ASN:H	8:J:65:PRO:HD2	1.81	0.43	
1:A:533:LYS:HE3	1:A:745:GLN:HE22	1.83	0.43	
1:A:642:CYS:O	1:A:645:LEU:HB3	2.19	0.43	
1:A:800:VAL:HG22	1:A:812:GLU:HB3	2.00	0.43	
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.99	0.43	
1:A:1152:ILE:HA	1:A:1192:LEU:O	2.18	0.43	
1:A:1328:TYR:CG	1:A:1329:THR:N	2.86	0.43	
2:B:548:GLY:N	2:B:612:GLU:OE2	2.51	0.43	
3:C:136:ASP:C	3:C:138:GLU:H	2.21	0.43	
3:C:148:ARG:HD2	8:J:61:LEU:O	2.19	0.43	
4:E:93:MET:HG3	4:E:97:VAL:HG23	2.00	0.43	
7:I:45:ARG:HG2	7:I:45:ARG:NH1	2.28	0.43	
1:A:276:LEU:HD13	1:A:292:ALA:HB3	2.01	0.43	
1:A:958:VAL:HG11	1:A:1049:ILE:HG23	2.00	0.43	
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.33	0.43	
1:A:1341:ILE:CG1	1:A:1376:THR:HG23	2.48	0.43	
1:A:1438:THR:CG2	2:B:1144:ALA:H	2.29	0.43	
2:B:785:TYR:CE2	2:B:795:ILE:HG12	2.53	0.43	
2:B:798:TYR:CD2	8:J:4:PRO:HG3	2.54	0.43	
2:B:973:ILE:O	2:B:975:GLN:HG3	2.18	0.43	
3:C:38:ILE:CG1	3:C:176:ILE:HD12	2.48	0.43	
5:F:116:ASP:O	5:F:120:ILE:HG13	2.18	0.43	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:79:GLY:HA3	1:A:245:PRO:CG	2.45	0.43	
1:A:313:GLN:HG2	1:A:322:VAL:HB	2.00	0.43	
1:A:446:ARG:HB2	1:A:487:MET:HE2	2.00	0.43	
1:A:774:ARG:HB2	1:A:797:LYS:HB3	2.00	0.43	
1:A:1104:ILE:HD13	1:A:1351:GLU:HB3	2.01	0.43	
2:B:46:GLN:HE21	2:B:496:ARG:NH1	2.16	0.43	
2:B:446:LEU:O	2:B:448:ILE:HG13	2.18	0.43	
2:B:979:LYS:HE2	2:B:1095:LEU:HD12	2.00	0.43	
3:C:185:LYS:HG2	3:C:213:PRO:HB3	2.00	0.43	
4:E:204:THR:CG2	4:E:205:SER:N	2.81	0.43	
5:F:109:VAL:HG23	5:F:124:GLU:HG2	2.00	0.43	
2:B:274:PRO:HG3	2:B:359:GLU:HB3	2.00	0.43	
2:B:327:ARG:NH2	2:B:371:GLU:HG2	2.34	0.43	
2:B:800:GLN:O	2:B:818:PRO:HB2	2.18	0.43	
3:C:242:GLN:NE2	3:C:246:ARG:HE	2.16	0.43	
1:A:881:GLN:CD	1:A:959:ASN:HA	2.39	0.43	
1:A:1264:GLU:HA	1:A:1267:MET:HE2	2.01	0.43	
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.59	0.43	
2:B:212:LEU:HD11	2:B:461:LEU:HD11	2.00	0.43	
2:B:860:MET:HA	2:B:964:VAL:O	2.18	0.43	
2:B:877:PRO:HB3	2:B:915:THR:CG2	2.48	0.43	
1:A:440:ASP:OD1	1:A:498:ARG:NH2	2.52	0.43	
1:A:605:MET:HE3	1:A:612:ILE:HG13	2.01	0.43	
1:A:1287:TYR:CD1	1:A:1305:VAL:HG21	2.54	0.43	
2:B:557:PHE:CZ	2:B:603:LEU:HD11	2.54	0.43	
2:B:561:TRP:O	2:B:590:HIS:HE1	2.02	0.43	
2:B:1222:ARG:H	2:B:1222:ARG:CD	2.21	0.43	
3:C:260:LEU:HD12	3:C:260:LEU:O	2.18	0.43	
4:E:22:MET:HA	4:E:187:TYR:CZ	2.54	0.43	
1:A:262:LEU:O	1:A:266:LEU:HG	2.19	0.43	
1:A:566:ILE:O	1:A:567:LYS:O	2.37	0.43	
1:A:1118:VAL:O	1:A:1118:VAL:HG23	2.18	0.43	
2:B:281:PRO:CG	2:B:284:ILE:HD12	2.46	0.43	
2:B:681:TRP:CH2	2:B:690:VAL:HG11	2.54	0.43	
2:B:796:LEU:O	2:B:799:PRO:HD3	2.18	0.43	
2:B:1212:ILE:O	2:B:1214:PRO:HD3	2.19	0.43	
3:C:58:LEU:HD22	3:C:62:PHE:CE2	2.53	0.43	
6:H:18:GLY:O	6:H:20:TYR:N	2.52	0.43	
7:I:19:ASP:OD1	7:I:22:ASN:HB2	2.19	0.43	
1:A:187:LYS:O	1:A:188:ASP:HB2	2.18	0.43	
1:A:329:LEU:C	1:A:331:GLY:H	2.21	0.43	



			Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
2:B:293:PRO:HG2	2:B:296:GLU:CB	2.47	0.43	
2:B:986:GLN:NE2	2:B:987:LYS:O	2.48	0.43	
3:C:43:THR:O	3:C:161:LYS:HA	2.19	0.43	
4:E:153:HIS:CG	4:E:184:VAL:HG11	2.54	0.43	
7:I:50:THR:HB	7:I:92:ARG:NH2	2.33	0.43	
3:C:63:ILE:O	3:C:67:LEU:HG	2.19	0.42	
3:C:169:LYS:NZ	10:L:70:ARG:HG2	2.34	0.42	
1:A:73:GLY:C	1:A:75:ASN:H	2.22	0.42	
1:A:550:LEU:HD13	1:A:556:TRP:CZ2	2.54	0.42	
1:A:914:GLU:C	1:A:916:GLY:N	2.72	0.42	
2:B:497:ARG:HG3	2:B:498:THR:H	1.84	0.42	
3:C:13:ALA:O	9:K:114:LEU:HB3	2.18	0.42	
1:A:914:GLU:O	1:A:916:GLY:N	2.52	0.42	
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.83	0.42	
2:B:268:THR:CG2	2:B:270:LYS:HE3	2.46	0.42	
2:B:281:PRO:HB3	2:B:320:ASP:OD2	2.19	0.42	
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.34	0.42	
4:E:77:SER:HG	4:E:105:PHE:HD2	1.64	0.42	
1:A:1173:HIS:NE2	1:A:1227:ILE:HG23	2.35	0.42	
2:B:225:VAL:HA	2:B:237:VAL:O	2.20	0.42	
2:B:424:LEU:O	2:B:428:ILE:HG13	2.19	0.42	
2:B:750:GLY:O	2:B:754:SER:HB2	2.19	0.42	
2:B:794:ASN:C	2:B:795:ILE:HD12	2.39	0.42	
9:K:78:THR:HG22	9:K:79:GLU:N	2.35	0.42	
1:A:38:PRO:C	1:A:39:GLU:HG3	2.38	0.42	
1:A:557:ASP:HA	9:K:26:LYS:HD2	2.02	0.42	
1:A:741:ASN:ND2	1:A:743:VAL:HB	2.34	0.42	
1:A:974:ASP:HA	6:H:136:LYS:HE2	2.01	0.42	
1:A:1436:ILE:O	1:A:1437:GLY:C	2.58	0.42	
2:B:760:ASP:OD1	2:B:760:ASP:N	2.53	0.42	
2:B:784:ASN:HB3	8:J:63:TYR:OH	2.19	0.42	
2:B:875:GLU:HG2	2:B:895:ASP:O	2.20	0.42	
2:B:953:LEU:CD2	2:B:955:THR:HG23	2.43	0.42	
2:B:983:ARG:HH11	2:B:1091:TYR:CB	2.32	0.42	
3:C:18:VAL:HG12	3:C:20:PHE:HD2	1.84	0.42	
9:K:58:PHE:HE2	9:K:74:ARG:HB3	1.84	0.42	
1:A:450:LEU:HD12	1:A:450:LEU:N	2.25	0.42	
1:A:636:GLU:OE2	1:A:962:ARG:HD3	2.19	0.42	
1:A:699:ALA:O	1:A:700:ASN:HB3	2.20	0.42	
1:A:853:ASP:OD1	1:A:855:THR:CB	2.66	0.42	
1:A:1008:GLN:O	1:A:1012:ARG:HG3	2.18	0.42	



	1 J	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
2:B:46:GLN:NE2	2:B:496:ARG:HB3	2.28	0.42	
2:B:244:LEU:HD11	2:B:366:GLN:HE22	1.85	0.42	
2:B:1023:VAL:HG12	2:B:1027:ILE:CD1	2.49	0.42	
4:E:16:PHE:CE2	4:E:20:LYS:HE2	2.54	0.42	
1:A:342:GLY:O	1:A:345:VAL:HG13	2.20	0.42	
1:A:808:LEU:HD12	1:A:808:LEU:N	2.34	0.42	
2:B:315:LYS:HE3	2:B:315:LYS:HB2	1.80	0.42	
2:B:586:TRP:NE1	2:B:588:GLY:O	2.52	0.42	
2:B:957:ASN:ND2	2:B:958:GLN:N	2.65	0.42	
3:C:57:VAL:O	3:C:57:VAL:CG1	2.67	0.42	
7:I:17:ARG:CG	7:I:28:GLU:HG2	2.48	0.42	
9:K:90:ALA:O	9:K:94:ILE:HG13	2.19	0.42	
1:A:551:TYR:CE1	9:K:74:ARG:HD3	2.55	0.42	
2:B:653:VAL:HG12	2:B:689:LEU:HD13	2.02	0.42	
2:B:654:ARG:H	2:B:657:HIS:HD2	1.67	0.42	
2:B:950:ASP:O	2:B:951:GLN:HB2	2.20	0.42	
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.40	0.42	
8:J:32:GLU:H	8:J:32:GLU:CD	2.23	0.42	
9:K:21:ILE:HG23	9:K:31:VAL:CG1	2.50	0.42	
1:A:92:HIS:CD2	1:A:94:GLY:H	2.38	0.42	
1:A:329:LEU:HD23	1:A:332:LYS:HB2	2.00	0.42	
2:B:102:VAL:HG11	2:B:122:LEU:HD13	2.01	0.42	
2:B:174:LEU:HD12	2:B:174:LEU:N	2.35	0.42	
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	2.01	0.42	
4:E:78:LEU:HD11	4:E:109:ILE:HG13	2.02	0.42	
1:A:2:VAL:O	1:A:2:VAL:HG13	2.20	0.42	
1:A:337:ARG:HH12	1:A:1403:GLU:HA	1.85	0.42	
2:B:383:ASN:O	2:B:387:LEU:HB2	2.20	0.42	
3:C:58:LEU:HD12	3:C:145:CYS:SG	2.60	0.42	
7:I:35:VAL:HG22	7:I:36:GLU:N	2.35	0.42	
1:A:834:THR:HG21	1:A:1077:THR:CA	2.47	0.41	
2:B:35:SER:HA	2:B:811:TYR:CE2	2.55	0.41	
2:B:844:SER:OG	2:B:996:ARG:N	2.43	0.41	
2:B:1002:THR:HG21	2:B:1006:ILE:HB	2.02	0.41	
3:C:42:PRO:HA	3:C:163:ILE:HD12	2.02	0.41	
3:C:43:THR:CG2	3:C:44:LEU:N	2.83	0.41	
6:H:97:MET:CE	6:H:142:LEU:HD23	2.50	0.41	
1:A:855:THR:CG2	1:A:857:ARG:HG3	2.43	0.41	
1:A:1115:SER:HA	1:A:1308:THR:O	2.21	0.41	
2:B:94:LYS:HD3	2:B:96:TYR:CZ	2.55	0.41	
2:B:858:SER:HA	2:B:966:VAL:O	2.20	0.41	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
4:E:204:THR:HG22	4:E:205:SER:N	2.36	0.41	
9:K:18:LYS:HE3	9:K:38:GLU:HG2	2.02	0.41	
1:A:391:LEU:HD23	1:A:400:PRO:O	2.20	0.41	
1:A:925:LEU:HD13	1:A:983:ILE:HD12	2.02	0.41	
1:A:975:HIS:ND1	1:A:1036:ARG:HG3	2.35	0.41	
1:A:1319:VAL:HG13	1:A:1320:PRO:HD2	2.03	0.41	
2:B:1163:CYS:SG	2:B:1165:ILE:HB	2.61	0.41	
3:C:166:GLU:HA	9:K:6:ARG:HB3	2.01	0.41	
4:E:59:SER:OG	4:E:81:GLU:HA	2.21	0.41	
4:E:88:VAL:HG21	4:E:110:PHE:CE2	2.55	0.41	
6:H:125:LEU:HB3	6:H:130:ARG:CZ	2.50	0.41	
8:J:52:THR:HG22	8:J:52:THR:O	2.19	0.41	
9:K:21:ILE:HD13	9:K:84:LYS:HE2	2.01	0.41	
1:A:103:CYS:SG	1:A:207:ILE:HG23	2.60	0.41	
1:A:369:SER:CB	9:K:2:ASN:HD21	2.33	0.41	
2:B:339:THR:CG2	2:B:343:ILE:HB	2.50	0.41	
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.49	0.41	
2:B:640:VAL:HG22	2:B:651:LEU:CD2	2.50	0.41	
3:C:35:ARG:HH11	9:K:41:THR:N	2.18	0.41	
3:C:265:MET:HE1	9:K:19:LEU:O	2.20	0.41	
4:E:94:LYS:O	4:E:98:ILE:HG13	2.20	0.41	
6:H:82:PRO:O	6:H:84:ALA:N	2.52	0.41	
1:A:63:ARG:HA	1:A:74:MET:HE2	2.02	0.41	
1:A:106:VAL:CG2	1:A:111:GLY:C	2.89	0.41	
1:A:246:VAL:O	1:A:328:ARG:NH2	2.54	0.41	
1:A:356:ASP:OD2	9:K:65:HIS:HE1	2.04	0.41	
1:A:396:PRO:HG3	1:A:416:ARG:HB3	2.02	0.41	
1:A:605:MET:CE	1:A:612:ILE:HG13	2.51	0.41	
1:A:1164:PRO:HG2	1:A:1165:GLU:H	1.85	0.41	
2:B:121:ASN:HA	2:B:207:GLY:CA	2.51	0.41	
2:B:235:SER:HA	2:B:261:ARG:NH2	2.35	0.41	
2:B:361:LEU:O	2:B:374:LYS:HE2	2.21	0.41	
2:B:875:GLU:O	2:B:877:PRO:HD3	2.21	0.41	
2:B:995:ARG:HD2	2:B:997:GLU:OE2	2.20	0.41	
3:C:22:LEU:CD2	9:K:101:LEU:HD21	2.50	0.41	
8:J:57:ILE:HA	8:J:60:PHE:CD2	2.55	0.41	
1:A:476:SER:N	1:A:477:PRO:HD2	2.36	0.41	
1:A:556:TRP:CH2	1:A:558:GLY:HA2	2.56	0.41	
2:B:242:SER:O	2:B:251:ILE:HA	2.19	0.41	
2:B:324:ILE:HD11	2:B:333:PHE:CG	2.56	0.41	
2:B:515:HIS:CD2	2:B:517:THR:H	2.23	0.41	



			Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:B:1159:ARG:HG3	2:B:1193:GLN:HE21	1.85	0.41	
7:I:16:PRO:HA	7:I:26:LEU:O	2.21	0.41	
9:K:65:HIS:CD2	9:K:66:PRO:HD2	2.55	0.41	
1:A:32:VAL:HG23	1:A:33:ALA:H	1.85	0.41	
1:A:406:ILE:HD12	1:A:406:ILE:N	2.36	0.41	
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.21	0.41	
2:B:123:THR:OG1	2:B:458:LYS:HE3	2.21	0.41	
2:B:757:PRO:HD3	2:B:983:ARG:HH21	1.86	0.41	
2:B:886:LYS:C	2:B:888:GLY:H	2.24	0.41	
2:B:1183:LYS:C	2:B:1185:CYS:H	2.24	0.41	
3:C:258:ILE:HG23	9:K:19:LEU:HD11	2.02	0.41	
6:H:5:LEU:HD11	6:H:135:LEU:HG	2.03	0.41	
1:A:81:PHE:HA	1:A:243:PRO:HD3	2.03	0.41	
1:A:186:LYS:HG2	1:A:187:LYS:H	1.86	0.41	
1:A:378:GLU:OE1	1:A:434:ARG:HD3	2.21	0.41	
2:B:115:GLN:HG2	2:B:193:LYS:CB	2.50	0.41	
2:B:339:THR:HG22	2:B:340:ALA:O	2.20	0.41	
2:B:870:ILE:HD11	2:B:919:SER:OG	2.21	0.41	
6:H:12:VAL:HG13	6:H:26:ILE:CG2	2.51	0.41	
6:H:113:ALA:HA	6:H:125:LEU:O	2.21	0.41	
7:I:98:VAL:CG2	7:I:111:THR:HG22	2.50	0.41	
7:I:103:CYS:SG	7:I:105:SER:HB2	2.60	0.41	
10:L:26:THR:C	10:L:27:LEU:HD23	2.41	0.41	
1:A:91:PHE:HZ	1:A:207:ILE:HG13	1.86	0.41	
1:A:220:THR:O	1:A:222:LEU:O	2.39	0.41	
1:A:313:GLN:CB	1:A:320:ARG:HB3	2.51	0.41	
1:A:590:ARG:HH11	1:A:590:ARG:HG2	1.86	0.41	
1:A:850:VAL:HG21	1:A:1058:VAL:HG21	2.03	0.41	
1:A:1027:ALA:O	1:A:1031:VAL:HG23	2.21	0.41	
1:A:1104:ILE:CD1	1:A:1351:GLU:HB3	2.51	0.41	
2:B:97:VAL:HG12	2:B:178:ASN:ND2	2.35	0.41	
2:B:129:PHE:CZ	2:B:166:PHE:HB2	2.56	0.41	
2:B:165:VAL:HG12	2:B:167:ILE:HG13	2.03	0.41	
2:B:351:TYR:CE2	2:B:355:ILE:HD11	2.55	0.41	
2:B:1006:ILE:HD11	8:J:43:ARG:CB	2.46	0.41	
3:C:40:GLU:OE2	3:C:254:LYS:NZ	2.44	0.41	
3:C:62:PHE:CE2	3:C:66:ARG:HD2	2.55	0.41	
3:C:163:ILE:CG2	3:C:165:LYS:H	2.33	0.41	
4:E:72:PHE:HE2	4:E:157:SER:HA	1.85	0.41	
6:H:15:VAL:HG22	6:H:26:ILE:HG12	2.03	0.41	
6:H:36:CYS:HA	6:H:126:GLU:O	2.21	0.41	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
8:J:39:LEU:HD23	8:J:39:LEU:HA	1.92	0.41	
8:J:41:LEU:HD22	8:J:46:CYS:HB3	2.02	0.41	
1:A:120:GLU:HG3	1:A:123:ARG:NH2	2.36	0.41	
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.36	0.41	
1:A:901:LEU:HA	1:A:907:THR:HG23	2.03	0.41	
1:A:946:VAL:CG2	4:E:201:LYS:HD2	2.45	0.41	
1:A:1059:HIS:CE1	5:F:155:LEU:HD22	2.45	0.41	
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.51	0.41	
2:B:795:ILE:HD12	2:B:795:ILE:N	2.36	0.41	
2:B:906:SER:O	2:B:907:GLY:C	2.58	0.41	
9:K:21:ILE:HG21	9:K:84:LYS:HE2	2.03	0.41	
1:A:24:PRO:O	1:A:28:ARG:HG3	2.21	0.40	
1:A:334:GLY:HA2	1:A:337:ARG:HB3	2.02	0.40	
1:A:463:ILE:HB	1:A:464:PRO:HD2	2.03	0.40	
1:A:473:SER:OG	1:A:522:GLY:O	2.23	0.40	
1:A:548:ASN:HA	9:K:60:ALA:HB1	2.02	0.40	
2:B:324:ILE:HG12	2:B:329:THR:CG2	2.45	0.40	
6:H:27:GLU:HA	6:H:38:LEU:O	2.20	0.40	
9:K:29:ASN:ND2	9:K:79:GLU:HA	2.35	0.40	
1:A:849:MET:HE1	1:A:1436:ILE:HA	2.00	0.40	
1:A:1120:LEU:HD21	1:A:1131:ALA:HA	2.02	0.40	
1:A:1150:SER:OG	7:I:46:HIS:HB3	2.21	0.40	
1:A:115:LEU:HD12	1:A:142:CYS:SG	2.61	0.40	
1:A:302:THR:HG23	1:A:306:ASN:ND2	2.36	0.40	
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.21	0.40	
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.21	0.40	
1:A:1345:ARG:NH1	1:A:1373:ASP:OD1	2.54	0.40	
2:B:217:ARG:HG2	2:B:218:SER:O	2.21	0.40	
4:E:201:LYS:HD3	4:E:201:LYS:HA	1.92	0.40	
9:K:18:LYS:HE3	9:K:38:GLU:CG	2.52	0.40	
1:A:305:ASP:O	1:A:308:ILE:HD11	2.21	0.40	
1:A:690:VAL:HG11	1:A:794:PRO:HD3	2.03	0.40	
1:A:1365:TYR:CD2	1:A:1365:TYR:C	2.94	0.40	
1:A:1376:THR:CG2	4:E:212:ARG:NH2	2.76	0.40	
2:B:344:LYS:HB2	2:B:347:LYS:HE2	2.02	0.40	
2:B:483:LEU:HD11	2:B:491:THR:HG23	2.04	0.40	
2:B:882:THR:HB	2:B:934:LYS:O	2.22	0.40	
2:B:1057:LYS:O	2:B:1061:GLU:HG3	2.21	0.40	
3:C:73:GLN:HA	3:C:133:ILE:HD11	2.02	0.40	
5:F:107:VAL:HG13	5:F:124:GLU:OE2	2.22	0.40	
1:A:298:PHE:CZ	1:A:312:PRO:HD3	2.57	0.40	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:A:333:GLU:O	1:A:337:ARG:HB2	2.22	0.40	
1:A:592:ASP:O	1:A:593:GLU:C	2.60	0.40	
1:A:901:LEU:CD2	1:A:907:THR:HG23	2.51	0.40	
2:B:259:TYR:HB2	2:B:268:THR:HG22	2.04	0.40	
2:B:311:LEU:HA	2:B:314:LEU:HD12	2.04	0.40	
2:B:840:ILE:HB	2:B:1011:ILE:HB	2.04	0.40	
2:B:996:ARG:NH2	3:C:174:ALA:O	2.54	0.40	
3:C:3:GLU:HB2	9:K:104:ASN:OD1	2.21	0.40	
3:C:250:THR:O	3:C:254:LYS:HG3	2.22	0.40	
6:H:32:THR:HB	6:H:33:GLN:H	1.54	0.40	
8:J:53:HIS:CG	8:J:54:VAL:N	2.90	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	А	1411/1733 (81%)	1250 (89%)	123~(9%)	38~(3%)	5	3
2	В	1074/1224~(88%)	950~(88%)	110 (10%)	14 (1%)	12	12
3	С	264/318~(83%)	236 (89%)	24 (9%)	4 (2%)	10	10
4	Е	213/215~(99%)	189 (89%)	22 (10%)	2(1%)	17	20
5	F	82/155~(53%)	76~(93%)	5~(6%)	1 (1%)	13	14
6	Η	129/146~(88%)	93~(72%)	21 (16%)	15 (12%)	0	0
7	Ι	120/122~(98%)	103 (86%)	17 (14%)	0	100	100
8	J	63/70~(90%)	59~(94%)	3~(5%)	1 (2%)	9	9
9	K	112/120~(93%)	106 (95%)	6 (5%)	0	100	100
10	L	44/70~(63%)	25~(57%)	16 (36%)	3(7%)	1	0
All	All	3512/4173 (84%)	3087 (88%)	347 (10%)	78 (2%)	6	5





All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	55	ASP
1	А	464	PRO
1	А	465	TYR
1	А	466	SER
1	А	567	LYS
1	А	593	GLU
1	А	1393	ASN
2	В	1222	ARG
6	Н	128	ASN
1	А	35	ILE
1	А	307	ASP
1	А	467	THR
1	А	525	GLN
1	А	1398	MET
2	В	646	LEU
2	В	879	ARG
2	В	887	HIS
3	С	4	GLU
3	С	231	ASN
4	Е	3	GLN
4	Е	50	MET
6	Н	18	GLY
6	Н	19	ARG
6	Н	61	SER
6	Н	78	SER
6	Н	105	GLU
6	Н	138	GLU
1	А	67	CYS
1	А	156	ASP
1	A	258	GLY
1	А	283	GLY
1	A	626	ASN
1	A	915	SER
1	А	958	VAL
1	А	1386	ARG
2	В	165	VAL
2	В	262	GLU
2	В	266	ALA
2	В	1190	ASP
3	С	90	ASP
3	С	137	LYS
5	F	73	ALA



Mol	Chain	Res	Type
6	Н	52	GLN
6	Н	81	PRO
6	Н	103	LYS
8	J	44	TYR
10	L	39	SER
1	А	72	GLU
1	А	188	ASP
1	А	194	ALA
1	А	196	GLU
1	А	248	PRO
1	А	752	LYS
1	А	764	CYS
2	В	864	LYS
2	В	1100	ASP
6	Н	62	SER
10	L	56	LEU
10	L	59	ALA
1	А	257	ARG
1	А	308	ILE
1	А	419	LYS
1	А	959	ASN
1	А	1402	PHE
2	В	90	ILE
2	В	1099	VAL
6	Н	83	GLN
6	Н	109	LYS
6	Н	139	ASN
1	А	250	ILE
6	Н	47	PHE
1	А	84	ILE
1	А	399	HIS
2	В	1214	PRO
1	А	61	ILE
2	В	1109	GLY
1	А	1114	PRO
1	А	400	PRO

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#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.



Mol	Chain	Chain Analysed Rotameric Outliers		Outliers	Percentiles		
1	А	1239/1520~(82%)	1180~(95%)	59~(5%)	25 36		
2	В	950/1061 (90%)	903~(95%)	47 (5%)	25 35		
3	С	234/274~(85%)	226~(97%)	8(3%)	37 51		
4	Ε	197/197~(100%)	191~(97%)	6 (3%)	41 57		
5	F	74/137~(54%)	71~(96%)	3~(4%)	30 43		
6	Н	117/128~(91%)	115~(98%)	2(2%)	60 76		
7	Ι	116/116~(100%)	109 (94%)	7~(6%)	19 26		
8	J	60/65~(92%)	52 (87%)	8 (13%)	4 4		
9	Κ	99/102~(97%)	93~(94%)	6~(6%)	18 25		
10	L	40/57~(70%)	35(88%)	5 (12%)	4 5		
All	All	3126/3657~(86%)	2975 (95%)	151 (5%)	25 36		

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

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	22	PHE
1	А	53	LEU
1	А	93	VAL
1	А	171	GLN
1	А	175	ARG
1	А	209	ASN
1	А	221	SER
1	А	385	ILE
1	А	386	ASP
1	А	434	ARG
1	А	446	ARG
1	А	449	SER
1	А	450	LEU
1	А	451	HIS
1	А	452	LYS
1	А	467	THR
1	А	472	LEU
1	А	474	VAL
1	А	475	THR
1	А	493	GLN
1	А	498	ARG
1	А	503	GLN



Mol	Chain	Res	Type
1	А	504	LEU
1	А	513	SER
1	А	535	THR
1	А	596	THR
1	А	597	LEU
1	А	618	GLU
1	А	622	VAL
1	А	626	ASN
1	А	666	ILE
1	А	672	ASP
1	А	756	ILE
1	А	769	SER
1	А	774	ARG
1	А	821	ARG
1	А	855	THR
1	А	858	ASN
1	А	873	MET
1	А	885	THR
1	А	903	ASN
1	А	919	ILE
1	А	920	LEU
1	А	940	ARG
1	А	1043	ASP
1	А	1048	ASN
1	А	1130	GLN
1	А	1166	ASP
1	А	1222	ASN
1	А	1277	GLU
1	А	1293	SER
1	А	1297	GLU
1	А	1309	ASP
1	А	1318	THR
1	A	1366	ARG
1	А	1372	VAL
1	A	1377	THR
1	A	1383	SER
1	A	1426	GLU
2	В	18	PHE
2	В	20	ASP
2	В	21	GLU
2	В	61	ASP
2	В	121	ASN



Mol	Chain	Res	Type
2	В	194	GLU
2	В	217	ARG
2	В	261	ARG
2	В	268	THR
2	В	313	MET
2	В	339	THR
2	В	357	GLN
2	В	366	GLN
2	В	372	SER
2	В	463	THR
2	В	466	TRP
2	В	485	ARG
2	В	496	ARG
2	В	540	SER
2	В	563	MET
2	В	567	GLU
2	В	589	VAL
2	В	612	GLU
2	В	636	PRO
2	В	641	GLU
2	В	644	GLU
2	В	737	THR
2	В	754	SER
2	В	790	ASP
2	В	806	THR
2	В	864	LYS
2	В	895	ASP
2	В	957	ASN
2	В	970	THR
2	В	997	GLU
2	В	999	MET
2	В	1007	VAL
2	В	1065	GLN
2	В	1097	HIS
2	В	1099	VAL
2	В	1145	SER
2	В	1150	ARG
2	В	1152	MET
2	В	1159	ARG
2	В	1186	ASP
2	В	1219	ASP
2	В	1222	ARG



Mol	Chain	Res	Type
3	С	23	SER
3	С	26	ASP
3	С	50	GLU
3	С	77	ILE
3	С	163	ILE
3	С	170	TRP
3	С	209	TYR
3	С	240	VAL
4	Е	104	ASN
4	Е	123	LEU
4	Е	146	HIS
4	Е	159	ASP
4	Е	196	VAL
4	Е	204	THR
5	F	79	ARG
5	F	82	THR
5	F	115	THR
6	Н	32	THR
6	Н	104	PHE
7	Ι	12	ASN
7	Ι	46	HIS
7	Ι	50	THR
7	Ι	61	ASP
7	Ι	84	VAL
7	Ι	87	GLN
7	Ι	111	THR
8	J	1	MET
8	J	3	VAL
8	J	7	CYS
8	J	14	VAL
8	J	28	ASP
8	J	37	SER
8	J	38	ARG
8	J	48	ARG
9	K	11	LEU
9	K	18	LYS
9	K	47	ARG
9	K	73	LEU
9	K	81	TYR
9	K	114	LEU
10	L	27	LEU
10	L	38	LEU



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Mol	Chain	Res	Type
10	L	42	ARG
10	L	50	ASP
10	L	64	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	64	ASN
1	А	68	GLN
1	А	83	HIS
1	А	92	HIS
1	А	171	GLN
1	А	313	GLN
1	А	390	GLN
1	А	394	ASN
1	А	397	ASN
1	А	479	ASN
1	А	503	GLN
1	А	517	ASN
1	А	660	ASN
1	А	736	ASN
1	А	741	ASN
1	А	742	ASN
1	А	745	GLN
1	А	757	ASN
1	А	768	GLN
1	А	854	ASN
1	А	858	ASN
1	А	903	ASN
1	А	906	HIS
1	А	926	GLN
1	А	994	GLN
1	А	1048	ASN
1	А	1052	GLN
1	А	1218	GLN
1	А	1265	ASN
1	А	1270	ASN
1	А	1364	ASN
1	А	1387	HIS
1	А	1432	GLN
2	В	46	GLN
2	В	178	ASN



Mol	Chain	Res	Type
2	В	215	GLN
2	В	236	HIS
2	В	255	GLN
2	В	325	GLN
2	В	363	HIS
2	В	366	GLN
2	В	465	ASN
2	В	484	ASN
2	В	513	GLN
2	В	515	HIS
2	В	516	ASN
2	В	518	HIS
2	В	587	HIS
2	В	590	HIS
2	В	657	HIS
2	В	706	GLN
2	В	734	HIS
2	В	744	HIS
2	В	786	ASN
2	В	957	ASN
2	В	1015	HIS
2	В	1062	HIS
2	В	1065	GLN
2	В	1084	GLN
2	В	1161	HIS
2	В	1176	ASN
2	В	1179	GLN
2	В	1187	ASN
2	В	1193	GLN
3	С	65	HIS
3	С	73	GLN
3	С	112	ASN
3	С	167	HIS
3	С	242	GLN
4	Е	101	GLN
4	Е	104	ASN
4	Е	113	GLN
4	Е	147	HIS
6	Н	11	GLN
6	Н	133	ASN
6	Н	134	ASN
7	Ι	12	ASN



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Mol	Chain	Res	Type
7	Ι	116	ASN
8	J	53	HIS
9	K	29	ASN
9	К	65	HIS
9	K	76	GLN
9	K	110	ASN
10	L	53	HIS

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 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	Type	Chain	Dog	Tink	Bo	ond leng	$_{\rm ths}$	B	ond ang	les
Moi Type Chain	nes Link		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2		
13	UTP	В	3571	12	22,30,30	1.40	3 (13%)	27,47,47	1.36	2 (7%)

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	UTP	В	3571	12	-	5/20/38/38	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	В	3571	UTP	C4-N3	4.38	1.40	1.33
13	В	3571	UTP	C6-N1	3.12	1.39	1.35
13	В	3571	UTP	PB-O1B	-2.09	1.45	1.55

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
13	В	3571	UTP	O4'-C1'-C2'	-4.26	100.70	106.93
13	В	3571	UTP	C5-C4-N3	-3.98	114.55	123.31

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	В	3571	UTP	PA-O3A-PB-O2B
13	В	3571	UTP	PB-O3B-PG-O2G
13	В	3571	UTP	PA-O3A-PB-O1B
13	В	3571	UTP	PB-O3B-PG-O1G
13	В	3571	UTP	PB-O3B-PG-O3G

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	В	3571	UTP	1	0

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





equivalents in the CSD to analyse the geometry.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

