

Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2021 – 03:18 pm BST

PDB ID	:	5FPH
Title	:	The GTPase domains of the immunity-related Irga6 dimerize in a parallel
		head-to-head fashion
Authors	:	Schulte, K.; Pawlowski, N.; Faelber, K.; Froehlich, C.; Howard, J.; Daumke,
		0.
Deposited on	:	2015-11-30
Resolution	:	3.20 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 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
EDS	:	2.23.1
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)	:	2.23.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.



Motria	Whole archive	Similar resolution		
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R_{free}	130704	1133 (3.20-3.20)		
Clashscore	141614	1253 (3.20-3.20)		
Ramachandran outliers	138981	1234 (3.20-3.20)		
Sidechain outliers	138945	1233 (3.20-3.20)		
RSRZ outliers	127900	1095 (3.20-3.20)		

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quali	ty of chain	
1	А	423	4% 52%	40%	• 7%
1	В	423	4%	47%	• 6%
1	С	423	49%	41%	• 8%
1	D	423	4% 50%	42%	• 6%
1	Е	423	3% 50%	41%	• 6%



Mol	Chain	Length	Quality of	f chain
			3%	
1	F	423	56%	36% • 7%
			2%	
1	G	423	52%	40% • 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GNP	А	501	-	-	Х	-
2	GNP	С	501	-	-	Х	-
2	GNP	Е	501	-	-	Х	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 22647 atoms, of which 24 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.

Mol	Chain	Residues		A	Atoms	5			ZeroOcc	AltConf	Trace
1	Δ	305	Total	С	Ν	Ο	\mathbf{S}	\mathbf{Se}	0	0	0
	A	595	3204	2062	522	606	4	10	0	0	0
1	В	306	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	\mathbf{Se}	0	0	0
	D	590	3204	2066	518	606	4	10	0	0	0
1	C	380	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	\mathbf{Se}	0	Ο	Ο
		009	3153	2033	514	592	4	10	0	0	0
1	а	306	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	\mathbf{Se}	0	0	0
	D	090	3193	2051	521	607	4	10	0	0	0
1	F	306	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	\mathbf{Se}	0	0	0
		090	3205	2065	521	605	4	10	0	0	0
1	F	304	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	\mathbf{Se}	0	0	0
L T	T,	094	3194	2055	521	604	4	10	0	0	0
1	C	200	Total	С	Ν	Ο	S	Se	0	0	0
	G	J99	3241	2086	527	614	4	10		U	U

• Molecule 1 is a protein called INTERFERON-INDUCIBLE GTPASE 1.

There are 98 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-9	GLY	-	expression tag	UNP Q9QZ85
А	-8	SER	-	expression tag	UNP Q9QZ85
А	-7	PRO	-	expression tag	UNP Q9QZ85
A	-6	GLY	-	expression tag	UNP Q9QZ85
А	-5	ILE	-	expression tag	UNP Q9QZ85
A	-4	PRO	-	expression tag	UNP Q9QZ85
A	-3	GLY	-	expression tag	UNP Q9QZ85
A	-2	SER	-	expression tag	UNP Q9QZ85
A	-1	THR	-	expression tag	UNP Q9QZ85
А	0	THR	-	expression tag	UNP Q9QZ85
A	31	GLU	ARG	engineered mutation	UNP Q9QZ85
А	32	GLU	LYS	engineered mutation	UNP Q9QZ85
А	176	GLU	LYS	engineered mutation	UNP Q9QZ85
А	246	GLU	LYS	engineered mutation	UNP Q9QZ85
В	-9	GLY	-	expression tag	UNP Q9QZ85



5FPH

Chain	Residue	Modelled	Actual	Comment	Reference
В	-8	SER	_	expression tag	UNP Q9QZ85
В	-7	PRO	_	expression tag	UNP Q9QZ85
В	-6	GLY	-	expression tag	UNP Q9QZ85
В	-5	ILE	-	expression tag	UNP Q9QZ85
В	-4	PRO	_	expression tag	UNP Q9QZ85
В	-3	GLY	-	expression tag	UNP Q9QZ85
В	-2	SER	-	expression tag	UNP Q9QZ85
В	-1	THR	-	expression tag	UNP Q9QZ85
В	0	THR	-	expression tag	UNP Q9QZ85
В	31	GLU	ARG	engineered mutation	UNP Q9QZ85
В	32	GLU	LYS	engineered mutation	UNP Q9QZ85
В	176	GLU	LYS	engineered mutation	UNP Q9QZ85
В	246	GLU	LYS	engineered mutation	UNP Q9QZ85
С	-9	GLY	-	expression tag	UNP Q9QZ85
С	-8	SER	-	expression tag	UNP Q9QZ85
С	-7	PRO	-	expression tag	UNP Q9QZ85
С	-6	GLY	-	expression tag	UNP Q9QZ85
С	-5	ILE	-	expression tag	UNP Q9QZ85
С	-4	PRO	-	expression tag	UNP Q9QZ85
С	-3	GLY	-	expression tag	UNP Q9QZ85
С	-2	SER	-	expression tag	UNP Q9QZ85
С	-1	THR	-	expression tag	UNP Q9QZ85
С	0	THR	-	expression tag	UNP Q9QZ85
C	31	GLU	ARG	engineered mutation	UNP Q9QZ85
C	32	GLU	LYS	engineered mutation	UNP Q9QZ85
C	176	GLU	LYS	engineered mutation	UNP Q9QZ85
C	246	GLU	LYS	engineered mutation	UNP Q9QZ85
D	-9	GLY	-	expression tag	UNP Q9QZ85
D	-8	SER	-	expression tag	UNP Q9QZ85
D	-7	PRO	-	expression tag	UNP Q9QZ85
D	-6	GLY	-	expression tag	UNP Q9QZ85
D	-5	ILE	-	expression tag	UNP Q9QZ85
D	-4	PRO	-	expression tag	UNP Q9QZ85
D	-3	GLY	-	expression tag	UNP Q9QZ85
D	-2	SER	-	expression tag	UNP Q9QZ85
D	-1	THR	-	expression tag	UNP Q9QZ85
D	0	THR	-	expression tag	UNP Q9QZ85
D	31	GLU	ARG	engineered mutation	UNP Q9QZ85
D	32	GLU	LYS	engineered mutation	UNP Q9QZ85
D	176	GLU	LYS	engineered mutation	UNP Q9QZ85
D	246	GLU	LYS	engineered mutation	UNP Q9QZ85
E	-9	GLY	-	expression tag	UNP Q9QZ85



nent	Reference
on tag	UNP Q9QZ85
1	UND OOOZOF

Chain	Residue	Modelled	Actual	Comment	Reference
Е	-8	SER	-	expression tag	UNP Q9QZ85
Е	-7	PRO	-	expression tag	UNP Q9QZ85
Е	-6	GLY	-	expression tag	UNP Q9QZ85
Е	-5	ILE	-	expression tag	UNP Q9QZ85
Е	-4	PRO	-	expression tag	UNP Q9QZ85
Е	-3	GLY	-	expression tag	UNP Q9QZ85
Е	-2	SER	-	expression tag	UNP Q9QZ85
E	-1	THR	-	expression tag	UNP Q9QZ85
Е	0	THR	-	expression tag	UNP Q9QZ85
Е	31	GLU	ARG	engineered mutation	UNP Q9QZ85
Е	32	GLU	LYS	engineered mutation	UNP Q9QZ85
Е	176	GLU	LYS	engineered mutation	UNP Q9QZ85
Е	246	GLU	LYS	engineered mutation	UNP Q9QZ85
F	-9	GLY	-	expression tag	UNP Q9QZ85
F	-8	SER	_	expression tag	UNP Q9QZ85
F	-7	PRO	_	expression tag	UNP Q9QZ85
F	-6	GLY	_	expression tag	UNP Q9QZ85
F	-5	ILE	_	expression tag	UNP Q9QZ85
F	-4	PRO	_	expression tag	UNP Q9QZ85
F	-3	GLY	_	expression tag	UNP Q9QZ85
F	-2	SER	_	expression tag	UNP Q9QZ85
F	-1	THR	_	expression tag	UNP Q9QZ85
F	0	THR	_	expression tag	UNP Q9QZ85
F	31	GLU	ARG	engineered mutation	UNP Q9QZ85
F	32	GLU	LYS	engineered mutation	UNP Q9QZ85
F	176	GLU	LYS	engineered mutation	UNP Q9QZ85
F	246	GLU	LYS	engineered mutation	UNP Q9QZ85
G	-9	GLY	_	expression tag	UNP Q9QZ85
G	-8	SER	-	expression tag	UNP Q9QZ85
G	-7	PRO	-	expression tag	UNP Q9QZ85
G	-6	GLY	-	expression tag	UNP Q9QZ85
G	-5	ILE	-	expression tag	UNP Q9QZ85
G	-4	PRO	-	expression tag	UNP Q9QZ85
G	-3	GLY	-	expression tag	UNP Q9QZ85
G	-2	SER	-	expression tag	UNP Q9QZ85
G	-1	THR	-	expression tag	UNP Q9QZ85
G	0	THR	-	expression tag	UNP Q9QZ85
G	31	GLU	ARG	engineered mutation	UNP Q9QZ85
G	32	GLU	LYS	engineered mutation	UNP Q9QZ85
G	176	GLU	LYS	engineered mutation	UNP Q9QZ85
G	246	GLU	LYS	engineered mutation	UNP Q9QZ85

 $\bullet\,$ Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter



code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	
9	Λ	1	Total	С	Ν	Ο	Р	0	0	
	Л	T	32	10	6	13	3	0	0	
9	В	1	Total	С	Ν	Ο	Р	0	0	
	D	I	32	10	6	13	3	0	0	
2	С	1	Total	С	Ν	Ο	Р	0	0	
	U	T	32	10	6	13	3	0		
2	F	1	Total	С	Ν	Ο	Р	0	0	
2	Ľ	T	32	10	6	13	3	0	0	
2	F	1	Total	С	Ν	Ο	Р	0	0	
2	Ľ	T	32	10	6	13	3	0	U	
2	G	1	Total	С	N	Ō	Р	0	0	
Z	G	T	32	10	6	13	3	0	U	

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	2	Total Mg 2 2	0	0
3	В	2	Total Mg 2 2	0	0
3	С	2	Total Mg 2 2	0	0
3	D	1	Total Mg 1 1	0	0
3	Е	2	Total Mg 2 2	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	2	Total Mg 2 2	0	0
3	G	2	Total Mg 2 2	0	0

• Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
4	C	1	Total	С	Η	Ν	Ο	0	0	
		L	20	4	12	1	3	0	U	
4	F	1	Total	С	Η	Ν	Ο	0	0	
4	Ľ		20	4	12	1	3			

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total O 1 1	0	0
5	В	2	Total O 2 2	0	0
5	С	1	Total O 1 1	0	0
5	D	1	Total O 1 1	0	0
5	F	2	$\begin{array}{cc} \text{Total} & \text{O} \\ 2 & 2 \end{array}$	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total O 1 1	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 and electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: INTERFERON-INDUCIBLE GTPASE 1







Y393 D396 M397 M397 H405 L406 K407 E408 E408 1409 N413





D339 D339 V3340 V3340 V3340 V3340 V3340 V3340 V344 V344 V355 V345 V355 V345 V355 V355 V355 V355 V355 V355 V355 V356 V355 V356 V355 V356 V355 V356 V355 V356 V36 V





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants	98.51Å 98.51 Å 1289.40 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Baselution (Å)	68.98 - 3.20	Depositor
	68.98 - 3.20	EDS
$\% { m Data \ completeness}$	$100.0\ (68.98-3.20)$	Depositor
(in resolution range)	$100.0\ (68.98-3.20)$	EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.00 ~({\rm at}~ 3.19 {\rm \AA})$	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
B B a	0.297 , 0.317	Depositor
It, It _{free}	0.297 , 0.316	DCC
\mathbf{R}_{free} test set	3215 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor ($Å^2$)	75.4	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.29 , 29.5	EDS
L-test for $twinning^2$	$ < L >=0.36, < L^2>=0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	22647	wwPDB-VP
Average B, all atoms $(Å^2)$	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.71% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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: TRS, MG, GNP

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

Mol Chai		Bond	lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.24	0/3258	0.43	0/4383	
1	В	0.24	0/3259	0.45	0/4386	
1	С	0.24	0/3204	0.42	0/4306	
1	D	0.24	0/3245	0.43	0/4366	
1	Е	0.23	0/3259	0.41	0/4383	
1	F	0.22	0/3247	0.41	0/4367	
1	G	0.23	0/3298	0.41	0/4439	
All	All	0.23	0/22770	0.42	0/30630	

There are no bond length outliers.

There are no bond angle outliers.

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	3204	0	3214	218	0
1	В	3204	0	3213	267	0
1	С	3153	0	3172	208	0
1	D	3193	0	3195	238	0
1	Е	3205	0	3204	176	0
1	F	3194	0	3191	176	0



5FPH

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3241	0	3247	158	0
2	А	32	0	13	18	0
2	В	32	0	13	8	0
2	С	32	0	13	11	0
2	Е	32	0	13	9	0
2	F	32	0	13	5	0
2	G	32	0	13	8	0
3	А	2	0	0	0	0
3	В	2	0	0	0	0
3	С	2	0	0	0	0
3	D	1	0	0	0	0
3	Е	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
4	С	8	12	12	1	0
4	Ε	8	12	12	1	0
5	А	1	0	0	1	0
5	В	2	0	0	1	0
5	С	1	0	0	0	0
5	D	1	0	0	0	0
5	F	2	0	0	0	0
5	G	1	0	0	0	0
All	All	22623	24	22538	1372	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 30.

All (1372) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ALA:HB1	1:A:127:LEU:HD11	1.23	1.11
1:C:173:MSE:HE2	1:D:141:LEU:HB3	1.26	1.10
1:B:78:THR:HG21	1:B:106:GLU:HG2	1.29	1.08
1:G:186:ASP:HA	1:G:189:ILE:HD11	1.36	1.06
1:C:181:VAL:HG13	1:C:230:LEU:HD21	1.40	1.04
1:B:233:LYS:HE2	1:B:233:LYS:HA	1.40	1.03
1:A:294:ILE:HG23	1:C:211:LEU:HD12	1.40	1.03
1:C:105:VAL:HG23	1:C:107:VAL:H	1.24	1.03
1:A:147:TYR:CE1	1:B:175:LYS:HG2	1.93	1.01
1:B:26:LYS:HE3	1:C:26:LYS:HE2	1.45	0.99
1:D:105:VAL:HG11	1:D:109:MSE:HB2	1.44	0.99



	lo uo puge	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlan (Å)
1:B:296:PBO:HB2	1:B:367:ILE:HD11	1 42	0.98
1:A:80:SER:HA	1:A:157:ALA:HB2	1.45	0.98
1:B:298:LEU:HD13	1:B:301:LEU:HD23	1 46	0.97
1:A:81:GLY:N	2:A:501:GNP:O1B	1.98	0.96
1:B:298:LEU:HD13	1:B:301:LEU:CD2	1.94	0.96
1:B:182:ARG:HD2	1:B:229:LEU:HD22	1.45	0.96
1:D:133:THR:HG23	1:D:134:ASN:H	1.31	0.96
1:A:146:PHE:HB2	1:A:152:PHE:HZ	1.31	0.94
1:B:104:VAL:HG22	1:B:106:GLU:H	1.31	0.94
1:C:330:LEU:HD13	1:C:405:LEU:HD11	1.47	0.92
1:B:298:LEU:HB2	1:B:364:SER:HA	1.51	0.91
1:B:189:ILE:HD11	1:B:206:LEU:HD11	1.50	0.91
1:E:302:LEU:HD21	1:G:223:ALA:H	1.36	0.91
1:D:243:LEU:HG	1:D:247:LEU:HD11	1.54	0.90
1:E:143:LYS:HE2	1:E:143:LYS:HA	1.54	0.90
1:D:244:MSE:HA	1:D:247:LEU:HD12	1.54	0.89
1:D:222:ILE:HA	1:F:303:ASP:OD2	1.72	0.89
1:B:235:VAL:HG22	1:B:266:ILE:HG21	1.53	0.88
1:A:214:VAL:HG13	1:A:224:GLU:HG2	1.56	0.88
1:F:302:LEU:HG	1:F:306:LEU:HD13	1.56	0.87
1:A:141:LEU:HB3	1:A:146:PHE:HE2	1.37	0.87
1:A:144:MSE:HE2	1:A:144:MSE:HA	1.56	0.87
1:E:109:MSE:HE3	1:E:133:THR:HA	1.55	0.86
1:B:344:MSE:HE1	1:B:408:GLU:HG3	1.57	0.86
1:C:105:VAL:HG23	1:C:107:VAL:N	1.91	0.85
1:C:241:PRO:HG3	1:C:266:ILE:HD12	1.59	0.85
1:D:111:ARG:HD2	1:D:125:TRP:CE3	2.12	0.84
1:B:358:THR:HA	1:B:361:GLU:HB2	1.56	0.84
1:D:336:ILE:CG2	1:D:340:GLN:HB3	2.08	0.84
1:B:210:ARG:NH2	1:B:239:ASP:OD2	2.11	0.84
1:E:330:LEU:HD11	1:E:405:LEU:HD21	1.60	0.84
1:C:260:MSE:HE2	1:C:273:LYS:HB3	1.60	0.83
1:C:84:SER:HA	1:C:102:THR:HG21	1.60	0.83
1:B:260:MSE:HE1	1:B:273:LYS:HG2	1.59	0.83
1:D:241:PRO:HG3	1:D:266:ILE:HD12	1.60	0.83
1:F:347:SER:HB2	1:F:348:PRO:HD3	1.61	0.83
1:E:302:LEU:HD21	1:G:223:ALA:N	1.94	0.83
1:E:74:VAL:HG12	1:E:82:LYS:HG3	1.61	0.82
1:D:301:LEU:HD11	1:D:363:LEU:HD12	1.60	0.82
1:A:347:SER:HB3	1:A:348:PRO:HD3	1.61	0.82
1:A:341:VAL:HA	1:A:344:MSE:HE2	1.62	0.81



	lous puge	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlan (Å)
1.B.334.TRP.HZ2	1.B.408.GLU.HB3	<u>1 44</u>	
1.E.302.LEU.HG	$1 \cdot F \cdot 306 \cdot L E U \cdot C D 1$	2 10	0.81
1.E.108.THB.HG22	1.F.110.GLU.H	1 45	0.81
1.E.146.PHE.HB2	$1 \cdot F \cdot 173 \cdot MSE \cdot HE1$	1.10	0.81
$1 \cdot A \cdot 147 \cdot TYB \cdot CD1$	1.B.175.LYS.HG2	2.17	0.80
$\frac{1 \cdot \text{E} \cdot 174 \cdot \text{MSE} \cdot \text{HE2}}{1 \cdot \text{E} \cdot 174 \cdot \text{MSE} \cdot \text{HE2}}$	1.E.173.MSE.HG3	1.61	0.80
1.B.347.SEB.HB2	1.B.348.PBO.HD3	1.64	0.80
$1 \cdot \text{E} \cdot 344 \cdot \text{MSE} \cdot \text{HE1}$	1.E.408.GLU.HG3	1.61	0.80
$1 \cdot A \cdot 147 \cdot TYB \cdot HE1$	1.B.175.LYS.HG2	1 43	0.80
1.D.111.ARG.HH12	1.D.145.LVS.HB2	1.10	0.80
1.D.285.GLU.HG2	1.D.388.PHE.HE1	1.10	0.80
$1 \cdot E \cdot 189 \cdot IL E \cdot HD11$	$1 \cdot E \cdot 206 \cdot L E U \cdot H D 21$	1.10	0.79
1.G·334·TRP·HE3	$1:\underline{C:336}:\underline{ILE:HD11}$	1.01	0.79
1:C:214:VAL:HG13	1:C:224:GLU:HB3	1.63	0.79
1.G.45.ABG.HH11	1.G·57·ALA·HB2	1.00	0.79
1.A.146.PHE.HB2	$1 \cdot A \cdot 152 \cdot PHE \cdot CZ$	2.18	0.79
1.A.306.LEU.HD11	1.A.359.ILE.HD13	1.65	0.78
$1 \cdot C \cdot 109 \cdot MSE \cdot HE1$	1.C·133·THB·HG21	1.65	0.78
$1 \cdot C \cdot 174 \cdot MSE \cdot HG2$	$1 \cdot D \cdot 174 \cdot MSE \cdot HG2$	1.63	0.78
1:F:241:PRO:HG3	1:F:266:ILE:HD12	1.64	0.78
1:D:334:TRP:O	1:D:336:ILE:N	$\frac{1.01}{2.15}$	0.78
1:D:143:LYS:HE2	1:D:143:LYS:HA	1.63	0.78
1:F:253:ILE:HD12	1:F:253:ILE:H	1 45	0.78
1:A:141:LEU:HB3	1:A:146:PHE:CE2	2.18	0.78
1:A:294:ILE:CG2	1:C:211:LEU:HD12	2.12	0.78
1:B:298:LEU:HG	1:B:364:SER:HA	1.66	0.78
1:B:78:THR:CG2	1:B:106:GLU:HG2	2.12	0.77
1:D:336:ILE:HG23	1:D:340:GLN:HB3	1.64	0.77
1:A:159:ARG:HG3	1:A:159:ARG:HH11	1.50	0.77
1:A:82:LYS:N	2:A:501:GNP:O1B	2.15	0.77
1:D:171:ILE:HG21	1:D:178:PHE:HB3	1.67	0.77
1:E:275:ARG:HH21	1:E:396:ASP:HA	1.48	0.76
1:F:336:ILE:HG23	1:F:340:GLN:HG3	1.67	0.76
1:C:90:ARG:NH2	1:C:98:GLY:O	2.19	0.76
1:D:133:THR:HG23	1:D:134:ASN:N	2.00	0.76
1:D:345:ILE:HD11	1:D:405:LEU:HD13	1.67	0.76
1:G:196:LYS:HE3	1:G:199:THR:HG23	1.67	0.76
2:B:501:GNP:H8	2:B:501:GNP:H5'2	1.66	0.76
1:B:210:ARG:HB3	1:D:294:ILE:HD11	1.68	0.75
1:B:220:ASN:HB2	1:B:222:ILE:HG12	1.69	0.75
1:D:111:ARG:NH1	1:D:145:LYS:HB2	2.01	0.75



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:251:LEU:HD23	1:A:252:PRO:HD2	1.67	0.75
1:B:376:TYR:HD2	1:C:373:ALA:HA	1.51	0.75
1:A:275:ARG:HH21	1:A:396:ASP:HA	1.51	0.74
1:B:26:LYS:HE3	1:C:26:LYS:CE	2.17	0.74
1:D:135:PHE:HB3	1:D:137:PRO:HD2	1.69	0.74
1:G:92:ILE:HD11	1:G:117:PRO:HG3	1.69	0.74
1:A:109:MSE:O	1:A:109:MSE:HG2	1.86	0.74
1:C:45:ARG:HH11	1:C:57:ALA:HB2	1.51	0.74
1:C:232:ASN:N	2:C:501:GNP:O6	2.20	0.74
1:C:210:ARG:N	1:C:229:LEU:HD11	2.02	0.74
1:E:174:MSE:HA	1:F:174:MSE:HG3	1.69	0.74
1:D:295:ILE:HD12	1:D:295:ILE:H	1.53	0.74
1:B:298:LEU:HB2	1:B:364:SER:CA	2.18	0.74
1:A:94:ASN:ND2	1:A:102:THR:OG1	2.21	0.74
1:B:298:LEU:CB	1:B:364:SER:HA	2.17	0.74
1:A:235:VAL:HG22	1:A:266:ILE:HG21	1.69	0.74
1:F:215:ASN:HA	1:F:218:ARG:HB3	1.68	0.74
1:B:334:TRP:CZ2	1:B:408:GLU:HB3	2.23	0.74
1:D:300:PHE:HA	1:D:360:GLN:NE2	2.03	0.73
1:G:251:LEU:HD23	1:G:252:PRO:HD2	1.71	0.73
1:A:111:ARG:NE	1:A:127:LEU:HD22	2.03	0.73
1:C:230:LEU:HD13	1:C:240:PHE:HE1	1.54	0.73
1:F:260:MSE:HE2	1:F:273:LYS:HB3	1.69	0.73
1:A:111:ARG:HH21	1:A:127:LEU:HD13	1.54	0.72
1:D:105:VAL:HG21	1:D:109:MSE:HG3	1.70	0.72
1:B:215:ASN:O	1:B:219:GLU:HG3	1.88	0.72
1:E:217:PHE:HD1	1:E:222:ILE:HD11	1.54	0.72
1:F:285:GLU:HG2	1:F:388:PHE:HE1	1.53	0.72
1:A:111:ARG:NH2	1:A:144:MSE:HB3	2.04	0.72
1:G:80:SER:HB3	1:G:155:ILE:HG22	1.71	0.72
2:A:501:GNP:H8	2:A:501:GNP:H5'1	1.69	0.72
1:B:78:THR:HG21	1:B:106:GLU:CG	2.15	0.72
1:A:241:PRO:HG3	1:A:266:ILE:HD12	1.72	0.72
1:G:189:ILE:HD12	1:G:190:THR:H	1.53	0.72
1:D:338:VAL:O	1:D:341:VAL:HG22	1.90	0.72
1:C:330:LEU:HD11	1:C:405:LEU:HD21	1.72	0.71
1:E:141:LEU:HB3	1:F:173:MSE:HE2	1.71	0.71
1:E:196:LYS:HD3	1:E:200:PHE:CD1	2.23	0.71
1:A:109:MSE:HE3	1:A:134:ASN:HD21	1.56	0.71
1:E:251:LEU:HD23	1:E:252:PRO:HD2	1.72	0.71
1:G:281:ARG:NH1	1:G:285:GLU:OE2	2.23	0.71



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlan (Å)
1:B:260:MSE:CE	1:B:273:LYS:HG2	2 21	0.71
1:B:235:VAL:CG2	1:B:266:ILE:HG21	2.20	0.71
1:E:171:ILE:HG21	1:E:178:PHE:HB3	1.72	0.71
1:B:172:SER:HB2	1:B:178:PHE:CE2	2.25	0.71
1:D:210:ARG:O	1:D:214:VAL:HG23	1.89	0.71
1:A:330:LEU:HD23	1:A:341:VAL:HG13	1.73	0.70
1:D:130:ILE:HD11	1:D:163:ASN:CG	2.11	0.70
1:A:214:VAL:CG1	1:A:224:GLU:HG2	2.21	0.70
1:A:82:LYS:H	2:A:501:GNP:PB	2.14	0.70
1:A:300:PHE:CZ	1:C:219:GLU:HA	2.26	0.70
1:C:171:ILE:HA	1:C:174:MSE:HE2	1.73	0.70
1:D:140:TYR:CE1	1:D:144:MSE:HG2	2.26	0.70
1:B:172:SER:HB2	1:B:178:PHE:HE2	1.57	0.70
1:G:186:ASP:OD2	2:G:501:GNP:N2	2.24	0.70
1:D:104:VAL:HG22	1:D:105:VAL:H	1.57	0.70
1:A:111:ARG:NH1	1:A:144:MSE:O	2.24	0.69
1:E:111:ARG:NH2	1:E:149:TYR:OH	2.25	0.69
1:B:235:VAL:CG1	1:B:266:ILE:HG22	2.22	0.69
1:C:330:LEU:CD1	1:C:405:LEU:HD21	2.22	0.69
1:D:162:LYS:O	1:D:166:ASP:N	2.23	0.69
1:A:81:GLY:H	2:A:501:GNP:PB	2.14	0.69
1:D:112:HIS:HD2	1:D:113:PRO:HD2	1.56	0.69
1:D:301:LEU:HD13	1:D:306:LEU:HD13	1.75	0.69
1:B:45:ARG:HH11	1:B:57:ALA:HB2	1.58	0.69
1:B:241:PRO:HG3	1:B:266:ILE:HD12	1.74	0.69
1:D:243:LEU:HG	1:D:247:LEU:CD1	2.22	0.69
1:B:341:VAL:HA	1:B:344:MSE:HG3	1.74	0.69
1:G:218:ARG:NE	1:G:224:GLU:OE2	2.24	0.69
1:F:298:LEU:HB2	1:F:386:GLU:OE2	1.93	0.69
1:C:147:TYR:HD2	1:C:148:GLU:HG3	1.57	0.69
1:E:51:ILE:HD12	1:E:51:ILE:H	1.57	0.69
1:G:275:ARG:HH21	1:G:396:ASP:HA	1.58	0.69
1:B:144:MSE:HA	1:B:144:MSE:HE2	1.74	0.69
1:C:160:PHE:O	1:C:216:THR:HG21	1.92	0.69
1:G:186:ASP:CA	1:G:189:ILE:HD11	2.20	0.69
1:G:241:PRO:HG3	1:G:266:ILE:HD12	1.75	0.68
1:F:251:LEU:HD23	1:F:252:PRO:HD2	1.74	0.68
1:B:189:ILE:HD11	1:B:206:LEU:CD1	2.23	0.68
1:D:275:ARG:HH21	1:D:396:ASP:HA	1.58	0.68
1:A:82:LYS:HG2	2:A:501:GNP:N3B	2.08	0.68
1:C:182:ARG:HG3	1:C:213:CYS:SG	2.34	0.68



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:341:VAL:HA	1:A:344:MSE:CE	2.22	0.68
1:D:136:PRO:HG2	1:D:137:PRO:HD3	1.75	0.68
1:G:301:LEU:HD21	1:G:306:LEU:HD13	1.75	0.68
1:B:298:LEU:HD13	1:B:301:LEU:HD21	1.76	0.68
1:C:36:GLN:O	1:C:40:ASN:ND2	2.27	0.68
1:F:165:ILE:HG12	1:F:217:PHE:CE2	2.29	0.68
1:F:210:ARG:HA	1:F:227:ILE:HD13	1.76	0.68
1:B:93:GLY:N	1:B:96:GLU:OE2	2.26	0.68
1:C:214:VAL:HG23	1:C:227:ILE:HG13	1.76	0.68
1:B:26:LYS:CE	1:C:26:LYS:HE2	2.21	0.68
1:F:45:ARG:HH11	1:F:57:ALA:HB2	1.58	0.67
1:A:94:ASN:HB3	1:A:102:THR:HG21	1.75	0.67
1:A:185:VAL:HG11	1:A:229:LEU:HB3	1.74	0.67
1:C:330:LEU:CD1	1:C:405:LEU:HD11	2.22	0.67
1:B:376:TYR:CD2	1:C:373:ALA:HA	2.30	0.67
1:E:336:ILE:CG2	1:E:340:GLN:HB3	2.24	0.67
1:A:102:THR:O	2:A:501:GNP:H5'2	1.94	0.67
1:B:104:VAL:HG22	1:B:106:GLU:N	2.09	0.67
1:C:66:ASP:O	1:C:121:ASN:ND2	2.27	0.67
1:D:214:VAL:HG12	1:D:218:ARG:HG3	1.76	0.67
1:A:203:GLU:N	1:A:203:GLU:OE1	2.28	0.67
1:C:83:SER:OG	2:C:501:GNP:O2G	2.13	0.67
1:C:214:VAL:CG2	1:C:227:ILE:HG13	2.24	0.67
1:A:171:ILE:O	1:A:174:MSE:HG2	1.94	0.67
1:F:66:ASP:O	1:F:121:ASN:ND2	2.28	0.67
1:B:375:GLY:HA3	1:C:375:GLY:N	2.10	0.66
1:B:251:LEU:HD23	1:B:252:PRO:HD2	1.76	0.66
1:G:136:PRO:HD2	1:G:139:THR:HB	1.78	0.66
1:B:105:VAL:HG13	1:B:107:VAL:HG13	1.78	0.66
1:A:94:ASN:HB3	1:A:102:THR:CG2	2.26	0.66
1:C:84:SER:HA	1:C:102:THR:CG2	2.25	0.66
1:E:241:PRO:HG3	1:E:266:ILE:CD1	2.26	0.66
1:A:106:GLU:O	1:A:107:VAL:HG12	1.96	0.66
1:B:298:LEU:CG	1:B:364:SER:HA	2.26	0.66
1:B:302:LEU:HD12	1:B:305:ASP:OD2	1.95	0.66
1:E:217:PHE:CD1	1:E:222:ILE:HD11	2.31	0.66
1:E:386:GLU:OE2	1:G:218:ARG:NH2	2.27	0.66
1:B:235:VAL:HG13	1:B:266:ILE:HG22	1.76	0.66
1:F:210:ARG:HA	1:F:227:ILE:CD1	2.26	0.66
1:F:241:PRO:HG3	1:F:266:ILE:CD1	2.25	0.66
1:G:257:HIS:NE2	1:G:281:ARG:HD2	2.10	0.66



	bus puge	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap(Å)
1:C:80:SEB:HA	1:C:157:ALA:HB2	1 76	0.65
1:C:173:MSE:HE1	1:D:146:PHE:HB2	1.76	0.65
1:A:171:ILE:HG21	1:A:178:PHE:HB3	1.77	0.65
1:C:251:LEU:HD23	1:C:252:PRO:HD2	1.76	0.65
1:D:244:MSE:HG2	1:D:263:LEU:HD13	1.77	0.65
1:E:241:PRO:HA	1:E:244:MSE:HE2	1.77	0.65
1:A:80:SER:CA	1:A:157:ALA:HB2	2.25	0.65
1:B:275:ARG:HH21	1:B:396:ASP:HA	1.60	0.65
1:D:217:PHE:O	1:D:221:GLY:N	2.30	0.65
1:E:41:LEU:HD11	1:E:45:ARG:NH1	2.11	0.65
1:F:180:PHE:HB2	1:F:226:PRO:O	1.97	0.65
1:C:85:PHE:CD2	1:C:155:ILE:HD11	2.32	0.65
1:E:141:LEU:HD13	1:E:174:MSE:CE	2.25	0.65
1:D:301:LEU:H	1:D:360:GLN:HG3	1.62	0.65
1:A:73:ALA:HB1	1:A:127:LEU:CD1	2.15	0.65
1:G:306:LEU:HG	1:G:310:LYS:NZ	2.10	0.65
1:G:347:SER:OG	1:G:348:PRO:HD3	1.97	0.65
1:B:116:HIS:CD2	1:B:262:SER:HB2	2.32	0.65
1:B:333:ASP:OD1	1:B:334:TRP:N	2.30	0.65
1:F:295:ILE:HG23	1:F:296:PRO:HD2	1.79	0.65
1:A:140:TYR:O	1:A:144:MSE:HG2	1.97	0.65
1:A:66:ASP:O	1:A:121:ASN:ND2	2.30	0.64
1:A:111:ARG:NH2	1:A:127:LEU:HD13	2.11	0.64
1:B:224:GLU:N	1:B:224:GLU:OE1	2.30	0.64
1:E:350:VAL:O	1:E:362:ARG:NH1	2.30	0.64
1:G:66:ASP:O	1:G:121:ASN:ND2	2.31	0.64
1:A:327:LEU:HB3	1:A:338:VAL:HG13	1.79	0.64
1:B:188:ASP:O	1:B:192:GLU:HG3	1.98	0.64
1:C:82:LYS:N	2:C:501:GNP:O2B	2.31	0.64
1:A:45:ARG:NH1	1:A:53:LEU:HB3	2.12	0.64
1:A:83:SER:N	2:A:501:GNP:O2B	2.19	0.64
1:B:291:LEU:HD13	1:B:378:LEU:CD2	2.28	0.64
1:C:85:PHE:HE2	1:C:153:ILE:HD13	1.61	0.64
1:D:218:ARG:HD2	1:F:300:PHE:HE2	1.61	0.64
1:E:182:ARG:HB3	1:E:229:LEU:HD22	1.79	0.64
1:F:80:SER:HA	1:F:157:ALA:HB2	1.78	0.64
1:A:285:GLU:HG2	1:A:388:PHE:HE1	1.62	0.64
1:G:109:MSE:HE3	1:G:135:PHE:CE2	2.32	0.64
1:B:106:GLU:O	1:B:107:VAL:HG22	1.98	0.64
1:D:358:THR:HG22	1:D:361:GLU:HG3	1.79	0.64
$1:\overline{\text{E:}330:\text{L}\text{EU:}\text{HD}13}$	1:E:405:LEU:HD11	1.80	0.64



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:209:ILE:HA	1:F:212:ASN:HD21	1.63	0.64
1:G:109:MSE:HE3	1:G:135:PHE:CZ	2.33	0.64
1:A:230:LEU:HD13	1:A:240:PHE:CE2	2.32	0.64
1:C:230:LEU:HB2	1:C:240:PHE:HD1	1.62	0.64
1:C:102:THR:O	2:C:501:GNP:H5'2	1.98	0.64
1:G:91:GLY:O	1:G:329:ARG:NH1	2.30	0.63
1:B:298:LEU:HD11	1:B:363:LEU:HB3	1.79	0.63
1:C:37:GLU:HA	1:C:40:ASN:HD21	1.62	0.63
1:E:43:GLU:HG2	1:F:44:LEU:HD11	1.81	0.63
1:E:235:VAL:HG22	1:E:266:ILE:HG21	1.80	0.63
1:D:130:ILE:CG2	1:D:167:ILE:HD11	2.28	0.63
1:A:146:PHE:CZ	1:B:173:MSE:HG3	2.33	0.63
1:A:299:THR:HG21	1:C:215:ASN:OD1	1.98	0.63
1:G:81:GLY:HA2	2:G:501:GNP:O1A	1.98	0.63
1:G:94:ASN:HB3	1:G:102:THR:HG21	1.80	0.63
1:D:105:VAL:CG1	1:D:109:MSE:HB2	2.25	0.63
1:D:113:PRO:HB3	1:D:125:TRP:CH2	2.33	0.63
1:A:339:ASP:OD1	1:A:339:ASP:N	2.28	0.63
1:E:34:ILE:HD11	1:E:38:ILE:HG21	1.81	0.63
1:A:146:PHE:HA	1:A:149:TYR:CE2	2.34	0.62
1:E:136:PRO:HD2	1:E:139:THR:HB	1.79	0.62
1:D:112:HIS:CD2	1:D:113:PRO:HD2	2.34	0.62
1:E:347:SER:OG	1:E:348:PRO:HD3	1.99	0.62
1:A:180:PHE:HB3	1:A:227:ILE:HD13	1.82	0.62
1:C:224:GLU:OE1	1:C:224:GLU:N	2.25	0.62
1:D:185:VAL:HG11	1:D:229:LEU:HB3	1.79	0.62
1:B:96:GLU:OE2	1:B:329:ARG:NH1	2.29	0.62
1:B:194:ASP:OD1	1:B:195:GLY:N	2.32	0.62
2:C:501:GNP:O2A	2:C:501:GNP:N3B	2.32	0.62
1:E:116:HIS:CD2	1:E:262:SER:HB2	2.35	0.62
1:A:165:ILE:HG12	1:A:217:PHE:CE1	2.35	0.62
1:C:173:MSE:CE	1:D:146:PHE:HB2	2.29	0.62
1:E:110:GLU:OE1	1:E:110:GLU:HA	1.99	0.62
1:F:90:ARG:NH1	1:F:114:TYR:HB3	2.14	0.62
1:G:337:GLU:HB2	1:G:340:GLN:HG2	1.81	0.62
1:D:141:LEU:HD12	1:D:141:LEU:H	1.65	0.62
1:F:109:MSE:HE3	1:F:133:THR:HA	1.81	0.62
1:F:252:PRO:HD2	1:F:255:LYS:HD3	1.81	0.61
1:G:141:LEU:HD22	1:G:146:PHE:CE2	2.35	0.61
1:A:116:HIS:CD2	1:A:262:SER:HB2	2.34	0.61
1:B:75:THR:HA	1:B:82:LYS:HZ2	1.64	0.61



	lous puge	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlan (Å)
1·B·327·LEU·HA	1.B.330.LEU.HB2	1.82	0.61
1:D:299:THR:OG1	1:D:386:GLU:OE2	2.09	0.61
1:A:251:LEU:CD2	1:A:252:PBO:HD2	2.30	0.61
1:D:218:ABG:HD3	1:F:301:LEU:HD22	1.82	0.61
1:F:186:ASP:OD2	2:F:501:GNP:N2	2.33	0.61
1:A:331:ALA:HA	1:A:336:ILE:O	2.00	0.61
1:E:45:ARG:HH11	1:E:57:ALA:HB2	1.66	0.61
1:F:336:ILE:CG2	1:F:340:GLN:HB2	2.30	0.61
1:G:214:VAL:HB	1:G:224:GLU:HG2	1.82	0.61
1:D:358:THR:HG23	1:D:361:GLU:H	1.65	0.61
1:B:74:VAL:CG1	1:B:82:LYS:HB2	2.31	0.61
1:D:143:LYS:C	1:D:144:MSE:HE2	2.21	0.61
1:B:298:LEU:HB2	1:B:364:SER:CB	2.30	0.61
1:D:104:VAL:HG13	1:D:105:VAL:N	2.15	0.61
1:D:92:ILE:CG2	1:D:99:ALA:HB2	2.31	0.60
1:E:232:ASN:HB2	2:E:501:GNP:N7	2.16	0.60
1:C:21:THR:HG21	1:C:43:GLU:OE1	2.00	0.60
1:C:165:ILE:HG12	1:C:217:PHE:CE1	2.36	0.60
1:D:104:VAL:HG22	1:D:105:VAL:N	2.16	0.60
1:E:109:MSE:CE	1:E:133:THR:HA	2.28	0.60
1:B:220:ASN:HB2	1:B:222:ILE:CG1	2.30	0.60
1:F:208:ASP:O	1:F:212:ASN:ND2	2.34	0.60
1:D:180:PHE:HE2	1:D:225:PRO:HG3	1.66	0.60
1:D:182:ARG:NH2	1:D:188:ASP:OD2	2.35	0.60
1:D:134:ASN:CG	1:D:135:PHE:H	2.04	0.60
1:G:189:ILE:HG23	1:G:205:VAL:CG1	2.31	0.60
1:B:327:LEU:HD23	1:B:330:LEU:HD12	1.84	0.60
1:A:251:LEU:HD23	1:A:252:PRO:CD	2.31	0.60
1:D:80:SER:HB3	1:D:155:ILE:HG22	1.83	0.60
1:C:230:LEU:HD22	1:C:240:PHE:CE1	2.36	0.60
1:G:298:LEU:HB3	1:G:364:SER:HA	1.83	0.60
1:A:94:ASN:HB3	1:A:102:THR:HB	1.83	0.60
1:B:193:ALA:HB2	1:B:200:PHE:CE1	2.36	0.60
1:C:80:SER:O	1:C:183:THR:OG1	2.20	0.60
1:C:97:GLU:HG3	1:C:98:GLY:N	2.16	0.60
1:D:300:PHE:HA	1:D:360:GLN:HE21	1.66	0.60
1:G:46:MSE:HG2	1:G:54:THR:HG21	1.84	0.60
1:A:94:ASN:HB3	1:A:102:THR:CB	2.31	0.59
1:E:146:PHE:HB2	1:F:173:MSE:CE	2.31	0.59
1:A:34:ILE:HD11	1:A:38:ILE:HG21	1.84	0.59
1:C:275:ARG:HH21	1:C:396:ASP:HA	1.66	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap(Å)
1:E:182:ABG:NH2	1:E:188:ASP:OD2	2.33	0.59
1:D:113:PRO:HB3	1:D:125:TRP:CZ3	2.37	0.59
1:F:336:ILE:HG23	1:F:340:GLN:CG	2.31	0.59
1:A:34:ILE:HD11	1:A:38:ILE:CG2	2.32	0.59
1:F:220:ASN:HB2	1:F:222:ILE:HG12	1.83	0.59
1:C:171:ILE:HG21	1:C:178:PHE:HB3	1.85	0.59
1:B:285:GLU:HG2	1:B:388:PHE:HE1	1.67	0.59
1:D:34:ILE:HD11	1:D:38:ILE:HG21	1.84	0.59
1:C:147:TYR:CD2	1:C:148:GLU:HG3	2.36	0.59
1:C:189:ILE:HG12	1:C:205:VAL:HG11	1.85	0.59
1:C:210:ARG:CA	1:C:229:LEU:HD11	2.32	0.59
1:E:66:ASP:O	1:E:121:ASN:ND2	2.35	0.59
1:A:115:LYS:HG2	1:A:123:VAL:HG22	1.84	0.59
1:A:313:MSE:HE3	1:A:317:ARG:HD2	1.85	0.59
1:B:266:ILE:HG13	1:B:267:THR:HG23	1.84	0.59
1:C:180:PHE:CE2	1:C:225:PRO:HG3	2.38	0.59
1:C:181:VAL:CG1	1:C:230:LEU:HD21	2.26	0.59
1:G:220:ASN:OD1	1:G:220:ASN:N	2.35	0.59
1:G:328:GLN:O	1:G:332:ARG:HG2	2.03	0.59
1:B:112:HIS:HD2	1:B:113:PRO:HD2	1.67	0.59
1:B:201:ASP:HB2	1:B:204:LYS:CB	2.33	0.59
1:C:241:PRO:HG3	1:C:266:ILE:CD1	2.31	0.59
1:A:20:PHE:HB2	1:A:287:PHE:CE2	2.38	0.58
1:A:86:ILE:HD12	1:A:124:PHE:HB3	1.84	0.58
1:B:298:LEU:HD23	1:B:367:ILE:HG21	1.85	0.58
1:E:141:LEU:HD13	1:E:174:MSE:HE1	1.85	0.58
1:G:196:LYS:CE	1:G:199:THR:HG23	2.33	0.58
1:A:207:GLN:O	1:A:211:LEU:HD13	2.03	0.58
1:C:230:LEU:HB2	1:C:240:PHE:CD1	2.38	0.58
1:D:143:LYS:O	1:D:144:MSE:HE2	2.04	0.58
1:D:146:PHE:HA	1:D:149:TYR:CD2	2.38	0.58
1:B:82:LYS:NZ	1:B:127:LEU:O	2.34	0.58
1:C:100:ALA:HB2	1:C:114:TYR:CZ	2.39	0.58
1:G:330:LEU:CD1	1:G:405:LEU:HD21	2.32	0.58
1:C:180:PHE:HE2	1:C:225:PRO:HG3	1.68	0.58
1:B:73:ALA:HB2	1:B:149:TYR:CG	2.38	0.58
1:A:298:LEU:HD12	1:C:211:LEU:CD1	2.34	0.58
1:B:201:ASP:HB2	1:B:204:LYS:HB2	1.84	0.58
1:B:298:LEU:CD1	1:B:301:LEU:HD23	2.28	0.58
1:B:298:LEU:HD12	1:B:363:LEU:HB2	1.86	0.58
1:C:141:LEU:HD21	1:C:170:ALA:HB1	1.85	0.58



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:189:ILE:HD11	1:E:206:LEU:CD2	2.31	0.58
1:F:210:ARG:HG2	1:F:227:ILE:HD13	1.85	0.58
1:G:201:ASP:HB2	1:G:204:LYS:HB2	1.86	0.58
1:D:286:GLY:HA2	1:D:388:PHE:CZ	2.38	0.58
1:E:155:ILE:HG23	1:E:183:THR:HG23	1.85	0.58
1:G:189:ILE:HD12	1:G:190:THR:N	2.19	0.58
1:A:106:GLU:HG2	1:A:107:VAL:N	2.18	0.58
1:D:214:VAL:HG13	1:D:224:GLU:CB	2.34	0.58
1:A:336:ILE:HD11	1:A:340:GLN:CB	2.32	0.58
1:B:251:LEU:HD23	1:B:252:PRO:CD	2.34	0.58
1:C:260:MSE:HE2	1:C:273:LYS:CB	2.33	0.58
1:D:20:PHE:HB2	1:D:287:PHE:CE2	2.39	0.58
1:A:241:PRO:HG3	1:A:266:ILE:CD1	2.33	0.57
1:C:94:ASN:HB2	1:C:102:THR:OG1	2.03	0.57
1:F:251:LEU:HD23	1:F:252:PRO:CD	2.33	0.57
1:G:251:LEU:CD2	1:G:252:PRO:HD2	2.33	0.57
1:C:347:SER:OG	1:C:348:PRO:HD3	2.02	0.57
1:D:162:LYS:HG2	1:D:166:ASP:OD2	2.04	0.57
1:E:162:LYS:O	1:E:165:ILE:HG22	2.04	0.57
1:E:251:LEU:HD23	1:E:252:PRO:CD	2.33	0.57
1:F:291:LEU:HD22	1:F:384:LEU:HD23	1.86	0.57
1:G:251:LEU:HD23	1:G:252:PRO:CD	2.33	0.57
1:C:70:LEU:HD12	1:C:150:ASP:OD2	2.04	0.57
1:E:251:LEU:CD2	1:E:252:PRO:HD2	2.34	0.57
1:A:230:LEU:HB2	1:A:240:PHE:CD2	2.39	0.57
1:B:221:GLY:HA2	1:D:302:LEU:CD1	2.35	0.57
1:B:306:LEU:HG	1:B:310:LYS:HE3	1.87	0.57
1:C:201:ASP:O	1:C:204:LYS:HG2	2.05	0.57
1:C:45:ARG:NH1	1:C:57:ALA:HB2	2.19	0.57
1:D:260:MSE:O	1:D:274:LYS:HE2	2.04	0.57
1:F:298:LEU:HD13	1:F:386:GLU:OE1	2.04	0.57
1:G:263:LEU:O	1:G:274:LYS:NZ	2.26	0.57
1:F:251:LEU:CD2	1:F:252:PRO:HD2	2.34	0.57
1:C:215:ASN:O	1:C:219:GLU:HG3	2.05	0.57
1:F:302:LEU:HD22	1:F:360:GLN:CG	2.35	0.57
1:B:361:GLU:O	1:B:364:SER:OG	2.14	0.57
1:D:111:ARG:HD2	1:D:125:TRP:CZ3	2.39	0.57
1:D:146:PHE:HA	1:D:149:TYR:CE2	2.40	0.57
1:A:146:PHE:HZ	1:B:173:MSE:HG3	1.70	0.57
1:B:251:LEU:CD2	1:B:252:PRO:HD2	2.35	0.57
1:C:105:VAL:HG12	2:C:501:GNP:O3G	2.03	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:E:241:PRO:HG3	1:E:266:ILE:HD12	1.87	0.57
1:F:286:GLY:HA2	1:F:388:PHE:CZ	2.39	0.57
1:A:310:LYS:HA	1:A:351:PHE:CE2	2.40	0.57
1:D:107:VAL:HG12	1:D:108:THR:H	1.70	0.57
1:D:104:VAL:HG13	1:D:105:VAL:H	1.71	0.56
1:E:28:ASN:OD1	1:E:29:THR:N	2.37	0.56
1:F:205:VAL:O	1:F:209:ILE:HG13	2.04	0.56
1:G:90:ARG:NH1	1:G:114:TYR:HB3	2.20	0.56
1:B:298:LEU:HG	1:B:363:LEU:O	2.05	0.56
1:C:189:ILE:HD11	1:C:206:LEU:HD21	1.86	0.56
1:C:260:MSE:CE	1:C:273:LYS:HB3	2.34	0.56
1:D:108:THR:HB	1:D:133:THR:OG1	2.06	0.56
1:D:218:ARG:HB3	1:F:300:PHE:HD2	1.70	0.56
1:D:330:LEU:HD21	1:D:409:ILE:HD11	1.86	0.56
1:E:108:THR:CG2	1:E:110:GLU:H	2.18	0.56
1:E:112:HIS:ND1	1:E:113:PRO:HD2	2.19	0.56
1:F:257:HIS:NE2	1:F:281:ARG:HD2	2.20	0.56
1:B:207:GLN:HG2	1:D:295:ILE:HD11	1.88	0.56
1:E:128:PRO:HD2	1:E:144:MSE:SE	2.56	0.56
1:A:90:ARG:NH1	1:A:114:TYR:HB3	2.21	0.56
1:E:214:VAL:HA	1:E:217:PHE:HD2	1.70	0.56
1:F:18:SER:O	1:F:21:THR:OG1	2.21	0.56
1:F:298:LEU:HD23	1:F:363:LEU:CB	2.35	0.56
1:A:336:ILE:HD11	1:A:340:GLN:HB3	1.88	0.56
1:A:227:ILE:HD12	1:A:228:PHE:H	1.70	0.56
1:F:217:PHE:CD1	1:F:225:PRO:HG3	2.40	0.56
1:D:130:ILE:HG21	1:D:167:ILE:HD11	1.86	0.56
1:D:339:ASP:OD1	1:D:339:ASP:N	2.37	0.56
1:F:46:MSE:HG2	1:F:54:THR:HG21	1.87	0.56
1:A:82:LYS:CB	1:A:155:ILE:HD12	2.36	0.56
1:C:136:PRO:HD2	1:C:139:THR:HB	1.87	0.56
1:C:251:LEU:HD23	1:C:252:PRO:CD	2.35	0.56
1:D:90:ARG:NH1	1:D:114:TYR:HB3	2.21	0.56
1:F:240:PHE:HB3	1:F:241:PRO:HD3	1.88	0.56
1:G:18:SER:O	1:G:21:THR:OG1	2.23	0.56
1:B:197:PRO:O	1:B:198:GLN:HB3	2.06	0.56
1:B:378:LEU:CD1	1:B:384:LEU:HG	2.36	0.56
1:D:336:ILE:HG23	1:D:340:GLN:CB	2.35	0.56
1:G:35:SER:OG	1:G:38:ILE:HD13	2.06	0.56
1:A:111:ARG:HE	1:A:127:LEU:HD22	1.71	0.55
1:A:111:ARG:CZ	1:A:144:MSE:HB3	2.35	0.55



	lo uo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:136:PRO:N	1:D:137:PRO:HD2	2.22	0.55
1:F:260:MSE:CE	1:F:273:LYS:HB3	2.34	0.55
1:G:90:ARG:NH2	1:G:98:GLY:O	2.38	0.55
1:B:153:ILE:HD13	1:B:179:TYR:HB2	1.86	0.55
1:D:299:THR:HG22	1:D:300:PHE:N	2.21	0.55
1:B:186:ASP:O	1:B:190:THR:OG1	2.22	0.55
1:D:344:MSE:SE	1:D:408:GLU:HG3	2.56	0.55
1:A:214:VAL:HG13	1:A:224:GLU:CG	2.33	0.55
1:C:172:SER:HB2	1:C:178:PHE:CE2	2.42	0.55
1:F:336:ILE:HG23	1:F:340:GLN:HB2	1.89	0.55
1:G:45:ARG:NH1	1:G:57:ALA:HB2	2.18	0.55
1:G:189:ILE:HG23	1:G:205:VAL:HG11	1.87	0.55
1:C:28:ASN:HB2	1:C:31:GLU:OE1	2.06	0.55
1:E:185:VAL:HG11	1:E:229:LEU:HB3	1.88	0.55
1:A:180:PHE:CD2	1:A:225:PRO:HG2	2.41	0.55
1:C:46:MSE:HG2	1:C:54:THR:HG21	1.87	0.55
1:C:85:PHE:CZ	1:C:89:LEU:HD11	2.40	0.55
1:C:128:PRO:HD2	1:C:144:MSE:SE	2.57	0.55
1:F:73:ALA:HB2	1:F:149:TYR:CD1	2.41	0.55
1:F:90:ARG:NH2	1:F:98:GLY:O	2.39	0.55
1:G:92:ILE:HD11	1:G:117:PRO:CG	2.36	0.55
1:A:82:LYS:O	1:A:86:ILE:HG12	2.06	0.55
1:B:230:LEU:HD22	1:B:240:PHE:CD2	2.42	0.55
1:C:75:THR:C	1:C:82:LYS:HE3	2.26	0.55
1:D:347:SER:N	1:D:348:PRO:CD	2.70	0.55
1:F:111:ARG:NH2	1:F:148:GLU:OE1	2.36	0.55
1:B:185:VAL:HG11	1:B:229:LEU:HB3	1.89	0.55
1:C:251:LEU:CD2	1:C:252:PRO:HD2	2.36	0.55
1:A:330:LEU:HD22	1:A:405:LEU:CD1	2.37	0.55
1:D:111:ARG:NH1	1:D:144:MSE:O	2.40	0.55
2:E:501:GNP:H3'	2:E:501:GNP:PA	2.47	0.55
1:B:328:GLN:O	1:B:332:ARG:HG2	2.07	0.55
1:C:42:ILE:HD13	1:C:58:ILE:HG12	1.89	0.55
1:E:106:GLU:O	1:E:107:VAL:HG12	2.06	0.55
1:E:106:GLU:OE1	1:E:107:VAL:N	2.39	0.55
1:F:317:ARG:HH22	1:F:324:GLU:HG3	1.71	0.55
1:A:82:LYS:HG2	2:A:501:GNP:PB	2.47	0.54
1:B:106:GLU:HĀ	1:B:106:GLU:OE1	2.06	0.54
1:G:106:GLU:HA	1:G:106:GLU:OE1	2.06	0.54
1:D:248:ILE:HG21	1:D:260:MSE:CE	2.36	0.54
1:F:26:LYS:NZ	1:G:26:LYS:HE2	2.22	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:235:VAL:HG22	1:G:266:ILE:HG21	1.88	0.54
1:C:101:LYS:HD2	1:C:101:LYS:O	2.07	0.54
1:D:347:SER:H	1:D:348:PRO:HD3	1.72	0.54
1:B:160:PHE:O	1:B:216:THR:HG21	2.08	0.54
1:B:185:VAL:HG22	1:B:230:LEU:O	2.08	0.54
1:C:152:PHE:CB	1:C:171:ILE:HD13	2.38	0.54
1:G:186:ASP:CG	2:G:501:GNP:HN21	2.11	0.54
1:E:285:GLU:HG2	1:E:388:PHE:HE1	1.73	0.54
1:B:187:SER:HA	1:B:190:THR:OG1	2.06	0.54
1:C:84:SER:N	1:C:102:THR:HG22	2.22	0.54
1:C:295:ILE:HG22	1:C:296:PRO:O	2.08	0.54
2:C:501:GNP:H3'	4:C:504:TRS:O3	2.07	0.54
1:D:336:ILE:HG22	1:D:337:GLU:O	2.08	0.54
1:E:104:VAL:HG11	2:E:501:GNP:O3G	2.08	0.54
1:F:217:PHE:CG	1:F:225:PRO:HG3	2.42	0.54
1:D:327:LEU:CD2	1:D:345:ILE:HG13	2.37	0.54
1:A:182:ARG:NH2	1:A:188:ASP:OD2	2.38	0.54
1:B:358:THR:O	1:B:362:ARG:HG3	2.08	0.54
1:B:112:HIS:CD2	1:B:113:PRO:HD2	2.43	0.54
1:B:330:LEU:CD1	1:B:405:LEU:HD21	2.38	0.54
1:C:285:GLU:HG2	1:C:388:PHE:HE1	1.73	0.54
1:A:18:SER:O	1:A:21:THR:OG1	2.27	0.53
1:A:78:THR:HG23	1:A:105:VAL:HG21	1.90	0.53
1:A:275:ARG:HH21	1:A:396:ASP:CA	2.20	0.53
1:D:328:GLN:O	1:D:332:ARG:HG2	2.07	0.53
1:E:185:VAL:HG22	1:E:230:LEU:O	2.08	0.53
1:A:92:ILE:HD11	1:A:117:PRO:HG2	1.90	0.53
1:A:144:MSE:HA	1:A:144:MSE:CE	2.34	0.53
1:A:165:ILE:HG12	1:A:217:PHE:HE1	1.71	0.53
1:A:188:ASP:O	1:A:192:GLU:HG3	2.08	0.53
1:C:185:VAL:HG22	1:C:230:LEU:O	2.08	0.53
1:D:105:VAL:CG2	1:D:109:MSE:HG3	2.36	0.53
1:D:301:LEU:HD11	1:D:363:LEU:CD1	2.36	0.53
1:G:260:MSE:O	1:G:274:LYS:HE2	2.08	0.53
1:B:182:ARG:HD3	1:B:185:VAL:HG12	1.89	0.53
1:B:291:LEU:HD13	1:B:378:LEU:HD21	1.91	0.53
1:G:301:LEU:HD22	1:G:363:LEU:HD12	1.89	0.53
1:A:338:VAL:O	1:A:342:GLU:HG3	2.08	0.53
1:B:74:VAL:HG12	1:B:82:LYS:HD2	1.89	0.53
1:C:82:LYS:NZ	1:C:127:LEU:O	2.33	0.53
1:E:44:LEU:HD21	1:F:43:GLU:OE1	2.09	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:260:MSE:HE2	1:F:273:LYS:CB	2.38	0.53
1:B:338:VAL:HA	1:B:341:VAL:HG23	1.90	0.53
1:D:285:GLU:HG2	1:D:388:PHE:CE1	2.34	0.53
1:B:155:ILE:HG12	1:B:181:VAL:HB	1.91	0.53
1:C:105:VAL:HG23	1:C:106:GLU:N	2.23	0.53
1:D:327:LEU:HD21	1:D:345:ILE:HG13	1.91	0.53
1:E:130:ILE:HD12	1:E:133:THR:OG1	2.09	0.53
1:A:322:VAL:HG21	1:A:398:VAL:HG13	1.90	0.53
1:A:336:ILE:CG1	1:A:340:GLN:HB2	2.39	0.53
1:D:202:LYS:H	1:D:202:LYS:HD2	1.73	0.53
1:D:207:GLN:O	1:D:211:LEU:HD23	2.08	0.53
2:E:501:GNP:H3'	2:E:501:GNP:O1A	2.08	0.53
1:F:16:LEU:N	1:F:17:PRO:CD	2.72	0.53
1:F:182:ARG:NH2	1:F:188:ASP:OD2	2.41	0.53
1:A:257:HIS:NE2	1:A:281:ARG:HD2	2.24	0.53
1:B:185:VAL:HG23	1:B:238:TYB:CE2	2.44	0.53
1:C:263:LEU:O	1:C:274:LYS:NZ	2.32	0.53
1:F:111:ARG:HH22	1:F:148:GLU:CD	2.12	0.53
1:A:82:LYS:HZ3	2:A:501:GNP:PG	2.32	0.53
1:C:34:ILE:HD11	1:C:38:ILE:HG21	1.91	0.53
1:F:201:ASP:OD2	1:F:204:LYS:N	2.41	0.53
1:G:184:LYS:HG2	2:G:501:GNP:C6	2.39	0.53
1:G:185:VAL:HG11	1:G:229:LEU:HB3	1.91	0.53
1:A:260:MSE:CE	1:A:273:LYS:HE2	2.39	0.53
1:C:85:PHE:CE2	1:C:153:ILE:HD13	2.43	0.53
1:C:116:HIS:CD2	1:C:262:SER:HB2	2.44	0.53
1:D:260:MSE:CE	1:D:273:LYS:HE2	2.39	0.53
1:G:17:PRO:O	1:G:21:THR:HG23	2.09	0.53
1:E:104:VAL:HG22	1:E:105:VAL:N	2.24	0.52
1:F:45:ARG:NH1	1:F:57:ALA:HB2	2.24	0.52
1:B:152:PHE:HB2	1:B:171:ILE:HD13	1.91	0.52
1:C:44:LEU:HA	1:D:44:LEU:HD13	1.91	0.52
1:C:82:LYS:HA	1:C:155:ILE:HD12	1.92	0.52
1:D:138:ASN:N	1:D:138:ASN:OD1	2.40	0.52
1:E:18:SER:O	1:E:21:THR:OG1	2.23	0.52
1:G:323:ASP:O	1:G:327:LEU:HG	2.10	0.52
1:C:252:PRO:HD2	1:C:255:LYS:HD3	1.90	0.52
1:D:205:VAL:O	1:D:209:ILE:HG13	2.10	0.52
1:D:341:VAL:O	1:D:345:ILE:HG12	2.09	0.52
1:G:306:LEU:HG	1:G:310:LYS:HZ2	1.73	0.52
1:B:94:ASN:HB3	1:B:102:THR:OG1	2.10	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:132:SER:O	1:D:133:THR:HG22	2.09	0.52
1:E:174:MSE:HE2	1:F:173:MSE:CG	2.38	0.52
1:E:302:LEU:HD21	1:G:223:ALA:CA	2.39	0.52
1:A:171:ILE:HA	1:A:174:MSE:HE3	1.90	0.52
1:F:295:ILE:CG2	1:F:296:PRO:HD2	2.38	0.52
1:C:83:SER:N	2:C:501:GNP:O2B	2.42	0.52
1:C:109:MSE:CE	1:C:133:THR:HG21	2.37	0.52
1:C:301:LEU:HD22	1:C:301:LEU:O	2.10	0.52
1:D:240:PHE:CB	1:D:241:PRO:HD3	2.40	0.52
1:A:111:ARG:CD	1:A:127:LEU:HD22	2.39	0.52
1:A:146:PHE:HA	1:A:149:TYR:CD2	2.45	0.52
1:B:221:GLY:CA	1:D:302:LEU:HD11	2.40	0.52
1:B:291:LEU:HD13	1:B:378:LEU:HD23	1.92	0.52
1:A:111:ARG:NH1	1:A:149:TYR:OH	2.42	0.52
1:A:159:ARG:HH11	1:A:159:ARG:CG	2.22	0.52
1:B:18:SER:O	1:B:21:THR:OG1	2.26	0.52
1:B:155:ILE:HA	1:B:181:VAL:O	2.10	0.52
1:E:323:ASP:O	1:E:327:LEU:HG	2.10	0.52
1:F:275:ARG:HH21	1:F:396:ASP:HA	1.75	0.52
1:A:92:ILE:HG21	1:A:99:ALA:HB2	1.92	0.52
1:A:293:ASN:O	1:C:207:GLN:HG3	2.09	0.52
1:C:128:PRO:HD2	1:C:144:MSE:CE	2.39	0.52
1:G:81:GLY:N	2:G:501:GNP:O1B	2.40	0.52
1:A:323:ASP:O	1:A:327:LEU:HG	2.10	0.52
1:B:146:PHE:CZ	1:B:176:GLU:HG3	2.45	0.52
1:D:151:PHE:CD2	1:D:251:LEU:HD11	2.45	0.52
1:D:168:ALA:HB2	1:D:180:PHE:HZ	1.75	0.52
1:E:336:ILE:HG21	1:E:340:GLN:HB3	1.92	0.52
1:G:94:ASN:HB3	1:G:102:THR:CG2	2.40	0.52
1:A:92:ILE:CG2	1:A:99:ALA:HB2	2.40	0.51
1:A:336:ILE:HG12	1:A:340:GLN:HB2	1.91	0.51
1:B:350:VAL:HG23	1:B:351:PHE:CD2	2.45	0.51
1:C:299:THR:HB	1:C:364:SER:HB3	1.92	0.51
1:E:107:VAL:O	1:E:107:VAL:HG13	2.10	0.51
1:E:291:LEU:HD22	1:E:384:LEU:HD23	1.92	0.51
1:G:286:GLY:HA2	1:G:388:PHE:CZ	2.45	0.51
1:B:111:ARG:NH1	1:B:148:GLU:OE1	2.33	0.51
1:B:336:ILE:HG23	1:B:337:GLU:N	2.25	0.51
1:D:214:VAL:HG13	1:D:224:GLU:HB2	1.91	0.51
1:D:235:VAL:HG22	1:D:266:ILE:HG21	1.92	0.51
1:G:42:ILE:HD13	1:G:58:ILE:HG12	1.92	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:180:PHE:HD2	1:A:225:PRO:HG2	1.72	0.51
1:D:218:ARG:CB	1:F:300:PHE:HD2	2.23	0.51
1:D:311:LYS:NZ	1:D:311:LYS:HB3	2.25	0.51
1:D:393:TYR:CE2	1:D:397:MSE:HE3	2.46	0.51
1:E:252:PRO:HD2	1:E:255:LYS:HD2	1.93	0.51
1:E:345:ILE:HB	1:E:401:ASP:CG	2.31	0.51
1:B:221:GLY:HA2	1:D:302:LEU:HD13	1.93	0.51
1:A:137:PRO:HA	1:A:140:TYR:HB3	1.93	0.51
1:B:82:LYS:HA	1:B:155:ILE:HD12	1.93	0.51
1:D:105:VAL:HG21	1:D:109:MSE:CG	2.39	0.51
1:F:73:ALA:HB2	1:F:149:TYR:CG	2.46	0.51
1:A:251:LEU:HD22	1:A:255:LYS:HB2	1.92	0.51
1:A:333:ASP:OD2	1:A:412:ARG:HD2	2.09	0.51
2:B:501:GNP:H5'2	2:B:501:GNP:C8	2.39	0.51
1:C:230:LEU:HD22	1:C:240:PHE:CD1	2.46	0.51
1:D:58:ILE:HG22	1:D:288:ALA:HB2	1.93	0.51
1:D:188:ASP:O	1:D:192:GLU:HG3	2.11	0.51
1:F:291:LEU:CD2	1:F:384:LEU:HD23	2.39	0.51
1:B:324:GLU:O	1:B:328:GLN:HG3	2.11	0.51
1:E:182:ARG:HB3	1:E:229:LEU:CD2	2.41	0.51
1:F:302:LEU:HD22	1:F:360:GLN:CB	2.41	0.51
1:G:281:ARG:O	1:G:285:GLU:HG3	2.10	0.51
1:B:233:LYS:HE2	1:B:233:LYS:CA	2.22	0.51
1:B:306:LEU:O	1:B:310:LYS:HG3	2.10	0.51
1:B:377:LEU:HD12	1:B:384:LEU:HD12	1.92	0.51
1:C:116:HIS:HB3	1:C:119:ILE:O	2.11	0.51
1:C:214:VAL:HG13	1:C:224:GLU:CB	2.37	0.51
1:D:151:PHE:HD2	1:D:251:LEU:HD11	1.75	0.51
1:G:82:LYS:HA	1:G:155:ILE:CD1	2.41	0.51
1:A:330:LEU:HD23	1:A:341:VAL:CG1	2.40	0.50
1:B:341:VAL:HA	1:B:344:MSE:CG	2.41	0.50
1:C:206:LEU:H	1:C:206:LEU:HD22	1.76	0.50
1:D:260:MSE:HE3	1:D:273:LYS:HE2	1.93	0.50
1:E:141:LEU:HD13	1:E:174:MSE:HE3	1.93	0.50
1:G:140:TYR:CE1	1:G:144:MSE:HE3	2.47	0.50
1:G:201:ASP:CB	1:G:204:LYS:HB2	2.41	0.50
1:A:233:LYS:NZ	2:A:501:GNP:N3	2.59	0.50
1:B:298:LEU:HG	1:B:363:LEU:C	2.31	0.50
1:B:299:THR:HB	1:B:300:PHE:CD1	2.46	0.50
1:C:109:MSE:HE1	1:C:133:THR:CG2	2.39	0.50
$1:C:225:PR\overline{O:HB2}$	1:C:226:PRO:HD2	1.94	0.50



	bus puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:46:MSE:HG2	1:E:54:THR:HG21	1.92	0.50
1:E:205:VAL:O	1:E:209:ILE:HG13	2.11	0.50
1:F:305:ASP:N	1:F:305:ASP:OD1	2.44	0.50
1:F:323:ASP:O	1:F:327:LEU:HG	2.10	0.50
1:G:201:ASP:HB3	1:G:204:LYS:H	1.75	0.50
1:A:182:ARG:HB3	1:A:229:LEU:HD22	1.94	0.50
1:A:185:VAL:HG22	1:A:230:LEU:O	2.11	0.50
1:A:78:THR:HA	2:A:501:GNP:O1G	2.11	0.50
1:B:104:VAL:HG11	2:B:501:GNP:O3G	2.11	0.50
1:D:218:ARG:HD3	1:F:301:LEU:CD2	2.41	0.50
1:E:286:GLY:HA2	1:E:388:PHE:CZ	2.46	0.50
1:A:159:ARG:HG3	1:A:159:ARG:NH1	2.24	0.50
1:C:141:LEU:HG	1:C:146:PHE:CD2	2.46	0.50
1:D:130:ILE:HG23	1:D:167:ILE:HD11	1.93	0.50
1:F:77:GLU:HG2	1:F:78:THR:N	2.26	0.50
1:A:107:VAL:HG13	1:A:107:VAL:O	2.11	0.50
1:G:82:LYS:CB	1:G:155:ILE:HD12	2.42	0.50
1:G:335:GLU:OE2	1:G:412:ARG:NE	2.39	0.50
1:A:80:SER:O	1:A:184:LYS:HE3	2.11	0.50
1:A:296:PRO:HB3	1:A:386:GLU:HG2	1.94	0.50
1:B:46:MSE:HG2	1:B:54:THR:HG21	1.94	0.50
1:C:210:ARG:HB2	1:C:229:LEU:HD11	1.92	0.50
1:D:92:ILE:HG21	1:D:99:ALA:HB2	1.94	0.50
1:D:257:HIS:NE2	1:D:281:ARG:HD2	2.27	0.50
1:E:275:ARG:HH21	1:E:396:ASP:CA	2.21	0.50
1:B:105:VAL:HG13	1:B:107:VAL:CG1	2.42	0.50
1:C:111:ARG:HA	1:C:126:ASP:O	2.10	0.50
1:D:150:ASP:OD1	1:D:255:LYS:HE2	2.12	0.50
1:E:263:LEU:O	1:E:274:LYS:NZ	2.26	0.50
1:B:31:GLU:N	1:B:31:GLU:OE1	2.44	0.50
1:B:66:ASP:O	1:B:121:ASN:ND2	2.45	0.50
1:B:203:GLU:OE1	1:D:381:ASN:ND2	2.28	0.50
1:B:291:LEU:HD22	1:B:384:LEU:HD23	1.94	0.50
1:D:286:GLY:HA2	1:D:388:PHE:CE2	2.46	0.50
1:D:299:THR:HG22	1:D:300:PHE:H	1.77	0.50
1:F:227:ILE:HD11	1:F:229:LEU:HD21	1.94	0.50
1:G:275:ARG:HH21	1:G:396:ASP:CA	2.25	0.50
1:G:296:PRO:O	1:G:367:ILE:HG12	2.12	0.50
1:C:184:LYS:HE2	2:C:501:GNP:O4'	2.12	0.49
1:G:301:LEU:CD2	1:G:306:LEU:HD13	2.42	0.49
$1:G:306:\overline{\text{LEU:HG}}$	1:G:310:LYS:HZ1	1.76	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:160:PHE:CE2	1:B:180:PHE:HD2	2.30	0.49
1:B:210:ARG:HB3	1:D:294:ILE:CD1	2.40	0.49
1:D:295:ILE:CG2	1:D:296:PRO:HD2	2.42	0.49
1:A:82:LYS:N	2:A:501:GNP:PB	2.83	0.49
1:B:365:ARG:O	1:B:369:GLU:HG3	2.11	0.49
1:C:85:PHE:CE2	1:C:153:ILE:HG21	2.48	0.49
1:C:130:ILE:HB	1:C:167:ILE:HD11	1.94	0.49
1:C:257:HIS:NE2	1:C:281:ARG:HD2	2.27	0.49
1:C:295:ILE:HG23	1:C:296:PRO:HD2	1.93	0.49
1:E:45:ARG:NH1	1:E:57:ALA:HB2	2.27	0.49
1:A:173:MSE:CE	1:B:142:GLU:HG3	2.42	0.49
1:C:222:ILE:O	1:C:223:ALA:HB3	2.12	0.49
1:D:309:LEU:HD21	1:D:387:ILE:HG13	1.93	0.49
1:F:42:ILE:O	1:F:46:MSE:HG3	2.12	0.49
1:B:107:VAL:O	1:B:107:VAL:HG23	2.13	0.49
1:B:181:VAL:HG13	1:B:230:LEU:HD21	1.95	0.49
1:B:298:LEU:HG	1:B:364:SER:CA	2.41	0.49
1:C:354:THR:HB	1:C:358:THR:HG21	1.95	0.49
1:E:201:ASP:OD2	1:E:204:LYS:N	2.45	0.49
1:D:58:ILE:CG2	1:D:288:ALA:HB2	2.42	0.49
1:D:70:LEU:HD12	1:D:150:ASP:OD2	2.13	0.49
1:D:154:ILE:HB	1:D:180:PHE:CD1	2.48	0.49
1:D:248:ILE:HG13	1:D:260:MSE:CE	2.43	0.49
1:E:294:ILE:HD11	1:G:210:ARG:HB3	1.94	0.49
1:C:34:ILE:HD11	1:C:38:ILE:CD1	2.43	0.49
1:D:101:LYS:HG2	1:D:102:THR:O	2.13	0.49
1:D:218:ARG:HD2	1:F:300:PHE:CE2	2.44	0.49
1:E:335:GLU:OE1	1:E:335:GLU:N	2.46	0.49
1:G:133:THR:HB	1:G:135:PHE:CD2	2.47	0.49
1:G:185:VAL:HG22	1:G:230:LEU:O	2.13	0.49
1:A:252:PRO:HD2	1:A:255:LYS:HD3	1.94	0.49
1:D:141:LEU:H	1:D:141:LEU:CD1	2.25	0.49
1:D:358:THR:CG2	1:D:361:GLU:HG3	2.42	0.49
1:G:73:ALA:HB2	1:G:149:TYR:CG	2.48	0.49
1:E:58:ILE:CG2	1:E:288:ALA:HB2	2.42	0.49
1:F:306:LEU:HD23	1:F:306:LEU:C	2.33	0.49
1:G:116:HIS:CD2	1:G:262:SER:HB2	2.48	0.49
1:G:315:PHE:O	1:G:319:VAL:HG23	2.13	0.49
1:B:184:LYS:HG2	2:B:501:GNP:C5	2.43	0.48
1:C:217:PHE:O	1:C:221:GLY:N	2.45	0.48
1:C:220:ASN:HB3	1:C:222:ILE:HG12	1.94	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:83:SER:HB2	1:D:102:THR:HG22	1.94	0.48
1:D:154:ILE:HG21	1:D:180:PHE:HE1	1.77	0.48
1:F:317:ARG:NH2	1:F:324:GLU:HG3	2.28	0.48
1:B:377:LEU:HD12	1:B:384:LEU:CD1	2.43	0.48
1:C:84:SER:CA	1:C:102:THR:CG2	2.90	0.48
1:D:90:ARG:NH2	1:D:98:GLY:O	2.46	0.48
1:E:184:LYS:HE2	2:E:501:GNP:C8	2.43	0.48
1:E:286:GLY:HA2	1:E:388:PHE:CE1	2.48	0.48
1:G:138:ASN:HA	1:G:141:LEU:HG	1.95	0.48
1:A:139:THR:HG22	1:A:143:LYS:HG3	1.94	0.48
1:B:298:LEU:CD1	1:B:363:LEU:HB3	2.43	0.48
1:C:34:ILE:HD11	1:C:38:ILE:HD12	1.94	0.48
1:C:286:GLY:HA2	1:C:388:PHE:CZ	2.48	0.48
1:A:82:LYS:HB2	1:A:155:ILE:HD12	1.95	0.48
1:A:338:VAL:HG12	1:A:342:GLU:HG3	1.94	0.48
1:B:214:VAL:HA	1:B:217:PHE:HD2	1.77	0.48
1:D:115:LYS:HG2	1:D:123:VAL:HG22	1.94	0.48
1:D:180:PHE:CE2	1:D:225:PRO:HG3	2.46	0.48
1:D:224:GLU:OE1	1:D:224:GLU:N	2.36	0.48
1:E:315:PHE:O	1:E:319:VAL:HG23	2.12	0.48
1:G:204:LYS:O	1:G:207:GLN:HG2	2.14	0.48
1:A:82:LYS:HA	1:A:155:ILE:CD1	2.44	0.48
1:B:283:TRP:HZ3	1:B:377:LEU:HD13	1.77	0.48
1:E:184:LYS:HE2	2:E:501:GNP:N9	2.29	0.48
1:F:209:ILE:HA	1:F:212:ASN:ND2	2.26	0.48
1:D:182:ARG:HB3	1:D:229:LEU:HD22	1.96	0.48
1:E:230:LEU:HD22	1:E:240:PHE:CD2	2.48	0.48
1:F:253:ILE:H	1:F:253:ILE:CD1	2.21	0.48
1:G:221:GLY:C	1:G:222:ILE:HG12	2.32	0.48
1:A:134:ASN:OD1	1:A:134:ASN:N	2.47	0.48
1:B:341:VAL:O	1:B:344:MSE:HG3	2.13	0.48
1:D:107:VAL:HG12	1:D:108:THR:N	2.27	0.48
1:E:218:ARG:HH22	1:E:224:GLU:HB2	1.79	0.48
1:E:230:LEU:HD13	1:E:240:PHE:CE2	2.49	0.48
1:F:286:GLY:HA2	1:F:388:PHE:CE1	2.48	0.48
1:F:309:LEU:HD21	1:F:387:ILE:HG13	1.95	0.48
1:G:295:ILE:HD13	1:G:383:PHE:CZ	2.49	0.48
1:A:44:LEU:HA	1:B:44:LEU:HD13	1.95	0.48
1:A:253:ILE:HD13	1:A:256:ARG:CZ	2.44	0.48
1:B:368:GLN:O	1:B:372:LEU:HD23	2.14	0.48
1:D:209:ILE:HB	1:D:229:LEU:HD11	1.94	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:324:GLU:O	1:D:328:GLN:HG3	2.14	0.48
1:G:95:GLU:N	1:G:95:GLU:OE1	2.46	0.48
1:D:82:LYS:O	1:D:86:ILE:HG13	2.13	0.48
1:E:44:LEU:HD11	1:F:43:GLU:HG2	1.96	0.48
1:E:241:PRO:HA	1:E:244:MSE:CE	2.41	0.48
1:B:45:ARG:NH1	1:B:57:ALA:HB2	2.24	0.48
1:B:241:PRO:HG3	1:B:266:ILE:CD1	2.41	0.48
1:B:283:TRP:CZ3	1:B:377:LEU:HB3	2.49	0.48
1:D:323:ASP:O	1:D:327:LEU:HG	2.14	0.48
1:E:43:GLU:OE1	1:F:44:LEU:HD21	2.14	0.48
1:E:358:THR:HG22	1:E:361:GLU:HG3	1.96	0.48
1:G:336:ILE:HB	1:G:340:GLN:HB2	1.96	0.48
1:A:271:ILE:HG22	1:A:399:THR:HG23	1.96	0.47
1:B:303:ASP:OD1	1:B:303:ASP:N	2.46	0.47
1:D:218:ARG:CB	1:F:300:PHE:CD2	2.97	0.47
1:E:186:ASP:OD1	1:E:187:SER:N	2.47	0.47
1:F:165:ILE:HG21	1:F:222:ILE:HG13	1.96	0.47
1:A:130:ILE:O	1:A:133:THR:HG22	2.14	0.47
1:A:295:ILE:HG12	1:A:383:PHE:CZ	2.49	0.47
1:B:179:TYR:CE2	1:B:247:LEU:HD23	2.49	0.47
1:G:322:VAL:HG21	1:G:398:VAL:HG13	1.95	0.47
1:G:345:ILE:HG13	1:G:348:PRO:CD	2.44	0.47
1:A:233:LYS:HZ3	2:A:501:GNP:C2	2.27	0.47
1:A:336:ILE:HD11	1:A:340:GLN:HB2	1.96	0.47
1:B:31:GLU:O	1:B:280:GLN:NE2	2.32	0.47
1:D:275:ARG:HH21	1:D:396:ASP:CA	2.26	0.47
1:D:347:SER:N	1:D:348:PRO:HD3	2.29	0.47
1:E:358:THR:HG23	1:E:361:GLU:H	1.79	0.47
1:F:31:GLU:O	1:F:280:GLN:NE2	2.33	0.47
1:F:336:ILE:HG23	1:F:340:GLN:CB	2.44	0.47
1:G:92:ILE:HG21	1:G:99:ALA:HB2	1.96	0.47
1:G:144:MSE:HB2	1:G:146:PHE:CE1	2.49	0.47
1:B:178:PHE:CE1	1:B:180:PHE:HE1	2.32	0.47
1:C:145:LYS:HE2	1:C:147:TYR:OH	2.14	0.47
1:G:251:LEU:HD22	1:G:255:LYS:HB2	1.97	0.47
1:A:184:LYS:HG2	2:A:501:GNP:C5	2.44	0.47
1:A:315:PHE:O	1:A:319:VAL:HG23	2.15	0.47
1:B:34:ILE:HD11	1:B:39:LEU:HD21	1.96	0.47
1:D:87:ASN:OD1	1:D:100:ALA:N	2.48	0.47
1:E:104:VAL:HG22	1:E:105:VAL:H	1.77	0.47
1:E:251:LEU:HD22	1:E:255:LYS:HB2	1.96	0.47



	lo uo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:146:PHE:HA	1:F:149:TYR:CD2	2.50	0.47
1:E:342:GLU:O	1:E:345:ILE:HG12	2.14	0.47
1:C:83:SER:OG	1:C:126:ASP:OD2	2.33	0.47
1:C:147:TYR:O	1:C:148:GLU:HB2	2.13	0.47
1:C:185:VAL:HG22	1:C:230:LEU:C	2.35	0.47
1:C:337:GLU:O	1:C:341:VAL:HG23	2.14	0.47
1:D:111:ARG:HD3	1:D:149:TYR:OH	2.15	0.47
1:D:141:LEU:HG	1:D:146:PHE:CD2	2.50	0.47
1:E:165:ILE:HD11	1:E:222:ILE:HD13	1.97	0.47
1:F:299:THR:HG23	1:F:300:PHE:CE2	2.50	0.47
1:G:171:ILE:HG21	1:G:178:PHE:HB3	1.96	0.47
1:A:298:LEU:HD12	1:C:211:LEU:HD13	1.97	0.47
1:A:300:PHE:HE1	1:C:218:ARG:C	2.17	0.47
1:D:218:ARG:HB2	1:F:300:PHE:CD2	2.50	0.47
1:E:393:TYR:CE2	1:E:397:MSE:HE3	2.49	0.47
1:F:80:SER:HB3	1:F:155:ILE:HG22	1.96	0.47
1:A:45:ARG:HH11	1:A:53:LEU:HB3	1.76	0.47
1:A:385:LYS:HB2	1:A:388:PHE:CE2	2.50	0.47
1:C:214:VAL:CG1	1:C:224:GLU:HB3	2.39	0.47
1:C:296:PRO:HG2	1:C:376:TYR:HE1	1.80	0.47
1:F:329:ARG:HG3	1:F:330:LEU:N	2.30	0.47
1:G:189:ILE:CG2	1:G:205:VAL:HG11	2.45	0.47
1:A:125:TRP:CD1	1:A:149:TYR:HE1	2.33	0.47
1:A:180:PHE:HE2	1:A:225:PRO:HG3	1.80	0.47
1:B:298:LEU:CD1	1:B:363:LEU:CB	2.93	0.47
1:B:336:ILE:CG1	1:B:337:GLU:H	2.27	0.47
1:D:28:ASN:HB2	1:D:31:GLU:OE1	2.15	0.47
1:D:295:ILE:HG23	1:D:296:PRO:HD2	1.97	0.47
1:D:315:PHE:O	1:D:319:VAL:HG23	2.15	0.47
1:D:368:GLN:O	1:D:372:LEU:HD23	2.15	0.47
1:E:152:PHE:HB2	1:E:171:ILE:HD13	1.97	0.47
1:F:136:PRO:HD2	1:F:139:THR:HB	1.97	0.47
1:F:165:ILE:HG12	1:F:217:PHE:CZ	2.50	0.47
1:G:73:ALA:HB2	1:G:149:TYR:CD1	2.49	0.47
1:A:105:VAL:HG23	2:A:501:GNP:O3G	2.15	0.46
1:A:385:LYS:HB2	1:A:388:PHE:CD2	2.50	0.46
1:D:206:LEU:HD22	1:D:238:TYR:CE1	2.50	0.46
1:E:313:MSE:HE3	1:E:347:SER:HB2	1.98	0.46
1:F:302:LEU:HG	1:F:306:LEU:HD12	1.92	0.46
1:G:20:PHE:HB2	1:G:287:PHE:CE2	2.50	0.46
1:B:205:VAL:O	1:B:209:ILE:HG13	$2.\overline{15}$	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:378:LEU:HD12	1:B:378:LEU:N	2.31	0.46
1:F:157:ALA:HB1	1:F:184:LYS:HD2	1.97	0.46
1:B:82:LYS:CB	1:B:155:ILE:HD12	2.46	0.46
1:B:341:VAL:CA	1:B:344:MSE:HG3	2.43	0.46
1:C:107:VAL:O	1:C:107:VAL:HG13	2.15	0.46
1:C:188:ASP:O	1:C:192:GLU:HG3	2.16	0.46
1:C:297:SER:HB3	1:C:368:GLN:HG2	1.97	0.46
1:C:393:TYR:CE2	1:C:397:MSE:HE3	2.50	0.46
1:D:116:HIS:CD2	1:D:262:SER:HB2	2.50	0.46
1:D:135:PHE:C	1:D:137:PRO:HD2	2.36	0.46
1:D:263:LEU:O	1:D:274:LYS:NZ	2.32	0.46
1:F:185:VAL:HG11	1:F:229:LEU:HB3	1.97	0.46
1:F:338:VAL:O	1:F:341:VAL:HG22	2.15	0.46
1:G:286:GLY:HA2	1:G:388:PHE:CE2	2.51	0.46
1:C:317:ARG:HA	1:C:322:VAL:HG22	1.97	0.46
1:D:202:LYS:HD2	1:D:202:LYS:N	2.30	0.46
1:E:210:ARG:O	1:E:214:VAL:HG22	2.15	0.46
1:E:354:THR:HG22	1:E:362:ARG:NH2	2.31	0.46
1:G:24:PHE:CE2	1:G:39:LEU:HD21	2.51	0.46
1:B:171:ILE:HG21	1:B:178:PHE:HB3	1.96	0.46
1:B:186:ASP:OD1	2:B:501:GNP:N1	2.43	0.46
1:D:95:GLU:OE1	1:D:95:GLU:N	2.48	0.46
1:F:393:TYR:CE2	1:F:397:MSE:HE3	2.50	0.46
1:G:28:ASN:HB2	1:G:31:GLU:CD	2.36	0.46
1:G:115:LYS:HG2	1:G:123:VAL:HG22	1.98	0.46
1:G:130:ILE:HD11	1:G:137:PRO:HA	1.97	0.46
1:A:175:LYS:HZ3	1:B:147:TYR:HB2	1.81	0.46
1:B:315:PHE:O	1:B:319:VAL:HG23	2.16	0.46
1:F:188:ASP:O	1:F:192:GLU:HG2	2.15	0.46
1:G:324:GLU:OE1	1:G:328:GLN:NE2	2.47	0.46
2:G:501:GNP:O5'	2:G:501:GNP:H8	2.16	0.46
1:A:138:ASN:OD1	1:B:138:ASN:ND2	2.47	0.46
1:B:298:LEU:HD12	1:B:363:LEU:CB	2.46	0.46
1:C:86:ILE:HG23	1:C:124:PHE:CB	2.46	0.46
1:D:244:MSE:CA	1:D:247:LEU:HD12	2.37	0.46
1:E:322:VAL:HG21	1:E:398:VAL:HG13	1.97	0.46
1:F:215:ASN:OD1	1:F:216:THR:N	2.49	0.46
1:A:80:SER:O	1:A:183:THR:OG1	2.19	0.46
1:C:150:ASP:OD1	1:C:255:LYS:HE2	2.15	0.46
1:D:141:LEU:HA	1:D:146:PHE:CE2	2.50	0.46
1:G:241:PRO:HG3	1:G:266:ILE:CD1	2.43	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlan(Å)
1.C.152.PHE.HB2	1.C.171.ILE.HD13	1.98	0.46
$1 \cdot C \cdot 179 \cdot TYB \cdot CZ$	1.C.247.LEU.HD23	2.51	0.10
1.C.368.GLN.O	1:C:372:LEU:HD13	2.01	0.10
1.D.185.VAL.:HG22	1.0.972.010.11010	2.16	0.10
1.G.298.LEU.H	$1 \cdot G \cdot 367 \cdot ILE \cdot HG21$	1.80	0.10
$1 \cdot \Delta \cdot 135 \cdot \text{PHE} \cdot \text{CE}2$	$1 \cdot \Delta \cdot 1/3 \cdot I \sqrt{S \cdot HE2}$	2.51	0.40
$1 \cdot 1 \cdot 1 \cdot 1 \cdot 1 \cdot 1 \cdot 2 \cdot 1 \cdot 1 \cdot 1 \cdot $	$1 \cdot \Delta \cdot 220 \cdot \text{LEU} \cdot \text{CD}2$	2.01	0.40
1:M:102:M:CO:HD3 1:D:182:ABG:HB3	1.N.229.LEU.CD2	2.40	0.40
1.E.301.LEU.HD22	1.E.363.LEU.CD1	2.40	0.40
$1 \cdot E \cdot 179 \cdot T \vee B \cdot C Z$	1.E.000.EEU.0D1	2.40	0.40
1.F.286.CLV.HA2	1.F.388.PHF.CF2	2.51	0.40
1.F.200.011.IIA2	1.F.366.I HE.0E2	2.51	0.40
1.D.42.IEE.O	1.B.238.TVB.OH	2.11	0.45
$\frac{1.0.109.1109.11012}{1.0.994.11 \text{ F}\cdot\text{N}}$	1.D.230.1110.011 1.C.204.ILF.HD12	2.10	0.45
1.0.294.IDD.IN	1.U.294.IDD.IID12	2.51	0.45
1.E.77.GLU.UE2	1.E.101.E15.IID2	2.15	0.45
1.F.298.LEU.IID23	$\frac{1.11.503.1100.11103}{2.000000000000000000000000000000000000$	2.16	0.45
1.G.75.1III.IIG25	2.G.301.GN1.05G	2.10	0.45
1.G.252.1 KO.HD2	1.G.205.LIS.IID5	1.96	0.45
1.D.275.ARG.IIII21	1.D.390.ABF.OA	2.25	0.45
	1.D.329.Ang.nD3 $1.D.114.TVD.CE1$	2.10	0.45
1.D.100.ALA.IIA	1.D.114.11R.OD1 $1.D.960.MCF.UF1$	1.02	0.45
1.D.240.ILE.IIGI3	1.C.972.IVS.UF2	1.90	0.45
1.G.200.MBE.OE	1.G.275.L15.HE2	2.47	0.45
	1.4.197.I FU.HD99	1.97	0.45
1.A.111.AnG.nG2	$\frac{1.A.127.LEU.HD22}{1.D.150.ASD.OD2}$	2.97	0.45
	1.D.100.ASF.0D2	2.10	0.45
1.D.190.L15.HG2	1.D.190.L15.U	2.10	0.45
1:D:222:ILE:IIG12	$1:D:222:ILE:\Pi$	1.09	0.45
1.D.90.CED.O	2.E.301.GNF.04	2.40	0.45
1.D.00.5EIV.O	1.D.106.IVC.UD9	2.33	0.45
	1.D.190.L15.IID2	1.07	0.45
1.D.201.ASF.IID2		1.99	0.45
1.C.95.DUF.UF9	1.D.301.LEU.HA	1.03	0.45
$1: \bigcirc :00: P \square \square \square \square \square \square \square$	1:0:100:1LE:IIG21	1.01	0.45
1:D:2I:FHE:HE2	$1:D:270:GLN:\PiA$	1.81	0.45
$1.D.140.F\Pi E.\Pi DI$	$1.D.149.11K.\Pi E2$	1.00	0.45
1.D:214:VAL:UGI	I:D:210:AKG:HE	<u></u> りた1	0.45
1:E:100:ALA:HB2	1.C.919.ADC.NU1	2.01	0.45
1:E:300:PHE:U	1.E.218:AKG:NH1	2.49	0.45
1:F:209:ILE:HB	1:F:229:LEU:UD1	2.47	0.45
1:G:260:MSE:HE3	1:G:273:LYS:HE2	1.98	0.45



Interstomic Clash				
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:73:ALA:HB2	1:B:149:TYR:CD1	2.52	0.45	
1:B:335:GLU:O	1:B:336:ILE:HB	2.17	0.45	
1:C:172:SER:HB2	1:C:178:PHE:HE2	1.81	0.45	
1:C:326:SER:O	1:C:329:ARG:HG3	2.16	0.45	
1:E:173:MSE:HE1	1:F:142:GLU:HB2	1.98	0.45	
1:F:244:MSE:SE	1:F:263:LEU:HB3	2.67	0.45	
1:B:58:ILE:HD13	1:B:287:PHE:HB3	1.98	0.45	
1:B:378:LEU:HD11	1:B:384:LEU:HG	1.98	0.45	
1:D:267:THR:HA	1:D:406:LEU:HD21	1.99	0.45	
1:E:336:ILE:CG2	1:E:340:GLN:CB	2.95	0.45	
1:G:165:ILE:O	1:G:169:LYS:HG3	2.16	0.45	
1:G:378:LEU:HD11	1:G:384:LEU:HG	1.99	0.45	
1:B:220:ASN:CB	1:B:222:ILE:HD11	2.47	0.45	
1:B:266:ILE:HG13	1:B:267:THR:N	2.32	0.45	
1:C:261:VAL:O	1:C:319:VAL:HG13	2.16	0.45	
1:C:315:PHE:O	1:C:319:VAL:HG23	2.17	0.45	
1:D:23:TYR:CE2	1:D:27:PHE:HE1	2.34	0.45	
1:F:150:ASP:OD1	1:F:255:LYS:HE2	2.17	0.45	
1:F:217:PHE:CD2	1:F:225:PRO:HB3	2.52	0.45	
1:F:302:LEU:HD22	1:F:360:GLN:HB3	1.97	0.45	
1:F:317:ARG:HA	1:F:322:VAL:CG2	2.47	0.45	
1:G:335:GLU:CD	1:G:412:ARG:HE	2.18	0.45	
1:A:300:PHE:CE1	1:C:219:GLU:HA	2.51	0.45	
1:B:185:VAL:HG22	1:B:230:LEU:C	2.37	0.45	
1:D:68:SER:OG	1:D:258:ASN:OD1	2.35	0.45	
1:D:104:VAL:CG2	1:D:105:VAL:H	2.23	0.45	
1:E:260:MSE:O	1:E:274:LYS:HE2	2.17	0.45	
1:E:358:THR:CG2	1:E:361:GLU:HG3	2.47	0.45	
1:A:17:PRO:O	1:A:21:THR:HG23	2.17	0.45	
1:A:116:HIS:HB3	1:A:119:ILE:O	2.17	0.45	
1:A:260:MSE:O	1:A:274:LYS:HE2	2.17	0.45	
1:A:275:ARG:O	1:A:279:LYS:HG3	2.17	0.45	
1:C:235:VAL:HG22	1:C:266:ILE:HG21	1.99	0.45	
1:D:294:ILE:HD12	1:D:294:ILE:N	2.31	0.45	
1:D:326:SER:O	1:D:330:LEU:HD13	2.17	0.45	
1:F:165:ILE:CG2	1:F:222:ILE:HG21	2.47	0.45	
1:F:165:ILE:HG23	1:F:222:ILE:HG21	1.99	0.45	
1:G:145:LYS:HD2	1:G:147:TYR:OH	2.17	0.45	
1:A:331:ALA:O	1:A:335:GLU:HA	2.16	0.45	
1:B:17:PRO:O	1:B:21:THR:HG23	2.16	0.45	
1:B:90:ARG:NH1	1:B:114:TYR:HB3	2.31	0.45	



A 4 1	A 4 5 775 D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:44:LEU:HD21	1:D:43:GLU:OE1	2.16	0.45
1:C:205:VAL:O	1:C:209:ILE:HG13	2.16	0.45
1:C:211:LEU:O	1:C:215:ASN:N	2.50	0.45
1:D:111:ARG:HB3	1:D:127:LEU:HD22	1.98	0.45
1:D:130:ILE:HG22	1:D:140:TYR:CE2	2.52	0.45
1:D:241:PRO:HG3	1:D:266:ILE:CD1	2.40	0.45
1:F:209:ILE:HB	1:F:229:LEU:HD11	1.99	0.45
1:F:302:LEU:HD21	1:F:360:GLN:HA	1.98	0.45
1:G:159:ARG:HH12	1:G:161:LYS:HA	1.82	0.45
1:A:43:GLU:OE1	1:B:44:LEU:HD21	2.17	0.44
1:A:203:GLU:HB3	1:A:206:LEU:HD23	1.99	0.44
1:D:92:ILE:HG22	1:D:99:ALA:HB2	1.99	0.44
1:F:82:LYS:HB2	2:F:501:GNP:O2G	2.18	0.44
1:B:212:ASN:O	1:B:215:ASN:HB3	2.16	0.44
1:C:141:LEU:HA	1:C:146:PHE:CD2	2.52	0.44
1:C:345:ILE:HG13	1:C:348:PRO:CD	2.46	0.44
1:D:133:THR:CG2	1:D:134:ASN:N	2.71	0.44
1:D:135:PHE:CB	1:D:137:PRO:HD2	2.43	0.44
1:E:130:ILE:HD13	1:E:140:TYR:CG	2.52	0.44
1:F:146:PHE:HA	1:F:149:TYR:CE2	2.53	0.44
1:F:220:ASN:CB	1:F:222:ILE:HG12	2.46	0.44
1:F:344:MSE:CE	1:F:408:GLU:HG3	2.43	0.44
1:G:235:VAL:HG13	1:G:266:ILE:HG22	1.99	0.44
1:A:34:ILE:HD11	1:A:38:ILE:HB	1.98	0.44
1:D:348:PRO:O	1:D:352:LYS:HG3	2.17	0.44
1:E:146:PHE:HA	1:E:149:TYR:CE2	2.52	0.44
1:E:301:LEU:N	1:E:301:LEU:HD12	2.32	0.44
1:F:243:LEU:O	1:F:247:LEU:HG	2.18	0.44
1:A:105:VAL:CG2	2:A:501:GNP:PG	3.06	0.44
1:C:210:ARG:HB2	1:C:229:LEU:CD1	2.48	0.44
1:D:70:LEU:HD12	1:D:150:ASP:CG	2.38	0.44
1:E:106:GLU:HB3	1:E:107:VAL:H	1.56	0.44
1:F:234:ASN:CG	1:F:237:HIS:HD1	2.20	0.44
1:G:154:ILE:HD12	1:G:180:PHE:CE1	2.53	0.44
1:G:354:THR:HG21	1:G:362:ARG:NH2	2.32	0.44
1:C:105:VAL:HG11	2:C:501:GNP:O1G	2.17	0.44
1:C:184:LYS:HE2	2:C:501:GNP:C1'	2.47	0.44
1:D:214:VAL:O	1:D:218:ARG:HG3	2.16	0.44
1:F:287:PHE:CZ	1:F:378:LEU:HD21	2.52	0.44
1:F:339:ASP:N	1:F:339:ASP:OD1	2.51	0.44
1:F:352:LYS:O	1:F:362:ARG:NH2	2.42	0.44



		Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
1:B:170:ALA:O	1:B:174:MSE:HG3	2.18	0.44	
1:C:100:ALA:HB2	1:C:114:TYR:CE1	2.52	0.44	
1:D:113:PRO:HD3	1:D:125:TRP:CZ3	2.53	0.44	
1:D:130:ILE:HG13	1:D:131:GLY:N	2.32	0.44	
1:D:313:MSE:HG2	1:D:351:PHE:HE2	1.82	0.44	
1:F:80:SER:O	1:F:183:THR:OG1	2.32	0.44	
1:F:116:HIS:CD2	1:F:262:SER:HB2	2.53	0.44	
1:F:315:PHE:O	1:F:319:VAL:HG23	2.18	0.44	
1:B:159:ARG:NH1	1:B:159:ARG:HB2	2.31	0.44	
1:B:252:PRO:HD2	1:B:255:LYS:HD2	2.00	0.44	
1:C:180:PHE:CE2	1:C:225:PRO:CG	3.00	0.44	
1:E:130:ILE:CG2	1:E:163:ASN:HB3	2.48	0.44	
1:E:275:ARG:O	1:E:279:LYS:HG3	2.18	0.44	
1:E:385:LYS:HB2	1:E:388:PHE:CE2	2.53	0.44	
1:F:116:HIS:HA	1:F:117:PRO:HD3	1.90	0.44	
1:G:74:VAL:CG1	1:G:82:LYS:HB2	2.48	0.44	
1:G:227:ILE:HD12	1:G:228:PHE:H	1.83	0.44	
1:G:305:ASP:O	1:G:309:LEU:HG	2.18	0.44	
1:G:340:GLN:O	1:G:344:MSE:HG3	2.17	0.44	
1:A:46:MSE:HG2	1:A:54:THR:HG21	2.00	0.44	
1:A:313:MSE:O	1:A:317:ARG:HG3	2.18	0.44	
1:A:393:TYR:CE2	1:A:397:MSE:HE3	2.52	0.44	
1:B:378:LEU:HD13	1:B:384:LEU:HG	1.99	0.44	
1:C:105:VAL:CG2	1:C:106:GLU:N	2.81	0.44	
1:C:181:VAL:CG1	1:C:230:LEU:HD11	2.48	0.44	
1:D:136:PRO:N	1:D:137:PRO:CD	2.80	0.44	
1:E:92:ILE:HD11	1:E:117:PRO:HG2	1.98	0.44	
1:F:305:ASP:O	1:F:308:THR:HB	2.18	0.44	
1:B:322:VAL:HG21	1:B:398:VAL:HG13	2.00	0.44	
1:F:31:GLU:N	1:F:31:GLU:OE1	2.51	0.44	
1:G:275:ARG:O	1:G:279:LYS:HG3	2.18	0.44	
1:B:96:GLU:CD	1:B:329:ARG:HH22	2.21	0.43	
1:B:96:GLU:H	1:B:96:GLU:HG3	1.67	0.43	
1:B:106:GLU:HB3	1:B:107:VAL:H	1.42	0.43	
1:D:218:ARG:CD	1:F:301:LEU:HD22	2.47	0.43	
1:G:266:ILE:HG13	1:G:267:THR:HG23	2.00	0.43	
1:B:20:PHE:HB2	1:B:287:PHE:CE2	2.53	0.43	
1:B:257:HIS:NE2	1:B:281:ARG:HD2	2.33	0.43	
1:C:109:MSE:HE1	1:C:135:PHE:CZ	2.53	0.43	
1:D:34:ILE:HD11	1:D:38:ILE:CG2	2.46	0.43	
1:E:20:PHE:HB2	1:E:287:PHE:CE2	2.52	0.43	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:E:155:ILE:HG12	1:E:181:VAL:HB	1.99	0.43	
1:B:31:GLU:HG2	1:B:276:GLN:OE1	2.17	0.43	
1:B:35:SER:O	1:B:38:ILE:HG22	2.17	0.43	
1:B:45:ARG:HH11	1:B:57:ALA:CB	2.27	0.43	
1:B:83:SER:CB	2:B:501:GNP:HNB3	2.32	0.43	
1:B:182:ARG:HD3	1:B:185:VAL:CG1	2.49	0.43	
1:B:206:LEU:HD12	1:B:206:LEU:N	2.33	0.43	
1:D:307:GLU:O	1:D:311:LYS:HG2	2.19	0.43	
1:E:116:HIS:HB3	1:E:119:ILE:O	2.19	0.43	
1:F:322:VAL:HG21	1:F:398:VAL:HG13	1.99	0.43	
1:G:320:PHE:HB3	1:G:402:ALA:HB2	2.01	0.43	
1:A:337:GLU:H	1:A:337:GLU:HG2	1.67	0.43	
1:A:354:THR:HG22	1:A:355:ASP:N	2.33	0.43	
1:B:152:PHE:CB	1:B:171:ILE:HD13	2.48	0.43	
1:B:283:TRP:HZ3	1:B:377:LEU:HB3	1.83	0.43	
1:D:31:GLU:OE1	1:D:31:GLU:N	2.51	0.43	
1:D:168:ALA:HB2	1:D:180:PHE:CZ	2.53	0.43	
1:D:209:ILE:HB	1:D:229:LEU:CD1	2.48	0.43	
1:E:128:PRO:HG2	1:E:144:MSE:HE1	1.99	0.43	
1:F:72:VAL:HG22	1:F:151:PHE:CZ	2.53	0.43	
1:B:207:GLN:CG	1:D:295:ILE:HD11	2.48	0.43	
1:B:327:LEU:HD23	1:B:330:LEU:CD1	2.48	0.43	
1:C:136:PRO:HD2	1:C:139:THR:CB	2.49	0.43	
1:E:234:ASN:ND2	1:E:237:HIS:HB2	2.33	0.43	
1:E:267:THR:HA	1:E:406:LEU:HD21	2.01	0.43	
1:E:356:GLU:OE1	1:E:356:GLU:N	2.46	0.43	
1:E:385:LYS:HB2	1:E:388:PHE:CD2	2.53	0.43	
1:F:102:THR:O	2:F:501:GNP:N3B	2.47	0.43	
1:G:45:ARG:O	1:G:48:LYS:HB2	2.18	0.43	
1:G:165:ILE:HG12	1:G:217:PHE:CE1	2.53	0.43	
1:A:227:ILE:HD12	1:A:228:PHE:N	2.34	0.43	
1:A:268:ASP:OD1	1:A:403:LYS:HG2	2.17	0.43	
1:C:75:THR:OG1	1:C:76:GLY:N	2.52	0.43	
1:F:80:SER:N	2:F:501:GNP:O1B	2.51	0.43	
1:G:268:ASP:OD1	1:G:406:LEU:HD23	2.19	0.43	
1:C:323:ASP:O	1:C:327:LEU:HG	2.19	0.43	
1:C:367:ILE:CD1	1:C:386:GLU:HG3	2.48	0.43	
1:E:336:ILE:HG22	1:E:337:GLU:N	2.33	0.43	
1:F:185:VAL:HG22	1:F:230:LEU:O	2.18	0.43	
1:F:214:VAL:O	1:F:218:ARG:N	2.43	0.43	
1:G:127:LEU:HA	1:G:128:PRO:HD3	1.88	0.43	



	Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlan (Å)
1:G:324:GLU:O	1:G:328:GLN:HG3	2.18	0.43
1:A:34:ILE:CG2	1:A:39:LEU:HD21	2.49	0.43
1:A:159:ARG:CG	1:A:159:ARG:NH1	2.80	0.43
1:B:51:ILE:HG22	1:B:55:ASN:ND2	2.33	0.43
1:B:207:GLN:OE1	1:D:295:ILE:HD11	2.18	0.43
1:B:222:ILE:O	1:B:223:ALA:HB3	2.18	0.43
1:B:347:SER:O	1:B:350:VAL:HG22	2.19	0.43
1:D:46:MSE:HG2	1:D:54:THR:HG21	2.01	0.43
1:G:116:HIS:HA	1:G:117:PRO:HD3	1.88	0.43
1:A:42:ILE:O	1:A:46:MSE:HG3	2.19	0.43
1:A:260:MSE:HE3	1:A:273:LYS:HE2	2.01	0.43
1:A:298:LEU:O	1:A:299:THR:OG1	2.31	0.43
1:B:275:ARG:O	1:B:279:LYS:HG3	2.18	0.43
1:C:243:LEU:O	1:C:247:LEU:HG	2.18	0.43
1:D:141:LEU:HA	1:D:146:PHE:CD2	2.53	0.43
1:E:59:SER:O	1:E:63:LYS:HG3	2.19	0.43
1:E:215:ASN:O	1:E:219:GLU:HG3	2.19	0.43
1:F:21:THR:HG21	1:F:43:GLU:CD	2.39	0.43
1:F:298:LEU:HB3	1:F:364:SER:HA	2.00	0.43
1:A:135:PHE:HE2	1:A:143:LYS:HE2	1.84	0.43
1:B:300:PHE:O	1:B:301:LEU:HD22	2.18	0.43
1:C:42:ILE:O	1:C:46:MSE:HG3	2.18	0.43
1:C:80:SER:HB2	1:C:156:SER:HA	2.00	0.43
1:E:15:ASP:HB2	1:E:17:PRO:HD2	2.00	0.43
1:F:136:PRO:HD2	1:F:139:THR:CB	2.49	0.43
1:G:257:HIS:CE1	1:G:281:ARG:HD2	2.53	0.43
1:A:44:LEU:HD11	1:B:43:GLU:HG2	2.01	0.42
1:A:113:PRO:HB3	1:A:125:TRP:CZ2	2.54	0.42
1:B:235:VAL:HG11	1:B:266:ILE:HG22	1.96	0.42
1:B:317:ARG:HA	1:B:322:VAL:CG2	2.49	0.42
1:B:330:LEU:HD11	1:B:405:LEU:HD21	2.00	0.42
1:C:385:LYS:HB2	1:C:388:PHE:CE2	2.54	0.42
1:D:107:VAL:CG1	1:D:108:THR:H	2.30	0.42
1:D:135:PHE:CB	1:D:136:PRO:HD2	2.49	0.42
1:D:162:LYS:HA	1:D:165:ILE:HB	2.00	0.42
1:E:45:ARG:HH11	1:E:57:ALA:CB	2.30	0.42
1:E:225:PRO:HA	1:E:226:PRO:HD3	1.94	0.42
1:E:344:MSE:HB2	1:E:344:MSE:HE3	1.72	0.42
1:F:301:LEU:HD13	1:F:301:LEU:HA	1.76	0.42
1:A:80:SER:C	1:A:184:LYS:HE3	2.39	0.42
1:A:146:PHE:HA	1:A:149:TYR:HE2	1.83	0.42



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:74:VAL:HG11	1:B:82:LYS:HB2	2.01	0.42	
1:B:81:GLY:HA2	2:B:501:GNP:O3A	2.18	0.42	
1:C:291:LEU:HD22	1:C:384:LEU:HD23	2.01	0.42	
1:D:51:ILE:HG22	1:D:55:ASN:ND2	2.35	0.42	
1:E:49:GLY:O	1:E:51:ILE:HD12	2.18	0.42	
1:G:206:LEU:HD12	1:G:206:LEU:HA	1.77	0.42	
1:G:222:ILE:HG22	1:G:222:ILE:O	2.19	0.42	
1:B:263:LEU:O	1:B:274:LYS:NZ	2.33	0.42	
1:E:145:LYS:HB3	1:E:147:TYR:HD1	1.83	0.42	
1:E:196:LYS:HD3	1:E:200:PHE:CE1	2.53	0.42	
1:E:301:LEU:HD22	1:E:363:LEU:HD13	2.01	0.42	
1:G:82:LYS:HA	1:G:155:ILE:HD12	2.02	0.42	
1:A:173:MSE:HE1	1:B:142:GLU:HG3	2.01	0.42	
1:B:16:LEU:HD13	1:B:379:PRO:HD2	2.00	0.42	
1:B:263:LEU:HA	1:B:264:PRO:HD3	1.91	0.42	
1:B:286:GLY:HA2	1:B:388:PHE:CZ	2.53	0.42	
1:B:327:LEU:HA	1:B:330:LEU:HD12	2.01	0.42	
1:B:367:ILE:HG23	1:B:368:GLN:N	2.35	0.42	
1:E:230:LEU:HD13	1:E:240:PHE:HE2	1.83	0.42	
1:E:243:LEU:O	1:E:247:LEU:HG	2.19	0.42	
1:E:324:GLU:O	1:E:328:GLN:HG2	2.19	0.42	
1:F:187:SER:OG	2:F:501:GNP:N2	2.52	0.42	
1:F:303:ASP:O	1:F:306:LEU:HB3	2.20	0.42	
1:A:323:ASP:OD1	1:A:323:ASP:N	2.52	0.42	
1:B:240:PHE:N	1:B:241:PRO:CD	2.83	0.42	
1:B:298:LEU:CB	1:B:364:SER:CA	2.89	0.42	
1:C:146:PHE:HA	1:C:149:TYR:HE2	1.85	0.42	
1:E:51:ILE:HG22	1:E:55:ASN:ND2	2.35	0.42	
1:G:336:ILE:HB	1:G:340:GLN:CB	2.50	0.42	
1:C:260:MSE:HE2	1:C:273:LYS:CG	2.49	0.42	
1:D:295:ILE:HD12	1:D:295:ILE:N	2.27	0.42	
1:D:352:LYS:O	1:D:359:ILE:HD11	2.20	0.42	
1:G:368:GLN:O	1:G:372:LEU:HD23	2.19	0.42	
1:A:37:GLU:HB3	1:B:37:GLU:OE2	2.20	0.42	
1:A:206:LEU:HD22	1:A:206:LEU:N	2.34	0.42	
1:B:31:GLU:OE2	1:B:273:LYS:HE3	2.20	0.42	
1:B:105:VAL:O	1:B:105:VAL:HG22	2.20	0.42	
1:B:326:SER:O	1:B:330:LEU:N	2.45	0.42	
1:C:206:LEU:HD22	1:C:206:LEU:N	2.35	0.42	
1:E:309:LEU:HD21	1:E:387:ILE:HG13	2.02	0.42	
1:F:16:LEU:HG	1:F:17:PRO:HD3	2.01	0.42	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:26:LYS:CE	1:G:26:LYS:HE2	2.50	0.42
1:B:31:GLU:HA	1:B:277:PHE:CE1	2.55	0.42
1:B:283:TRP:CZ3	1:B:377:LEU:HD13	2.54	0.42
1:B:337:GLU:O	1:B:340:GLN:HB2	2.19	0.42
1:C:31:GLU:HG2	1:C:273:LYS:HG3	2.02	0.42
1:D:111:ARG:H	1:D:111:ARG:HG3	1.61	0.42
1:D:153:ILE:HD13	1:D:179:TYR:HB2	2.02	0.42
1:D:185:VAL:HG22	1:D:230:LEU:C	2.40	0.42
1:D:286:GLY:HA2	1:D:388:PHE:CE1	2.54	0.42
1:D:357:GLU:OE1	1:D:357:GLU:N	2.52	0.42
1:F:174:MSE:O	1:F:174:MSE:HG2	2.20	0.42
1:F:298:LEU:CD2	1:F:363:LEU:HB3	2.49	0.42
1:G:72:VAL:HG22	1:G:151:PHE:CZ	2.54	0.42
1:D:154:ILE:HG21	1:D:180:PHE:CE1	2.54	0.42
1:E:109:MSE:HE1	1:E:132:SER:O	2.19	0.42
1:G:152:PHE:CB	1:G:171:ILE:HD13	2.50	0.42
1:B:38:ILE:O	1:B:42:ILE:HG13	2.20	0.42
1:B:270:VAL:O	1:B:274:LYS:HG3	2.20	0.42
1:C:107:VAL:HG23	1:C:132:SER:HB2	2.02	0.42
1:C:385:LYS:HB2	1:C:388:PHE:CD2	2.55	0.42
1:D:334:TRP:C	1:D:336:ILE:N	2.72	0.42
1:E:34:ILE:HD11	1:E:38:ILE:CD1	2.50	0.42
1:F:251:LEU:HD22	1:F:255:LYS:HB2	2.01	0.42
1:A:205:VAL:O	1:A:209:ILE:HG13	2.20	0.41
1:A:206:LEU:HB3	1:A:210:ARG:NH1	2.35	0.41
1:B:330:LEU:HD22	1:B:405:LEU:HD11	2.00	0.41
1:B:352:LYS:O	1:B:362:ARG:NH1	2.52	0.41
1:C:230:LEU:CB	1:C:240:PHE:HD1	2.31	0.41
1:C:305:ASP:O	1:C:309:LEU:HG	2.20	0.41
1:E:174:MSE:HE1	1:F:173:MSE:HE3	2.01	0.41
1:E:295:ILE:HG22	1:E:297:SER:H	1.85	0.41
1:F:154:ILE:HD12	1:F:180:PHE:CE1	2.55	0.41
1:F:263:LEU:HA	1:F:264:PRO:HD3	1.90	0.41
1:G:74:VAL:HG12	1:G:82:LYS:HB2	2.02	0.41
1:B:345:ILE:HB	1:B:401:ASP:CG	2.39	0.41
1:C:16:LEU:HB2	1:C:17:PRO:HD3	2.02	0.41
1:C:45:ARG:HH11	1:C:57:ALA:CB	2.27	0.41
1:D:275:ARG:O	1:D:279:LYS:HG3	2.20	0.41
1:E:41:LEU:HD13	1:E:41:LEU:C	2.41	0.41
1:E:58:ILE:HG22	1:E:288:ALA:HB2	2.02	0.41
1:G:82:LYS:NZ	1:G:127:LEU:O	2.49	0.41



	ous puge	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:G:189:ILE:HG23	1:G:205:VAL:HG12	2.01	0.41	
1:A:28:ASN:HB2	1:A:31:GLU:CD	2.40	0.41	
1:A:165:ILE:HG12	1:A:217:PHE:CD1	2.56	0.41	
1:B:156:SER:OG	1:B:159:ARG:O	2.39	0.41	
1:C:275:ARG:O	1:C:279:LYS:HG3	2.20	0.41	
1:E:65:ILE:O	1:E:68:SER:OG	2.37	0.41	
1:E:146:PHE:CD1	1:E:149:TYR:HE2	2.37	0.41	
1:E:152:PHE:CB	1:E:171:ILE:HD13	2.50	0.41	
1:E:211:LEU:C	1:E:211:LEU:HD23	2.40	0.41	
1:F:28:ASN:HB2	1:F:31:GLU:OE1	2.20	0.41	
1:F:260:MSE:HE2	1:F:273:LYS:CG	2.50	0.41	
1:A:34:ILE:HD11	1:A:38:ILE:CB	2.50	0.41	
1:A:150:ASP:CG	1:A:255:LYS:HE2	2.41	0.41	
1:A:158:THR:OG1	1:A:159:ARG:N	2.53	0.41	
1:C:281:ARG:HG2	1:C:281:ARG:HH11	1.85	0.41	
1:C:337:GLU:HB2	1:C:340:GLN:HG2	2.03	0.41	
1:D:202:LYS:HA	1:D:205:VAL:HG22	2.02	0.41	
1:E:358:THR:OG1	1:E:359:ILE:N	2.53	0.41	
1:E:359:ILE:HG13	1:E:360:GLN:N	2.35	0.41	
1:F:182:ARG:HB3	1:F:229:LEU:HD22	2.02	0.41	
1:G:334:TRP:CE3	1:G:336:ILE:HD11	2.39	0.41	
1:A:28:ASN:ND2	1:A:31:GLU:OE2	2.54	0.41	
1:A:38:ILE:O	1:A:42:ILE:HG13	2.20	0.41	
1:A:206:LEU:HD22	1:A:206:LEU:H	1.85	0.41	
1:B:281:ARG:HG2	1:B:281:ARG:HH11	1.85	0.41	
1:C:240:PHE:N	1:C:241:PRO:CD	2.84	0.41	
1:D:281:ARG:HG2	1:D:281:ARG:HH11	1.85	0.41	
1:E:102:THR:HB	2:E:501:GNP:O3'	2.21	0.41	
1:F:137:PRO:O	1:F:141:LEU:HG	2.20	0.41	
1:F:330:LEU:HD12	1:F:330:LEU:C	2.40	0.41	
1:G:330:LEU:HD11	1:G:405:LEU:HD21	2.01	0.41	
1:G:393:TYR:CE2	1:G:397:MSE:HE3	2.56	0.41	
1:A:281:ARG:HH11	1:A:281:ARG:HG2	1.86	0.41	
1:B:82:LYS:HE2	2:B:501:GNP:O1G	2.21	0.41	
1:B:176:GLU:HA	5:B:602:HOH:O	2.19	0.41	
1:C:210:ARG:CB	1:C:229:LEU:HD11	2.50	0.41	
1:D:161:LYS:O	1:D:165:ILE:HG13	2.20	0.41	
1:E:31:GLU:O	1:E:280:GLN:NE2	2.37	0.41	
1:E:368:GLN:O	1:E:372:LEU:HD23	2.21	0.41	
2:E:501:GNP:O3'	4:E:504:TRS:O3	2.15	0.41	
1:G:113:PRO:HB3	1:G:125:TRP:CH2	2.56	0.41	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:G:182:ARG:HB3	1:G:229:LEU:HD22	2.02	0.41	
1:A:111:ARG:NH1	1:A:149:TYR:CE2	2.89	0.41	
1:A:286:GLY:HA2	1:A:388:PHE:CZ	2.55	0.41	
1:D:141:LEU:HD12	1:D:141:LEU:N	2.34	0.41	
1:D:218:ARG:CD	1:F:301:LEU:CD2	2.98	0.41	
1:E:143:LYS:HE2	1:E:143:LYS:CA	2.36	0.41	
1:E:362:ARG:HD3	1:E:366:TYR:OH	2.21	0.41	
1:A:185:VAL:HG22	1:A:230:LEU:C	2.40	0.41	
1:A:309:LEU:HD13	1:A:390:LEU:HD13	2.03	0.41	
1:A:372:LEU:HD13	1:A:372:LEU:HA	1.93	0.41	
1:B:28:ASN:HB2	1:B:31:GLU:OE1	2.21	0.41	
1:B:140:TYR:O	1:B:144:MSE:HG2	2.19	0.41	
1:B:153:ILE:CD1	1:B:179:TYR:HB2	2.51	0.41	
1:B:198:GLN:HG2	1:B:199:THR:N	2.35	0.41	
1:B:235:VAL:O	1:B:240:PHE:HB3	2.20	0.41	
1:B:260:MSE:HE1	1:B:277:PHE:CD1	2.55	0.41	
1:D:152:PHE:HB2	1:D:171:ILE:HD13	2.02	0.41	
1:F:222:ILE:O	1:F:223:ALA:HB3	2.21	0.41	
1:F:302:LEU:HD12	1:F:302:LEU:HA	1.73	0.41	
1:G:83:SER:HB2	2:G:501:GNP:O2B	2.20	0.41	
1:A:44:LEU:HD13	1:B:44:LEU:CA	2.51	0.41	
1:A:82:LYS:NZ	2:A:501:GNP:PG	2.94	0.41	
1:B:34:ILE:HD11	1:B:39:LEU:CD2	2.51	0.41	
1:B:70:LEU:HD22	1:B:259:PHE:HB2	2.03	0.41	
1:B:377:LEU:HB2	1:B:378:LEU:HD12	2.02	0.41	
1:C:155:ILE:HG12	1:C:181:VAL:HB	2.03	0.41	
1:C:286:GLY:HA2	1:C:388:PHE:CE1	2.56	0.41	
1:D:303:ASP:OD1	1:D:303:ASP:N	2.54	0.41	
1:D:311:LYS:HB3	1:D:311:LYS:HZ2	1.85	0.41	
1:E:35:SER:HB3	1:E:253:ILE:HD12	2.03	0.41	
1:E:53:LEU:HD11	1:G:29:THR:HG21	2.03	0.41	
1:E:105:VAL:HG12	1:E:105:VAL:O	2.20	0.41	
1:E:266:ILE:HG13	1:E:267:THR:HG23	2.03	0.41	
1:E:295:ILE:HG23	1:E:296:PRO:HD2	2.02	0.41	
1:F:281:ARG:HH11	1:F:281:ARG:HG2	1.85	0.41	
1:G:16:LEU:N	1:G:17:PRO:CD	2.84	0.41	
1:G:136:PRO:CD	1:G:139:THR:HB	2.49	0.41	
1:G:327:LEU:HD22	1:G:341:VAL:CG1	2.50	0.41	
1:A:74:VAL:O	1:A:127:LEU:N	2.36	0.41	
1:A:176:GLU:HG3	5:A:2001:HOH:O	2.21	0.41	
1:A:251:LEU:HD22	1:A:255:LYS:CB	2.51	0.41	



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:16:LEU:N	1:B:17:PRO:CD	2.84	0.41
1:B:189:ILE:HD13	1:B:202:LYS:HG3	2.02	0.41
1:B:199:THR:HG22	1:B:199:THR:O	2.20	0.41
1:B:305:ASP:O	1:B:309:LEU:HG	2.21	0.41
1:C:68:SER:O	1:C:121:ASN:HB3	2.21	0.41
1:C:173:MSE:O	1:D:174:MSE:HE3	2.21	0.41
1:A:180:PHE:CE2	1:A:225:PRO:HG3	2.56	0.40
1:B:136:PRO:HG2	1:B:139:THR:OG1	2.21	0.40
1:B:230:LEU:HD22	1:B:240:PHE:CE2	2.56	0.40
1:C:211:LEU:C	1:C:211:LEU:HD23	2.41	0.40
1:D:17:PRO:O	1:D:21:THR:HG23	2.20	0.40
1:E:37:GLU:HB2	1:F:37:GLU:OE2	2.21	0.40
1:E:281:ARG:HG2	1:E:281:ARG:HH11	1.85	0.40
1:F:387:ILE:O	1:F:391:LYS:HG3	2.21	0.40
1:G:144:MSE:HB2	1:G:146:PHE:HE1	1.86	0.40
1:A:135:PHE:CD2	1:A:143:LYS:HD3	2.56	0.40
1:B:236:CYS:SG	1:B:266:ILE:HB	2.61	0.40
1:C:47:ARG:HH11	1:C:47:ARG:HG2	1.87	0.40
1:C:275:ARG:HH21	1:C:396:ASP:CA	2.31	0.40
1:D:42:ILE:O	1:D:46:MSE:HG3	2.20	0.40
1:E:359:ILE:O	1:E:363:LEU:HG	2.22	0.40
1:F:109:MSE:CE	1:F:133:THR:HA	2.47	0.40
1:A:189:ILE:HD11	1:A:206:LEU:HD21	2.04	0.40
1:A:301:LEU:HD12	1:A:301:LEU:N	2.37	0.40
1:C:204:LYS:HA	1:C:207:GLN:HB3	2.03	0.40
1:C:204:LYS:HE3	1:C:204:LYS:HB2	1.94	0.40
1:C:347:SER:N	1:C:348:PRO:CD	2.85	0.40
1:D:113:PRO:HB3	1:D:125:TRP:CZ2	2.56	0.40
1:E:342:GLU:O	1:E:345:ILE:N	2.54	0.40
1:F:215:ASN:O	1:F:219:GLU:N	2.37	0.40
1:G:51:ILE:HG22	1:G:55:ASN:ND2	2.36	0.40
1:A:111:ARG:CG	1:A:127:LEU:HD22	2.52	0.40
1:C:92:ILE:HG13	1:C:117:PRO:HG2	2.04	0.40
1:D:16:LEU:HB2	1:D:17:PRO:HD3	2.02	0.40
1:D:387:ILE:O	1:D:391:LYS:HG3	2.21	0.40
1:E:223:ALA:O	1:E:225:PRO:HD3	2.21	0.40
1:F:365:ARG:O	1:F:369:GLU:HG3	2.22	0.40
1:G:159:ARG:NH1	1:G:161:LYS:HG2	2.36	0.40
1:A:378:LEU:HD11	1:A:384:LEU:HG	2.04	0.40
1:B:202:LYS:HB2	1:B:202:LYS:HE3	1.88	0.40
1:B:220:ASN:HB3	1:B:222:ILE:HD11	2.04	0.40



Atom-1	Atom-2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:224:GLU:HA	1:B:225:PRO:HD3	1.79	0.40	
1:C:152:PHE:O	1:C:178:PHE:HA	2.21	0.40	
1:C:175:LYS:HA	1:C:175:LYS:HD3	1.80	0.40	
1:D:135:PHE:HB3	1:D:136:PRO:HD2	2.03	0.40	
1:E:330:LEU:CD1	1:E:405:LEU:HD11	2.51	0.40	
1:F:275:ARG:O	1:F:279:LYS:HG3	2.22	0.40	
1:F:298:LEU:HD23	1:F:363:LEU:HB2	2.03	0.40	
1:F:314:LYS:O	1:F:318:THR:HG23	2.21	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	389/423~(92%)	373~(96%)	16 (4%)	0	100	100
1	В	392/423~(93%)	378~(96%)	12 (3%)	2 (0%)	29	67
1	С	381/423~(90%)	369 (97%)	12 (3%)	0	100	100
1	D	392/423~(93%)	371~(95%)	18 (5%)	3~(1%)	19	58
1	Е	390/423~(92%)	377~(97%)	12 (3%)	1 (0%)	41	74
1	F	386/423~(91%)	369~(96%)	17 (4%)	0	100	100
1	G	397/423~(94%)	376 (95%)	19 (5%)	2(0%)	29	67
All	All	$2727/2961 \ (92\%)$	2613 (96%)	106 (4%)	8 (0%)	41	74

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	336	ILE
1	D	335	GLU
1	G	222	ILE



Continued from previous page...

Mol	Chain	Res	Type
1	D	104	VAL
1	D	107	VAL
1	G	107	VAL
1	В	107	VAL
1	Е	107	VAL

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.

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	otameric Outliers		Percentiles		
1	А	361/374~(96%)	350~(97%)	11 (3%)	41	73		
1	В	360/374~(96%)	343~(95%)	17~(5%)	26	62		
1	С	355/374~(95%)	345~(97%)	10~(3%)	43	74		
1	D	358/374~(96%)	351~(98%)	7 (2%)	55	80		
1	Е	359/374~(96%)	350~(98%)	9 (2%)	47	77		
1	F	359/374~(96%)	348~(97%)	11 (3%)	40	72		
1	G	365/374~(98%)	355~(97%)	10 (3%)	44	75		
All	All	2517/2618~(96%)	2442 (97%)	75 (3%)	41	73		

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	101	LYS
1	А	106	GLU
1	А	109	MSE
1	А	132	SER
1	А	134	ASN
1	А	159	ARG
1	А	222	ILE
1	А	240	PHE
1	А	300	PHE
1	А	334	TRP
1	А	339	ASP
1	В	96	GLU



Mol	Chain	Res	Type
1	В	106	GLU
1	В	107	VAL
1	В	108	THR
1	В	182	ARG
1	В	190	THR
1	В	240	PHE
1	В	298	LEU
1	В	299	THR
1	В	300	PHE
1	В	301	LEU
1	В	303	ASP
1	В	304	SER
1	В	334	TRP
1	В	335	GLU
1	В	336	ILE
1	В	344	MSE
1	С	101	LYS
1	С	102	THR
1	С	106	GLU
1	С	218	ARG
1	С	220	ASN
1	С	240	PHE
1	С	300	PHE
1	С	301	LEU
1	С	313	MSE
1	С	329	ARG
1	D	111	ARG
1	D	132	SER
1	D	251	LEU
1	D	300	PHE
1	D	335	GLU
1	D	337	GLU
1	D	339	ASP
1	E	107	VAL
1	E	109	MSE
1	E	110	GLU
1	E	111	ARG
1	E	135	PHE
1	E	196	LYS
1	E	240	PHE
1	E	337	GLU
1	E	340	GLN



Mol	Chain	Res	Type
1	F	109	MSE
1	F	138	ASN
1	F	297	SER
1	F	300	PHE
1	F	301	LEU
1	F	305	ASP
1	F	307	GLU
1	F	337	GLU
1	F	339	ASP
1	F	340	GLN
1	F	360	GLN
1	G	108	THR
1	G	189	ILE
1	G	194	ASP
1	G	199	THR
1	G	202	LYS
1	G	203	GLU
1	G	204	LYS
1	G	206	LEU
1	G	220	ASN
1	G	240	PHE

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

Mol	Chain	\mathbf{Res}	Type
1	А	94	ASN
1	С	40	ASN
1	С	87	ASN
1	D	360	GLN
1	F	212	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 21 ligands modelled in this entry, 13 are monoatomic - leaving 8 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	Tune	Chain	Dog	Tink	Bond lengths		Bond angles			
	or Type Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
2	GNP	А	501	3	28,34,34	2.58	11 (39%)	30,54,54	2.71	11 (36%)
2	GNP	Е	501	3	28,34,34	2.58	8 (28%)	30,54,54	2.24	8 (26%)
4	TRS	Е	504	-	7,7,7	0.38	0	9,9,9	0.31	0
2	GNP	G	501	3	28,34,34	2.61	10(35%)	30,54,54	2.21	8 (26%)
2	GNP	В	501	3	28,34,34	2.61	8 (28%)	30,54,54	2.26	9 (30%)
2	GNP	F	501	3	28,34,34	2.61	8 (28%)	30,54,54	2.22	9 (30%)
2	GNP	С	501	3	28,34,34	2.67	10 (35%)	30,54,54	2.36	7 (23%)
4	TRS	С	504	-	7,7,7	0.33	0	9,9,9	0.62	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.

Mol	Type	Chain	\mathbf{Res}	Link	Chirals	Torsions	Rings
2	GNP	А	501	3	-	11/17/38/38	0/3/3/3
2	GNP	Е	501	3	-	8/17/38/38	0/3/3/3
4	TRS	Е	504	-	-	0/9/9/9	-
2	GNP	G	501	3	-	10/17/38/38	0/3/3/3
2	GNP	В	501	3	-	4/17/38/38	0/3/3/3
2	GNP	F	501	3	-	9/17/38/38	0/3/3/3
2	GNP	С	501	3	-	6/17/38/38	0/3/3/3
4	TRS	С	504	-	-	3/9/9/9	-



5FPH

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	GNP	C4-N9	-7.45	1.37	1.47
2	G	501	GNP	C4-N9	-7.35	1.37	1.47
2	В	501	GNP	C4-N9	-7.32	1.38	1.47
2	A	501	GNP	C4-N9	-7.26	1.38	1.47
2	F	501	GNP	C4-N9	-7.26	1.38	1.47
2	Е	501	GNP	C4-N9	-7.15	1.38	1.47
2	G	501	GNP	C5-C6	-6.43	1.41	1.52
2	С	501	GNP	C5-C6	-6.41	1.41	1.52
2	В	501	GNP	C5-C6	-6.34	1.41	1.52
2	F	501	GNP	C5-C6	-6.34	1.41	1.52
2	Е	501	GNP	C5-C6	-6.34	1.41	1.52
2	А	501	GNP	C5-C6	-6.29	1.42	1.52
2	С	501	GNP	PB-O3A	-5.60	1.52	1.59
2	F	501	GNP	PB-O3A	-5.17	1.52	1.59
2	В	501	GNP	PB-O3A	-5.14	1.52	1.59
2	Е	501	GNP	PB-O3A	-5.09	1.52	1.59
2	G	501	GNP	PB-O3A	-5.01	1.52	1.59
2	А	501	GNP	PB-O3A	-4.54	1.53	1.59
2	А	501	GNP	C6-N1	4.06	1.39	1.33
2	G	501	GNP	C6-N1	4.03	1.39	1.33
2	В	501	GNP	C6-N1	4.00	1.39	1.33
2	F	501	GNP	C6-N1	3.96	1.39	1.33
2	С	501	GNP	C6-N1	3.94	1.39	1.33
2	Е	501	GNP	C6-N1	3.93	1.39	1.33
2	А	501	GNP	PB-O2B	-3.75	1.46	1.56
2	С	501	GNP	PB-O2B	-3.42	1.47	1.56
2	F	501	GNP	PG-01G	3.35	1.51	1.46
2	G	501	GNP	PG-01G	3.30	1.51	1.46
2	В	501	GNP	PG-01G	3.20	1.51	1.46
2	E	501	GNP	PG-01G	3.19	1.51	1.46
2	В	501	GNP	PB-O2B	-3.11	1.48	1.56
2	С	501	GNP	PG-01G	3.10	1.51	1.46
2	F	501	GNP	PB-O2B	-3.08	1.48	1.56
2	E	501	GNP	PB-O2B	-3.08	1.48	1.56
2	G	501	GNP	PB-O2B	-3.07	1.48	1.56
2	A	501	GNP	PG-01G	2.96	1.50	1.46
2	C	501	GNP	C5-C4	-2.45	1.37	1.53
2	B	501	GNP	C5-C4	-2.43	1.38	1.53
2	A	501	GNP	<u>C5-C4</u>	-2.42	1.38	1.53
2	E	501	GNP	C5-C4	-2.42	1.38	1.53
2	G	501	GNP	C5-C4	-2.41	1.38	1.53
2	F	501	GNP	C5-C4	-2.41	1.38	1.53

All (55) bond length outliers are listed below:



5FPH

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
2	Е	501	GNP	C8-N9	-2.30	1.37	1.45
2	С	501	GNP	C8-N9	-2.28	1.37	1.45
2	G	501	GNP	C8-N9	-2.27	1.37	1.45
2	F	501	GNP	C8-N9	-2.26	1.37	1.45
2	А	501	GNP	C8-N9	-2.26	1.37	1.45
2	С	501	GNP	PG-O2G	-2.25	1.50	1.56
2	В	501	GNP	C8-N9	-2.23	1.38	1.45
2	А	501	GNP	PG-N3B	-2.21	1.57	1.63
2	А	501	GNP	PG-O2G	-2.16	1.50	1.56
2	А	501	GNP	PG-O3G	-2.11	1.51	1.56
2	C	501	GNP	PG-O3G	-2.05	1.51	1.56
2	G	501	GNP	PG-O3G	-2.03	1.51	1.56
2	G	501	GNP	PG-O2G	-2.01	1.51	1.56

Continued from previous page...

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
2	С	501	GNP	C4-C5-N7	6.38	110.92	102.46
2	Е	501	GNP	C4-C5-N7	6.36	110.89	102.46
2	F	501	GNP	C4-C5-N7	6.23	110.72	102.46
2	G	501	GNP	C4-C5-N7	6.20	110.68	102.46
2	В	501	GNP	C4-C5-N7	6.20	110.67	102.46
2	А	501	GNP	C4-C5-N7	6.15	110.61	102.46
2	А	501	GNP	O1B-PB-N3B	-5.73	103.33	111.77
2	G	501	GNP	C5-C6-N1	-5.29	111.66	118.19
2	F	501	GNP	C5-C6-N1	-5.25	111.72	118.19
2	В	501	GNP	C5-C6-N1	-5.25	111.72	118.19
2	А	501	GNP	C5-C6-N1	-5.23	111.74	118.19
2	Е	501	GNP	C5-C6-N1	-5.21	111.76	118.19
2	С	501	GNP	C5-C6-N1	-5.14	111.85	118.19
2	С	501	GNP	O2B-PB-O1B	4.97	120.35	109.92
2	А	501	GNP	O1G-PG-N3B	-4.61	104.98	111.77
2	С	501	GNP	PA-O3A-PB	-4.55	116.58	132.62
2	А	501	GNP	O2B-PB-O1B	4.54	119.43	109.92
2	А	501	GNP	O6-C6-C5	4.18	128.39	119.86
2	F	501	GNP	O6-C6-C5	4.14	128.30	119.86
2	В	501	GNP	O6-C6-C5	4.14	128.30	119.86
2	А	501	GNP	PA-O3A-PB	-4.11	118.14	132.62
2	G	501	GNP	O6-C6-C5	4.10	128.22	119.86
2	E	501	GNP	O6-C6-C5	4.09	128.21	119.86
2	С	501	GNP	O6-C6-C5	4.04	128.10	119.86
2	В	501	GNP	O2B-PB-O1B	3.91	118.12	109.92



Mol	Chain	\mathbf{Res}	Type	\mathbf{Atoms}	$Z = Observed(^{o})$		$Ideal(^{o})$
2	G	501	GNP	O2B-PB-O1B	3.87	118.04	109.92
2	F	501	GNP	O2B-PB-O1B	3.77	117.83	109.92
2	Е	501	GNP	O2B-PB-O1B	3.70	117.68	109.92
2	В	501	GNP	O3G-PG-O1G	-3.69	104.19	113.45
2	С	501	GNP	O3G-PG-O2G	3.63	117.30	107.64
2	А	501	GNP	O3G-PG-O2G	3.61	117.25	107.64
2	G	501	GNP	O3G-PG-O1G	-3.44	104.80	113.45
2	Е	501	GNP	O3G-PG-O1G	-3.38	104.95	113.45
2	F	501	GNP	O3G-PG-O1G	-3.37	104.97	113.45
2	С	501	GNP	O3G-PG-O1G	-3.37	104.98	113.45
2	F	501	GNP	PA-O3A-PB	-3.32	120.93	132.62
2	В	501	GNP	PA-O3A-PB	-3.29	121.03	132.62
2	G	501	GNP	PA-O3A-PB	-3.23	121.24	132.62
2	В	501	GNP	O3G-PG-O2G	3.22	116.22	107.64
2	F	501	GNP	O3G-PG-O2G	3.14	116.01	107.64
2	Е	501	GNP	O3G-PG-O2G	3.13	115.97	107.64
2	G	501	GNP	O3G-PG-O2G	2.97	115.56	107.64
2	А	501	GNP	O3G-PG-O1G	-2.79	106.44	113.45
2	Е	501	GNP	O1G-PG-N3B	-2.60	107.94	111.77
2	В	501	GNP	O1G-PG-N3B	-2.57	107.98	111.77
2	Е	501	GNP	PA-O3A-PB	-2.51	123.78	132.62
2	A	501	GNP	O3A-PB-N3B	2.43	113.33	106.59
2	F	501	GNP	O1G-PG-N3B	-2.17	108.58	111.77
2	А	501	GNP	O6-C6-N1	-2.10	119.87	122.69
2	F	501	GNP	O6-C6-N1	-2.02	119.98	122.69
2	В	501	GNP	O6-C6-N1	-2.02	119.98	122.69
2	G	501	GNP	O1G-PG-N3B	-2.01	108.80	111.77

There are no chirality outliers.

Mol	Chain	\mathbf{Res}	Type	Atoms
2	А	501	GNP	PA-O3A-PB-O1B
2	А	501	GNP	PA-O3A-PB-O2B
2	А	501	GNP	C5'-O5'-PA-O1A
2	А	501	GNP	C5'-O5'-PA-O2A
2	А	501	GNP	O4'-C1'-N9-C4
2	А	501	GNP	C2'-C1'-N9-C8
2	А	501	GNP	C2'-C1'-N9-C4
2	В	501	GNP	PB-N3B-PG-O1G
2	В	501	GNP	PG-N3B-PB-O1B
2	В	501	GNP	C2'-C1'-N9-C4

All (51) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	С	501	GNP	PB-N3B-PG-O1G
2	С	501	GNP	PG-N3B-PB-O1B
2	С	501	GNP	PG-N3B-PB-O3A
2	С	501	GNP	O4'-C1'-N9-C4
2	С	501	GNP	C2'-C1'-N9-C8
2	С	501	GNP	C2'-C1'-N9-C4
2	Е	501	GNP	PB-N3B-PG-O1G
2	Е	501	GNP	PG-N3B-PB-O1B
2	Е	501	GNP	C5'-O5'-PA-O3A
2	Е	501	GNP	C5'-O5'-PA-O2A
2	Е	501	GNP	C2'-C1'-N9-C8
2	F	501	GNP	PB-N3B-PG-O1G
2	F	501	GNP	PG-N3B-PB-O1B
2	F	501	GNP	PA-O3A-PB-O1B
2	F	501	GNP	PA-O3A-PB-O2B
2	F	501	GNP	C5'-O5'-PA-O1A
2	F	501	GNP	O4'-C1'-N9-C4
2	F	501	GNP	C2'-C1'-N9-C8
2	F	501	GNP	C2'-C1'-N9-C4
2	G	501	GNP	PB-N3B-PG-O1G
2	G	501	GNP	PG-N3B-PB-O1B
2	G	501	GNP	PG-N3B-PB-O3A
2	G	501	GNP	PA-O3A-PB-O1B
2	G	501	GNP	PA-O3A-PB-O2B
2	G	501	GNP	C5'-O5'-PA-O1A
2	G	501	GNP	C5'-O5'-PA-O2A
2	G	501	GNP	O4'-C1'-N9-C4
2	G	501	GNP	C2'-C1'-N9-C4
4	С	504	TRS	C3-C-C1-O1
4	С	504	TRS	N-C-C1-O1
2	А	501	GNP	C3'-C4'-C5'-O5'
2	А	501	GNP	O4'-C4'-C5'-O5'
2	E	501	GNP	C4'-C5'-O5'-PA
2	G	501	GNP	C5'-O5'-PA-O3A
4	С	504	TRS	C2-C-C1-O1
2	E	501	GNP	C5'-O5'-PA-O1A
2	F	501	GNP	C4'-C5'-O5'-PA
2	В	501	GNP	O4'-C4'-C5'-O5'
2	A	501	GNP	C5'-O5'-PA-O3A
2	A	501	GNP	PB-N3B-PG-O1G
2	Е	501	GNP	PG-N3B-PB-O3A

Continued from previous page...

There are no ring outliers.



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	501	GNP	18	0
2	Е	501	GNP	9	0
4	Е	504	TRS	1	0
2	G	501	GNP	8	0
2	В	501	GNP	8	0
2	F	501	GNP	5	0
2	С	501	GNP	11	0
4	С	504	TRS	1	0

8 monomers are involved in 59 short contacts:

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)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	< RSRZ >	#RSRZ>2	$OWAB(A^2)$	Q<0.9
1	А	385/423~(91%)	0.22	17 (4%) 34 21	39, 68, 108, 144	0
1	В	386/423~(91%)	0.30	15 (3%) 39 25	38, 67, 104, 126	0
1	С	379/423~(89%)	0.28	13 (3%) 45 29	38, 64, 103, 126	0
1	D	386/423~(91%)	0.36	19 (4%) 29 17	38, 67, 112, 137	0
1	Е	386/423~(91%)	0.20	14 (3%) 42 27	36, 62, 99, 135	0
1	F	384/423~(90%)	0.31	14 (3%) 42 27	37, 65, 98, 111	0
1	G	389/423~(91%)	0.17	7 (1%) 68 55	33, 59, 95, 147	0
All	All	2695/2961~(91%)	0.26	99 (3%) 41 26	33, 65, 103, 147	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	98	GLY	6.2
1	D	131	GLY	6.0
1	С	297	SER	5.2
1	D	134	ASN	4.9
1	С	194	ASP	4.7
1	G	198	GLN	4.6
1	А	334	TRP	4.6
1	D	298	LEU	4.4
1	С	106	GLU	4.3
1	А	97	GLU	4.3
1	D	345	ILE	4.2
1	D	353	PRO	4.1
1	В	199	THR	4.1
1	С	335	GLU	4.0
1	А	268	ASP	4.0
1	Е	301	LEU	3.9
1	G	199	THR	3.8



Mol	Chain	Res	Type	RSRZ
1	А	198	GLN	3.6
1	Е	137	PRO	3.6
1	В	134	ASN	3.4
1	G	200	PHE	3.4
1	С	296	PRO	3.4
1	F	131	GLY	3.4
1	С	159	ARG	3.3
1	В	340	GLN	3.3
1	D	106	GLU	3.3
1	С	138	ASN	3.3
1	D	354	THR	3.2
1	G	134	ASN	3.1
1	В	126	ASP	3.1
1	F	157	ALA	3.1
1	В	95	GLU	3.1
1	А	29	THR	3.1
1	А	235	VAL	3.0
1	Е	297	SER	3.0
1	F	372	LEU	3.0
1	D	297	SER	2.9
1	А	199	THR	2.9
1	D	352	LYS	2.9
1	Е	138	ASN	2.9
1	Е	268	ASP	2.8
1	С	231	SER	2.8
1	С	102	THR	2.8
1	Е	98	GLY	2.8
1	D	335	GLU	2.8
1	F	137	PRO	2.8
1	F	99	ALA	2.7
1	В	339	ASP	2.7
1	F	326	SER	2.7
1	F	98	GLY	2.7
1	D	268	ASP	2.6
1	G	408	GLU	2.6
1	F	138	ASN	2.6
1	А	320	PHE	2.6
1	В	198	GLN	2.6
1	Е	189	ILE	2.6
1	Е	223	ALA	2.5
1	F	225	PRO	2.5
1	F	222	ILE	2.5



Mol	Chain	Res	Type	RSRZ
1	Е	361	GLU	2.5
1	А	329	ARG	2.5
1	С	186	ASP	2.5
1	С	304	SER	2.5
1	D	218	ARG	2.5
1	Е	298	LEU	2.5
1	В	29	THR	2.4
1	F	413	ASN	2.4
1	А	215	ASN	2.4
1	А	203	GLU	2.4
1	С	148	GLU	2.4
1	С	222	ILE	2.4
1	В	330	LEU	2.3
1	В	352	LYS	2.3
1	В	399	THR	2.3
1	G	103	GLY	2.3
1	А	324	GLU	2.3
1	F	92	ILE	2.3
1	В	147	TYR	2.3
1	Ε	356	GLU	2.3
1	А	335	GLU	2.2
1	В	97	GLU	2.2
1	D	130	ILE	2.2
1	D	357	GLU	2.2
1	E	413	ASN	2.2
1	D	126	ASP	2.2
1	G	223	ALA	2.2
1	D	192	GLU	2.1
1	A	124	PHE	2.1
1	F	298	LEU	2.1
1	E	300	PHE	2.1
1	D	97	GLU	2.1
1	A	126	ASP	2.1
1	F	14	ASN	2.1
1	D	356	GLU	2.1
1	B	333	ASP	2.1
1	A	195	GLY	2.0
1	A	399	THR	2.0
1	B	229	LEU	2.0
1	E	118	ASN	2.0

Continued from previous page...



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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B} ext{-factors}({ m \AA}^2)$	Q<0.9
4	TRS	Е	504	8/8	0.55	0.28	79,109,138,138	0
2	GNP	А	501	32/32	0.69	0.24	60,80,100,116	32
3	MG	А	503	1/1	0.73	0.23	38,38,38,38	0
4	TRS	С	504	8/8	0.81	0.20	81,99,142,142	0
3	MG	В	502	1/1	0.81	0.50	$110,\!110,\!110,\!110$	0
2	GNP	Е	501	32/32	0.87	0.25	34,67,79,88	32
2	GNP	В	501	32/32	0.88	0.23	56,69,88,95	32
2	GNP	С	501	32/32	0.89	0.21	46,63,84,91	32
3	MG	F	503	1/1	0.89	0.20	36,36,36,36	0
3	MG	Е	502	1/1	0.90	0.14	44,44,44,44	0
2	GNP	F	501	32/32	0.90	0.18	49,66,77,80	32
2	GNP	G	501	32/32	0.90	0.21	44,59,74,79	32
3	MG	В	503	1/1	0.90	0.23	44,44,44,44	0
3	MG	G	502	1/1	0.95	0.08	43,43,43,43	0
3	MG	F	502	1/1	0.95	0.17	71,71,71,71	0
3	MG	А	502	1/1	0.95	0.50	91,91,91,91	0
3	MG	G	503	1/1	0.96	0.19	43,43,43,43	0
3	MG	Е	503	1/1	0.96	0.21	20,20,20,20	0
3	MG	D	501	1/1	0.96	0.28	32,32,32,32	0
3	MG	С	503	1/1	0.97	0.20	30,30,30,30	0
3	MG	С	502	1/1	0.99	0.11	68,68,68,68	0

6.5 Other polymers (i)

There are no such residues in this entry.

