

Full wwPDB X-ray Structure Validation Report (i)

Sep 5, 2023 – 01:07 PM EDT

PDB ID	:	3TUI
Title	:	Inward facing conformations of the MetNI methionine ABC transporter: CY5
		native crystal form
Authors	:	Johnson, E.; Nguyen, P.T.; Rees, D.C.
Deposited on	:	2011-09-16
Resolution	:	2.90 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
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 2.90 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.



Motrie	Whole archive	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	Quality	v of chain
1	А	217	.% 53%	47%
1	В	217	4%	52% •
1	Е	217	4% 50%	48% •
1	F	217	3% 52%	47% •
2	С	366	54%	40% · 6%



Mol	Chain	Length	Quality of chain					
2	D	366	5%	37%	• 6%			
2	G	366	4%	43%	• 6%			
2	Н	366	3% 49%	44%	• 6%			



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17386 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	216	Total	С	Ν	0	\mathbf{S}	0	0	0
1	A	210	1627	1079	266	272	10	0	0	0
1	р	216	Total	С	Ν	0	S	0	0	0
1	D	210	1627	1079	266	272	10	0	0	0
1	F	216	Total	С	Ν	0	S	0	0	0
1		210	1627	1079	266	272	10	0		
1 F	216	Total	С	Ν	0	S	0	0	0	
	r	210	1627	1079	266	272	10	0	0	0

• Molecule 1 is a protein called D-methionine transport system permease protein metI.

• Molecule 2 is a protein called Methionine import ATP-binding protein MetN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
0	C	344	Total	С	Ν	0	\mathbf{S}	0	0	0
	U		2661	1670	471	508	12	0	0	0
0	П	343	Total	С	Ν	0	S	0	0	0
	D		2651	1664	468	507	12	0	0	
0	C	949	Total	С	Ν	0	S	0	0	0
	G	343	2651	1664	468	507	12	0	0	0
9	2 H	II 944	Total	С	Ν	0	S	0	0	0
		044	2661	1670	471	508	12	U		0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	-22	MET	-	expression tag	UNP P30750
С	-21	GLY	-	expression tag	UNP P30750
С	-20	HIS	-	expression tag	UNP P30750
С	-19	HIS	-	expression tag	UNP P30750
С	-18	HIS	-	expression tag	UNP P30750
С	-17	HIS	-	expression tag	UNP P30750
С	-16	HIS	-	expression tag	UNP P30750
С	-15	HIS	-	expression tag	UNP P30750



Chain	Residue	Modelled	Actual	Comment	Reference
С	-14	-14 HIS		expression tag	UNP P30750
С	-13	HIS	-	expression tag	UNP P30750
С	-12	HIS	-	expression tag	UNP P30750
С	С -11		-	expression tag	UNP P30750
С	-10	SER	-	expression tag	UNP P30750
С	-9	SER	-	expression tag	UNP P30750
С	-8	GLY	-	expression tag	UNP P30750
С	-7	HIS	-	expression tag	UNP P30750
С	-6	ILE	-	expression tag	UNP P30750
С	-5	ASP	-	expression tag	UNP P30750
С	-4	ASP	-	expression tag	UNP P30750
С	-3	ASP	-	expression tag	UNP P30750
С	-2	ASP	-	expression tag	UNP P30750
С	-1	LYS	-	expression tag	UNP P30750
С	0	HIS	-	expression tag	UNP P30750
С	166	GLN	GLU	engineered mutation	UNP P30750
D	-22	MET	-	expression tag	UNP P30750
D	-21	GLY	-	expression tag	UNP P30750
D	-20	HIS	-	expression tag	UNP P30750
D	-19	HIS	-	expression tag	UNP P30750
D	-18	HIS	-	expression tag	UNP P30750
D	-17	HIS	-	expression tag	UNP P30750
D	-16	HIS	-	expression tag	UNP P30750
D	-15	HIS	-	expression tag	UNP P30750
D	-14	HIS	-	expression tag	UNP P30750
D	-13	HIS	-	expression tag	UNP P30750
D	-12	HIS	-	expression tag	UNP P30750
D	-11	HIS	-	expression tag	UNP P30750
D	-10	SER	-	expression tag	UNP P30750
D	-9	SER	-	expression tag	UNP P30750
D	-8	GLY	-	expression tag	UNP P30750
D	-7	HIS	-	expression tag	UNP P30750
D	-6	ILE	-	expression tag	UNP P30750
D	-5	ASP	-	expression tag	UNP P30750
D	-4	ASP	-	expression tag	UNP P30750
D	-3	ASP	-	expression tag	UNP P30750
D	-2	ASP	-	expression tag	UNP P30750
D	-1	LYS	-	expression tag	UNP P30750
D	0	HIS	-	expression tag	UNP P30750
D	166	GLN	GLU	engineered mutation	UNP P30750
G	-22	MET	-	expression tag	UNP P30750
G	-21	GLY	-	expression tag	UNP P30750



Chain	nain Residue Modelled Actu		Actual	Comment	Reference
G	-20	HIS	-	expression tag	UNP P30750
G	-19	HIS	-	expression tag	UNP P30750
G	-18	HIS	-	expression tag	UNP P30750
G	-17	HIS	-	expression tag	UNP P30750
G	-16	HIS	-	expression tag	UNP P30750
G	-15	HIS	-	expression tag	UNP P30750
G	-14	HIS	-	expression tag	UNP P30750
G	-13	HIS	-	expression tag	UNP P30750
G	-12	HIS	-	expression tag	UNP P30750
G	-11	HIS	-	expression tag	UNP P30750
G	-10	SER	-	expression tag	UNP P30750
G	-9	SER	-	expression tag	UNP P30750
G	-8	GLY	-	expression tag	UNP P30750
G	-7	HIS	-	expression tag	UNP P30750
G	-6	ILE	-	expression tag	UNP P30750
G	-5	ASP	-	expression tag	UNP P30750
G	-4	ASP	-	expression tag	UNP P30750
G	-3	ASP	-	expression tag	UNP P30750
G	-2	ASP	-	expression tag	UNP P30750
G	-1	LYS	-	expression tag	UNP P30750
G	0	HIS	-	expression tag	UNP P30750
G	166	GLN	GLU	engineered mutation	UNP P30750
Η	-22	MET	-	expression tag	UNP P30750
H	-21	GLY	-	expression tag	UNP P30750
H	-20	HIS	-	expression tag	UNP P30750
H	-19	HIS	-	expression tag	UNP P30750
H	-18	HIS	-	expression tag	UNP P30750
H	-17	HIS	-	expression tag	UNP P30750
H	-16	HIS	-	expression tag	UNP P30750
H	-15	HIS	-	expression tag	UNP P30750
H	-14	HIS	-	expression tag	UNP P30750
H	-13	HIS	-	expression tag	UNP P30750
H	-12	HIS	-	expression tag	UNP P30750
Н	-11	HIS	-	expression tag	UNP P30750
H	-10	SER	-	expression tag	UNP P30750
H	-9	SER	-	expression tag	UNP P30750
H	-8	GLY	-	expression tag	UNP P30750
H	-7	HIS	-	expression tag	UNP P30750
H	-6	ILE	-	expression tag	UNP P30750
H	-5	ASP	-	expression tag	UNP P30750
H	-4	ASP	-	expression tag	UNP P30750
H	-3	ASP	-	expression tag	UNP P30750



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Chain	Chain Residue Modelle		Actual	Comment	Reference
Н	-2	ASP	-	expression tag	UNP P30750
Н	-1	LYS	-	expression tag	UNP P30750
Н	0	HIS	-	expression tag	UNP P30750
Н	166	GLN	GLU	engineered mutation	UNP P30750

• Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf			
2	С	1	Total	С	Ν	0	Р	0	0			
0	U	1	27	10	5	10	2	0	0			
2	Л	1	Total	С	Ν	Ο	Р	0	0			
0	D	D	D	D	L	27	10	5	10	2	0	0
2	С	1	Total	С	Ν	Ο	Р	0	0			
0	G	1	27	10	5	10	2	0	0			
9	ц	1	Total	С	Ν	Ο	Р	0	0			
3	п	1	27	10	5	10	2	0				

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	20	TotalO2020	0	0
4	В	19	Total O 19 19	0	0
4	С	17	Total O 17 17	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	20	TotalO2020	0	0
4	Е	12	Total O 12 12	0	0
4	F	11	Total O 11 11	0	0
4	G	23	TotalO2323	0	0
4	Н	24	TotalO2424	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: D-methionine transport system permease protein metI













4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	83.43Å 140.08Å 150.07Å	Dopositor
a, b, c, α , β , γ	90.00° 96.39° 90.00°	Depositor
Bosolution (Å)	29.61 - 2.90	Depositor
Resolution (A)	29.61 - 2.66	EDS
% Data completeness	97.9 (29.61-2.90)	Depositor
(in resolution range)	84.7(29.61-2.66)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) > 1$	3.76 (at 2.64\AA)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
P. P.	0.240 , 0.303	Depositor
n, n_{free}	0.236 , 0.295	DCC
R_{free} test set	4130 reflections (4.95%)	wwPDB-VP
Wilson B-factor $(Å^2)$	50.0	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.28 , 67.0	EDS
L-test for $twinning^2$	$ L > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17386	wwPDB-VP
Average B, all atoms $(Å^2)$	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.65% 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: ADP

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

Mal	Chain	Bond lengths		Bond angles	
MOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.52	0/1660	0.73	0/2267
1	В	0.57	0/1660	0.75	0/2267
1	Е	0.51	0/1660	0.67	0/2267
1	F	0.48	0/1660	0.68	1/2267~(0.0%)
2	С	0.47	0/2701	0.68	0/3662
2	D	0.48	0/2690	0.72	2/3647~(0.1%)
2	G	0.48	0/2690	0.71	3/3647~(0.1%)
2	Н	0.48	0/2701	0.70	1/3662~(0.0%)
All	All	0.49	0/17422	0.71	7/23686~(0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	В	0	1
2	G	0	1
2	Н	0	2
All	All	0	4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	G	47	LEU	CA-CB-CG	6.71	130.73	115.30
2	D	196	LEU	CA-CB-CG	6.43	130.10	115.30
2	G	196	LEU	CA-CB-CG	5.76	128.55	115.30
2	D	282	LEU	CB-CG-CD2	-5.34	101.92	111.00
1	F	17	LEU	CA-CB-CG	5.30	127.48	115.30



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	G	4	LEU	CA-CB-CG	5.15	127.14	115.30
2	Н	196	LEU	CA-CB-CG	5.09	127.01	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	118	GLY	Peptide
2	G	12	HIS	Peptide
2	Н	113	PRO	Peptide
2	Н	132	ASP	Peptide

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	1627	0	1746	109	0
1	В	1627	0	1746	123	0
1	Е	1627	0	1746	110	0
1	F	1627	0	1746	103	0
2	С	2661	0	2714	143	0
2	D	2651	0	2707	122	0
2	G	2651	0	2707	140	0
2	Н	2661	0	2714	145	0
3	С	27	0	12	2	0
3	D	27	0	12	1	0
3	G	27	0	12	3	0
3	Н	27	0	12	4	0
4	А	20	0	0	0	0
4	В	19	0	0	3	0
4	С	17	0	0	1	0
4	D	20	0	0	2	0
4	Ε	12	0	0	0	0
4	F	11	0	0	0	0
4	G	23	0	0	1	0
4	Н	24	0	0	4	0
All	All	17386	0	17874	954	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 27.

All (954) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom_1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:163:MET:SD	1:B:69:ILE:HG21	1.91	1.10
2:C:164:CYS:HB2	2:C:196:LEU:HD13	1.33	1.10
1:A:121:GLU:OE2	2:C:49:ARG:NH1	1.91	1.03
1:E:119:LEU:HD21	2:G:94:LEU:HD23	1.36	1.02
2:G:53:LEU:HB2	2:G:81:ARG:HH11	1.28	0.99
2:G:1:MET:HG3	2:G:2:ILE:HG22	1.43	0.98
2:D:82:ARG:HH21	2:D:110:ASP:HB2	1.30	0.96
1:F:73:VAL:O	1:F:76:ILE:HG13	1.66	0.95
2:G:53:LEU:HD11	2:G:69:LEU:HB3	1.48	0.94
1:F:155:ILE:HB	1:F:203:ILE:HD11	1.50	0.94
2:D:319:THR:HG22	2:D:321:GLN:H	1.32	0.93
1:A:85:THR:HG22	1:A:87:ILE:H	1.31	0.93
1:F:129:THR:H	1:F:132:GLN:HE21	1.05	0.92
1:F:13:VAL:HA	1:F:172:LEU:HD11	1.49	0.91
2:G:148:ARG:NH1	4:G:358:HOH:O	2.05	0.89
1:B:119:LEU:O	1:B:123:SER:HB2	1.73	0.89
1:A:154:LEU:HB3	1:A:203:ILE:HD11	1.54	0.88
2:C:220:ILE:HD12	2:C:234:THR:HG21	1.56	0.88
2:H:3:LYS:HG3	2:H:27:HIS:HD2	1.37	0.87
2:H:244:THR:HG23	2:H:245:LEU:HD13	1.54	0.87
2:D:4:LEU:HD22	2:D:62:VAL:HG22	1.54	0.86
1:B:115:ILE:HD11	1:B:138:LEU:HD23	1.56	0.85
2:D:9:LYS:HA	2:D:58:THR:HG22	1.57	0.85
1:E:5:MET:O	1:E:8:LEU:HB3	1.74	0.85
2:G:185:ASP:O	2:G:189:ARG:HG2	1.76	0.85
2:G:31:GLY:H	2:G:193:THR:HG23	1.40	0.84
2:H:107:LEU:HB3	2:H:112:THR:HG21	1.58	0.84
2:C:0:HIS:ND1	2:C:27:HIS:HB3	1.92	0.84
2:D:235:PRO:O	2:D:239:LYS:HG2	1.78	0.84
2:H:286:THR:HG22	2:H:292:VAL:HG21	1.58	0.83
2:H:48:ILE:HD11	2:H:163:LEU:HB3	1.61	0.83
2:D:22:ASN:N	2:D:217:GLY:O	2.10	0.83
2:G:248:ASP:O	2:G:249:ILE:HG22	1.79	0.83
1:A:129:THR:H	1:A:132:GLN:HE21	1.26	0.82
2:C:164:CYS:HB2	2:C:196:LEU:CD1	2.08	0.82
1:A:69:ILE:HD12	1:A:163:MET:CE	2.10	0.81
2:H:253:TYR:OH	2:H:315:GLU:OE2	1.97	0.81



	to de pagem	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:C:195:LEU:HD12	2:C:196:LEU:H	1.46	0.81	
1:B:85:THR:HG22	1:B:86:SER:N	1.95	0.80	
2:D:128:VAL:O	2:D:148:ARG:HD3	1.81	0.80	
1:E:32:LEU:HB3	1:E:33:PRO:HD3	1.63	0.80	
2:H:147:GLN:O	2:H:151:ILE:HG13	1.80	0.80	
1:B:20:THR:CG2	1:B:154:LEU:HD12	2.11	0.80	
1:A:32:LEU:HB3	1:A:33:PRO:HD3	1.61	0.80	
2:C:316:MET:CE	2:C:326:ALA:HB3	2.10	0.80	
2:G:229:PHE:HA	2:G:241:ILE:CD1	2.11	0.80	
1:B:45:GLN:O	4:B:247:HOH:O	2.00	0.80	
2:C:62:VAL:HG12	2:C:69:LEU:HD12	1.64	0.80	
1:E:41:THR:CG2	1:E:53:TYR:HB2	2.12	0.80	
1:B:94:VAL:HB	1:B:95:PRO:HD3	1.64	0.79	
2:H:272:GLU:HB2	2:H:336:LYS:HB3	1.65	0.79	
1:A:179:TYR:HB3	1:A:188:VAL:HG11	1.63	0.79	
2:G:73:SER:HB2	2:G:76:GLU:HB2	1.64	0.79	
1:B:210:ILE:O	1:B:214:VAL:HG23	1.82	0.79	
1:E:69:ILE:HG23	1:E:70:ILE:HD12	1.62	0.79	
1:E:163:MET:SD	1:F:69:ILE:HG21	2.21	0.79	
2:D:285:GLU:HG3	2:D:289:ARG:HD2	1.65	0.79	
1:F:38:LEU:HD21	1:F:106:ARG:HH21	1.48	0.78	
2:D:34:TYR:OH	2:D:212:ALA:HB2	1.83	0.78	
2:H:288:ARG:HD2	4:H:349:HOH:O	1.84	0.78	
2:H:286:THR:HG22	2:H:292:VAL:CG2	2.13	0.78	
1:B:188:VAL:HA	1:B:191:THR:HG22	1.63	0.77	
2:C:130:LEU:HD11	2:C:148:ARG:HB2	1.67	0.77	
1:E:69:ILE:HD12	1:F:163:MET:HA	1.67	0.77	
2:H:164:CYS:HB2	2:H:196:LEU:HB3	1.67	0.77	
2:G:185:ASP:OD1	2:G:188:ARG:NH1	2.17	0.77	
1:F:139:LEU:HB2	1:F:140:PRO:HD3	1.67	0.76	
1:F:129:THR:H	1:F:132:GLN:NE2	1.83	0.76	
2:H:1:MET:HB3	2:H:193:THR:HG21	1.65	0.76	
2:G:110:ASP:O	2:G:112:THR:HG23	1.85	0.76	
1:A:185:ASN:HB3	1:A:188:VAL:HG12	1.68	0.76	
1:B:207:GLY:HA2	1:B:210:ILE:HG22	1.66	0.76	
1:F:13:VAL:HA	1:F:172:LEU:CD1	2.16	0.75	
2:C:316:MET:HE3	2:C:326:ALA:HB3	1.69	0.75	
1:A:75:MET:HA	1:A:78:PHE:HD2	1.51	0.75	
2:G:123:GLU:O	2:G:126:SER:N	2.19	0.75	
2:G:299:ALA:HB2	2:G:312:MET:HG3	1.67	0.75	
2:D:205:LYS:HD3	2:D:244:THR:HG21	1.69	0.75	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:G:31:GLY:H	2:G:193:THR:CG2	1.99	0.74	
2:H:220:ILE:HG22	2:H:234:THR:HG21	1.67	0.74	
2:H:247:LEU:HD12	2:H:313:LEU:HG	1.68	0.74	
1:B:132:GLN:O	1:B:136:LYS:HB2	1.86	0.74	
2:D:237:ALA:O	2:D:241:ILE:HG12	1.88	0.74	
2:G:107:LEU:HD21	2:G:156:ALA:HB1	1.69	0.74	
1:F:129:THR:N	1:F:132:GLN:HE21	1.85	0.73	
2:H:270:ARG:HB2	2:H:340:LEU:HD11	1.70	0.73	
1:E:123:SER:HA	1:E:126:MET:HE3	1.69	0.73	
2:H:103:VAL:O	2:H:106:PRO:HD2	1.88	0.73	
2:G:53:LEU:CB	2:G:81:ARG:HH11	2.01	0.73	
2:G:100:PHE:HD2	2:G:134:HIS:HE2	1.37	0.73	
2:D:49:ARG:NH2	2:D:165:ASP:OD2	2.22	0.73	
1:B:41:THR:HG22	1:B:53:TYR:HB2	1.69	0.73	
1:E:23:SER:HB2	1:E:157:LEU:HD13	1.69	0.73	
2:G:45:SER:HA	2:G:48:ILE:HG22	1.71	0.72	
1:F:13:VAL:CA	1:F:172:LEU:HD11	2.17	0.72	
2:G:99:VAL:CG1	2:G:141:LEU:HD11	2.20	0.72	
1:B:2:SER:CB	1:B:4:PRO:HD2	2.19	0.72	
1:B:19:MET:HE3	1:B:169:ALA:HB1	1.71	0.72	
1:B:204:GLN:O	1:B:208:ASP:HB2	1.90	0.72	
2:G:1:MET:HB2	2:G:65:ASP:H	1.54	0.72	
2:C:283:LEU:O	2:C:286:THR:HG22	1.90	0.72	
1:B:179:TYR:O	1:B:184:TYR:N	2.23	0.72	
2:D:319:THR:HB	2:D:322:ASP:H	1.55	0.72	
1:A:69:ILE:HD12	1:A:163:MET:HE2	1.72	0.71	
2:C:163:LEU:HD23	2:C:195:LEU:HB3	1.73	0.71	
2:G:229:PHE:HA	2:G:241:ILE:HD13	1.71	0.71	
1:A:132:GLN:O	1:A:136:LYS:HB2	1.90	0.71	
1:A:149:ALA:HA	1:A:152:ILE:HG22	1.72	0.71	
2:C:220:ILE:HD11	2:C:236:LEU:HD23	1.71	0.71	
2:G:29:PRO:HB2	2:G:32:GLN:HG3	1.72	0.71	
1:E:119:LEU:HD21	2:G:94:LEU:CD2	2.15	0.71	
1:E:115:ILE:HD12	1:E:138:LEU:HD23	1.73	0.70	
1:F:2:SER:HB3	1:F:4:PRO:HD2	1.72	0.70	
2:H:303:TYR:CE2	2:H:308:LYS:HB2	2.26	0.70	
1:E:143:LEU:HD23	1:E:214:VAL:HG13	1.71	0.70	
2:D:319:THR:HG22	2:D:320:GLN:N	2.07	0.70	
2:G:304:ALA:O	2:G:307:VAL:HG12	1.91	0.70	
2:H:319:THR:HG23	2:H:322:ASP:HB2	1.73	0.70	
2:G:100:PHE:HD2	2:G:134:HIS:NE2	1.90	0.70	



	A	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:103:VAL:HG21	2:C:125:LEU:HD11	1.74	0.70
2:H:144:GLY:HA2	2:H:179:ILE:HD11	1.72	0.70
2:H:285:GLU:OE2	2:H:289:ARG:NE	2.24	0.70
1:E:39:TYR:HA	1:E:42:ARG:HG3	1.73	0.70
1:B:39:TYR:CD1	1:B:113:LEU:HD23	2.26	0.69
2:D:212:ALA:HB1	2:D:219:LEU:HD23	1.74	0.69
2:G:36:VAL:HB	2:G:197:ILE:HG22	1.72	0.69
2:H:262:PHE:CD1	2:H:263:THR:N	2.60	0.69
1:B:61:ASN:ND2	4:B:221:HOH:O	2.24	0.69
1:E:94:VAL:HB	1:E:95:PRO:HD3	1.74	0.69
2:G:146:LYS:O	2:G:149:VAL:HG12	1.91	0.69
2:G:200:GLU:HB2	2:G:203:VAL:HG23	1.74	0.69
2:H:97:ARG:NH2	2:H:108:GLU:OE2	2.25	0.69
1:E:41:THR:HG22	1:E:53:TYR:HB2	1.74	0.69
1:B:9:LEU:HA	1:B:175:ILE:HD13	1.74	0.69
1:E:167:VAL:HG12	1:E:167:VAL:O	1.93	0.69
1:A:23:SER:HA	1:A:97:THR:HG22	1.75	0.68
1:B:2:SER:HB3	1:B:4:PRO:HD2	1.75	0.68
2:D:112:THR:HG22	2:D:116:GLU:HB3	1.74	0.68
1:B:20:THR:HG22	1:B:154:LEU:HD12	1.73	0.68
2:C:196:LEU:HD12	2:C:197:ILE:N	2.07	0.68
1:E:28:PHE:HD1	1:E:104:ILE:HD13	1.59	0.68
2:G:89:GLN:HB2	2:G:166:GLN:HB2	1.73	0.68
1:F:92:ALA:HB2	1:F:169:ALA:HB1	1.76	0.68
1:E:45:GLN:O	1:E:48:ALA:HB2	1.94	0.68
1:A:163:MET:SD	1:B:69:ILE:CG2	2.78	0.67
2:H:29:PRO:HG2	2:H:32:GLN:OE1	1.95	0.67
1:B:115:ILE:HG13	1:B:115:ILE:O	1.95	0.67
1:B:134:VAL:HA	1:B:138:LEU:HB2	1.76	0.67
1:E:28:PHE:CD1	1:E:104:ILE:HD13	2.29	0.67
2:G:9:LYS:HE2	2:G:56:ARG:O	1.94	0.67
1:A:69:ILE:HD12	1:A:163:MET:HE3	1.76	0.67
1:F:119:LEU:O	1:F:123:SER:OG	2.09	0.67
2:G:4:LEU:HD11	2:G:51:VAL:HG22	1.76	0.67
1:A:75:MET:HA	1:A:78:PHE:CD2	2.30	0.67
1:E:92:ALA:O	1:E:95:PRO:HD2	1.94	0.67
1:F:178:GLN:O	1:F:182:ILE:HG13	1.95	0.67
2:G:45:SER:O	2:G:49:ARG:HD2	1.95	0.67
2:G:245:LEU:HD12	2:G:300:GLN:HB3	1.75	0.67
1:A:68:PHE:CZ	1:A:96:LEU:HD12	2.30	0.66
1:A:211:VAL:O	1:A:214:VAL:HG22	1.95	0.66



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:H:53:LEU:HD12	2:H:69:LEU:HB3	1.78	0.66
2:G:142:SER:OG	2:G:145:GLN:HG2	1.95	0.66
2:H:201:MET:CE	2:H:240:PHE:HB3	2.25	0.66
2:H:293:ASN:HB2	2:H:317:HIS:HB2	1.77	0.66
1:B:62:ILE:O	1:B:65:SER:OG	2.13	0.66
2:C:299:ALA:CB	2:C:312:MET:HG2	2.26	0.66
1:A:40:VAL:O	1:A:45:GLN:HB3	1.96	0.66
2:D:293:ASN:HB2	2:D:317:HIS:HB2	1.77	0.66
2:G:82:ARG:HG2	2:G:82:ARG:HH11	1.60	0.66
1:B:216:ARG:O	4:B:5032:HOH:O	2.13	0.66
1:B:118:GLY:O	2:D:92:ASN:OD1	2.14	0.66
2:G:248:ASP:O	2:G:249:ILE:CG2	2.44	0.66
1:B:127:GLY:HA3	2:D:82:ARG:HH12	1.61	0.66
2:D:142:SER:HB2	2:D:145:GLN:HG3	1.78	0.66
2:H:3:LYS:HG3	2:H:27:HIS:CD2	2.26	0.65
1:B:151:THR:HG21	1:B:204:GLN:HG3	1.78	0.65
2:H:256:ARG:O	2:H:257:LEU:HD12	1.97	0.65
2:H:302:ASP:HB2	2:H:309:PHE:CZ	2.31	0.65
1:F:92:ALA:CB	1:F:169:ALA:HB1	2.26	0.65
2:G:229:PHE:HA	2:G:241:ILE:HD11	1.79	0.65
2:G:282:LEU:O	2:G:286:THR:HG23	1.95	0.65
1:A:200:VAL:HA	1:A:203:ILE:HG22	1.78	0.65
2:D:100:PHE:HD2	2:D:134:HIS:CD2	2.14	0.65
2:H:295:ASN:HB2	2:H:315:GLU:HB2	1.79	0.65
2:D:45:SER:O	2:D:49:ARG:HG2	1.96	0.65
1:E:163:MET:HG2	1:F:163:MET:CE	2.27	0.65
2:D:37:ILE:HD13	2:D:201:MET:SD	2.37	0.65
1:E:41:THR:HG21	1:E:53:TYR:HB2	1.79	0.65
2:H:142:SER:N	2:H:145:GLN:OE1	2.28	0.65
1:A:23:SER:OG	1:A:96:LEU:HB3	1.97	0.64
2:H:105:LEU:HB3	2:H:106:PRO:HD3	1.79	0.64
1:E:5:MET:CE	1:E:188:VAL:HG21	2.27	0.64
2:H:48:ILE:HG23	2:H:49:ARG:N	2.11	0.64
2:G:197:ILE:O	2:G:198:THR:HB	1.96	0.64
2:C:214:ILE:HG13	2:C:218:GLU:O	1.96	0.64
2:C:220:ILE:CD1	2:C:236:LEU:HD23	2.27	0.64
1:F:41:THR:HA	1:F:48:ALA:HA	1.78	0.64
1:A:179:TYR:HB3	1:A:188:VAL:CG1	2.28	0.64
1:B:85:THR:CG2	1:B:86:SER:N	2.60	0.64
1:A:41:THR:HG21	1:A:52:LEU:HD12	1.79	0.63
2:D:7:ILE:HG22	2:D:21:LEU:HD13	1.80	0.63



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:D:175:THR:HG23	4:D:347:HOH:O	1.99	0.63
2:D:285:GLU:HG3	2:D:289:ARG:CD	2.28	0.63
2:G:44:LYS:HE3	3:G:2503:ADP:O3B	1.98	0.63
2:C:195:LEU:HD12	2:C:196:LEU:N	2.12	0.63
2:C:292:VAL:HG11	2:C:316:MET:CE	2.28	0.63
1:F:18:ALA:O	1:F:22:VAL:HG23	1.98	0.63
1:F:37:LEU:HD11	1:F:52:LEU:HD21	1.80	0.63
1:A:144:PRO:HB3	1:A:214:VAL:HG21	1.79	0.63
1:A:200:VAL:O	1:A:203:ILE:HG22	1.99	0.63
2:D:24:VAL:HG13	2:D:219:LEU:HD12	1.81	0.63
2:G:224:THR:O	2:G:228:VAL:HG23	1.99	0.62
2:G:296:ILE:HG12	2:G:314:THR:HG22	1.81	0.62
2:D:205:LYS:HG2	2:D:229:PHE:CZ	2.33	0.62
1:F:47:ILE:O	1:F:47:ILE:HG13	1.99	0.62
2:C:27:HIS:O	2:C:29:PRO:HD3	1.99	0.62
2:C:316:MET:HE1	2:C:326:ALA:HB3	1.81	0.62
1:F:80:ARG:HB2	1:F:86:SER:HB3	1.82	0.62
2:H:45:SER:HB2	3:H:2502:ADP:O2A	1.99	0.62
1:A:154:LEU:HB3	1:A:203:ILE:CD1	2.27	0.62
2:G:11:PHE:HB2	2:G:18:ILE:HG22	1.80	0.62
2:H:148:ARG:HD2	4:H:350:HOH:O	1.99	0.62
1:B:13:VAL:HG22	1:B:172:LEU:HD11	1.80	0.62
2:C:2:ILE:HG12	2:C:28:VAL:HB	1.80	0.62
1:E:2:SER:O	1:E:5:MET:N	2.33	0.62
2:G:187:ASN:ND2	2:G:192:LEU:O	2.30	0.62
1:B:3:GLU:N	1:B:4:PRO:CD	2.62	0.62
2:C:37:ILE:HG12	2:C:240:PHE:CE2	2.35	0.62
1:E:32:LEU:HB3	1:E:33:PRO:CD	2.30	0.62
2:H:220:ILE:CG2	2:H:234:THR:HG21	2.28	0.62
2:H:303:TYR:OH	2:H:308:LYS:HE2	2.00	0.62
1:F:134:VAL:HA	1:F:138:LEU:HD12	1.82	0.62
2:D:214:ILE:HA	2:D:219:LEU:HA	1.82	0.61
1:E:69:ILE:HB	1:E:163:MET:HE2	1.80	0.61
2:H:112:THR:HG23	2:H:117:VAL:HG22	1.82	0.61
2:C:73:SER:HB2	2:C:76:GLU:HG2	1.81	0.61
2:C:0:HIS:ND1	2:C:27:HIS:CB	2.64	0.61
2:D:33:ILE:HD13	2:D:207:ILE:HB	1.83	0.61
2:H:45:SER:HB2	3:H:2502:ADP:PA	2.40	0.61
1:B:32:LEU:HB3	1:B:33:PRO:HD3	1.83	0.61
2:D:234:THR:HG22	2:D:236:LEU:H	1.65	0.61
1:B:36:VAL:O	1:B:40:VAL:HG22	2.01	0.60



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:G:179:ILE:O	2:G:182:LEU:HB3	2.01	0.60
2:G:272:GLU:HB2	2:G:336:LYS:HB3	1.83	0.60
2:H:11:PHE:HB3	3:H:2502:ADP:C2	2.36	0.60
2:C:299:ALA:HB1	2:C:312:MET:HG2	1.82	0.60
2:G:236:LEU:O	2:G:239:LYS:HB2	2.01	0.60
2:H:201:MET:HE3	2:H:240:PHE:HB3	1.84	0.60
2:C:315:GLU:HG3	2:C:317:HIS:NE2	2.16	0.60
2:D:4:LEU:CD2	2:D:62:VAL:HG22	2.27	0.60
1:A:128:ALA:HB2	2:C:109:LEU:HD13	1.83	0.60
1:F:129:THR:OG1	1:F:132:GLN:HG3	2.02	0.60
2:G:166:GLN:HB3	2:G:169:SER:HB2	1.84	0.60
2:D:8:THR:HG23	2:D:22:ASN:HA	1.83	0.60
2:H:89:GLN:HG3	2:H:169:SER:HB3	1.84	0.60
1:B:85:THR:HG22	1:B:86:SER:H	1.65	0.60
2:C:206:ARG:HG2	2:C:207:ILE:HG23	1.84	0.60
2:G:296:ILE:HA	2:G:314:THR:HG22	1.83	0.60
2:H:144:GLY:O	2:H:148:ARG:HG3	2.00	0.60
1:B:39:TYR:CE1	1:B:113:LEU:HD23	2.37	0.60
2:C:172:ASP:O	2:C:176:THR:HG23	2.02	0.60
1:A:28:PHE:CD1	1:A:104:ILE:HD13	2.37	0.59
1:E:163:MET:HE2	1:F:163:MET:HG2	1.84	0.59
1:F:2:SER:O	1:F:6:MET:HG2	2.02	0.59
1:A:92:ALA:O	1:A:95:PRO:HG2	2.02	0.59
1:F:46:ILE:HD11	1:F:120:ILE:HG23	1.84	0.59
1:A:2:SER:HB2	1:A:4:PRO:HD2	1.83	0.59
1:F:151:THR:O	1:F:155:ILE:HG22	2.02	0.59
1:F:36:VAL:HG12	1:F:112:LEU:HD11	1.83	0.59
2:H:200:GLU:O	2:H:203:VAL:HG12	2.03	0.59
1:B:87:ILE:HG13	1:B:168:GLY:O	2.02	0.59
2:C:103:VAL:O	2:C:106:PRO:HD2	2.02	0.59
2:H:319:THR:CG2	2:H:322:ASP:HB2	2.32	0.59
2:G:105:LEU:N	2:G:106:PRO:HD2	2.18	0.59
1:B:216:ARG:HG2	2:D:139:SER:HB2	1.85	0.59
2:H:123:GLU:HG3	2:H:124:LEU:HD13	1.83	0.59
1:B:207:GLY:HA2	1:B:210:ILE:CG2	2.33	0.59
2:C:44:LYS:HE3	3:C:2500:ADP:O1B	2.02	0.59
1:E:59:ILE:HG13	1:E:60:VAL:N	2.18	0.59
1:A:163:MET:HE1	1:B:163:MET:O	2.03	0.58
2:G:296:ILE:HG12	2:G:314:THR:CG2	2.32	0.58
2:C:293:ASN:HB2	2:C:317:HIS:HB2	1.85	0.58
2:H:89:GLN:HB2	2:H:166:GLN:HB2	1.84	0.58



	t i c	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:H:164:CYS:HB2	2:H:196:LEU:CB	2.33	0.58
1:A:80:ARG:O	1:A:84:GLY:N	2.34	0.58
2:C:1:MET:HE2	2:C:160:LYS:HB3	1.84	0.58
2:C:171:LEU:HB2	2:C:176:THR:HG22	1.85	0.58
1:A:93:ILE:O	1:A:97:THR:HG23	2.03	0.58
1:A:94:VAL:N	1:A:95:PRO:HD2	2.17	0.58
1:A:185:ASN:HB3	1:A:188:VAL:CG1	2.34	0.58
2:D:319:THR:HG22	2:D:321:GLN:N	2.13	0.58
2:H:328:ALA:O	2:H:332:GLU:HG2	2.03	0.58
1:B:78:PHE:O	1:B:81:VAL:HG12	2.03	0.58
2:G:103:VAL:O	2:G:106:PRO:HD2	2.04	0.58
2:C:1:MET:CE	2:C:160:LYS:HB3	2.33	0.58
2:D:82:ARG:O	2:D:157:SER:OG	2.21	0.58
2:D:266:VAL:HG21	2:D:317:HIS:CE1	2.39	0.58
2:G:99:VAL:HG12	2:G:141:LEU:HD11	1.86	0.58
2:H:229:PHE:CZ	2:H:244:THR:HG21	2.38	0.58
2:G:68:GLU:OE1	2:G:68:GLU:HA	2.04	0.58
2:H:64:VAL:O	2:H:67:GLN:HG2	2.04	0.58
1:A:26:PHE:O	1:A:30:ILE:HG22	2.04	0.58
2:C:1:MET:HG3	2:C:2:ILE:HG23	1.86	0.58
2:C:231:HIS:N	2:C:232:PRO:HD3	2.19	0.58
2:D:21:LEU:HA	2:D:217:GLY:CA	2.34	0.58
1:F:2:SER:C	1:F:4:PRO:HD2	2.24	0.58
2:H:151:ILE:O	2:H:155:LEU:HG	2.04	0.58
2:C:56:ARG:NH1	2:C:70:THR:O	2.37	0.57
2:G:327:ILE:O	2:G:331:GLN:HG3	2.04	0.57
1:A:17:LEU:HD21	1:A:199:LEU:HD11	1.85	0.57
2:D:174:ALA:O	2:D:177:ARG:HB2	2.04	0.57
2:G:114:LYS:HE2	2:G:118:LYS:HE3	1.84	0.57
1:B:89:LEU:HD12	1:B:90:GLN:N	2.20	0.57
2:C:72:LEU:HG	2:C:76:GLU:HB2	1.86	0.57
2:C:196:LEU:HD12	2:C:197:ILE:H	1.67	0.57
2:D:73:SER:HB2	2:D:76:GLU:HB2	1.86	0.57
1:E:63:PHE:HB3	1:E:102:PRO:HG2	1.86	0.57
2:G:9:LYS:HE3	2:G:55:GLU:HG3	1.86	0.57
2:C:292:VAL:HG11	2:C:316:MET:HE2	1.86	0.57
1:E:163:MET:HG2	1:F:163:MET:HE2	1.86	0.57
1:B:2:SER:O	1:B:6:MET:HG2	2.04	0.57
2:C:312:MET:HE1	4:D:351:HOH:O	2.04	0.57
2:G:125:LEU:O	2:G:130:LEU:N	2.38	0.57
1:A:163:MET:HG2	1:B:163:MET:HE2	1.85	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:282:LEU:O	2:C:286:THR:HB	2.04	0.57
2:G:329:TRP:O	2:G:333:HIS:HD2	1.87	0.57
1:E:37:LEU:HA	1:E:40:VAL:HG22	1.85	0.57
1:B:178:GLN:OE1	1:B:182:ILE:HD12	2.04	0.57
2:H:267:PRO:HB2	2:H:269:LEU:HD11	1.87	0.57
1:B:115:ILE:CD1	1:B:138:LEU:HD23	2.34	0.56
2:G:298:SER:HB3	2:G:313:LEU:HB2	1.86	0.56
2:H:119:ARG:O	2:H:122:THR:OG1	2.18	0.56
2:D:34:TYR:CD1	2:D:34:TYR:C	2.78	0.56
1:A:92:ALA:O	1:A:95:PRO:HD2	2.05	0.56
2:C:147:GLN:O	2:C:151:ILE:HG13	2.06	0.56
1:A:154:LEU:CB	1:A:203:ILE:HD11	2.31	0.56
2:D:7:ILE:N	2:D:24:VAL:O	2.36	0.56
2:C:5:SER:HB2	2:C:61:SER:HB3	1.87	0.56
1:E:46:ILE:HD12	1:E:46:ILE:H	1.71	0.56
2:G:45:SER:HA	2:G:48:ILE:CG2	2.34	0.56
2:H:286:THR:CG2	2:H:292:VAL:HG21	2.33	0.56
2:D:20:ALA:O	2:D:43:GLY:HA3	2.06	0.56
2:D:50:CYS:O	2:D:62:VAL:HG21	2.06	0.56
2:H:68:GLU:OE2	2:H:70:THR:OG1	2.22	0.56
2:C:211:VAL:O	2:C:211:VAL:HG13	2.06	0.56
1:E:130:PRO:HA	1:E:133:ILE:HD12	1.87	0.56
1:A:137:VAL:O	1:A:140:PRO:HD2	2.06	0.56
2:C:145:GLN:O	2:C:149:VAL:HG23	2.06	0.56
1:E:78:PHE:O	1:E:81:VAL:HG22	2.06	0.56
2:H:124:LEU:HD23	2:H:156:ALA:HA	1.87	0.56
1:A:76:ILE:HB	1:A:77:PRO:HD3	1.87	0.55
1:E:42:ARG:HH21	1:E:113:LEU:HD11	1.71	0.55
1:B:42:ARG:HD3	1:B:113:LEU:HD21	1.87	0.55
1:E:68:PHE:CZ	1:E:96:LEU:HD23	2.41	0.55
1:F:3:GLU:N	1:F:4:PRO:CD	2.70	0.55
1:F:137:VAL:O	1:F:141:GLU:HB2	2.06	0.55
1:B:118:GLY:HA2	1:B:121:GLU:HB2	1.86	0.55
2:D:31:GLY:O	2:D:187:ASN:ND2	2.37	0.55
1:E:46:ILE:HG21	1:E:130:PRO:HG3	1.87	0.55
2:G:89:GLN:HG3	2:G:169:SER:HB3	1.87	0.55
2:H:94:LEU:HD12	2:H:97:ARG:HD2	1.88	0.55
2:C:52:ASN:HB3	2:C:54:LEU:HG	1.88	0.55
2:D:168:THR:HB	2:D:176:THR:HG23	1.88	0.55
1:E:19:MET:CE	1:E:161:SER:HB2	2.36	0.55
1:B:85:THR:CG2	1:B:86:SER:H	2.18	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:163:LEU:CD2	2:C:195:LEU:HB3	2.35	0.55
2:G:168:THR:HA	2:G:171:LEU:HD12	1.89	0.55
1:A:30:ILE:O	1:A:33:PRO:HD2	2.07	0.55
2:G:124:LEU:HD23	2:G:152:ALA:O	2.06	0.55
1:B:9:LEU:HA	1:B:175:ILE:CD1	2.37	0.55
2:G:48:ILE:HD13	2:G:197:ILE:HG12	1.89	0.55
1:A:121:GLU:CD	2:C:49:ARG:NH1	2.60	0.55
2:C:9:LYS:HE3	2:C:10:VAL:O	2.07	0.55
2:D:72:LEU:CD1	2:D:76:GLU:HB3	2.37	0.55
2:G:46:THR:OG1	3:G:2503:ADP:O1A	2.24	0.55
2:H:105:LEU:O	2:H:108:GLU:HB2	2.07	0.55
1:E:119:LEU:HD11	2:G:93:LEU:O	2.06	0.54
2:G:330:LEU:O	2:G:333:HIS:O	2.25	0.54
2:H:248:ASP:O	2:H:250:PRO:HD3	2.07	0.54
1:A:39:TYR:HE1	1:A:113:LEU:HD23	1.72	0.54
2:D:91:PHE:CD1	2:D:91:PHE:N	2.74	0.54
2:G:168:THR:HB	2:G:176:THR:HG23	1.89	0.54
1:A:13:VAL:HA	1:A:172:LEU:HD11	1.90	0.54
1:B:9:LEU:HD11	1:B:191:THR:HG23	1.89	0.54
2:G:29:PRO:O	2:G:32:GLN:HB2	2.07	0.54
2:H:322:ASP:HA	2:H:325:ALA:HB3	1.87	0.54
2:C:138:PRO:HA	2:C:141:LEU:HD12	1.90	0.54
1:E:129:THR:HG22	1:E:131:MET:H	1.71	0.54
2:H:83:GLN:OE1	2:H:160:LYS:HE2	2.07	0.54
1:E:80:ARG:HB2	1:E:86:SER:HB2	1.89	0.54
1:E:115:ILE:HD13	1:E:141:GLU:HB3	1.90	0.54
1:F:210:ILE:O	1:F:214:VAL:HG12	2.08	0.54
1:B:92:ALA:O	1:B:95:PRO:HD2	2.08	0.54
1:E:147:VAL:HG23	1:E:211:VAL:HG22	1.90	0.54
1:F:100:ALA:HA	1:F:103:PHE:CE2	2.42	0.54
2:H:215:SER:HB3	2:H:220:ILE:HD11	1.89	0.54
2:D:72:LEU:HD13	2:D:76:GLU:HB3	1.90	0.54
1:E:58:ALA:O	1:E:62:ILE:HG12	2.08	0.54
1:F:38:LEU:HD21	1:F:106:ARG:NH2	2.22	0.54
2:G:37:ILE:HG12	2:G:240:PHE:CE2	2.43	0.54
2:G:244:THR:HG23	2:G:245:LEU:HD22	1.90	0.54
2:H:229:PHE:HZ	2:H:244:THR:HG21	1.71	0.54
1:B:15:GLU:OE1	1:B:89:LEU:HD23	2.08	0.54
1:B:101:ALA:N	1:B:102:PRO:HD2	2.23	0.54
1:F:167:VAL:HG12	1:F:167:VAL:O	2.08	0.54
2:G:296:ILE:HD13	2:G:312:MET:SD	2.48	0.54



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:G:312:MET:HG2	2:G:314:THR:HG23	1.90	0.54
1:E:120:ILE:O	1:E:123:SER:OG	2.19	0.53
1:B:118:GLY:HA2	1:B:121:GLU:CB	2.38	0.53
1:B:155:ILE:HD11	1:B:204:GLN:HB2	1.88	0.53
2:D:199:HIS:CE1	2:D:200:GLU:HG3	2.42	0.53
1:E:137:VAL:O	1:E:141:GLU:HB2	2.07	0.53
2:C:15:THR:HG23	2:C:16:ARG:HG2	1.89	0.53
1:E:30:ILE:HG13	1:E:31:GLY:N	2.24	0.53
1:E:71:LEU:O	1:E:75:MET:HG2	2.07	0.53
2:D:100:PHE:CD2	2:D:134:HIS:CD2	2.96	0.53
1:F:134:VAL:HG22	1:F:138:LEU:HD12	1.90	0.53
1:A:121:GLU:CD	2:C:49:ARG:HH12	2.10	0.53
1:B:216:ARG:N	1:B:216:ARG:HD2	2.24	0.53
1:B:184:TYR:CG	1:B:184:TYR:O	2.62	0.53
2:C:150:ALA:HB1	4:C:356:HOH:O	2.08	0.53
2:C:319:THR:HG22	2:C:321:GLN:H	1.71	0.53
2:D:6:ASN:H	2:D:25:SER:HB3	1.74	0.53
2:G:123:GLU:O	2:G:126:SER:HB2	2.09	0.53
2:G:142:SER:H	2:G:145:GLN:HE21	1.57	0.53
2:G:285:GLU:HG3	2:G:289:ARG:HE	1.74	0.53
2:H:48:ILE:CG2	2:H:49:ARG:N	2.71	0.53
2:H:198:THR:HG21	2:H:203:VAL:HG13	1.88	0.53
2:C:48:ILE:HD11	2:C:163:LEU:HD22	1.91	0.53
2:D:164:CYS:HB2	2:D:196:LEU:CB	2.39	0.53
1:F:127:GLY:O	2:H:78:THR:HG23	2.09	0.53
2:G:2:ILE:H	2:G:64:VAL:HA	1.74	0.53
2:D:164:CYS:HB2	2:D:196:LEU:HB3	1.90	0.53
1:E:28:PHE:HD1	1:E:104:ILE:CD1	2.21	0.53
1:E:134:VAL:HA	1:E:138:LEU:HB2	1.90	0.53
2:G:52:ASN:O	2:G:53:LEU:HB2	2.09	0.53
2:C:199:HIS:CE1	2:C:200:GLU:HG3	2.44	0.53
2:C:241:ILE:O	2:C:244:THR:HG22	2.08	0.53
2:D:180:LEU:HD23	2:D:183:LEU:HD12	1.90	0.53
2:H:201:MET:HE2	2:H:240:PHE:HB3	1.90	0.52
2:H:39:ALA:O	2:H:44:LYS:NZ	2.43	0.52
1:B:96:LEU:CD2	1:B:160:TYR:HB3	2.40	0.52
2:C:1:MET:HE2	2:C:161:VAL:HG23	1.91	0.52
2:D:319:THR:CG2	2:D:320:GLN:N	2.72	0.52
1:E:92:ALA:C	1:E:95:PRO:HD2	2.29	0.52
1:F:209:ARG:HA	1:F:209:ARG:NE	2.24	0.52
1:B:207:GLY:CA	1:B:210:ILE:HG22	2.37	0.52



	to do pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:104:ALA:HB2	2:D:121:VAL:HG21	1.92	0.52
2:D:336:LYS:HZ2	2:D:336:LYS:HB3	1.75	0.52
1:F:32:LEU:HB3	1:F:33:PRO:HD3	1.91	0.52
2:G:24:VAL:HG13	2:G:219:LEU:HD22	1.92	0.52
2:H:206:ARG:NH2	4:H:353:HOH:O	2.35	0.52
2:D:245:LEU:CD2	2:D:302:ASP:HB2	2.40	0.52
1:A:155:ILE:HG12	1:A:200:VAL:HG13	1.92	0.52
1:E:134:VAL:HG23	1:E:135:ARG:N	2.23	0.52
1:B:78:PHE:HA	1:B:81:VAL:HG12	1.92	0.52
1:B:115:ILE:HD11	1:B:138:LEU:CD2	2.34	0.52
2:C:181:GLU:OE2	2:C:206:ARG:NH1	2.43	0.52
2:C:205:LYS:NZ	2:C:302:ASP:OD2	2.38	0.52
2:C:245:LEU:HB3	2:C:300:GLN:HG2	1.92	0.52
1:E:30:ILE:HG13	1:E:31:GLY:H	1.74	0.52
1:E:5:MET:O	1:E:8:LEU:CB	2.55	0.52
1:F:118:GLY:O	2:H:92:ASN:ND2	2.43	0.52
2:H:241:ILE:O	2:H:244:THR:HG22	2.10	0.52
2:H:8:THR:O	2:H:58:THR:HB	2.10	0.51
1:B:133:ILE:HG22	1:B:138:LEU:HD12	1.91	0.51
2:D:245:LEU:HD21	2:D:302:ASP:HB2	1.92	0.51
1:E:17:LEU:HD21	1:E:199:LEU:HD22	1.93	0.51
2:G:45:SER:CA	2:G:48:ILE:HG22	2.40	0.51
2:G:46:THR:N	3:G:2503:ADP:O1A	2.27	0.51
2:H:100:PHE:HD2	2:H:134:HIS:HE1	1.58	0.51
1:F:132:GLN:O	1:F:136:LYS:HB2	2.11	0.51
1:F:177:TYR:CE1	1:F:181:TYR:CD2	2.98	0.51
2:H:295:ASN:O	2:H:314:THR:HA	2.10	0.51
2:D:329:TRP:O	2:D:333:HIS:HD2	1.92	0.51
2:H:262:PHE:HD1	2:H:263:THR:O	1.92	0.51
1:A:3:GLU:N	1:A:4:PRO:HD2	2.25	0.51
1:B:36:VAL:HG12	1:B:112:LEU:HD11	1.91	0.51
2:D:1:MET:HB2	2:D:193:THR:HG21	1.92	0.51
2:H:145:GLN:O	2:H:149:VAL:HG23	2.11	0.51
2:C:295:ASN:HB3	2:C:315:GLU:HG2	1.92	0.51
2:G:285:GLU:CG	2:G:289:ARG:HE	2.23	0.51
1:F:134:VAL:HA	1:F:138:LEU:HB2	1.91	0.51
1:F:182:ILE:HG13	1:F:183:GLY:H	1.75	0.51
2:G:177:ARG:HH21	2:G:206:ARG:HH22	1.59	0.51
1:F:143:LEU:HD23	1:F:214:VAL:HG21	1.92	0.51
2:H:247:LEU:HD21	2:H:311:ILE:O	2.10	0.51
2:D:4:LEU:O	2:D:25:SER:HA	2.10	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:162:ALA:C	1:F:69:ILE:HD11	2.31	0.51
1:A:143:LEU:N	1:A:144:PRO:HD2	2.26	0.51
2:G:146:LYS:O	2:G:149:VAL:CG1	2.57	0.51
1:E:39:TYR:O	1:E:42:ARG:HB2	2.11	0.50
2:G:99:VAL:HG11	2:G:141:LEU:HD11	1.90	0.50
2:H:7:ILE:HG23	2:H:57:PRO:HB3	1.93	0.50
2:H:10:VAL:HG12	2:H:19:GLN:HG3	1.93	0.50
2:C:234:THR:HG23	2:C:235:PRO:HD2	1.93	0.50
1:A:64:ARG:HB2	1:A:102:PRO:HB2	1.92	0.50
1:A:92:ALA:O	1:A:96:LEU:HB2	2.11	0.50
2:G:168:THR:CB	2:G:176:THR:HG23	2.41	0.50
2:G:200:GLU:HB2	2:G:203:VAL:CG2	2.39	0.50
1:B:11:ARG:O	1:B:15:GLU:HG2	2.12	0.50
1:B:151:THR:CG2	1:B:204:GLN:HG3	2.40	0.50
2:C:128:VAL:HG11	2:C:152:ALA:HB2	1.93	0.50
2:C:227:GLU:O	2:C:230:SER:O	2.30	0.50
2:G:208:CYS:O	2:G:225:VAL:HG21	2.11	0.50
1:A:45:GLN:HG3	1:A:46:ILE:H	1.77	0.50
2:G:5:SER:HB2	2:G:61:SER:HB3	1.93	0.50
2:G:22:ASN:HB3	2:G:218:GLU:OE1	2.12	0.50
2:G:91:PHE:CD1	2:G:91:PHE:N	2.71	0.50
1:A:68:PHE:CZ	1:A:96:LEU:CD1	2.94	0.50
2:C:164:CYS:CB	2:C:196:LEU:HD13	2.24	0.50
2:C:240:PHE:O	2:C:243:SER:OG	2.17	0.50
2:D:36:VAL:HB	2:D:197:ILE:HG22	1.93	0.50
1:F:155:ILE:HG12	1:F:155:ILE:O	2.10	0.50
2:D:9:LYS:HD3	2:D:56:ARG:O	2.12	0.50
1:F:15:GLU:HG2	1:F:89:LEU:HD21	1.94	0.50
2:G:100:PHE:HD2	2:G:134:HIS:CD2	2.29	0.50
2:G:241:ILE:O	2:G:244:THR:HG22	2.11	0.50
2:H:32:GLN:HE21	2:H:209:ASP:HB3	1.77	0.50
2:H:113:PRO:HG2	2:H:116:GLU:HG3	1.94	0.50
1:B:2:SER:C	1:B:4:PRO:HD2	2.32	0.49
1:B:35:GLY:HA3	1:B:108:VAL:HB	1.93	0.49
1:B:123:SER:HA	1:B:126:MET:HE3	1.93	0.49
2:C:2:ILE:CG2	2:C:161:VAL:HG21	2.41	0.49
2:C:270:ARG:HB3	2:C:340:LEU:HD11	1.94	0.49
2:D:172:ASP:O	2:D:176:THR:N	2.30	0.49
2:G:37:ILE:HD13	2:G:201:MET:SD	2.52	0.49
2:C:94:LEU:HD12	2:C:97:ARG:HD2	1.94	0.49
2:C:310:GLY:C	2:C:311:ILE:HG13	2.33	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:329:TRP:CE2	2:D:333:HIS:NE2	2.80	0.49
1:A:196:LEU:HD13	1:B:70:ILE:HG13	1.94	0.49
1:B:185:ASN:HB3	1:B:188:VAL:HG22	1.95	0.49
2:C:7:ILE:HD11	2:C:61:SER:O	2.11	0.49
1:A:101:ALA:N	1:A:102:PRO:HD2	2.28	0.49
2:C:130:LEU:HD13	2:C:149:VAL:HG22	1.94	0.49
2:H:131:GLY:O	2:H:133:LYS:N	2.44	0.49
2:H:184:LYS:HD2	2:H:207:ILE:HG22	1.92	0.49
1:B:103:PHE:CE2	1:B:156:THR:HG21	2.48	0.49
1:E:131:MET:O	1:E:134:VAL:HG22	2.13	0.49
2:G:209:ASP:O	2:G:225:VAL:HG23	2.12	0.49
2:H:174:ALA:HA	2:H:177:ARG:HH11	1.76	0.49
1:A:184:TYR:CZ	1:A:186:ALA:HA	2.48	0.49
1:E:78:PHE:O	1:E:82:ILE:HG12	2.13	0.49
2:G:76:GLU:HG2	2:G:79:LYS:NZ	2.28	0.49
2:D:1:MET:HE2	2:D:161:VAL:HG23	1.94	0.49
1:E:4:PRO:O	1:E:8:LEU:HB2	2.13	0.49
1:E:5:MET:HE2	1:E:188:VAL:HG21	1.95	0.49
2:H:52:ASN:ND2	2:H:54:LEU:HG	2.27	0.49
1:A:23:SER:HB3	1:A:157:LEU:HD13	1.95	0.49
2:D:285:GLU:HG3	2:D:289:ARG:NE	2.27	0.49
2:G:30:ALA:HA	2:G:193:THR:CG2	2.43	0.49
2:H:52:ASN:HD22	2:H:54:LEU:HG	1.76	0.49
1:B:71:LEU:O	1:B:75:MET:HG3	2.13	0.49
2:D:82:ARG:NH2	2:D:110:ASP:HB2	2.13	0.49
2:D:182:LEU:O	2:D:186:ILE:HG13	2.12	0.49
2:G:226:SER:HB2	2:G:307:VAL:HG11	1.94	0.49
1:B:12:GLY:HA2	1:B:15:GLU:HG3	1.93	0.49
1:F:13:VAL:HG23	1:F:14:TRP:N	2.28	0.49
1:E:13:VAL:HG22	1:E:172:LEU:HD11	1.93	0.48
1:F:119:LEU:HD23	2:H:94:LEU:HD22	1.94	0.48
1:A:130:PRO:O	1:A:133:ILE:HG13	2.13	0.48
2:C:299:ALA:HB2	2:C:312:MET:HG2	1.93	0.48
1:F:89:LEU:N	1:F:89:LEU:HD12	2.28	0.48
2:G:155:LEU:HD11	2:G:186:ILE:HD12	1.95	0.48
2:H:198:THR:HG21	2:H:203:VAL:CG1	2.43	0.48
1:A:115:ILE:HD13	1:A:141:GLU:HB2	1.96	0.48
1:B:17:LEU:HD21	1:B:199:LEU:HD11	1.95	0.48
1:B:49:ASN:HB2	1:B:52:LEU:HB3	1.95	0.48
1:B:143:LEU:HD23	1:B:214:VAL:HG11	1.95	0.48
1:B:199:LEU:O	1:B:203:ILE:HG12	2.13	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:198:THR:HG21	2:D:203:VAL:CG2	2.43	0.48
1:A:5:MET:HE3	1:A:8:LEU:HD23	1.95	0.48
1:B:100:ALA:O	1:B:103:PHE:HB3	2.13	0.48
2:C:296:ILE:HG22	2:C:314:THR:HG22	1.95	0.48
3:C:2500:ADP:H5'1	3:C:2500:ADP:H8	1.78	0.48
1:F:89:LEU:CD1	1:F:89:LEU:H	2.26	0.48
2:G:2:ILE:HG12	2:G:2:ILE:O	2.14	0.48
2:H:44:LYS:HB3	2:H:197:ILE:HB	1.94	0.48
2:H:88:PHE:O	2:H:90:HIS:O	2.31	0.48
1:B:120:ILE:O	1:B:123:SER:HB3	2.13	0.48
2:H:124:LEU:CD2	2:H:156:ALA:HA	2.44	0.48
2:C:99:VAL:HG12	2:C:141:LEU:HD11	1.96	0.48
2:C:243:SER:O	2:C:244:THR:C	2.51	0.48
2:G:186:ILE:HG22	2:G:189:ARG:HH11	1.78	0.48
2:H:121:VAL:HG12	2:H:125:LEU:HD12	1.96	0.48
1:B:210:ILE:O	1:B:210:ILE:CG1	2.62	0.48
2:C:293:ASN:OD1	2:D:288:ARG:NH1	2.45	0.48
2:D:13:GLN:OE1	2:D:14:GLY:N	2.47	0.48
2:D:170:ALA:O	2:D:171:LEU:HG	2.14	0.48
2:G:227:GLU:O	2:G:231:HIS:HB2	2.14	0.48
1:A:39:TYR:CE1	1:A:113:LEU:HD23	2.48	0.47
2:C:49:ARG:HG2	2:C:54:LEU:HB2	1.96	0.47
1:E:101:ALA:HB3	1:E:102:PRO:HD3	1.95	0.47
2:C:4:LEU:O	2:C:25:SER:HA	2.14	0.47
1:E:52:LEU:O	1:E:56:VAL:N	2.30	0.47
1:F:41:THR:HG21	1:F:52:LEU:HD23	1.96	0.47
1:A:12:GLY:O	1:A:16:THR:N	2.42	0.47
1:B:104:ILE:O	1:B:107:MET:N	2.48	0.47
1:B:127:GLY:HA3	2:D:82:ARG:NH1	2.28	0.47
2:C:48:ILE:CD1	2:C:163:LEU:HD22	2.43	0.47
2:C:274:THR:O	2:C:278:VAL:HG23	2.14	0.47
2:H:32:GLN:NE2	2:H:209:ASP:HB3	2.29	0.47
1:A:1:MET:SD	1:A:6:MET:HG3	2.55	0.47
1:A:120:ILE:CD1	1:A:138:LEU:HD11	2.44	0.47
2:D:24:VAL:HG13	2:D:219:LEU:CD1	2.44	0.47
2:D:248:ASP:O	2:D:250:PRO:HD3	2.14	0.47
2:D:327:ILE:HG23	2:D:337:VAL:HG11	1.95	0.47
1:E:65:SER:OG	1:F:200:VAL:HG11	2.14	0.47
1:F:5:MET:O	1:F:8:LEU:HB2	2.15	0.47
2:H:53:LEU:HD12	2:H:69:LEU:CB	2.43	0.47
2:H:267:PRO:HD2	2:H:316:MET:O	2.15	0.47



	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:67:PRO:HB3	1:B:159:GLY:HA2	1.96	0.47
1:B:68:PHE:HE1	1:B:95:PRO:O	1.98	0.47
1:E:104:ILE:CG1	1:E:153:THR:HG21	2.45	0.47
2:C:297:ILE:O	2:C:298:SER:HB3	2.15	0.47
1:E:143:LEU:HB3	1:E:144:PRO:HD3	1.97	0.47
2:G:214:ILE:HG13	2:G:218:GLU:O	2.14	0.47
1:A:104:ILE:HD11	1:A:153:THR:HG21	1.95	0.47
2:C:79:LYS:HA	2:C:82:ARG:HG2	1.97	0.47
2:C:104:ALA:O	2:C:107:LEU:N	2.47	0.47
2:D:296:ILE:HG12	2:D:312:MET:CE	2.45	0.47
1:E:57:SER:O	1:E:61:ASN:HB2	2.14	0.47
1:E:179:TYR:HA	1:E:183:GLY:O	2.15	0.47
1:F:76:ILE:HB	1:F:77:PRO:CD	2.45	0.47
2:H:262:PHE:HD1	2:H:263:THR:N	2.10	0.47
1:A:124:ARG:O	2:C:81:ARG:HD3	2.16	0.46
1:B:177:TYR:CE1	1:B:181:TYR:HD2	2.33	0.46
2:D:118:LYS:O	2:D:122:THR:OG1	2.23	0.46
1:E:19:MET:HE3	1:E:161:SER:HB2	1.97	0.46
2:H:42:ALA:HB1	2:H:214:ILE:HG12	1.98	0.46
1:B:129:THR:O	1:B:133:ILE:HG13	2.13	0.46
2:G:180:LEU:HA	2:G:180:LEU:HD23	1.67	0.46
2:H:118:LYS:O	2:H:122:THR:HG23	2.15	0.46
1:B:188:VAL:HA	1:B:191:THR:CG2	2.40	0.46
2:C:2:ILE:HG22	2:C:64:VAL:HG13	1.98	0.46
2:D:224:THR:HG22	2:D:225:VAL:N	2.31	0.46
1:E:139:LEU:HB2	1:E:140:PRO:HD3	1.98	0.46
1:F:34:VAL:O	1:F:38:LEU:HB2	2.15	0.46
1:F:128:ALA:HA	1:F:132:GLN:NE2	2.31	0.46
2:G:45:SER:O	2:G:48:ILE:HG22	2.15	0.46
1:A:139:LEU:N	1:A:140:PRO:CD	2.78	0.46
2:D:3:LYS:NZ	2:D:27:HIS:HB2	2.31	0.46
2:D:280:ALA:CB	2:D:282:LEU:HG	2.46	0.46
1:F:77:PRO:O	1:F:81:VAL:HG23	2.15	0.46
1:F:179:TYR:O	1:F:184:TYR:N	2.48	0.46
2:G:83:GLN:HA	2:G:159:PRO:HA	1.98	0.46
1:B:210:ILE:O	1:B:210:ILE:HG12	2.14	0.46
1:F:89:LEU:O	1:F:92:ALA:N	2.41	0.46
2:H:128:VAL:HG11	2:H:152:ALA:HB2	1.96	0.46
1:B:2:SER:CA	1:B:4:PRO:HD2	2.45	0.46
1:B:57:SER:OG	1:B:106:ARG:NH2	2.39	0.46
2:C:231:HIS:N	2:C:232:PRO:CD	2.78	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:25:PHE:CE1	1:E:29:VAL:HG21	2.50	0.46
1:E:104:ILE:HG12	1:E:153:THR:HG21	1.98	0.46
1:F:38:LEU:HD13	1:F:56:VAL:HG12	1.98	0.46
2:G:9:LYS:HD3	2:G:57:PRO:HA	1.97	0.46
2:G:165:ASP:HA	2:G:197:ILE:HD11	1.97	0.46
1:A:129:THR:OG1	1:A:132:GLN:HG3	2.16	0.46
1:E:100:ALA:O	1:E:103:PHE:HB2	2.15	0.46
1:F:52:LEU:O	1:F:56:VAL:HG23	2.15	0.46
2:H:251:GLU:HG3	2:H:252:ASP:H	1.80	0.46
1:A:40:VAL:HA	1:A:45:GLN:HG2	1.98	0.46
1:A:170:GLY:HA2	1:A:174:GLN:OE1	2.16	0.46
2:C:99:VAL:CG1	2:C:141:LEU:HD11	2.46	0.46
2:C:45:SER:O	2:C:48:ILE:HG22	2.16	0.46
1:E:78:PHE:CE1	1:E:82:ILE:HD11	2.51	0.46
1:F:19:MET:CE	1:F:161:SER:OG	2.64	0.46
2:G:180:LEU:HD23	2:G:183:LEU:HD12	1.97	0.46
2:H:32:GLN:HG2	2:H:209:ASP:OD2	2.16	0.46
2:H:303:TYR:CZ	2:H:308:LYS:HG3	2.51	0.46
1:B:12:GLY:O	1:B:15:GLU:N	2.49	0.45
1:A:179:TYR:HA	1:A:183:GLY:O	2.16	0.45
2:C:234:THR:HG22	2:C:237:ALA:H	1.81	0.45
1:E:141:GLU:OE2	2:G:95:SER:HB2	2.16	0.45
2:G:107:LEU:HD12	2:G:120:ARG:HH21	1.81	0.45
2:G:245:LEU:HD11	2:G:302:ASP:HB2	1.97	0.45
1:B:32:LEU:HA	1:B:108:VAL:HG21	1.99	0.45
1:B:188:VAL:CA	1:B:191:THR:HG22	2.38	0.45
2:C:84:ILE:HA	2:C:161:VAL:O	2.16	0.45
2:C:236:LEU:HD11	2:C:240:PHE:HE1	1.82	0.45
2:C:298:SER:HA	2:D:299:ALA:O	2.15	0.45
2:D:180:LEU:HD11	2:D:203:VAL:HG12	1.97	0.45
2:D:319:THR:HG22	2:D:320:GLN:H	1.77	0.45
2:H:94:LEU:HD12	2:H:97:ARG:CD	2.47	0.45
1:A:1:MET:SD	1:A:6:MET:CG	3.05	0.45
1:A:155:ILE:CG1	1:A:203:ILE:CG2	2.95	0.45
2:H:2:ILE:HB	2:H:28:VAL:HB	1.97	0.45
2:H:118:LYS:HG3	4:H:358:HOH:O	2.16	0.45
2:H:309:PHE:HE2	2:H:311:ILE:HG12	1.82	0.45
1:A:12:GLY:C	1:A:172:LEU:HG	2.37	0.45
1:A:142:ALA:O	1:A:145:GLY:N	2.50	0.45
2:D:11:PHE:CE2	2:D:20:ALA:HB2	2.52	0.45
1:E:167:VAL:O	1:E:167:VAL:CG1	2.64	0.45



	A L O	Interatomic	Clash
Atom-1	Atom-1 Atom-2		overlap (Å)
1:A:129:THR:H	1:A:132:GLN:NE2	2.05	0.45
2:D:26:LEU:HD21	2:D:28:VAL:HG23	1.99	0.45
2:D:252:ASP:O	2:D:256:ARG:HB2	2.16	0.45
2:D:253:TYR:O	2:D:257:LEU:N	2.50	0.45
2:G:329:TRP:CE2	2:G:333:HIS:NE2	2.84	0.45
1:A:5:MET:SD	1:A:8:LEU:HD23	2.57	0.45
2:C:1:MET:CE	2:C:161:VAL:HG23	2.46	0.45
2:D:46:THR:N	3:D:2501:ADP:O1A	2.37	0.45
2:D:205:LYS:HG2	2:D:229:PHE:CE2	2.51	0.45
2:D:260:GLU:HB2	2:D:261:PRO:HD2	1.98	0.45
1:F:198:ILE:O	1:F:202:LEU:HB2	2.17	0.45
2:H:286:THR:O	2:H:292:VAL:HG22	2.17	0.45
2:D:99:VAL:HG22	2:D:141:LEU:HD21	1.99	0.45
2:D:112:THR:HB	2:D:117:VAL:CG1	2.47	0.45
1:E:134:VAL:CG2	1:E:135:ARG:N	2.80	0.45
1:F:3:GLU:N	1:F:4:PRO:HD2	2.32	0.45
2:H:172:ASP:HB2	2:H:175:THR:OG1	2.17	0.45
1:B:143:LEU:CD2	1:B:214:VAL:HG11	2.47	0.44
1:E:163:MET:CE	1:F:163:MET:HG2	2.46	0.44
1:F:64:ARG:HD2	1:F:103:PHE:HB3	1.98	0.44
2:G:31:GLY:N	2:G:193:THR:CG2	2.73	0.44
2:H:45:SER:O	2:H:49:ARG:HD2	2.16	0.44
1:A:137:VAL:HG22	2:C:94:LEU:HD11	1.99	0.44
2:C:187:ASN:O	2:C:191:GLY:HA2	2.16	0.44
1:E:28:PHE:O	1:E:30:ILE:N	2.50	0.44
2:H:73:SER:OG	2:H:76:GLU:HG3	2.17	0.44
2:H:120:ARG:O	2:H:124:LEU:HB2	2.17	0.44
1:A:9:LEU:HD23	1:A:175:ILE:HD13	1.98	0.44
1:A:127:GLY:O	2:C:78:THR:HG23	2.17	0.44
1:B:184:TYR:O	1:B:184:TYR:CD1	2.70	0.44
2:C:62:VAL:CG1	2:C:69:LEU:HD12	2.42	0.44
2:C:228:VAL:O	2:C:232:PRO:HG3	2.18	0.44
2:C:278:VAL:HG13	2:C:301:MET:SD	2.58	0.44
2:D:168:THR:CB	2:D:176:THR:HG23	2.46	0.44
1:E:141:GLU:OE2	2:G:95:SER:N	2.41	0.44
1:A:177:TYR:O	1:A:181:TYR:HB3	2.18	0.44
1:B:89:LEU:O	1:B:92:ALA:N	2.50	0.44
2:C:71:THR:HG23	2:C:71:THR:O	2.18	0.44
2:D:1:MET:HE3	2:D:64:VAL:HG13	1.99	0.44
2:D:234:THR:HG23	2:D:235:PRO:HD2	1.99	0.44
2:G:82:ARG:HG2	2:G:82:ARG:NH1	2.28	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:207:GLY:O	1:B:211:VAL:HG23	2.18	0.44
2:D:289:ARG:NH1	2:D:329:TRP:HE1	2.15	0.44
2:G:9:LYS:HE3	2:G:55:GLU:CG	2.48	0.44
2:G:10:VAL:HA	2:G:18:ILE:O	2.18	0.44
2:G:52:ASN:HB3	2:G:54:LEU:HG	1.99	0.44
2:G:82:ARG:CZ	2:G:110:ASP:HB2	2.47	0.44
1:A:155:ILE:HG13	1:A:203:ILE:CG2	2.48	0.44
2:C:221:GLU:OE1	2:C:234:THR:HB	2.17	0.44
2:C:232:PRO:HG3	2:C:241:ILE:HD13	1.98	0.44
2:D:319:THR:H	2:D:322:ASP:HB2	1.83	0.44
1:E:51:LYS:O	1:E:54:ARG:HB3	2.18	0.44
2:H:72:LEU:HG	2:H:76:GLU:HB2	1.99	0.44
1:A:18:ALA:O	1:A:22:VAL:HG23	2.18	0.44
1:A:32:LEU:HB3	1:A:33:PRO:CD	2.41	0.44
1:B:83:VAL:HG21	1:B:91:ALA:HA	2.00	0.44
2:C:301:MET:SD	2:C:310:GLY:HA3	2.58	0.44
2:D:319:THR:HB	2:D:322:ASP:HB2	1.99	0.44
1:E:2:SER:O	1:E:3:GLU:C	2.53	0.44
1:E:106:ARG:HA	1:E:106:ARG:HD3	1.89	0.44
1:E:115:ILE:CD1	1:E:141:GLU:HB3	2.48	0.44
2:H:112:THR:CG2	2:H:117:VAL:HG22	2.47	0.44
1:A:163:MET:HE2	1:B:163:MET:HA	2.00	0.44
2:C:249:ILE:HD12	2:C:249:ILE:H	1.82	0.44
2:C:343:VAL:O	2:C:343:VAL:HG22	2.17	0.44
2:G:137:TYR:O	2:G:140:ASN:N	2.50	0.44
2:C:53:LEU:HD12	2:C:69:LEU:HB3	2.00	0.44
2:C:144:GLY:O	2:C:148:ARG:HG3	2.17	0.44
1:F:78:PHE:CZ	1:F:82:ILE:HD11	2.53	0.44
2:H:4:LEU:O	2:H:25:SER:HA	2.18	0.44
2:H:267:PRO:HG3	2:H:323:THR:HG21	1.99	0.44
1:B:119:LEU:HD13	2:D:94:LEU:CD2	2.48	0.43
2:C:173:PRO:O	2:C:177:ARG:HG3	2.18	0.43
2:D:21:LEU:HA	2:D:217:GLY:HA3	1.98	0.43
1:E:59:ILE:HG13	1:E:60:VAL:H	1.81	0.43
1:B:139:LEU:HB2	1:B:140:PRO:HD3	1.99	0.43
2:C:15:THR:HG23	2:C:16:ARG:N	2.33	0.43
1:E:41:THR:HG23	1:E:49:ASN:O	2.18	0.43
1:F:70:ILE:HD12	1:F:70:ILE:N	2.33	0.43
1:F:155:ILE:HD12	1:F:200:VAL:HG13	2.01	0.43
2:G:72:LEU:HB3	2:G:77:LEU:HD12	2.00	0.43
2:G:245:LEU:HB3	2:G:247:LEU:HD13	2.00	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:H:52:ASN:HD22	2:H:54:LEU:CD1	2.31	0.43
2:H:280:ALA:HA	2:H:281:PRO:HD3	1.91	0.43
1:A:5:MET:HE2	1:A:188:VAL:HG23	2.00	0.43
1:B:23:SER:HB2	1:B:157:LEU:HD13	2.01	0.43
2:C:105:LEU:N	2:C:106:PRO:HD2	2.33	0.43
1:F:13:VAL:CG1	1:F:172:LEU:HD11	2.47	0.43
1:B:147:VAL:HG11	1:B:210:ILE:HG23	1.99	0.43
2:C:1:MET:HB2	2:C:30:ALA:HB2	2.00	0.43
2:C:48:ILE:HG23	2:C:49:ARG:N	2.34	0.43
2:G:13:GLN:O	2:G:16:ARG:N	2.49	0.43
2:G:35:GLY:O	2:G:211:VAL:HG23	2.18	0.43
2:H:18:ILE:N	2:H:18:ILE:HD12	2.34	0.43
2:H:79:LYS:O	2:H:82:ARG:HB2	2.18	0.43
1:B:41:THR:O	1:B:48:ALA:HA	2.18	0.43
1:B:177:TYR:CE1	1:B:181:TYR:CD2	3.06	0.43
2:C:244:THR:HG23	2:C:245:LEU:H	1.83	0.43
2:D:273:PHE:HE1	2:D:312:MET:HG2	1.84	0.43
1:F:42:ARG:O	1:F:45:GLN:CB	2.66	0.43
1:A:76:ILE:HD12	1:A:86:SER:OG	2.19	0.43
1:A:155:ILE:CG1	1:A:203:ILE:HG23	2.49	0.43
1:F:100:ALA:HB2	1:F:157:LEU:HD21	2.01	0.43
1:A:139:LEU:HB2	1:A:140:PRO:HD3	2.00	0.43
2:C:234:THR:HG22	2:C:236:LEU:N	2.34	0.43
1:F:158:VAL:HG12	1:F:159:GLY:N	2.33	0.43
2:G:100:PHE:CD1	2:G:100:PHE:C	2.92	0.43
2:H:106:PRO:HG2	2:H:153:ARG:HG2	2.01	0.43
2:C:124:LEU:HD11	2:C:156:ALA:HA	2.01	0.43
1:E:85:THR:OG1	1:E:87:ILE:HG13	2.19	0.43
1:E:177:TYR:CE1	1:E:181:TYR:HD2	2.37	0.43
2:G:260:GLU:HA	2:G:261:PRO:HD3	1.84	0.43
2:H:33:ILE:HD11	2:H:187:ASN:HB2	2.01	0.43
1:B:167:VAL:O	1:B:167:VAL:HG23	2.19	0.43
1:A:23:SER:CB	1:A:157:LEU:HD13	2.49	0.42
1:F:46:ILE:CD1	1:F:133:ILE:HD13	2.49	0.42
2:D:107:LEU:HB3	2:D:117:VAL:HG12	2.01	0.42
1:E:77:PRO:O	1:E:81:VAL:HG13	2.19	0.42
1:E:178:GLN:HA	1:E:182:ILE:HD12	2.00	0.42
1:F:133:ILE:HG22	1:F:138:LEU:HG	1.99	0.42
2:G:55:GLU:OE1	2:G:55:GLU:HA	2.20	0.42
2:D:329:TRP:O	2:D:333:HIS:CD2	2.72	0.42
2:H:83:GLN:HA	2:H:159:PRO:HA	2.01	0.42



	Interatomic Clash					
Atom-1	Atom-2	distance (Å)	overlap (Å)			
1:A:23:SER:HA	1:A:97:THR:CG2	2.46	0.42			
1:A:92:ALA:O	1:A:95:PRO:CG	2.67	0.42			
2:C:124:LEU:HD13	2:C:152:ALA:O	2.19	0.42			
1:F:13:VAL:HG12	1:F:172:LEU:HD11	2.01	0.42			
1:F:155:ILE:HG13	1:F:200:VAL:HG22	2.01	0.42			
2:G:2:ILE:HG23	2:G:28:VAL:HB	2.01	0.42			
1:A:122:ALA:O	1:A:125:ALA:HB3	2.20	0.42			
1:A:137:VAL:HG12	1:A:138:LEU:HD12	2.01	0.42			
2:C:110:ASP:OD1	2:C:110:ASP:O	2.37	0.42			
2:C:296:ILE:O	2:C:296:ILE:HD12	2.19	0.42			
2:D:10:VAL:CG1	2:D:17:THR:HG23	2.50	0.42			
2:D:186:ILE:HG21	2:D:192:LEU:HD23	2.02	0.42			
1:F:76:ILE:N	1:F:77:PRO:HD2	2.34	0.42			
1:F:83:VAL:HG21	1:F:91:ALA:HB2	2.01	0.42			
1:F:176:GLY:O	1:F:189:MET:HE1	2.19	0.42			
2:C:128:VAL:HB	2:C:148:ARG:HB3	2.01	0.42			
2:D:63:LEU:O	2:D:63:LEU:HD12	2.20	0.42			
2:D:98:THR:HG22	2:D:137:TYR:CE1	2.55	0.42			
1:F:89:LEU:N	1:F:89:LEU:CD1	2.82	0.42			
2:G:301:MET:SD	2:G:310:GLY:HA3	2.59	0.42			
2:H:141:LEU:HB3	2:H:145:GLN:HB2	2.02	0.42			
2:H:269:LEU:N	2:H:269:LEU:HD12	2.34	0.42			
2:H:319:THR:HG23	2:H:322:ASP:CB	2.48	0.42			
1:B:27:GLY:O	1:B:31:GLY:N	2.42	0.42			
1:E:30:ILE:HD11	1:E:101:ALA:HB2	2.00	0.42			
2:G:164:CYS:HB2	2:G:196:LEU:HB2	2.01	0.42			
2:H:53:LEU:HD23	2:H:55:GLU:O	2.19	0.42			
2:H:267:PRO:HB2	2:H:269:LEU:CD1	2.49	0.42			
1:A:128:ALA:HB2	2:C:109:LEU:CD1	2.47	0.42			
1:A:157:LEU:HD23	1:A:157:LEU:HA	1.57	0.42			
1:A:163:MET:HG2	1:B:163:MET:CE	2.48	0.42			
1:B:9:LEU:HD11	1:B:191:THR:CG2	2.49	0.42			
1:B:193:LEU:O	1:B:197:VAL:HG23	2.19	0.42			
2:D:107:LEU:O	2:D:110:ASP:O	2.37	0.42			
2:D:172:ASP:HB3	2:D:175:THR:H	1.84	0.42			
1:E:6:MET:HE2	1:E:6:MET:HB2	1.93	0.42			
1:E:22:VAL:HG12	1:E:22:VAL:O	2.19	0.42			
1:E:32:LEU:HD12	1:E:108:VAL:HG21	2.02	0.42			
2:G:295:ASN:HB3	2:G:315:GLU:HG3	2.01	0.42			
2:H:247:LEU:HD13	2:H:298:SER:HB3	2.02	0.42			
2:C:2:ILE:HG21	2:C:161:VAL:HG21	2.02	0.42			



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:105:LEU:O	2:C:109:LEU:HG	2.20	0.42
2:D:37:ILE:O	2:D:214:ILE:HG22	2.19	0.42
1:E:75:MET:O	1:E:79:THR:N	2.36	0.42
1:F:68:PHE:CZ	1:F:96:LEU:HD23	2.55	0.42
1:F:180:GLY:HA3	1:F:189:MET:CE	2.49	0.42
2:C:79:LYS:HA	2:C:79:LYS:HD3	1.86	0.42
1:E:133:ILE:O	1:E:137:VAL:HG22	2.20	0.42
1:F:11:ARG:O	1:F:15:GLU:HG3	2.20	0.42
1:F:70:ILE:HD12	1:F:70:ILE:H	1.85	0.42
1:A:5:MET:CE	1:A:8:LEU:HD23	2.50	0.41
1:B:133:ILE:HG22	1:B:138:LEU:CD1	2.50	0.41
2:C:164:CYS:O	2:C:197:ILE:HG13	2.20	0.41
1:E:28:PHE:CD1	1:E:104:ILE:CD1	2.98	0.41
1:E:41:THR:OG1	1:E:52:LEU:HD11	2.19	0.41
1:E:163:MET:SD	1:F:69:ILE:CG2	3.03	0.41
1:F:40:VAL:O	1:F:46:ILE:O	2.38	0.41
2:H:91:PHE:CD2	2:H:91:PHE:N	2.88	0.41
2:H:119:ARG:HA	2:H:122:THR:OG1	2.19	0.41
1:B:2:SER:HB2	1:B:5:MET:H	1.84	0.41
1:B:39:TYR:HD1	1:B:113:LEU:HD23	1.82	0.41
2:D:121:VAL:HG12	2:D:125:LEU:HD12	2.03	0.41
1:F:62:ILE:O	1:F:65:SER:HB3	2.19	0.41
2:H:45:SER:CB	3:H:2502:ADP:O2A	2.66	0.41
1:B:83:VAL:HG12	1:B:85:THR:H	1.85	0.41
1:B:101:ALA:O	1:B:104:ILE:HB	2.21	0.41
2:C:270:ARG:HG2	2:C:340:LEU:HD21	2.03	0.41
2:C:321:GLN:HG3	2:C:322:ASP:N	2.35	0.41
1:E:69:ILE:HG23	1:E:70:ILE:CD1	2.43	0.41
2:H:94:LEU:N	2:H:94:LEU:HD23	2.35	0.41
1:B:143:LEU:HD23	1:B:214:VAL:CG1	2.50	0.41
2:C:8:THR:HG23	2:C:21:LEU:O	2.20	0.41
2:D:34:TYR:CE1	2:D:35:GLY:O	2.73	0.41
2:H:54:LEU:HD23	2:H:54:LEU:HA	1.61	0.41
1:A:41:THR:HA	1:A:47:ILE:O	2.20	0.41
1:A:82:ILE:HG23	1:A:83:VAL:HG23	2.01	0.41
2:C:116:GLU:O	2:C:120:ARG:N	2.42	0.41
1:E:23:SER:CB	1:E:157:LEU:HD13	2.44	0.41
1:E:32:LEU:CB	1:E:33:PRO:HD3	2.43	0.41
2:H:162:LEU:HB2	2:H:192:LEU:HD11	2.02	0.41
1:B:119:LEU:O	1:B:123:SER:CB	2.56	0.41
2:C:182:LEU:HD13	2:C:186:ILE:CD1	2.50	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:D:9:LYS:N	2:D:21:LEU:HD12	2.36	0.41
1:F:22:VAL:O	1:F:26:PHE:HD2	2.04	0.41
1:A:72:LEU:HD22	1:A:167:VAL:HG21	2.03	0.41
2:C:103:VAL:HG21	2:C:125:LEU:CD1	2.47	0.41
1:E:23:SER:OG	1:E:96:LEU:CB	2.69	0.41
1:E:137:VAL:HG23	1:E:138:LEU:N	2.35	0.41
1:E:176:GLY:O	1:E:180:GLY:HA3	2.21	0.41
1:F:36:VAL:O	1:F:39:TYR:N	2.54	0.41
2:G:172:ASP:OD1	2:G:175:THR:HG22	2.21	0.41
2:G:257:LEU:HD13	2:G:268:MET:CE	2.49	0.41
1:B:76:ILE:HB	1:B:77:PRO:HD3	2.03	0.41
2:C:53:LEU:CD2	2:C:57:PRO:HD3	2.51	0.41
2:D:112:THR:CG2	2:D:116:GLU:HB3	2.49	0.41
1:F:46:ILE:HD13	1:F:133:ILE:HD13	2.02	0.41
2:H:33:ILE:O	2:H:209:ASP:N	2.53	0.41
2:H:272:GLU:HA	2:H:311:ILE:HG22	2.02	0.41
1:A:163:MET:HG2	1:B:163:MET:HG2	2.02	0.41
1:B:68:PHE:CZ	1:B:96:LEU:HD23	2.56	0.41
1:B:112:LEU:HD22	1:B:138:LEU:HD22	2.03	0.41
2:C:53:LEU:HD23	2:C:53:LEU:HA	1.88	0.41
2:C:292:VAL:HG11	2:C:316:MET:HE3	2.01	0.41
1:E:193:LEU:HD11	1:F:66:ILE:HD13	2.02	0.41
1:F:83:VAL:HG21	1:F:91:ALA:CB	2.50	0.41
2:G:211:VAL:O	2:G:211:VAL:HG13	2.20	0.41
2:G:247:LEU:HD11	2:G:300:GLN:HB2	2.03	0.41
2:H:0:HIS:HA	2:H:28:VAL:O	2.21	0.41
2:C:201:MET:O	2:C:204:VAL:HB	2.21	0.41
2:D:172:ASP:OD1	2:D:173:PRO:HD2	2.20	0.41
1:F:129:THR:O	1:F:132:GLN:N	2.53	0.41
2:G:181:GLU:O	2:G:185:ASP:N	2.40	0.41
2:H:195:LEU:HD12	2:H:196:LEU:N	2.35	0.41
2:H:228:VAL:HG12	2:H:241:ILE:HD11	2.01	0.41
1:A:32:LEU:CB	1:A:33:PRO:HD3	2.41	0.40
1:A:137:VAL:C	1:A:140:PRO:HD2	2.41	0.40
1:B:42:ARG:CD	1:B:113:LEU:HD21	2.51	0.40
2:C:3:LYS:HG3	2:C:27:HIS:CD2	2.56	0.40
1:E:6:MET:C	1:E:8:LEU:N	2.74	0.40
1:F:122:ALA:O	1:F:126:MET:HG3	2.21	0.40
1:F:180:GLY:HA3	1:F:189:MET:HE1	2.02	0.40
1:A:23:SER:CA	1:A:97:THR:HG22	2.47	0.40
2:D:182:LEU:O	2:D:182:LEU:HD12	2.21	0.40



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:73:VAL:O	1:E:74:TRP:C	2.59	0.40
2:H:33:ILE:HG12	2:H:194:ILE:HB	2.04	0.40
2:H:37:ILE:CD1	2:H:201:MET:HA	2.51	0.40
2:C:319:THR:HG22	2:C:320:GLN:N	2.35	0.40
2:D:120:ARG:HH12	2:D:158:ASN:HD22	1.70	0.40
1:F:2:SER:CB	1:F:4:PRO:HD2	2.44	0.40
2:H:262:PHE:CD1	2:H:263:THR:O	2.73	0.40
1:A:92:ALA:O	1:A:95:PRO:CD	2.68	0.40
2:D:270:ARG:HH22	2:D:272:GLU:CD	2.25	0.40
1:E:69:ILE:HG23	1:E:70:ILE:H	1.87	0.40
2:H:51:VAL:HG11	2:H:163:LEU:HD21	2.03	0.40
2:H:128:VAL:O	2:H:148:ARG:NE	2.45	0.40
2:C:216:ASN:OD1	2:C:216:ASN:N	2.54	0.40
1:F:20:THR:HG22	1:F:154:LEU:CD2	2.52	0.40
2:G:216:ASN:O	2:G:218:GLU:HG2	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	214/217~(99%)	206 (96%)	8 (4%)	0	100	100
1	В	214/217~(99%)	201 (94%)	12 (6%)	1 (0%)	29	61
1	Е	214/217~(99%)	202 (94%)	12 (6%)	0	100	100
1	F	214/217~(99%)	202 (94%)	12 (6%)	0	100	100
2	С	342/366~(93%)	330 (96%)	12 (4%)	0	100	100
2	D	341/366~(93%)	334 (98%)	7 (2%)	0	100	100
2	G	341/366~(93%)	330 (97%)	11 (3%)	0	100	100
2	Н	342/366~(93%)	328 (96%)	14 (4%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2222/2332~(95%)	2133 (96%)	88 (4%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	46	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	171/172~(99%)	171 (100%)	0	100	100
1	В	171/172~(99%)	169 (99%)	2 (1%)	71	91
1	Ε	171/172~(99%)	169 (99%)	2(1%)	71	91
1	F	171/172~(99%)	169 (99%)	2 (1%)	71	91
2	С	299/319~(94%)	292 (98%)	7 (2%)	50	80
2	D	298/319~(93%)	290~(97%)	8 (3%)	44	77
2	G	298/319~(93%)	293~(98%)	5 (2%)	60	86
2	Н	299/319~(94%)	295~(99%)	4 (1%)	69	90
All	All	1878/1964~(96%)	1848 (98%)	30 (2%)	62	86

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	2	SER
1	В	154	LEU
2	С	23	ASN
2	С	26	LEU
2	С	49	ARG
2	С	102	ASN
2	С	223	ASP
2	С	244	THR
2	С	286	THR



Mol	Chain	Res	Type
2	D	7	ILE
2	D	72	LEU
2	D	91	PHE
2	D	102	ASN
2	D	134	HIS
2	D	182	LEU
2	D	196	LEU
2	D	219	LEU
1	E	28	PHE
1	Е	69	ILE
1	F	155	ILE
1	F	158	VAL
2	G	107	LEU
2	G	192	LEU
2	G	196	LEU
2	G	202	ASP
2	G	300	GLN
2	Н	47	LEU
2	Н	195	LEU
2	Н	196	LEU
2	Н	245	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	61	ASN
1	А	132	GLN
1	В	61	ASN
2	С	27	HIS
2	С	166	GLN
2	С	199	HIS
2	D	111	ASN
1	F	132	GLN
1	F	190	ASN
2	G	145	GLN
2	G	333	HIS
2	Н	27	HIS
2	Н	52	ASN
2	Н	134	HIS
2	Н	166	GLN



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)

4 ligands are modelled in this entry.

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

Mal	I Trupe Chain Beg		Tink	Bond lengths			Bond angles										
IVIOI	туре	Unam	nes	nes	nes	nes	nes	nes	res	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	Н	2502	-	24,29,29	1.33	3 (12%)	29,45,45	1.48	6 (20%)							
3	ADP	D	2501	-	24,29,29	1.04	2 (8%)	29,45,45	1.43	4 (13%)							
3	ADP	С	2500	-	24,29,29	1.10	1 (4%)	29,45,45	1.35	5 (17%)							
3	ADP	G	2503	-	24,29,29	1.04	2 (8%)	29,45,45	1.32	4 (13%)							

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
3	ADP	Н	2502	-	-	2/12/32/32	0/3/3/3
3	ADP	D	2501	-	-	2/12/32/32	0/3/3/3
3	ADP	С	2500	-	-	5/12/32/32	0/3/3/3
3	ADP	G	2503	-	-	3/12/32/32	0/3/3/3



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
3	Н	2502	ADP	C5-C4	3.42	1.50	1.40
3	С	2500	ADP	C5-C4	2.97	1.48	1.40
3	Н	2502	ADP	C2-N3	2.97	1.36	1.32
3	D	2501	ADP	C5-C4	2.72	1.48	1.40
3	G	2503	ADP	C5-C4	2.63	1.47	1.40
3	Н	2502	ADP	O4'-C1'	2.54	1.44	1.41
3	G	2503	ADP	O4'-C1'	2.14	1.44	1.41
3	D	2501	ADP	O4'-C1'	2.11	1.44	1.41

All (8) bond length outliers are listed below:

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	Н	2502	ADP	N3-C2-N1	-3.50	123.22	128.68
3	D	2501	ADP	C3'-C2'-C1'	3.47	106.20	100.98
3	Н	2502	ADP	C2'-C3'-C4'	3.42	109.28	102.64
3	D	2501	ADP	C4-C5-N7	-3.18	106.09	109.40
3	G	2503	ADP	N3-C2-N1	-3.07	123.88	128.68
3	С	2500	ADP	N3-C2-N1	-2.98	124.03	128.68
3	D	2501	ADP	N3-C2-N1	-2.89	124.17	128.68
3	G	2503	ADP	C3'-C2'-C1'	2.88	105.32	100.98
3	С	2500	ADP	C4-C5-N7	-2.68	106.60	109.40
3	С	2500	ADP	PA-O3A-PB	-2.58	123.96	132.83
3	С	2500	ADP	C3'-C2'-C1'	2.49	104.72	100.98
3	G	2503	ADP	C4-C5-N7	-2.47	106.83	109.40
3	Н	2502	ADP	O2'-C2'-C3'	-2.40	104.06	111.82
3	D	2501	ADP	PA-O3A-PB	-2.35	124.77	132.83
3	С	2500	ADP	C2-N1-C6	2.29	122.67	118.75
3	Н	2502	ADP	N6-C6-N1	2.22	123.17	118.57
3	Н	2502	ADP	C2-N1-C6	2.03	122.23	118.75
3	G	2503	ADP	C2'-C3'-C4'	2.03	106.58	102.64
3	Н	2502	ADP	O3'-C3'-C2'	-2.01	105.31	111.82

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	С	2500	ADP	PA-O3A-PB-O2B
3	С	2500	ADP	C5'-O5'-PA-O2A
3	С	2500	ADP	C5'-O5'-PA-O3A
3	G	2503	ADP	PA-O3A-PB-O3B
3	G	2503	ADP	C5'-O5'-PA-O1A



	5	1	1 5	
Mol	Chain	Res	Type	Atoms
3	С	2500	ADP	O4'-C4'-C5'-O5'
3	D	2501	ADP	O4'-C4'-C5'-O5'
3	G	2503	ADP	C5'-O5'-PA-O3A
3	Н	2502	ADP	PB-O3A-PA-O2A
3	Н	2502	ADP	PB-O3A-PA-O1A
3	D	2501	ADP	PB-O3A-PA-O2A
3	С	2500	ADP	PA-O3A-PB-O3B

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There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Н	2502	ADP	4	0
3	D	2501	ADP	1	0
3	С	2500	ADP	2	0
3	G	2503	ADP	3	0

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













5.7 Other polymers (i)

There are no such residues in this entry.



5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 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	$\langle RSRZ \rangle$	#RSRZ>2		$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	А	216/217~(99%)	-0.21	3 (1%) 75	75	18, 58, 105, 130	0
1	В	216/217~(99%)	-0.13	8 (3%) 41	37	17, 55, 103, 131	0
1	Ε	216/217~(99%)	0.07	9 (4%) 36	32	31, 65, 100, 137	0
1	F	216/217~(99%)	-0.02	6 (2%) 53	49	30, 63, 117, 150	0
2	С	344/366~(93%)	0.14	25 (7%) 15	11	18, 65, 117, 161	0
2	D	343/366~(93%)	0.03	19 (5%) 25	21	22, 68, 115, 159	0
2	G	343/366~(93%)	-0.01	15 (4%) 34	30	23, 61, 112, 140	0
2	Н	344/366~(93%)	0.01	12 (3%) 44	38	21, 66, 122, 162	0
All	All	2238/2332 (95%)	0.00	97 (4%) 35	31	17, 63, 116, 162	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	17	THR	8.3
2	С	13	GLN	8.3
2	D	12	HIS	6.7
2	D	13	GLN	6.6
2	Н	251	GLU	6.5
2	С	14	GLY	6.1
2	D	115	ASP	5.3
2	С	16	ARG	5.2
1	Ε	51	LYS	4.9
2	С	15	THR	4.7
1	F	84	GLY	4.6
2	С	18	ILE	4.5
2	D	16	ARG	4.2
2	G	114	LYS	3.9
1	F	184	TYR	3.8
2	G	15	THR	3.8



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Mol	Chain	Res	Type	RSRZ	
2	D	114	LYS	3.7	
2	D	15	THR	3.7	
2	С	17	THR	3.6	
2	Н	252	ASP	3.5	
2	С	115	ASP	3.5	
1	Е	84	GLY	3.5	
1	F	192	VAL	3.5	
2	G	164	CYS	3.4	
2	G	163	LEU	3.3	
2	G	66	GLY	3.3	
2	Н	132	ASP	3.2	
2	D	14	GLY	3.2	
2	D	216	ASN	3.2	
1	Е	47	ILE	3.2	
2	G	85	GLY	3.2	
2	G	115	ASP	3.1	
1	Е	49	ASN	3.1	
2	С	12	HIS	3.1	
1	В	4	PRO	3.0	
1	Е	41	THR	3.0	
1	В	82	ILE	3.0	
2	G	16	ARG	3.0	
1	Е	80	ARG	2.9	
1	В	7	TRP	2.8	
2	С	289	ARG	2.8	
2	D	113	PRO	2.8	
2	G	71	THR	2.8	
1	А	82	ILE	2.7	
2	С	264	ASP	2.7	
2	Н	246	HIS	2.7	
1	Ε	52	LEU	2.7	
2	С	154	ALA	2.7	
2	Н	248	ASP	2.7	
2	G	86	MET	2.6	
2	С	85	GLY	2.6	
1	В	81	VAL	2.6	
2	D	164	CYS	2.6	
2	С	321	GLN	2.5	
2	С	263	THR	2.5	
2	D	71	THR	2.5	
2	С	118	LYS	2.5	
2	G	87	ILE	2.5	



Mol	Chain	Res	Type	RSRZ	
1	А	51	LYS	2.5	
2	Н	343	VAL	2.5	
2	С	251	GLU	2.4	
2	Н	276	GLN	2.4	
2	С	113	PRO	2.4	
1	В	84	GLY	2.4	
2	G	160	LYS	2.4	
1	F	85	THR	2.4	
1	F	188	VAL	2.4	
2	D	48	ILE	2.4	
2	Н	249	ILE	2.4	
2	G	111	ASN	2.4	
1	Е	40	VAL	2.3	
2	Н	254	GLN	2.3	
1	F	185	ASN	2.3	
2	С	119	ARG	2.3	
2	С	329	TRP	2.3	
1	В	209	ARG	2.3	
2	С	256	ARG	2.3	
1	В	1	MET	2.2	
2	С	123	GLU	2.2	
2	D	321	GLN	2.2	
2	D	220	ILE	2.2	
1	В	183	GLY	2.2	
2	Н	111	ASN	2.2	
1	Е	209	ARG	2.2	
2	С	116	GLU	2.2	
2	С	248	ASP	2.1	
2	С	114	LYS	2.1	
2	С	59	GLU	2.1	
2	D	19	GLN	2.1	
2	D	116	GLU	2.1	
2	D	235	PRO	2.1	
2	Н	150	ALA	2.1	
2	G	321	GLN	2.1	
2	Н	154	ALA	2.1	
2	G	295	ASN	2.0	
2	D	18	ILE	2.0	
1	А	77	PRO	2.0	

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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	B-factors(Å ²)	Q<0.9
3	ADP	С	2500	27/27	0.86	0.22	69,105,120,128	0
3	ADP	G	2503	27/27	0.87	0.28	77,120,138,143	0
3	ADP	D	2501	27/27	0.88	0.20	84,124,136,139	0
3	ADP	Н	2502	27/27	0.95	0.13	38,56,67,77	0

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)

There are no such residues in this entry.

