

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

#### Oct 25, 2023 – 02:55 PM EDT

PDB ID	:	2Z1B
Title	:	Crystal Structure of 5-aminolevulinic acid dehydratase (ALAD) from Mus
		musculs
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		moto, C.; Terada, T.; Shirozu, M.; Yokoyama, S.; RIKEN Structural Ge-
		nomics/Proteomics Initiative (RSGI)
Deposited on	:	2007-05-08
Resolution	:	3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

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

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

MolProbity Xtriage (Phenix) EDS Percentile statistics Refmac CCP4 Ideal geometry (protens)	::	4.02b-467 1.13 2.36 20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove) Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${igsimular resolution} \ (\# { m Entries, resolution range}({ m \AA}))$	
R <sub>free</sub>	130704	1149 (3.34-3.26)	
Clashscore	141614	1205 (3.34-3.26)	
Ramachandran outliers	138981	1183 (3.34-3.26)	
Sidechain outliers	138945	1182 (3.34-3.26)	
RSRZ outliers	127900	1115 (3.34-3.26)	

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 of chain	
1	А	330	% <b>2</b> 9%	49%	10% 12%
1	В	330	27%	56%	14% •
1	С	330	20%	54%	13% • 13%
1	D	330	3% 22%	55%	12% • 10%



## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9223 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	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	200	Total	С	Ν	0	$\mathbf{S}$	0	0	0
	A	290	2230	1428	387	400	15	0	0	0
1	D	200	Total	С	Ν	0	S	0	0	0
	I D	520	2445	1557	426	445	17	0	0	U
1	1 0	000	Total	С	Ν	0	S	0	0	0
	200	2217	1420	385	398	14	0		0	
1 D	206	Total	С	Ν	0	S	0	0	0	
	296	2274	1454	397	408	15	0	0	0	

• Molecule 1 is a protein called Delta-aminolevulinic acid dehydratase.

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	12	Total O 12 12	0	0
2	В	20	TotalO2020	0	0
2	С	15	Total O 15 15	0	0
2	D	10	Total         O           10         10	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: Delta-aminolevulinic acid dehydratase



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• Molecule 1: Delta-aminolevulinic acid dehydratase









## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants	240.92Å 240.92Å 103.94Å	Deneiten
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
$\mathbf{B}_{\mathrm{ascolution}}\left(\overset{\mathrm{A}}{\mathbf{\lambda}}\right)$	43.40 – 3.30	Depositor
Resolution (A)	47.72 - 3.29	EDS
% Data completeness	88.7 (43.40-3.30)	Depositor
(in resolution range)	95.4 (47.72-3.29)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$< I/\sigma(I) > 1$	$3.79 (at 3.33 \text{\AA})$	Xtriage
Refinement program	CNS 1.1	Depositor
B B a	0.278 , $0.353$	Depositor
It, Itfree	0.266 , $0.335$	DCC
$R_{free}$ test set	2400 reflections $(8.75%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	98.3	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31,90.0	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	9223	wwPDB-VP
Average B, all atoms $(Å^2)$	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.

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



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

## 5 Model quality (i)

## 5.1 Standard geometry (i)

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	
	Ullaili	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.33	0/2278	0.57	0/3091
1	В	0.34	0/2500	0.61	0/3394
1	С	0.31	0/2264	0.57	0/3071
1	D	0.32	0/2323	0.56	0/3151
All	All	0.32	0/9365	0.58	0/12707

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	2230	0	2252	229	0
1	В	2445	0	2452	303	0
1	С	2217	0	2240	352	0
1	D	2274	0	2297	324	0
2	А	12	0	0	3	0
2	В	20	0	0	5	0
2	С	15	0	0	4	0
2	D	10	0	0	5	0
All	All	9223	0	9241	1127	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 61.



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A 1 - 1		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:227:PRO:HG2	1:A:230:ALA:HB2	1.35	1.09
1:A:5:SER:HB2	1:B:240:ARG:HG3	1.39	1.03
1:A:242:ILE:HD13	1:A:271:LEU:HD11	1.40	1.03
1:C:227:PRO:HG2	1:C:230:ALA:HB2	1.40	1.03
1:C:255:LEU:HD11	1:D:256:PRO:HA	1.40	1.02
1:C:84:ARG:HH21	1:C:84:ARG:HB2	1.24	1.00
1:A:255:LEU:HD11	1:B:256:PRO:HA	1.42	0.99
1:C:262:ARG:NH2	1:C:310:ALA:HA	1.81	0.96
1:D:227:PRO:HG2	1:D:230:ALA:HB2	1.45	0.94
1:C:233:LEU:HD12	1:D:20:GLN:HG2	1.51	0.93
1:C:201:ALA:HB2	1:C:225:GLN:HB3	1.50	0.92
1:D:77:LEU:HA	1:D:118:ALA:HB3	1.50	0.92
1:C:32:ILE:HD11	1:C:314:ILE:HG23	1.54	0.89
1:C:149:ARG:HB3	1:C:149:ARG:HH11	1.33	0.89
1:A:99:SER:HB2	1:A:100:PRO:HD2	1.54	0.87
1:D:145:GLU:HA	1:D:148:GLN:HE21	1.38	0.87
1:B:45:GLN:HB2	1:B:55:ARG:HB2	1.57	0.87
1:A:224:TYR:HA	1:B:11:TYR:HE2	1.38	0.86
1:B:226:LEU:HD12	1:B:226:LEU:H	1.40	0.86
1:B:273:LEU:H	1:B:313:ASP:HB2	1.39	0.86
1:D:39:ASP:O	1:D:41:PRO:HD3	1.75	0.86
1:B:35:ILE:HD11	1:B:78:ILE:HG13	1.57	0.85
1:B:116:LEU:HD23	1:C:15:LEU:HB3	1.59	0.85
1:B:39:ASP:O	1:B:41:PRO:HD3	1.76	0.84
1:D:199:LYS:HD2	1:D:205:TYR:OH	1.78	0.84
1:C:47:ILE:HG22	1:C:50:LEU:H	1.40	0.83
1:A:84:ARG:HH21	1:A:84:ARG:HB2	1.40	0.83
1:A:260:MET:O	1:A:264:VAL:HG22	1.79	0.82
1:C:253:PRO:HD2	1:C:257:TYR:CE2	2.14	0.82
1:B:47:ILE:HD11	1:B:55:ARG:HG3	1.59	0.82
1:C:265:LYS:HE3	1:C:265:LYS:HA	1.62	0.82
1:C:259:ASP:HA	1:D:259:ASP:HA	1.62	0.81
1:B:27:SER:H	1:B:30:ASN:ND2	1.79	0.81
1:D:207:PRO:HB2	1:D:279:SER:HB2	1.59	0.81
1:A:123:LEU:HD21	1:A:150:LEU:HD13	1.60	0.81
1:D:306:ALA:HA	1:D:309:ARG:NH1	1.96	0.81
1:D:66:ARG:O	1:D:70:GLU:HG2	1.82	0.80
1:C:168:SER:HB2	1:C:199:LYS:HE3	1.62	0.80
1:C:84:ARG:HB2	1:C:84:ARG:NH2	1.97	0.80
1:D:221:ARG:HB2	1:D:222:ARG:HH11	1.46	0.80

All (1127) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:240:ARG:HH21	1:B:7:LEU:HD12	1.45	0.79
1:D:216:PRO:HD3	1:D:221:ARG:HH21	1.46	0.79
1:C:265:LYS:HE2	1:C:269:PRO:HA	1.65	0.79
1:B:27:SER:H	1:B:30:ASN:HD21	1.29	0.79
1:D:117:VAL:HG11	1:D:162:CYS:HA	1.65	0.79
1:A:32:ILE:HD13	1:A:314:ILE:HG22	1.65	0.79
1:C:33:TYR:HB3	1:C:76:VAL:HG12	1.64	0.79
1:D:279:SER:HA	1:D:318:TYR:HE2	1.48	0.78
1:C:11:TYR:O	1:C:13:HIS:N	2.16	0.78
1:B:39:ASP:OD1	1:B:82:PRO:HA	1.84	0.78
1:C:297:ARG:HA	2:C:332:HOH:O	1.83	0.78
1:B:8:HIS:HB3	1:C:189:ASN:HB2	1.66	0.77
1:D:170:MET:HA	1:D:174:ARG:NH1	1.98	0.77
1:A:102:ILE:O	1:A:105:VAL:HG12	1.84	0.77
1:C:149:ARG:HB3	1:C:149:ARG:NH1	1.98	0.77
1:B:105:VAL:HG13	1:B:106:ARG:H	1.49	0.77
1:C:106:ARG:NH1	1:C:160:ALA:HA	2.00	0.77
1:D:110:LYS:HE2	1:D:110:LYS:HA	1.67	0.77
1:B:250:MET:HA	1:B:274:ALA:O	1.86	0.76
1:A:95:ASP:HA	1:A:99:SER:HB3	1.67	0.76
1:A:262:ARG:O	1:A:265:LYS:HB3	1.85	0.76
1:C:167:PRO:HB2	1:C:174:ARG:HD2	1.67	0.76
1:C:260:MET:HE3	1:D:309:ARG:HE	1.51	0.76
1:B:207:PRO:HB2	1:B:279:SER:HB2	1.68	0.76
1:A:323:LEU:O	1:A:327:LEU:HD13	1.85	0.75
1:D:277:GLN:NE2	1:D:303:THR:HG21	2.01	0.75
1:C:29:SER:HA	1:C:74:ARG:HG3	1.69	0.75
1:B:320:ALA:HB3	1:B:321:PRO:HD3	1.69	0.74
1:C:77:LEU:HD23	1:C:118:ALA:O	1.87	0.74
1:D:77:LEU:HA	1:D:118:ALA:CB	2.16	0.74
1:A:5:SER:HB2	1:B:240:ARG:CG	2.15	0.74
1:C:205:TYR:CE1	1:C:252:LYS:HE2	2.22	0.74
1:A:227:PRO:CG	1:A:230:ALA:HB2	2.17	0.73
1:C:73:LEU:H	1:C:324:LEU:HD13	1.53	0.73
1:D:154:ALA:HB1	1:D:165:VAL:HG11	1.69	0.73
1:B:101:THR:HG23	1:B:102:ILE:H	1.54	0.73
1:D:117:VAL:HG12	1:D:119:CYS:SG	2.28	0.73
1:B:151:ALA:HA	1:B:178:ILE:HD13	1.70	0.73
1:C:259:ASP:HB2	1:D:262:ARG:HB2	1.71	0.73
1:A:74:ARG:HB3	1:A:74:ARG:NH1	2.03	0.73
1:C:201:ALA:HB2	1:C:225:GLN:CB	2.19	0.73



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:239:ALA:O	1:A:243:GLN:HG3	1.88	0.73
1:C:258:LEU:HB3	1:D:258:LEU:HB3	1.70	0.73
1:D:157:TYR:HB3	1:D:162:CYS:HB2	1.70	0.73
1:D:33:TYR:HB3	1:D:76:VAL:HG12	1.70	0.72
1:B:179:LYS:O	1:B:183:LEU:HD23	1.90	0.72
1:D:205:TYR:CE1	1:D:252:LYS:HE2	2.23	0.72
1:A:146:SER:HB2	1:A:147:ARG:NH2	2.04	0.72
1:B:154:ALA:HB2	1:B:178:ILE:HD12	1.71	0.72
1:C:320:ALA:HB3	1:C:321:PRO:HD3	1.71	0.72
1:D:75:CYS:HB2	1:D:116:LEU:HB3	1.72	0.71
1:D:255:LEU:HD23	1:D:303:THR:HG23	1.72	0.71
1:D:275:VAL:HG12	1:D:315:ILE:HG12	1.72	0.71
1:C:275:VAL:HG12	1:C:315:ILE:HA	1.72	0.71
1:D:250:MET:HG2	1:D:251:VAL:H	1.55	0.71
1:C:193:VAL:H	1:C:247:ASP:HB2	1.55	0.71
1:A:76:VAL:HG13	1:A:115:LEU:HD11	1.72	0.71
1:C:32:ILE:HD13	1:C:316:ILE:HG12	1.72	0.71
1:C:99:SER:HB2	1:C:100:PRO:HD2	1.73	0.71
1:A:46:PRO:C	1:A:47:ILE:HD12	2.11	0.71
1:C:306:ALA:HA	1:C:309:ARG:CZ	2.20	0.71
1:B:53:VAL:HG12	1:B:54:ALA:N	2.07	0.70
1:B:233:LEU:HA	1:B:236:ARG:HB2	1.74	0.70
1:A:199:LYS:HE2	1:A:252:LYS:HZ3	1.57	0.70
1:A:253:PRO:HD2	1:A:257:TYR:CE2	2.27	0.70
1:A:166:ALA:HB2	1:A:194:MET:HB3	1.72	0.70
1:C:227:PRO:HG2	1:C:230:ALA:CB	2.21	0.70
1:B:40:VAL:HG12	1:B:43:ASP:HB3	1.74	0.69
1:B:267:LYS:HE2	1:B:268:HIS:HE1	1.57	0.69
1:D:76:VAL:O	1:D:118:ALA:HB3	1.92	0.69
1:B:182:LEU:HD13	1:B:191:VAL:HB	1.74	0.69
1:C:255:LEU:HD23	1:D:255:LEU:HD12	1.74	0.69
1:C:284:MET:HB3	1:D:284:MET:HB3	1.74	0.69
1:D:155:LEU:HD23	1:D:155:LEU:O	1.92	0.69
1:A:233:LEU:HD23	1:A:233:LEU:O	1.93	0.69
1:A:289:ALA:C	1:A:291:ALA:H	1.96	0.69
1:B:17:ARG:O	1:B:21:THR:HG22	1.92	0.69
1:C:32:ILE:N	1:C:32:ILE:HD12	2.08	0.69
1:C:105:VAL:HG13	1:C:106:ARG:N	2.08	0.69
1:D:222:ARG:N	1:D:222:ARG:HD2	2.08	0.69
1:B:231:ARG:HG3	1:B:260:MET:HE1	1.75	0.69
1:D:279:SER:HA	1:D:318:TYR:CE2	2.28	0.69



	louo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:233:LEU:HD12	1:B:20:GLN:CG	2.22	0.68
1:C:260:MET:HE1	1:D:309:ARG:HG2	1.74	0.68
1:A:224:TYR:HA	1:B:11:TYR:CE2	2.24	0.68
1:B:174:ARG:O	1:B:178:ILE:HG12	1.92	0.68
1:B:38:THR:HG21	1:B:45:GLN:HE22	1.58	0.68
1:D:77:LEU:HD23	1:D:118:ALA:HB1	1.75	0.68
1:D:205:TYR:HE1	1:D:252:LYS:HE2	1.57	0.68
1:B:288:GLY:O	1:B:293:ALA:HB3	1.92	0.68
1:C:54:ALA:HB3	1:C:56:TYR:CZ	2.29	0.68
1:A:320:ALA:HB3	1:A:321:PRO:HD3	1.73	0.68
1:C:44:VAL:O	1:C:46:PRO:HD3	1.93	0.68
1:A:278:VAL:HG22	1:A:281:GLU:OE2	1.94	0.67
1:C:11:TYR:CD1	1:C:11:TYR:N	2.61	0.67
1:D:33:TYR:H	1:D:76:VAL:HA	1.60	0.67
1:C:50:LEU:HB3	1:C:53:VAL:HG21	1.76	0.67
1:B:53:VAL:HG12	1:B:54:ALA:H	1.59	0.67
1:C:106:ARG:HH11	1:C:160:ALA:HA	1.56	0.67
1:D:250:MET:HA	1:D:274:ALA:O	1.94	0.67
1:D:149:ARG:HA	1:D:152:GLU:HB2	1.77	0.67
1:D:107:LEU:O	1:D:110:LYS:N	2.27	0.67
1:C:226:LEU:HD12	1:C:226:LEU:H	1.60	0.67
1:D:176:GLU:HB2	1:D:244:GLU:HG2	1.76	0.67
1:A:33:TYR:HB2	1:A:320:ALA:CB	2.24	0.67
1:A:35:ILE:HD12	1:A:76:VAL:HB	1.77	0.67
1:C:289:ALA:C	1:C:291:ALA:H	1.97	0.67
1:D:250:MET:HG2	1:D:251:VAL:N	2.09	0.67
1:B:267:LYS:HE2	1:B:268:HIS:CE1	2.29	0.67
1:C:239:ALA:O	1:C:242:ILE:HG22	1.94	0.66
1:B:38:THR:HG21	1:B:45:GLN:NE2	2.09	0.66
1:C:155:LEU:HD23	1:C:155:LEU:O	1.96	0.66
1:D:155:LEU:HD21	1:D:159:LYS:HE3	1.77	0.66
1:B:105:VAL:HG13	1:B:106:ARG:N	2.09	0.66
1:B:303:THR:HG22	1:B:307:PHE:HE2	1.60	0.66
1:B:308:ARG:NH2	1:B:313:ASP:HA	2.11	0.66
1:D:35:ILE:HD11	1:D:78:ILE:HA	1.77	0.66
1:C:11:TYR:N	1:C:11:TYR:HD1	1.94	0.66
1:A:249:LEU:HB2	1:A:273:LEU:HD23	1.78	0.66
1:A:289:ALA:O	1:A:291:ALA:N	2.28	0.66
1:B:61:LEU:HD23	1:B:108:LEU:HD21	1.77	0.66
1:C:273:LEU:HD22	1:C:274:ALA:H	1.61	0.66
1:B:304:MET:SD	1:B:315:ILE:HG21	2.36	0.66



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:D:228:PRO:O	1:D:230:ALA:N	2.28	0.66
1:A:47:ILE:HG22	1:A:49:SER:H	1.59	0.65
1:A:159:LYS:HG2	1:A:187:LEU:HD11	1.78	0.65
1:B:15:LEU:HD11	1:B:19:TRP:HE1	1.61	0.65
1:B:92:SER:HA	1:B:95:ASP:HB2	1.78	0.65
1:D:306:ALA:HA	1:D:309:ARG:HH12	1.59	0.65
1:A:49:SER:O	1:A:51:PRO:HD3	1.96	0.65
1:D:66:ARG:N	1:D:67:PRO:HD2	2.12	0.65
1:C:233:LEU:HD12	1:D:20:GLN:CG	2.23	0.65
1:B:185:HIS:O	1:B:187:LEU:HG	1.96	0.65
1:D:242:ILE:C	1:D:242:ILE:HD13	2.17	0.65
1:B:50:LEU:HB3	1:B:53:VAL:HG21	1.78	0.65
1:B:43:ASP:N	1:B:60:GLN:HE21	1.95	0.64
1:D:13:HIS:HE1	1:D:15:LEU:HB3	1.61	0.64
1:D:280:GLY:O	1:D:284:MET:HG3	1.96	0.64
1:B:50:LEU:HB3	1:B:53:VAL:CG2	2.28	0.64
1:D:276:TYR:HE1	1:D:278:VAL:HA	1.62	0.64
1:C:11:TYR:HB2	1:C:17:ARG:HG2	1.79	0.64
1:C:174:ARG:O	1:C:178:ILE:HG13	1.97	0.64
1:B:235:LEU:HD13	1:B:267:LYS:HD3	1.79	0.64
1:C:105:VAL:HG13	1:C:106:ARG:H	1.61	0.64
1:C:282:PHE:HD2	1:C:318:TYR:HB2	1.64	0.63
1:A:47:ILE:HG21	1:A:211:ALA:HB2	1.80	0.63
1:B:58:VAL:O	1:B:61:LEU:HB2	1.97	0.63
1:A:233:LEU:HD12	1:B:20:GLN:HG2	1.79	0.63
1:B:173:GLY:O	1:B:176:GLU:HB3	1.99	0.63
1:C:150:LEU:HD21	1:C:169:ASP:OD2	1.98	0.63
1:C:192:SER:HA	1:C:247:ASP:OD2	1.98	0.63
1:B:43:ASP:H	1:B:60:GLN:HE21	1.47	0.63
1:B:66:ARG:HD2	2:B:347:HOH:O	1.99	0.63
1:B:308:ARG:HE	1:B:308:ARG:HA	1.64	0.63
1:A:173:GLY:HA2	1:A:244:GLU:OE1	1.99	0.62
1:D:216:PRO:HD3	1:D:221:ARG:NH2	2.14	0.62
1:A:49:SER:HB3	1:A:207:PRO:HA	1.80	0.62
1:B:46:PRO:HA	1:B:54:ALA:CB	2.29	0.62
1:B:66:ARG:O	1:B:70:GLU:HG2	2.00	0.62
1:D:176:GLU:O	1:D:180:ALA:HB2	1.99	0.62
1:A:74:ARG:HB3	1:A:74:ARG:HH11	1.64	0.62
1:B:296:LEU:HG	1:B:300:VAL:CG2	2.30	0.62
1:C:282:PHE:CD2	1:C:318:TYR:HB2	2.35	0.62
1:B:123:LEU:HD23	1:B:130:GLY:H	1.62	0.62



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:133:GLY:O	1:B:134:LEU:HB2	1.99	0.62
1:B:194:MET:HA	1:B:248:MET:HG2	1.82	0.62
1:B:274:ALA:HB2	1:B:314:ILE:HB	1.81	0.62
1:C:322:GLN:HB2	1:C:326:TRP:CH2	2.35	0.62
1:A:50:LEU:HD21	1:A:279:SER:HB2	1.82	0.62
1:D:277:GLN:HG3	1:D:281:GLU:OE1	1.99	0.62
1:D:320:ALA:O	1:D:324:LEU:HG	1.99	0.62
1:A:278:VAL:CG2	1:A:281:GLU:HG3	2.30	0.62
1:C:301:LEU:HD11	1:C:326:TRP:HB3	1.82	0.62
1:B:101:THR:HG23	1:B:102:ILE:N	2.15	0.62
1:C:313:ASP:O	1:C:314:ILE:HD12	1.99	0.62
1:A:95:ASP:CG	1:A:153:VAL:HG13	2.20	0.62
1:B:227:PRO:HG2	1:B:230:ALA:CB	2.30	0.62
1:C:266:ASP:O	1:C:269:PRO:HD3	1.99	0.62
1:D:47:ILE:HD12	1:D:210:ASP:O	2.00	0.62
1:D:221:ARG:HB2	1:D:222:ARG:NH1	2.14	0.62
1:D:99:SER:OG	1:D:101:THR:HG22	2.00	0.61
1:C:256:PRO:HA	1:D:255:LEU:HD11	1.82	0.61
1:D:81:VAL:HG11	1:D:212:ALA:HA	1.82	0.61
1:D:99:SER:HB3	1:D:102:ILE:HG12	1.82	0.61
1:B:54:ALA:HB3	1:B:56:TYR:CE1	2.36	0.61
1:C:306:ALA:HA	1:C:309:ARG:NH1	2.15	0.61
1:B:7:LEU:O	1:B:10:GLY:N	2.34	0.61
1:B:11:TYR:O	1:B:13:HIS:N	2.32	0.61
1:B:224:TYR:O	1:B:225:GLN:HB2	2.00	0.61
1:C:77:LEU:HA	1:C:118:ALA:HB3	1.82	0.61
1:D:19:TRP:C	1:D:21:THR:H	2.04	0.61
1:A:55:ARG:HH21	1:A:212:ALA:N	1.98	0.61
1:D:153:VAL:HG12	1:D:157:TYR:HE1	1.65	0.61
1:B:122:CYS:SG	1:B:129:HIS:CE1	2.94	0.61
1:C:297:ARG:HG3	1:C:326:TRP:CD1	2.36	0.61
1:D:110:LYS:HA	1:D:110:LYS:CE	2.30	0.61
1:A:56:TYR:H	1:A:56:TYR:HD1	1.47	0.61
1:A:73:LEU:HD12	2:A:341:HOH:O	2.00	0.61
1:B:99:SER:OG	1:B:101:THR:HG22	2.00	0.61
1:C:111:THR:HG22	1:C:112:PHE:CE1	2.36	0.61
1:A:116:LEU:HD13	1:A:163:GLN:HB2	1.83	0.61
1:B:26:VAL:HG22	1:B:308:ARG:HG3	1.81	0.61
1:C:170:MET:HE1	1:C:174:ARG:HH21	1.64	0.61
1:D:242:ILE:HD13	1:D:242:ILE:O	2.00	0.61
1:B:41:PRO:O	1:B:43:ASP:N	2.34	0.60



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:C:32:ILE:CD1	1:C:314:ILE:HG23	2.31	0.60
1:C:102:ILE:HA	1:C:105:VAL:HG12	1.83	0.60
1:C:226:LEU:HD12	1:C:226:LEU:N	2.16	0.60
1:C:292:GLY:O	1:C:294:PHE:N	2.34	0.60
1:D:35:ILE:CD1	1:D:78:ILE:HA	2.31	0.60
1:B:273:LEU:O	1:B:314:ILE:N	2.34	0.60
1:C:17:ARG:O	1:C:21:THR:HG22	2.01	0.60
1:D:60:GLN:O	1:D:60:GLN:HG3	2.01	0.60
1:C:54:ALA:HB3	1:C:56:TYR:CE1	2.37	0.60
1:C:20:GLN:NE2	1:D:233:LEU:HG	2.17	0.60
1:B:101:THR:HG21	1:B:157:TYR:CZ	2.37	0.60
1:D:51:PRO:O	1:D:53:VAL:HG23	2.01	0.60
1:A:278:VAL:HG22	1:A:281:GLU:HG3	1.83	0.60
1:B:282:PHE:CD2	1:B:318:TYR:HB2	2.37	0.60
1:D:75:CYS:CB	1:D:116:LEU:HB3	2.31	0.60
1:A:78:ILE:HD11	1:A:108:LEU:HD12	1.82	0.59
1:B:227:PRO:HG2	1:B:230:ALA:HB2	1.82	0.59
1:C:33:TYR:CD1	1:C:320:ALA:HB3	2.37	0.59
1:C:314:ILE:C	1:C:315:ILE:HD12	2.22	0.59
1:D:65:LEU:O	1:D:69:VAL:HG23	2.02	0.59
1:A:280:GLY:O	1:A:284:MET:HB2	2.02	0.59
1:B:91:GLY:C	1:B:93:ALA:H	2.05	0.59
1:B:273:LEU:N	1:B:313:ASP:HB2	2.16	0.59
1:C:281:GLU:HA	1:C:284:MET:CE	2.31	0.59
1:C:306:ALA:HA	1:C:309:ARG:NH2	2.17	0.59
1:D:145:GLU:HA	1:D:148:GLN:NE2	2.14	0.59
1:A:240:ARG:NH2	1:B:7:LEU:HD12	2.16	0.59
1:C:287:HIS:ND1	1:D:291:ALA:HB1	2.18	0.59
1:D:22:ALA:O	1:D:24:SER:N	2.32	0.59
1:D:221:ARG:HA	1:D:224:TYR:CZ	2.37	0.59
1:B:64:MET:HG3	1:B:65:LEU:HD23	1.84	0.59
1:C:200:PHE:N	1:C:200:PHE:HD1	1.98	0.59
1:C:323:LEU:O	1:C:327:LEU:HD13	2.02	0.59
1:B:110:LYS:NZ	1:B:110:LYS:HA	2.17	0.59
1:B:296:LEU:HG	1:B:300:VAL:HG23	1.85	0.59
1:C:273:LEU:HD13	1:C:274:ALA:N	2.17	0.59
1:D:277:GLN:HE21	1:D:303:THR:HG21	1.68	0.59
1:C:38:THR:HG23	1:C:55:ARG:HB3	1.84	0.59
1:C:251:VAL:HG12	1:C:252:LYS:N	2.18	0.59
1:D:236:ARG:HG3	1:D:236:ARG:HH11	1.67	0.59
1:A:257:TYR:CD1	1:B:309:ARG:NH1	2.70	0.59



	i i i i i i i i i i i i i i i i i i i	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:32:ILE:HB	1:C:316:ILE:HG23	1.85	0.59
1:D:39:ASP:OD1	1:D:82:PRO:HA	2.02	0.59
1:D:105:VAL:HG21	1:D:162:CYS:H	1.65	0.59
1:D:153:VAL:HG12	1:D:157:TYR:CE1	2.38	0.59
1:B:25:THR:O	1:B:308:ARG:HD2	2.02	0.59
1:C:111:THR:HG22	1:C:112:PHE:CD1	2.38	0.58
1:C:75:CYS:HB2	1:C:116:LEU:O	2.04	0.58
1:C:301:LEU:HD11	1:C:326:TRP:CB	2.33	0.58
1:B:47:ILE:HD12	1:B:211:ALA:HA	1.85	0.58
1:C:32:ILE:HG23	1:C:75:CYS:SG	2.43	0.58
1:D:38:THR:HG23	1:D:55:ARG:HB3	1.86	0.58
1:C:41:PRO:O	1:C:43:ASP:N	2.36	0.58
1:C:149:ARG:HH11	1:C:149:ARG:CB	2.10	0.58
1:A:56:TYR:CD1	1:A:56:TYR:N	2.70	0.58
1:C:200:PHE:N	1:C:200:PHE:CD1	2.67	0.58
1:C:257:TYR:O	1:C:261:VAL:HG23	2.04	0.58
1:D:56:TYR:N	1:D:56:TYR:CD1	2.71	0.58
1:A:174:ARG:O	1:A:178:ILE:HD13	2.03	0.58
1:B:75:CYS:SG	1:B:116:LEU:HB3	2.43	0.58
1:D:22:ALA:C	1:D:24:SER:H	2.07	0.58
1:D:169:ASP:O	1:D:170:MET:HB2	2.04	0.58
1:D:307:PHE:CB	1:D:315:ILE:HD11	2.34	0.58
1:C:41:PRO:HB3	1:C:59:ASN:H	1.68	0.58
1:B:122:CYS:C	1:B:123:LEU:HD22	2.24	0.58
1:B:201:ALA:HB2	1:B:225:GLN:O	2.03	0.58
1:A:173:GLY:HA2	1:A:244:GLU:CD	2.24	0.57
1:C:207:PRO:HG3	1:D:293:ALA:HB1	1.85	0.57
1:C:226:LEU:H	1:C:226:LEU:CD1	2.15	0.57
1:C:321:PRO:HB2	1:C:322:GLN:OE1	2.04	0.57
1:C:255:LEU:CD1	1:D:256:PRO:HA	2.25	0.57
1:D:278:VAL:O	1:D:281:GLU:HB2	2.04	0.57
1:A:182:LEU:HD22	1:A:187:LEU:O	2.04	0.57
1:B:226:LEU:H	1:B:226:LEU:CD1	2.15	0.57
1:C:116:LEU:HD22	1:C:163:GLN:OE1	2.04	0.57
1:C:209:ARG:HH11	1:C:209:ARG:HG2	1.69	0.57
1:B:77:LEU:HA	1:B:118:ALA:O	2.05	0.57
1:C:28:ALA:O	1:C:74:ARG:HG2	2.04	0.57
1:B:22:ALA:O	1:B:23:ALA:HB3	2.05	0.57
1:C:84:ARG:HH21	1:C:84:ARG:CB	2.09	0.57
1:D:157:TYR:HD1	1:D:157:TYR:H	1.52	0.57
1:B:15:LEU:HD11	1:B:19:TRP:NE1	2.19	0.57



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:C:23:ALA:O	1:C:24:SER:HB3	2.05	0.57
1:C:109:ARG:NH1	1:C:163:GLN:NE2	2.52	0.57
1:C:236:ARG:HG3	1:C:236:ARG:HH11	1.69	0.57
1:D:167:PRO:HB2	1:D:174:ARG:HE	1.69	0.57
1:A:116:LEU:HD11	1:A:164:VAL:HG23	1.86	0.57
1:A:233:LEU:HD12	1:B:20:GLN:CD	2.25	0.57
1:B:95:ASP:OD1	1:B:153:VAL:HG22	2.05	0.57
1:C:253:PRO:HB3	1:C:278:VAL:HG22	1.86	0.57
1:D:281:GLU:HB3	2:D:340:HOH:O	2.04	0.57
1:C:24:SER:HA	1:C:308:ARG:HB3	1.86	0.57
1:A:55:ARG:HH21	1:A:211:ALA:C	2.08	0.56
1:C:198:ALA:HB1	1:C:200:PHE:HE1	1.70	0.56
1:D:14:PRO:HA	1:D:17:ARG:CZ	2.35	0.56
1:B:91:GLY:O	1:B:93:ALA:N	2.38	0.56
1:C:205:TYR:HB3	1:C:209:ARG:NH1	2.21	0.56
1:A:95:ASP:OD2	1:A:153:VAL:HG13	2.04	0.56
1:A:259:ASP:OD1	1:A:260:MET:N	2.38	0.56
1:B:194:MET:O	1:B:194:MET:HG2	2.05	0.56
1:B:255:LEU:HB3	1:B:256:PRO:HD3	1.86	0.56
1:C:166:ALA:O	1:C:196:TYR:HE1	1.87	0.56
1:C:207:PRO:CG	1:D:293:ALA:HB1	2.35	0.56
1:A:27:SER:H	1:A:30:ASN:HD22	1.53	0.56
1:A:155:LEU:HD12	1:A:181:ALA:HB1	1.87	0.56
1:A:235:LEU:HD21	1:A:263:GLU:HB3	1.87	0.56
1:C:240:ARG:O	1:C:244:GLU:HG3	2.05	0.56
1:A:240:ARG:HD3	1:A:244:GLU:OE2	2.05	0.56
1:B:196:TYR:CD2	1:B:250:MET:SD	2.98	0.56
1:B:43:ASP:N	1:B:60:GLN:NE2	2.54	0.56
1:C:226:LEU:HD23	1:C:234:ALA:HA	1.88	0.56
1:D:233:LEU:O	1:D:236:ARG:HB2	2.06	0.56
1:D:242:ILE:HA	1:D:246:ALA:HB3	1.87	0.56
1:C:257:TYR:HA	1:D:309:ARG:HH21	1.70	0.56
1:D:11:TYR:C	1:D:13:HIS:H	2.09	0.56
1:D:287:HIS:O	1:D:291:ALA:HB2	2.05	0.56
1:B:35:ILE:CD1	1:B:78:ILE:HG13	2.32	0.56
1:C:47:ILE:N	1:C:47:ILE:HD12	2.21	0.56
1:D:13:HIS:CE1	1:D:15:LEU:HB3	2.40	0.56
1:A:66:ARG:HH11	1:A:66:ARG:HG2	1.70	0.56
1:B:131:HIS:HD2	1:B:146:SER:HA	1.71	0.56
1:B:296:LEU:O	1:B:300:VAL:HG23	2.05	0.56
1:C:265:LYS:O	1:C:269:PRO:HD3	2.05	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:C:286:TRP:O	1:C:289:ALA:N	2.35	0.56
1:C:149:ARG:O	1:C:153:VAL:HG23	2.06	0.55
1:D:314:ILE:HG22	1:D:315:ILE:N	2.21	0.55
1:A:26:VAL:HG22	1:A:27:SER:N	2.22	0.55
1:B:136:SER:O	1:B:137:GLU:HB2	2.06	0.55
1:B:85:VAL:O	1:B:86:PRO:O	2.24	0.55
1:C:154:ALA:HA	1:C:157:TYR:CD1	2.42	0.55
1:D:260:MET:O	1:D:264:VAL:HG22	2.07	0.55
1:A:36:PHE:CD2	1:A:36:PHE:N	2.74	0.55
1:B:221:ARG:O	1:B:221:ARG:HG2	2.06	0.55
1:B:303:THR:HG22	1:B:307:PHE:CE2	2.41	0.55
1:C:255:LEU:HG	1:D:255:LEU:O	2.06	0.55
1:B:19:TRP:CD1	1:C:314:ILE:HD11	2.41	0.55
1:B:199:LYS:NZ	1:B:252:LYS:NZ	2.55	0.55
1:B:231:ARG:HB3	1:B:231:ARG:HH11	1.70	0.55
1:D:282:PHE:CD2	1:D:318:TYR:HB2	2.41	0.55
1:A:3:HIS:C	1:A:5:SER:H	2.11	0.55
1:C:197:SER:HB3	1:C:238:VAL:HG22	1.89	0.55
1:D:276:TYR:CE1	1:D:278:VAL:HA	2.41	0.55
1:C:47:ILE:HD13	1:C:53:VAL:HG12	1.89	0.55
1:C:252:LYS:HA	1:C:253:PRO:O	2.06	0.55
1:C:322:GLN:HB2	1:C:326:TRP:CZ3	2.42	0.55
1:A:17:ARG:O	1:A:21:THR:HG22	2.07	0.55
1:A:142:LEU:HD13	1:A:145:GLU:HG2	1.87	0.55
1:A:35:ILE:CD1	1:A:76:VAL:HB	2.37	0.54
1:C:265:LYS:HA	1:C:265:LYS:CE	2.34	0.54
1:A:307:PHE:HD2	1:A:315:ILE:HD13	1.71	0.54
1:B:169:ASP:HB3	1:B:171:MET:HG2	1.88	0.54
1:B:274:ALA:HA	1:B:314:ILE:O	2.07	0.54
1:C:116:LEU:HA	1:C:163:GLN:OE1	2.07	0.54
1:C:170:MET:HE1	1:C:174:ARG:NH2	2.22	0.54
2:C:333:HOH:O	1:D:262:ARG:HD2	2.07	0.54
1:D:254:GLY:O	1:D:257:TYR:N	2.37	0.54
1:D:323:LEU:O	1:D:325:LYS:N	2.40	0.54
1:A:54:ALA:HB3	1:A:56:TYR:CE1	2.42	0.54
1:B:13:HIS:CE1	1:B:15:LEU:H	2.24	0.54
1:C:277:GLN:HE22	1:C:285:LEU:HD11	1.72	0.54
1:A:40:VAL:HB	1:A:43:ASP:HB2	1.89	0.54
1:C:273:LEU:HD12	1:C:312:ALA:HA	1.89	0.54
1:C:305:THR:HG21	1:D:228:PRO:CB	2.38	0.54
1:B:39:ASP:OD2	1:B:85:VAL:HG23	2.08	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:32:ILE:HD11	1:C:314:ILE:CG2	2.33	0.54
1:A:123:LEU:N	1:A:123:LEU:HD22	2.22	0.54
1:B:85:VAL:HG13	1:B:86:PRO:HD2	1.90	0.54
1:A:316:ILE:HD12	1:A:316:ILE:N	2.23	0.54
1:C:275:VAL:CG1	1:C:315:ILE:HG13	2.38	0.54
1:D:102:ILE:HG22	1:D:102:ILE:O	2.07	0.54
1:C:11:TYR:O	1:C:16:LEU:HB3	2.08	0.54
1:C:58:VAL:C	1:C:60:GLN:H	2.10	0.54
1:A:257:TYR:HD1	1:B:309:ARG:NH1	2.06	0.54
1:B:105:VAL:HG23	1:B:117:VAL:HG11	1.90	0.54
1:C:99:SER:O	1:C:103:GLU:HG3	2.07	0.54
1:D:149:ARG:O	1:D:153:VAL:HG23	2.07	0.54
1:C:174:ARG:HG2	1:C:174:ARG:HH11	1.71	0.53
1:D:11:TYR:O	1:D:13:HIS:N	2.41	0.53
1:D:286:TRP:C	1:D:288:GLY:H	2.11	0.53
1:A:300:VAL:C	1:A:302:GLU:H	2.11	0.53
1:B:108:LEU:HD23	1:B:108:LEU:N	2.23	0.53
1:D:42:ASP:HA	1:D:60:GLN:HE21	1.73	0.53
1:D:158:ALA:HB1	1:D:187:LEU:HD13	1.90	0.53
1:B:183:LEU:HD13	1:B:188:GLY:HA3	1.91	0.53
1:C:51:PRO:O	1:C:53:VAL:HG23	2.07	0.53
1:C:157:TYR:HD1	1:C:157:TYR:H	1.57	0.53
1:D:301:LEU:O	1:D:304:MET:HB2	2.09	0.53
1:A:304:MET:C	1:A:306:ALA:H	2.11	0.53
1:B:59:ASN:O	1:B:61:LEU:N	2.41	0.53
1:D:238:VAL:CG1	1:D:249:LEU:HD13	2.39	0.53
1:C:253:PRO:HG3	1:C:278:VAL:HG11	1.90	0.53
1:A:305:THR:O	1:A:305:THR:HG22	2.09	0.53
1:B:8:HIS:CB	1:C:189:ASN:HB2	2.35	0.53
1:B:123:LEU:HB3	1:B:125:PRO:HD3	1.91	0.53
1:B:233:LEU:HD23	1:B:236:ARG:HG3	1.89	0.53
1:C:22:ALA:O	1:C:23:ALA:HB3	2.08	0.53
1:D:58:VAL:HG12	1:D:59:ASN:N	2.24	0.53
1:D:78:ILE:HB	1:D:118:ALA:O	2.09	0.53
1:C:147:ARG:HE	1:C:173:GLY:HA3	1.74	0.53
1:A:105:VAL:HG23	1:A:117:VAL:CG1	2.39	0.53
1:B:209:ARG:HH12	1:B:221:ARG:NH2	2.07	0.53
1:C:18:SER:HA	1:C:21:THR:CG2	2.39	0.53
1:C:35:ILE:O	1:C:35:ILE:HG13	2.08	0.53
1:A:105:VAL:HG23	1:A:117:VAL:HG11	1.91	0.53
1:C:287:HIS:CD2	1:C:287:HIS:H	2.27	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:D:202:SER:HB3	2:D:337:HOH:O	2.09	0.53
1:D:231:ARG:O	1:D:234:ALA:HB3	2.10	0.53
1:D:266:ASP:O	1:D:268:HIS:N	2.42	0.53
1:D:281:GLU:O	1:D:282:PHE:C	2.47	0.53
1:A:6:VAL:O	1:A:7:LEU:HD23	2.09	0.52
1:A:11:TYR:CD1	1:A:11:TYR:N	2.77	0.52
1:A:11:TYR:O	1:A:12:PHE:CG	2.63	0.52
1:B:260:MET:O	1:B:264:VAL:HG22	2.08	0.52
1:C:242:ILE:HG23	1:C:243:GLN:N	2.24	0.52
1:C:281:GLU:HA	1:C:284:MET:HE2	1.90	0.52
1:B:170:MET:CG	1:B:199:LYS:HB3	2.39	0.52
1:B:204:PHE:HB3	1:B:280:GLY:HA3	1.90	0.52
1:A:260:MET:HE3	1:B:309:ARG:HD2	1.90	0.52
1:A:11:TYR:HA	1:A:16:LEU:HB3	1.90	0.52
1:A:173:GLY:HA2	1:A:244:GLU:OE2	2.09	0.52
1:C:58:VAL:O	1:C:60:GLN:N	2.43	0.52
1:D:209:ARG:HG2	1:D:209:ARG:HH11	1.75	0.52
1:D:275:VAL:CG1	1:D:315:ILE:HG12	2.39	0.52
1:A:35:ILE:HD13	1:A:35:ILE:N	2.24	0.52
1:A:255:LEU:HD11	1:B:256:PRO:CA	2.30	0.52
1:B:147:ARG:O	1:B:150:LEU:HB3	2.08	0.52
1:B:317:THR:HG23	1:B:320:ALA:N	2.25	0.52
1:C:73:LEU:H	1:C:324:LEU:CD1	2.19	0.52
1:C:149:ARG:C	1:C:151:ALA:H	2.12	0.52
1:A:47:ILE:HD12	1:A:47:ILE:N	2.24	0.52
1:A:326:TRP:C	1:A:328:LYS:H	2.13	0.52
1:B:32:ILE:HB	1:B:316:ILE:HG12	1.92	0.52
1:B:207:PRO:O	1:B:210:ASP:HB2	2.10	0.52
1:D:320:ALA:HB3	1:D:321:PRO:HD3	1.92	0.52
1:A:199:LYS:HZ3	1:A:252:LYS:HE2	1.74	0.52
1:B:47:ILE:HD11	1:B:55:ARG:CG	2.34	0.52
1:B:176:GLU:N	1:B:244:GLU:OE1	2.43	0.52
1:B:280:GLY:O	1:B:284:MET:HG3	2.09	0.52
1:C:77:LEU:HA	1:C:118:ALA:O	2.10	0.52
1:C:178:ILE:O	1:C:181:ALA:HB3	2.09	0.52
1:B:273:LEU:O	1:B:313:ASP:N	2.43	0.51
1:C:275:VAL:HG11	1:C:315:ILE:HG13	1.92	0.51
1:B:73:LEU:HA	1:B:324:LEU:HD11	1.91	0.51
1:B:162:CYS:SG	1:B:163:GLN:N	2.83	0.51
1:C:12:PHE:CD1	1:C:12:PHE:C	2.84	0.51
1:B:133:GLY:O	1:B:134:LEU:CB	2.58	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:293:ALA:O	1:D:206:GLY:HA3	2.10	0.51
1:D:56:TYR:N	1:D:56:TYR:HD1	2.08	0.51
1:D:186:GLY:C	1:D:188:GLY:H	2.13	0.51
1:A:39:ASP:OD2	1:A:82:PRO:HA	2.11	0.51
1:A:265:LYS:HE2	1:A:269:PRO:HA	1.93	0.51
1:B:245:GLY:O	1:B:246:ALA:O	2.27	0.51
1:C:151:ALA:C	1:C:153:VAL:N	2.64	0.51
1:C:227:PRO:HA	2:C:340:HOH:O	2.11	0.51
1:D:197:SER:HB3	1:D:238:VAL:HA	1.92	0.51
1:A:242:ILE:HD13	1:A:271:LEU:CD1	2.27	0.51
1:C:233:LEU:HD23	1:C:233:LEU:O	2.11	0.51
1:A:66:ARG:N	1:A:67:PRO:HD2	2.26	0.51
1:A:78:ILE:HD11	1:A:108:LEU:CD1	2.41	0.51
1:B:296:LEU:HD23	1:B:326:TRP:HH2	1.76	0.51
1:A:164:VAL:HG22	1:A:192:SER:HB2	1.92	0.51
1:B:53:VAL:CG1	1:B:54:ALA:N	2.74	0.51
1:C:174:ARG:HH12	1:C:240:ARG:HH22	1.59	0.51
1:A:122:CYS:SG	1:A:123:LEU:N	2.83	0.51
1:A:199:LYS:O	1:A:225:GLN:HG2	2.11	0.51
1:B:68:LEU:O	1:B:71:ALA:N	2.43	0.51
1:D:282:PHE:HD2	1:D:318:TYR:HD2	1.58	0.51
1:B:122:CYS:SG	1:B:129:HIS:CG	3.04	0.51
1:D:78:ILE:N	1:D:118:ALA:O	2.39	0.51
1:D:97:GLU:HG2	1:D:98:ASP:N	2.26	0.51
1:D:242:ILE:HG23	1:D:243:GLN:N	2.26	0.51
1:B:122:CYS:SG	1:B:129:HIS:CD2	3.04	0.51
1:C:4:GLN:O	1:C:5:SER:HB3	2.11	0.51
1:D:272:PRO:HA	1:D:313:ASP:OD2	2.10	0.51
1:B:327:LEU:O	1:B:328:LYS:HD2	2.11	0.50
1:C:281:GLU:HA	1:C:284:MET:HE3	1.94	0.50
1:B:11:TYR:C	1:B:13:HIS:H	2.15	0.50
1:B:272:PRO:HG3	1:C:20:GLN:OE1	2.12	0.50
1:D:25:THR:HG23	1:D:25:THR:O	2.10	0.50
1:D:58:VAL:HG21	1:D:103:GLU:CD	2.31	0.50
1:A:95:ASP:OD1	1:A:153:VAL:HG13	2.12	0.50
1:A:257:TYR:HD1	1:B:309:ARG:NH2	2.10	0.50
1:A:323:LEU:C	1:A:325:LYS:N	2.64	0.50
1:D:64:MET:SD	1:D:64:MET:C	2.89	0.50
1:B:260:MET:HE2	1:B:260:MET:HA	1.93	0.50
1:C:66:ARG:N	1:C:67:PRO:HD2	2.26	0.50
1:A:7:LEU:HD12	1:B:240:ARG:HH21	1.77	0.50



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:90:GLN:HA	1:B:131:HIS:HE1	1.77	0.50
1:C:148:GLN:HG2	1:C:149:ARG:N	2.26	0.50
1:D:41:PRO:O	1:D:43:ASP:N	2.45	0.50
1:D:107:LEU:O	1:D:108:LEU:C	2.50	0.50
1:C:11:TYR:HA	1:C:16:LEU:O	2.12	0.50
1:C:12:PHE:HD1	1:C:12:PHE:O	1.95	0.50
1:C:310:ALA:O	1:C:312:ALA:N	2.45	0.50
1:D:236:ARG:HG3	1:D:236:ARG:NH1	2.26	0.50
1:A:38:THR:HG22	1:A:81:VAL:O	2.11	0.50
1:D:251:VAL:O	1:D:253:PRO:O	2.29	0.50
1:B:314:ILE:C	1:B:315:ILE:HD12	2.31	0.50
1:C:18:SER:HA	1:C:21:THR:HG22	1.94	0.50
1:C:105:VAL:HA	1:C:108:LEU:HD12	1.94	0.50
1:D:323:LEU:C	1:D:325:LYS:N	2.66	0.50
1:A:22:ALA:O	1:A:23:ALA:HB3	2.12	0.50
1:B:151:ALA:HA	1:B:178:ILE:CD1	2.40	0.50
1:B:199:LYS:HZ2	1:B:252:LYS:HZ3	1.60	0.50
1:B:105:VAL:CG1	1:B:106:ARG:H	2.22	0.49
1:C:50:LEU:HB3	1:C:53:VAL:CG2	2.41	0.49
1:A:277:GLN:O	1:A:277:GLN:HG2	2.12	0.49
1:B:104:ALA:O	1:B:108:LEU:HG	2.11	0.49
1:C:308:ARG:O	1:C:309:ARG:C	2.50	0.49
1:C:319:PHE:O	1:C:320:ALA:C	2.50	0.49
1:D:70:GLU:C	1:D:72:GLY:H	2.15	0.49
1:D:146:SER:O	1:D:150:LEU:HB2	2.11	0.49
1:D:282:PHE:HD2	1:D:318:TYR:HB2	1.75	0.49
1:A:263:GLU:C	1:A:265:LYS:H	2.15	0.49
1:B:262:ARG:O	1:B:262:ARG:HD3	2.12	0.49
1:D:279:SER:CA	1:D:318:TYR:HE2	2.21	0.49
1:C:20:GLN:HG2	1:D:233:LEU:HD12	1.93	0.49
1:C:197:SER:CB	1:C:238:VAL:HG22	2.43	0.49
1:C:327:LEU:O	1:C:328:LYS:C	2.50	0.49
1:D:196:TYR:O	1:D:198:ALA:N	2.45	0.49
1:D:282:PHE:HD2	1:D:318:TYR:CD2	2.30	0.49
1:A:147:ARG:O	1:A:150:LEU:N	2.43	0.49
1:C:205:TYR:CZ	1:C:252:LYS:HE2	2.48	0.49
1:D:226:LEU:HD12	1:D:226:LEU:H	1.77	0.49
1:D:258:LEU:O	1:D:261:VAL:N	2.40	0.49
1:B:94:ALA:HB2	1:B:124:CYS:SG	2.52	0.49
1:B:199:LYS:HZ2	1:B:252:LYS:NZ	2.10	0.49
1:B:321:PRO:C	1:B:323:LEU:H	2.15	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:C:84:ARG:HD3	1:C:84:ARG:N	2.28	0.49
1:C:289:ALA:C	1:C:291:ALA:N	2.65	0.49
1:C:307:PHE:HD2	1:C:315:ILE:CG1	2.26	0.49
1:D:72:GLY:O	1:D:324:LEU:HD22	2.13	0.49
1:C:198:ALA:HB1	1:C:200:PHE:CE1	2.47	0.49
1:B:61:LEU:C	1:B:63:GLU:H	2.16	0.49
1:B:154:ALA:HB1	1:B:178:ILE:HG23	1.95	0.49
1:B:315:ILE:HD12	1:B:315:ILE:N	2.27	0.49
1:C:56:TYR:CD1	1:C:56:TYR:N	2.80	0.49
1:C:122:CYS:O	1:C:122:CYS:SG	2.70	0.49
1:D:155:LEU:HD12	1:D:181:ALA:HB1	1.94	0.49
1:D:228:PRO:C	1:D:230:ALA:H	2.13	0.49
1:D:239:ALA:O	1:D:242:ILE:HG22	2.13	0.49
1:D:275:VAL:HG11	1:D:307:PHE:CD1	2.48	0.49
1:D:323:LEU:C	1:D:325:LYS:H	2.15	0.49
1:A:157:TYR:O	1:A:160:ALA:HB3	2.13	0.49
1:A:238:VAL:O	1:A:242:ILE:HG22	2.12	0.49
1:A:240:ARG:HH21	1:B:7:LEU:CD1	2.22	0.49
1:B:301:LEU:O	1:B:304:MET:N	2.46	0.49
1:D:36:PHE:O	1:D:56:TYR:N	2.46	0.49
1:A:121:VAL:HG11	1:A:154:ALA:HB2	1.94	0.49
1:A:204:PHE:HB3	1:A:280:GLY:HA3	1.95	0.49
1:C:119:CYS:HB3	1:C:157:TYR:CD2	2.48	0.49
1:C:205:TYR:HE1	1:C:252:LYS:HE2	1.76	0.49
1:C:325:LYS:C	1:C:327:LEU:H	2.16	0.48
1:D:33:TYR:O	1:D:77:LEU:N	2.46	0.48
1:D:258:LEU:HA	1:D:261:VAL:HG23	1.95	0.48
1:C:242:ILE:CG2	1:C:243:GLN:N	2.76	0.48
1:C:258:LEU:CB	1:D:258:LEU:HB3	2.42	0.48
1:D:307:PHE:HB3	1:D:315:ILE:HD11	1.93	0.48
1:A:99:SER:HB2	1:A:100:PRO:CD	2.36	0.48
1:B:53:VAL:CG1	1:B:54:ALA:H	2.24	0.48
1:B:91:GLY:C	1:B:93:ALA:N	2.67	0.48
1:C:104:ALA:O	1:C:107:LEU:HB3	2.13	0.48
1:C:175:VAL:HG11	1:C:246:ALA:HB2	1.95	0.48
1:C:258:LEU:HG	1:D:259:ASP:HB3	1.95	0.48
1:D:11:TYR:CB	1:D:17:ARG:HG2	2.43	0.48
1:D:314:ILE:HG22	1:D:315:ILE:H	1.78	0.48
1:A:302:GLU:HA	2:A:339:HOH:O	2.13	0.48
1:B:275:VAL:HG11	1:B:307:PHE:CD1	2.49	0.48
1:C:155:LEU:CD2	1:C:159:LYS:HE3	2.43	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:77:LEU:CD1	1:D:316:ILE:HD13	2.42	0.48
1:A:283:ALA:HB1	1:A:287:HIS:CE1	2.49	0.48
1:C:162:CYS:SG	1:C:163:GLN:N	2.86	0.48
1:C:259:ASP:CA	1:D:259:ASP:HA	2.39	0.48
1:D:282:PHE:C	1:D:282:PHE:CD1	2.87	0.48
1:C:149:ARG:HA	1:C:152:GLU:HG2	1.94	0.48
1:C:259:ASP:HB2	1:D:262:ARG:CB	2.42	0.48
1:A:37:VAL:HG12	1:A:38:THR:N	2.29	0.48
1:B:274:ALA:CB	1:B:314:ILE:HB	2.42	0.48
1:D:58:VAL:O	1:D:59:ASN:C	2.51	0.48
1:C:45:GLN:O	1:C:54:ALA:HA	2.14	0.48
1:C:110:LYS:O	1:C:110:LYS:HG2	2.14	0.48
1:D:199:LYS:HA	1:D:252:LYS:O	2.14	0.48
1:D:225:GLN:O	1:D:226:LEU:C	2.52	0.48
1:D:231:ARG:HG2	1:D:231:ARG:HH11	1.78	0.48
1:A:54:ALA:HB3	1:A:56:TYR:CZ	2.49	0.48
1:A:234:ALA:O	1:A:238:VAL:HG23	2.12	0.48
1:B:66:ARG:HB3	1:B:67:PRO:CD	2.44	0.48
1:B:182:LEU:O	1:B:188:GLY:N	2.45	0.48
1:D:308:ARG:C	1:D:310:ALA:H	2.18	0.48
1:A:169:ASP:OD1	1:A:174:ARG:HD2	2.13	0.48
1:B:8:HIS:C	1:B:10:GLY:H	2.18	0.48
1:D:179:LYS:HA	1:D:182:LEU:HD12	1.96	0.48
1:A:277:GLN:NE2	1:A:317:THR:OG1	2.47	0.47
1:A:306:ALA:HA	1:A:309:ARG:NH1	2.29	0.47
1:B:76:VAL:HG21	1:B:115:LEU:HD21	1.96	0.47
1:A:282:PHE:O	1:A:285:LEU:HB2	2.14	0.47
1:C:42:ASP:HA	1:C:60:GLN:HG2	1.96	0.47
1:C:64:MET:SD	1:C:65:LEU:HG	2.54	0.47
1:C:170:MET:HA	1:C:174:ARG:CZ	2.43	0.47
1:D:116:LEU:HD22	1:D:163:GLN:OE1	2.14	0.47
1:A:40:VAL:HB	1:A:43:ASP:CB	2.44	0.47
1:A:304:MET:C	1:A:306:ALA:N	2.68	0.47
1:B:154:ALA:CB	1:B:178:ILE:HG23	2.44	0.47
1:B:183:LEU:HD22	1:B:188:GLY:HA3	1.96	0.47
1:C:255:LEU:HD11	1:D:256:PRO:CA	2.28	0.47
1:C:312:ALA:HB1	1:C:315:ILE:HD11	1.95	0.47
1:D:258:LEU:O	1:D:261:VAL:HG23	2.14	0.47
1:D:322:GLN:O	1:D:326:TRP:HB2	2.14	0.47
1:A:259:ASP:OD2	1:B:310:ALA:HB2	2.15	0.47
1:B:7:LEU:O	1:B:8:HIS:C	2.52	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:43:ASP:H	1:B:60:GLN:NE2	2.10	0.47
1:B:109:ARG:HG3	1:B:161:GLY:O	2.14	0.47
1:B:293:ALA:O	1:B:294:PHE:HB3	2.14	0.47
1:C:34:PRO:HG2	1:C:318:TYR:CE1	2.49	0.47
1:C:251:VAL:CG1	1:C:252:LYS:N	2.77	0.47
1:C:287:HIS:CD2	1:C:287:HIS:N	2.82	0.47
1:A:253:PRO:HD2	1:A:257:TYR:CD2	2.49	0.47
1:B:86:PRO:C	1:B:87:LYS:HG3	2.35	0.47
1:D:158:ALA:CB	1:D:187:LEU:HD13	2.43	0.47
1:A:66:ARG:O	1:A:70:GLU:HG3	2.14	0.47
1:B:128:SER:OG	1:B:216:PRO:HB3	2.14	0.47
1:C:144:GLU:C	1:C:146:SER:H	2.16	0.47
1:C:299:ALA:O	1:C:302:GLU:N	2.43	0.47
1:C:311:GLY:O	1:C:312:ALA:C	2.52	0.47
1:A:99:SER:OG	1:A:102:ILE:HG12	2.15	0.47
1:A:285:LEU:HD13	1:A:300:VAL:HG22	1.97	0.47
1:B:99:SER:HB3	1:B:102:ILE:HG12	1.97	0.47
1:C:20:GLN:HG2	1:D:233:LEU:CD1	2.43	0.47
1:D:35:ILE:HD13	1:D:35:ILE:H	1.80	0.47
1:D:153:VAL:CG1	1:D:157:TYR:HE1	2.27	0.47
1:D:252:LYS:HA	1:D:253:PRO:O	2.15	0.47
1:C:153:VAL:O	1:C:155:LEU:N	2.48	0.47
1:A:19:TRP:O	1:A:22:ALA:HB2	2.15	0.47
1:A:190:ARG:HG3	1:A:190:ARG:HH11	1.80	0.47
1:C:24:SER:HA	1:C:308:ARG:HD3	1.95	0.47
1:C:202:SER:HB2	1:C:257:TYR:OH	2.15	0.47
1:D:196:TYR:HA	1:D:250:MET:HB3	1.97	0.47
1:B:105:VAL:CG1	1:B:106:ARG:N	2.78	0.47
1:B:295:ASP:OD2	1:B:297:ARG:N	2.41	0.47
1:C:11:TYR:C	1:C:13:HIS:N	2.68	0.47
1:C:35:ILE:HG12	1:C:77:LEU:O	2.15	0.47
1:C:105:VAL:CG1	1:C:106:ARG:H	2.27	0.47
1:C:253:PRO:HA	1:C:278:VAL:HG13	1.97	0.47
1:C:281:GLU:O	1:C:282:PHE:C	2.54	0.47
1:D:32:ILE:HG12	1:D:75:CYS:SG	2.55	0.47
1:D:277:GLN:NE2	1:D:303:THR:CG2	2.76	0.47
1:A:169:ASP:O	1:A:170:MET:HB2	2.16	0.46
1:A:320:ALA:O	1:A:324:LEU:HG	2.15	0.46
1:B:260:MET:HA	1:B:260:MET:CE	2.45	0.46
1:C:205:TYR:HB3	1:C:209:ARG:HH12	1.80	0.46
1:C:253:PRO:HB3	1:C:278:VAL:CG2	2.45	0.46



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:C:275:VAL:HG11	1:C:307:PHE:CD2	2.50	0.46
1:D:13:HIS:HE1	1:D:15:LEU:CB	2.27	0.46
1:D:81:VAL:CG1	1:D:212:ALA:HA	2.45	0.46
1:A:258:LEU:O	1:A:261:VAL:HB	2.15	0.46
1:B:66:ARG:HB3	1:B:67:PRO:HD3	1.98	0.46
1:C:20:GLN:HE21	1:D:233:LEU:HD11	1.80	0.46
1:C:32:ILE:HD13	1:C:316:ILE:CG1	2.43	0.46
1:C:205:TYR:CB	1:C:209:ARG:HH12	2.27	0.46
1:C:279:SER:O	1:C:282:PHE:HB3	2.15	0.46
1:D:122:CYS:HA	1:D:169:ASP:OD2	2.14	0.46
1:D:258:LEU:O	1:D:259:ASP:C	2.54	0.46
1:C:68:LEU:O	1:C:71:ALA:HB3	2.15	0.46
1:C:170:MET:HA	1:C:174:ARG:NH2	2.30	0.46
1:D:75:CYS:HB2	1:D:116:LEU:CB	2.43	0.46
1:D:262:ARG:HD3	1:D:262:ARG:C	2.35	0.46
1:A:12:PHE:CD1	1:A:12:PHE:C	2.88	0.46
1:A:306:ALA:HA	1:A:309:ARG:HH12	1.80	0.46
1:B:92:SER:HA	1:B:95:ASP:OD2	2.16	0.46
1:B:155:LEU:O	1:B:158:ALA:HB3	2.16	0.46
1:C:242:ILE:HD13	1:C:242:ILE:O	2.16	0.46
1:D:66:ARG:N	1:D:67:PRO:CD	2.77	0.46
1:D:253:PRO:HD2	1:D:257:TYR:CD2	2.50	0.46
1:A:31:LEU:C	1:A:32:ILE:HD12	2.35	0.46
1:A:239:ALA:O	1:A:242:ILE:HG23	2.16	0.46
1:B:19:TRP:CG	1:C:314:ILE:HD11	2.51	0.46
1:B:149:ARG:HB3	2:B:350:HOH:O	2.14	0.46
1:C:78:ILE:N	1:C:78:ILE:HD12	2.31	0.46
1:A:151:ALA:O	1:A:155:LEU:N	2.47	0.46
1:A:229:GLY:HA2	1:B:309:ARG:HD3	1.97	0.46
1:B:131:HIS:CD2	1:B:146:SER:HA	2.49	0.46
1:B:200:PHE:HB2	1:B:253:PRO:HD2	1.97	0.46
1:B:283:ALA:O	1:B:286:TRP:N	2.48	0.46
1:C:84:ARG:HD3	1:C:84:ARG:H	1.79	0.46
1:C:147:ARG:NE	1:C:173:GLY:HA3	2.30	0.46
1:D:200:PHE:C	1:D:202:SER:H	2.17	0.46
1:B:68:LEU:CD2	1:B:321:PRO:HB3	2.46	0.46
1:B:240:ARG:HD3	1:B:244:GLU:OE2	2.16	0.46
1:B:308:ARG:HH22	1:B:313:ASP:HA	1.80	0.46
1:C:123:LEU:N	1:C:123:LEU:HD22	2.31	0.46
1:A:313:ASP:C	1:A:314:ILE:HD13	2.35	0.46
1:B:196:TYR:CE2	1:B:250:MET:SD	3.09	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:200:PHE:HB2	1:B:253:PRO:CD	2.45	0.46
1:C:55:ARG:NH2	1:C:210:ASP:O	2.49	0.46
1:C:109:ARG:C	1:C:111:THR:H	2.18	0.46
1:D:235:LEU:O	1:D:236:ARG:C	2.54	0.46
1:D:307:PHE:HB2	1:D:315:ILE:HD11	1.98	0.46
1:C:284:MET:SD	1:D:285:LEU:HD23	2.56	0.46
1:C:323:LEU:O	1:C:325:LYS:N	2.48	0.46
1:D:238:VAL:HG13	1:D:249:LEU:HD13	1.97	0.46
1:A:50:LEU:O	1:A:53:VAL:HB	2.16	0.46
1:A:55:ARG:NH2	1:A:211:ALA:C	2.69	0.46
1:A:297:ARG:HG3	1:A:326:TRP:CD1	2.51	0.46
1:C:24:SER:HA	1:C:308:ARG:CB	2.46	0.46
1:C:105:VAL:CG1	1:C:106:ARG:N	2.76	0.46
1:C:190:ARG:O	1:C:190:ARG:HG2	2.15	0.46
1:D:183:LEU:C	1:D:183:LEU:HD13	2.36	0.46
1:D:193:VAL:H	1:D:247:ASP:HB2	1.81	0.46
1:D:253:PRO:HG3	2:D:337:HOH:O	2.15	0.46
1:D:319:PHE:O	1:D:323:LEU:HG	2.16	0.46
1:A:7:LEU:HD22	1:B:236:ARG:NH2	2.31	0.45
1:A:26:VAL:HG22	1:A:27:SER:H	1.81	0.45
1:A:230:ALA:HB1	1:A:233:LEU:HB3	1.98	0.45
1:A:326:TRP:C	1:A:328:LYS:N	2.70	0.45
1:B:13:HIS:NE2	1:C:116:LEU:HD23	2.32	0.45
1:C:47:ILE:HG21	1:C:50:LEU:HB2	1.98	0.45
1:C:83:SER:OG	1:C:84:ARG:HD3	2.15	0.45
1:C:298:THR:O	1:C:302:GLU:HB2	2.16	0.45
1:A:255:LEU:CD1	1:A:258:LEU:HD22	2.46	0.45
1:B:9:SER:HB3	1:C:189:ASN:HA	1.98	0.45
1:B:167:PRO:HB2	1:B:174:ARG:HE	1.81	0.45
1:C:235:LEU:HD23	1:C:235:LEU:N	2.30	0.45
1:C:265:LYS:O	1:C:269:PRO:CD	2.64	0.45
1:C:273:LEU:HD12	1:C:312:ALA:N	2.31	0.45
1:B:15:LEU:HD21	1:B:19:TRP:CZ2	2.51	0.45
1:C:265:LYS:CE	1:C:269:PRO:HA	2.41	0.45
1:C:273:LEU:HD22	1:C:274:ALA:N	2.29	0.45
1:C:279:SER:N	1:C:318:TYR:HE2	2.14	0.45
1:D:149:ARG:C	1:D:151:ALA:H	2.20	0.45
1:D:266:ASP:O	1:D:269:PRO:HD3	2.16	0.45
1:B:13:HIS:HA	1:B:14:PRO:HD2	1.73	0.45
1:B:179:LYS:HD3	1:B:193:VAL:CG2	2.47	0.45
1:B:242:ILE:HG23	1:B:243:GLN:N	2.30	0.45



	1.5	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:C:209:ARG:C	1:C:211:ALA:H	2.19	0.45
1:D:32:ILE:HD11	1:D:314:ILE:HG21	1.98	0.45
1:D:226:LEU:CD2	1:D:234:ALA:HA	2.47	0.45
1:D:300:VAL:O	1:D:304:MET:HG2	2.17	0.45
1:A:6:VAL:C	1:A:7:LEU:HD23	2.37	0.45
1:B:40:VAL:HG11	1:B:43:ASP:OD2	2.16	0.45
1:B:327:LEU:HD12	1:B:327:LEU:N	2.31	0.45
1:C:37:VAL:HG12	1:C:100:PRO:HB2	1.99	0.45
1:B:129:HIS:CE1	2:B:334:HOH:O	2.69	0.45
1:C:258:LEU:O	1:C:261:VAL:N	2.48	0.45
1:D:22:ALA:C	1:D:24:SER:N	2.70	0.45
1:D:61:LEU:HD23	1:D:107:LEU:HD23	1.97	0.45
1:D:222:ARG:N	1:D:222:ARG:CD	2.79	0.45
1:B:202:SER:OG	1:B:203:CYS:N	2.48	0.45
1:B:317:THR:HG23	1:B:320:ALA:H	1.81	0.45
1:C:58:VAL:C	1:C:60:GLN:N	2.70	0.45
1:C:151:ALA:C	1:C:153:VAL:H	2.19	0.45
1:C:240:ARG:HD2	1:C:240:ARG:C	2.36	0.45
1:C:262:ARG:O	1:C:265:LYS:HB3	2.16	0.45
1:A:121:VAL:O	1:A:167:PRO:HA	2.17	0.45
1:B:151:ALA:O	1:B:154:ALA:HB3	2.17	0.45
1:B:167:PRO:O	1:B:196:TYR:HD1	2.00	0.45
1:C:170:MET:H	1:C:170:MET:CE	2.30	0.45
1:C:299:ALA:O	1:C:303:THR:HG23	2.17	0.45
1:D:282:PHE:C	1:D:282:PHE:HD1	2.19	0.45
1:A:49:SER:C	1:A:51:PRO:HD3	2.38	0.45
1:C:179:LYS:HG3	1:C:183:LEU:HG	1.99	0.45
1:D:235:LEU:O	1:D:238:VAL:N	2.50	0.45
1:D:259:ASP:CG	1:D:260:MET:N	2.71	0.45
1:A:64:MET:O	1:A:64:MET:SD	2.75	0.45
1:A:202:SER:HB3	1:A:253:PRO:HG2	1.99	0.45
1:C:20:GLN:HE21	1:D:233:LEU:CG	2.30	0.45
1:C:255:LEU:N	1:C:256:PRO:CD	2.80	0.45
1:D:147:ARG:HA	2:D:338:HOH:O	2.17	0.45
1:D:233:LEU:O	1:D:234:ALA:C	2.56	0.45
1:D:242:ILE:C	1:D:242:ILE:CD1	2.85	0.45
1:B:227:PRO:HG2	1:B:230:ALA:HB3	1.99	0.44
1:C:305:THR:HG21	1:D:228:PRO:HB2	1.98	0.44
1:A:262:ARG:O	1:A:265:LYS:N	2.50	0.44
1:C:305:THR:HG21	1:D:228:PRO:HB3	1.99	0.44
1:D:44:VAL:HG23	1:D:44:VAL:O	2.16	0.44



	hi a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:193:VAL:O	1:A:247:ASP:HB2	2.16	0.44
1:A:257:TYR:HD1	1:B:309:ARG:HH22	1.64	0.44
1:C:11:TYR:O	1:C:12:PHE:C	2.56	0.44
1:C:12:PHE:C	1:C:12:PHE:HD1	2.18	0.44
1:C:285:LEU:HD12	1:C:319:PHE:HE2	1.82	0.44
1:D:157:TYR:C	1:D:162:CYS:HB3	2.38	0.44
1:D:255:LEU:CD2	1:D:303:THR:HG23	2.42	0.44
1:A:73:LEU:HA	2:A:341:HOH:O	2.17	0.44
1:B:33:TYR:CD1	1:B:320:ALA:HB3	2.53	0.44
1:B:38:THR:HG22	1:B:81:VAL:O	2.17	0.44
1:B:149:ARG:NE	2:B:350:HOH:O	2.50	0.44
1:C:37:VAL:HG13	1:C:57:GLY:HA2	1.99	0.44
1:C:153:VAL:HG12	1:C:157:TYR:HE1	1.82	0.44
1:C:201:ALA:HA	1:C:225:GLN:OE1	2.18	0.44
1:D:26:VAL:HG12	1:D:27:SER:N	2.33	0.44
1:D:237:ALA:O	1:D:240:ARG:N	2.49	0.44
1:A:276:TYR:O	1:A:278:VAL:N	2.50	0.44
1:B:13:HIS:CE1	1:C:116:LEU:HD23	2.52	0.44
1:B:26:VAL:HG22	1:B:308:ARG:CG	2.47	0.44
1:B:267:LYS:HB3	1:B:268:HIS:ND1	2.32	0.44
1:D:24:SER:OG	1:D:305:THR:HG23	2.18	0.44
1:D:42:ASP:O	1:D:43:ASP:HB2	2.18	0.44
1:D:105:VAL:CG2	1:D:162:CYS:H	2.31	0.44
1:D:254:GLY:O	1:D:255:LEU:C	2.56	0.44
1:B:90:GLN:HG2	1:B:131:HIS:CE1	2.52	0.44
1:B:153:VAL:O	1:B:156:ALA:HB3	2.18	0.44
1:B:252:LYS:HG3	1:B:278:VAL:CG1	2.47	0.44
1:C:170:MET:O	1:C:172:ASP:N	2.49	0.44
1:C:255:LEU:HD21	1:D:256:PRO:HA	1.99	0.44
1:C:258:LEU:C	1:C:260:MET:N	2.71	0.44
1:D:119:CYS:O	1:D:165:VAL:HA	2.18	0.44
1:A:284:MET:HG3	1:B:294:PHE:HZ	1.82	0.44
1:B:119:CYS:HB3	1:B:157:TYR:CD2	2.53	0.44
1:C:33:TYR:HE1	1:C:318:TYR:O	2.01	0.44
1:A:8:HIS:CE1	1:B:171:MET:HA	2.53	0.44
1:A:233:LEU:HD11	1:B:11:TYR:CD1	2.52	0.44
1:A:259:ASP:HA	1:B:259:ASP:HA	1.99	0.44
1:C:260:MET:HE3	1:D:309:ARG:NE	2.26	0.44
1:D:155:LEU:HD23	1:D:155:LEU:C	2.38	0.44
1:D:290:GLN:C	1:D:292:GLY:H	2.21	0.44
1:A:276:TYR:HA	1:A:316:ILE:HB	2.00	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:47:ILE:HD11	1:D:55:ARG:HG3	1.99	0.44
1:D:251:VAL:HG23	1:D:273:LEU:HD21	1.99	0.44
1:D:74:ARG:O	1:D:116:LEU:N	2.50	0.43
1:A:242:ILE:HD12	1:A:242:ILE:O	2.18	0.43
1:A:286:TRP:O	1:A:289:ALA:N	2.52	0.43
1:B:40:VAL:O	1:B:41:PRO:O	2.36	0.43
1:B:42:ASP:HA	1:B:60:GLN:HE21	1.83	0.43
1:B:65:LEU:HD12	1:B:112:PHE:CE2	2.53	0.43
1:D:46:PRO:HA	1:D:54:ALA:CB	2.48	0.43
1:D:199:LYS:HD3	1:D:252:LYS:HD3	1.99	0.43
1:B:40:VAL:CG1	1:B:43:ASP:HB3	2.45	0.43
1:B:49:SER:O	1:B:51:PRO:HD3	2.17	0.43
1:B:85:VAL:CG1	1:B:86:PRO:HD2	2.48	0.43
1:C:258:LEU:O	1:C:260:MET:N	2.52	0.43
1:A:55:ARG:NH2	1:A:211:ALA:HA	2.33	0.43
1:B:36:PHE:HB2	1:B:55:ARG:HA	2.01	0.43
1:B:64:MET:HG3	1:B:65:LEU:CD2	2.49	0.43
1:A:257:TYR:HD1	1:B:309:ARG:CZ	2.31	0.43
1:B:155:LEU:HD23	1:B:156:ALA:N	2.34	0.43
1:B:231:ARG:O	1:B:234:ALA:HB3	2.18	0.43
1:B:294:PHE:CD1	1:B:299:ALA:HB2	2.54	0.43
1:C:202:SER:OG	1:D:302:GLU:OE1	2.32	0.43
1:C:305:THR:O	1:C:306:ALA:C	2.57	0.43
1:C:325:LYS:C	1:C:327:LEU:N	2.72	0.43
1:D:209:ARG:C	1:D:211:ALA:H	2.21	0.43
1:D:260:MET:O	1:D:264:VAL:HG13	2.19	0.43
1:B:168:SER:HB3	1:B:196:TYR:CD1	2.54	0.43
1:C:74:ARG:NH1	1:C:74:ARG:HB3	2.34	0.43
1:A:40:VAL:CG1	1:A:43:ASP:HB2	2.49	0.43
1:A:147:ARG:HD3	1:A:147:ARG:HA	1.82	0.43
1:A:265:LYS:CE	1:A:269:PRO:HA	2.49	0.43
1:A:279:SER:N	1:A:318:TYR:HE2	2.17	0.43
1:B:250:MET:HG2	1:B:251:VAL:H	1.84	0.43
1:B:277:GLN:HG2	1:B:277:GLN:O	2.18	0.43
1:B:301:LEU:O	1:B:304:MET:HB2	2.19	0.43
1:C:61:LEU:O	1:C:63:GLU:N	2.39	0.43
1:C:203:CYS:O	1:C:205:TYR:N	2.51	0.43
1:D:11:TYR:C	1:D:13:HIS:N	2.71	0.43
1:D:54:ALA:HB3	1:D:56:TYR:CE1	2.54	0.43
1:D:167:PRO:HG2	1:D:178:ILE:HG13	1.99	0.43
1:D:235:LEU:HD13	1:D:267:LYS:HD3	2.00	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:55:ARG:NH2	1:A:212:ALA:N	2.65	0.43
1:A:249:LEU:CB	1:A:273:LEU:HD23	2.48	0.43
1:C:32:ILE:CD1	1:C:316:ILE:HG12	2.47	0.43
1:C:64:MET:SD	1:C:64:MET:C	2.97	0.43
1:D:21:THR:O	1:D:21:THR:HG23	2.19	0.43
1:A:118:ALA:HA	1:A:164:VAL:O	2.19	0.43
1:B:55:ARG:HD3	1:B:211:ALA:O	2.19	0.43
1:B:254:GLY:O	1:B:257:TYR:N	2.41	0.43
1:C:207:PRO:HG3	1:D:293:ALA:CB	2.47	0.43
1:A:289:ALA:C	1:A:291:ALA:N	2.63	0.43
1:A:62:GLU:O	1:A:62:GLU:HG3	2.19	0.42
1:A:255:LEU:HD12	1:A:258:LEU:HD22	2.00	0.42
1:B:295:ASP:OD2	1:B:295:ASP:C	2.58	0.42
1:C:11:TYR:C	1:C:13:HIS:H	2.22	0.42
1:C:81:VAL:HG21	1:C:211:ALA:O	2.19	0.42
1:C:170:MET:SD	1:C:174:ARG:NH2	2.92	0.42
1:D:158:ALA:N	1:D:162:CYS:HB3	2.34	0.42
1:A:11:TYR:O	1:A:12:PHE:CD2	2.72	0.42
1:A:300:VAL:C	1:A:302:GLU:N	2.72	0.42
1:B:12:PHE:CE2	1:B:16:LEU:HD23	2.53	0.42
1:B:47:ILE:HD11	1:B:55:ARG:NE	2.34	0.42
1:B:176:GLU:O	1:B:180:ALA:HB2	2.19	0.42
1:C:73:LEU:HD21	1:C:76:VAL:CG1	2.49	0.42
1:D:19:TRP:C	1:D:21:THR:N	2.71	0.42
1:D:122:CYS:C	1:D:123:LEU:HG	2.40	0.42
1:A:50:LEU:HB3	1:A:53:VAL:HB	2.00	0.42
1:A:65:LEU:C	1:A:67:PRO:HD2	2.38	0.42
1:A:251:VAL:O	1:A:275:VAL:HA	2.19	0.42
1:B:250:MET:HG2	1:B:251:VAL:N	2.34	0.42
1:C:41:PRO:O	1:C:57:GLY:HA3	2.18	0.42
1:C:257:TYR:CD1	1:D:309:ARG:NH2	2.87	0.42
1:D:35:ILE:HD13	1:D:77:LEU:O	2.19	0.42
1:D:117:VAL:HB	1:D:163:GLN:H	1.84	0.42
1:D:276:TYR:CD2	1:D:316:ILE:HG21	2.55	0.42
1:A:176:GLU:HB2	1:A:244:GLU:HB3	2.02	0.42
1:A:232:GLY:C	1:A:234:ALA:N	2.73	0.42
1:B:309:ARG:O	1:B:309:ARG:HG2	2.18	0.42
1:D:58:VAL:HG21	1:D:103:GLU:OE1	2.20	0.42
1:D:99:SER:HB3	1:D:102:ILE:CG1	2.48	0.42
1:D:276:TYR:C	1:D:276:TYR:CD1	2.92	0.42
1:D:286:TRP:C	1:D:288:GLY:N	2.72	0.42



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:255:LEU:HG	1:B:255:LEU:CD1	2.49	0.42
1:B:123:LEU:HD23	1:B:130:GLY:N	2.31	0.42
1:B:177:ALA:HA	1:B:180:ALA:HB3	2.00	0.42
1:C:102:ILE:HA	1:C:105:VAL:CG1	2.49	0.42
1:C:286:TRP:C	1:C:288:GLY:N	2.73	0.42
1:D:227:PRO:O	1:D:228:PRO:O	2.38	0.42
1:D:259:ASP:CG	1:D:260:MET:H	2.23	0.42
1:A:174:ARG:HG2	1:A:174:ARG:HH11	1.85	0.42
1:A:277:GLN:HE22	1:A:319:PHE:HD2	1.67	0.42
1:B:41:PRO:O	1:B:42:ASP:C	2.55	0.42
1:B:50:LEU:O	1:B:51:PRO:C	2.57	0.42
1:C:33:TYR:CD1	1:C:321:PRO:HD3	2.55	0.42
1:C:265:LYS:HD2	1:C:311:GLY:HA2	2.02	0.42
1:D:232:GLY:O	1:D:233:LEU:C	2.57	0.42
1:A:170:MET:HE3	1:A:174:ARG:NH2	2.34	0.42
1:A:226:LEU:HD12	1:A:226:LEU:N	2.35	0.42
1:B:33:TYR:CD1	1:B:321:PRO:HD3	2.55	0.42
1:B:38:THR:OG1	1:B:45:GLN:NE2	2.53	0.42
1:B:46:PRO:HA	1:B:54:ALA:HB2	1.99	0.42
1:B:262:ARG:NH2	1:B:309:ARG:O	2.52	0.42
1:C:38:THR:HG23	1:C:55:ARG:CB	2.48	0.42
1:C:74:ARG:O	1:C:115:LEU:HD12	2.20	0.42
1:D:116:LEU:HD11	1:D:164:VAL:HG21	2.00	0.42
1:D:120:ASP:OD1	1:D:121:VAL:N	2.53	0.42
1:D:155:LEU:HD23	1:D:159:LYS:HG3	2.01	0.42
1:D:167:PRO:HB3	1:D:174:ARG:HD2	2.01	0.42
1:B:237:ALA:O	1:B:240:ARG:N	2.52	0.42
1:C:8:HIS:C	1:C:10:GLY:H	2.23	0.42
1:C:147:ARG:HE	1:C:173:GLY:CA	2.32	0.42
1:C:149:ARG:C	1:C:151:ALA:N	2.73	0.42
1:C:207:PRO:HD3	1:D:293:ALA:O	2.20	0.42
1:C:282:PHE:C	1:C:282:PHE:CD1	2.93	0.42
1:D:176:GLU:HB2	1:D:244:GLU:CG	2.47	0.42
1:A:147:ARG:NE	1:A:147:ARG:CA	2.83	0.42
1:A:193:VAL:N	1:A:247:ASP:OD2	2.45	0.42
1:A:197:SER:HB3	1:A:238:VAL:HG22	2.02	0.42
1:C:61:LEU:HD23	1:C:108:LEU:HD21	2.02	0.42
1:D:19:TRP:O	1:D:21:THR:N	2.52	0.42
1:B:73:LEU:HD12	1:B:324:LEU:HD11	2.02	0.42
1:B:200:PHE:HE1	1:B:257:TYR:HB3	1.85	0.42
1:C:255:LEU:CD2	1:D:255:LEU:HD12	2.47	0.42



	A de la construction de la const	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:13:HIS:O	1:D:17:ARG:HG3	2.20	0.42
1:D:266:ASP:C	1:D:268:HIS:N	2.72	0.42
1:B:209:ARG:HH12	1:B:221:ARG:HH22	1.68	0.41
1:C:121:VAL:HB	1:C:167:PRO:HA	2.00	0.41
1:C:151:ALA:O	1:C:153:VAL:N	2.52	0.41
1:C:258:LEU:C	1:C:260:MET:H	2.22	0.41
1:C:289:ALA:O	1:C:291:ALA:N	2.46	0.41
1:D:44:VAL:O	1:D:46:PRO:HD3	2.20	0.41
1:D:78:ILE:CG2	1:D:79:PHE:N	2.83	0.41
1:D:166:ALA:O	1:D:196:TYR:CE1	2.73	0.41
1:A:47:ILE:C	1:A:49:SER:H	2.23	0.41
1:A:151:ALA:HB2	1:A:178:ILE:HD12	2.02	0.41
1:A:195:SER:O	1:A:197:SER:N	2.53	0.41
1:A:295:ASP:OD2	1:A:296:LEU:N	2.53	0.41
1:B:16:LEU:HD12	1:B:16:LEU:HA	1.91	0.41
1:B:74:ARG:HB3	1:C:15:LEU:HD22	2.02	0.41
1:B:77:LEU:HD23	1:B:118:ALA:O	2.20	0.41
1:B:90:GLN:HA	1:B:131:HIS:CE1	2.55	0.41
1:B:226:LEU:HA	1:B:227:PRO:HD2	1.93	0.41
1:C:175:VAL:HG22	1:C:195:SER:HB2	2.02	0.41
1:C:258:LEU:HB3	1:D:259:ASP:H	1.85	0.41
1:D:77:LEU:HD12	1:D:316:ILE:HD13	2.02	0.41
1:D:253:PRO:HA	1:D:278:VAL:HG13	2.01	0.41
1:A:252:LYS:HA	1:A:253:PRO:C	2.40	0.41
1:C:34:PRO:HG2	1:C:318:TYR:CD1	2.55	0.41
1:C:233:LEU:HD11	1:D:11:TYR:CD1	2.55	0.41
1:D:33:TYR:HA	1:D:34:PRO:HD3	1.75	0.41
1:D:36:PHE:HB2	1:D:55:ARG:HA	2.02	0.41
1:D:120:ASP:CG	1:D:121:VAL:N	2.73	0.41
1:A:35:ILE:HD13	1:A:35:ILE:H	1.83	0.41
1:B:296:LEU:HG	1:B:300:VAL:HG21	2.02	0.41
1:C:20:GLN:HE21	1:D:233:LEU:CD1	2.34	0.41
1:C:80:GLY:HA3	1:C:101:THR:HG23	2.02	0.41
1:D:70:GLU:C	1:D:72:GLY:N	2.74	0.41
1:D:171:MET:O	1:D:172:ASP:C	2.57	0.41
1:A:326:TRP:O	1:A:328:LYS:N	2.53	0.41
1:B:199:LYS:HZ1	1:B:252:LYS:HZ1	1.67	0.41
1:C:44:VAL:O	1:C:44:VAL:HG12	2.20	0.41
1:C:228:PRO:HD3	2:C:340:HOH:O	2.20	0.41
1:A:143:SER:C	1:A:145:GLU:H	2.22	0.41
1:B:62:GLU:HB2	1:B:111:THR:HG21	2.01	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:255:LEU:O	1:B:255:LEU:HD13	2.20	0.41
1:C:33:TYR:CE1	1:C:318:TYR:O	2.73	0.41
1:C:323:LEU:C	1:C:325:LYS:N	2.72	0.41
1:D:14:PRO:N	1:D:17:ARG:NH1	2.68	0.41
1:D:75:CYS:SG	1:D:76:VAL:N	2.94	0.41
1:D:270:GLU:H	1:D:270:GLU:HG2	1.69	0.41
1:B:42:ASP:O	1:B:43:ASP:HB2	2.21	0.41
1:B:231:ARG:HG3	1:B:260:MET:CE	2.48	0.41
1:B:323:LEU:O	1:B:326:TRP:N	2.52	0.41
1:C:73:LEU:HD21	1:C:76:VAL:HG13	2.03	0.41
1:D:39:ASP:OD1	1:D:39:ASP:N	2.53	0.41
1:D:117:VAL:HB	1:D:163:GLN:HB2	2.02	0.41
1:D:308:ARG:C	1:D:310:ALA:N	2.72	0.41
1:A:15:LEU:O	1:A:18:SER:N	2.54	0.41
1:A:17:ARG:HD3	1:B:222:ARG:O	2.21	0.41
1:A:77:LEU:C	1:A:77:LEU:HD23	2.41	0.41
1:A:102:ILE:O	1:A:105:VAL:N	2.54	0.41
1:A:112:PHE:HA	1:A:113:PRO:HD2	1.95	0.41
1:A:152:GLU:HG3	1:A:153:VAL:N	2.35	0.41
1:A:199:LYS:HE2	1:A:252:LYS:NZ	2.32	0.41
1:B:129:HIS:CE1	2:B:342:HOH:O	2.74	0.41
1:C:157:TYR:O	1:C:160:ALA:HB3	2.20	0.41
1:C:197:SER:HB2	1:C:198:ALA:H	1.58	0.41
1:C:262:ARG:NH2	1:C:309:ARG:O	2.53	0.41
1:D:221:ARG:C	1:D:223:CYS:H	2.24	0.41
1:A:15:LEU:O	1:A:16:LEU:C	2.59	0.41
1:A:33:TYR:HB2	1:A:320:ALA:HB2	2.00	0.41
1:A:147:ARG:NH1	1:A:171:MET:HB2	2.36	0.41
1:A:197:SER:HB2	1:A:250:MET:O	2.21	0.41
1:B:122:CYS:O	1:B:123:LEU:HD13	2.21	0.41
1:B:207:PRO:HB2	1:B:279:SER:CB	2.47	0.41
1:B:296:LEU:HD23	1:B:326:TRP:CH2	2.54	0.41
1:B:308:ARG:HA	1:B:308:ARG:NE	2.33	0.41
1:C:8:HIS:HA	1:C:11:TYR:CE1	2.56	0.41
1:C:73:LEU:HD12	1:C:74:ARG:H	1.85	0.41
1:C:112:PHE:HA	1:C:113:PRO:HD2	1.88	0.41
1:C:171:MET:O	1:C:172:ASP:C	2.59	0.41
1:C:174:ARG:HG3	1:C:175:VAL:H	1.86	0.41
1:C:205:TYR:O	1:C:206:GLY:C	2.59	0.41
1:C:273:LEU:HD12	1:C:312:ALA:CA	2.51	0.41
1:C:315:ILE:HD12	1:C:315:ILE:N	2.36	0.41



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:C:319:PHE:O	1:C:322:GLN:HG2	2.21	0.41
1:C:325:LYS:O	1:C:327:LEU:N	2.53	0.41
1:D:20:GLN:OE1	1:D:20:GLN:HA	2.21	0.41
1:D:175:VAL:HG23	2:D:336:HOH:O	2.20	0.41
1:D:255:LEU:N	1:D:256:PRO:CD	2.84	0.41
1:A:32:ILE:HD13	1:A:314:ILE:CG2	2.45	0.41
1:A:84:ARG:HH21	1:A:84:ARG:CB	2.23	0.41
1:C:238:VAL:CG1	1:C:249:LEU:HD13	2.51	0.41
1:D:13:HIS:CE1	1:D:15:LEU:H	2.38	0.41
1:D:57:GLY:O	1:D:61:LEU:HB2	2.21	0.41
1:D:97:GLU:HG2	1:D:98:ASP:OD2	2.21	0.41
1:D:156:ALA:O	1:D:157:TYR:C	2.59	0.41
1:D:161:GLY:O	1:D:162:CYS:C	2.58	0.41
1:D:193:VAL:O	1:D:195:SER:N	2.49	0.41
1:A:319:PHE:O	1:A:320:ALA:C	2.59	0.40
1:B:38:THR:HG22	1:B:81:VAL:HB	2.02	0.40
1:B:38:THR:CG2	1:B:45:GLN:HE22	2.29	0.40
1:B:192:SER:HA	1:B:247:ASP:OD2	2.21	0.40
1:C:273:LEU:HD13	1:C:273:LEU:C	2.42	0.40
1:D:32:ILE:HB	1:D:316:ILE:HG12	2.01	0.40
1:D:264:VAL:HG23	1:D:265:LYS:N	2.37	0.40
1:A:57:GLY:O	1:A:60:GLN:N	2.55	0.40
1:A:124:CYS:HA	1:A:125:PRO:HD2	1.98	0.40
1:A:166:ALA:CB	1:A:194:MET:O	2.69	0.40
1:B:13:HIS:CD2	1:C:116:LEU:HD23	2.57	0.40
1:B:205:TYR:OH	1:B:253:PRO:HD3	2.22	0.40
1:B:323:LEU:O	1:B:327:LEU:HD13	2.20	0.40
1:C:322:GLN:O	1:C:325:LYS:HB3	2.21	0.40
1:D:205:TYR:HE1	1:D:252:LYS:CE	2.30	0.40
1:D:221:ARG:HA	1:D:224:TYR:OH	2.21	0.40
1:D:325:LYS:HB2	1:D:325:LYS:NZ	2.36	0.40
1:B:179:LYS:HD3	1:B:193:VAL:HG21	2.02	0.40
1:C:47:ILE:CD1	1:C:54:ALA:HA	2.52	0.40
1:C:194:MET:HG3	1:C:248:MET:HG3	2.03	0.40
1:C:261:VAL:HG13	1:C:273:LEU:HD11	2.03	0.40
1:C:323:LEU:HA	1:C:326:TRP:HE3	1.86	0.40
1:D:33:TYR:HE1	1:D:318:TYR:O	2.04	0.40
1:D:149:ARG:C	1:D:151:ALA:N	2.74	0.40
1:D:214:SER:O	1:D:215:SER:HB3	2.20	0.40
1:D:225:GLN:O	1:D:226:LEU:O	2.39	0.40
1:A:66:ARG:HG2	1:A:66:ARG:NH1	2.35	0.40



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:304:MET:O	1:A:306:ALA:N	2.54	0.40
1:B:15:LEU:O	1:B:16:LEU:C	2.60	0.40
1:B:84:ARG:HG3	1:B:84:ARG:O	2.21	0.40
1:B:153:VAL:HG12	1:B:157:TYR:CE1	2.57	0.40
1:C:95:ASP:HB3	1:C:153:VAL:HA	2.04	0.40
1:C:238:VAL:HG11	1:C:249:LEU:HD13	2.02	0.40
1:D:105:VAL:O	1:D:109:ARG:HB2	2.22	0.40
1:D:122:CYS:SG	1:D:123:LEU:N	2.93	0.40
1:D:147:ARG:O	1:D:148:GLN:C	2.60	0.40
1:D:186:GLY:O	1:D:188:GLY:N	2.54	0.40
1:D:285:LEU:HD12	1:D:319:PHE:HE2	1.86	0.40
1:A:177:ALA:O	1:A:180:ALA:HB3	2.21	0.40
1:A:234:ALA:C	1:A:236:ARG:N	2.75	0.40
1:B:27:SER:C	1:B:29:SER:H	2.24	0.40
1:B:37:VAL:HA	1:B:56:TYR:O	2.21	0.40
1:B:75:CYS:SG	1:B:76:VAL:N	2.95	0.40
1:B:282:PHE:O	1:B:283:ALA:C	2.60	0.40
1:C:43:ASP:O	1:C:44:VAL:HG23	2.22	0.40
1:C:306:ALA:CB	1:C:309:ARG:HH22	2.35	0.40
1:D:110:LYS:CE	1:D:110:LYS:CA	2.99	0.40
1:D:166:ALA:O	1:D:196:TYR:HE1	2.04	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	ntiles
1	А	282/330~(86%)	196 (70%)	68 (24%)	18 (6%)	1	9
1	В	316/330~(96%)	203 (64%)	80 (25%)	33 (10%)	0	3
1	С	280/330~(85%)	179 (64%)	60 (21%)	41 (15%)	0	1
1	D	290/330~(88%)	178 (61%)	79 (27%)	33 (11%)	0	2



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1168/1320~(88%)	756~(65%)	287~(25%)	125 (11%)	0 3

All (125) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	58	VAL
1	А	226	LEU
1	А	278	VAL
1	А	290	GLN
1	В	12	PHE
1	В	41	PRO
1	В	42	ASP
1	В	58	VAL
1	В	59	ASN
1	В	86	PRO
1	В	92	SER
1	В	134	LEU
1	В	220	ASP
1	В	225	GLN
1	В	226	LEU
1	В	246	ALA
1	В	298	THR
1	С	5	SER
1	С	12	PHE
1	С	24	SER
1	С	39	ASP
1	С	42	ASP
1	С	58	VAL
1	С	73	LEU
1	С	82	PRO
1	C	122	CYS
1	С	206	GLY
1	С	293	ALA
1	C	311	GLY
1	C	312	ALA
1	D	12	PHE
1	D	41	PRO
1	D	42	ASP
1	D	58	VAL
1	D	115	LEU
1	D	228	PRO
1	А	82	PRO



Mol	Chain	Res	Tvpe
1	A	197	SER.
1	A	264	VAL
1	A	275	VAL
1	R	43	ASP
1	B	88	ASP
1	B	147	ARG
1	B	211	ALA
1	C	41	PRO
1	C	44	VAL
1	C	59	ASN
1	C	83	SER
1	C	154	ALA
1	C	172	ASP
1	C	186	GLY
1	C	204	PHE
1	C	278	VAL
1	D	5	SER
1	D	20	GLN
1	D	21	THR
1	D	59	ASN
1	D	143	SER
1	D	162	CYS
1	D	187	LEU
1	D	197	SER
1	D	226	LEU
1	D	229	GLY
1	D	232	GLY
1	D	267	LYS
1	D	293	ALA
1	D	324	LEU
1	А	209	ARG
1	В	8	HIS
1	В	56	TYR
1	В	60	GLN
1	В	130	GLY
1	В	133	GLY
1	В	136	SER
1	В	278	VAL
1	В	294	PHE
1	В	309	ARG
1	С	9	SER
1	С	150	LEU
	1	L	



1         C         170         MET           1         C         184         LYS           1         C         228         PRO           1         C         324         LEU           1         D         194         MET           1         D         234         ALA           1         D         234         ALA           1         B         9         SER           1         B         154         ALA           1         C         30         ASN           1         C         270         GLU           1         C         307         PHE           1         C         320         ALA           1         C         320         ALA           1         C         320         ALA           1         D         292         GLY           1         A         41         PRO           1         A         327         LEU           1         A         327         LEU           1         A         326         TRP           1         A         326	Mol	Chain	Res	Type
1         C         184         LYS           1         C         228         PRO           1         C         324         LEU           1         D         194         MET           1         D         234         ALA           1         A         8         HIS           1         B         9         SER           1         B         154         ALA           1         C         30         ASN           1         C         270         GLU           1         C         307         PHE           1         C         320         ALA           1         C         320         ALA           1         C         320         ALA           1         D         213         GLN           1         D         292         GLY           1         A         41         PRO           1         A         327         LEU           1         A         327         LEU           1         B         322         GLN           1         C         326	1	С	170	MET
1         C         228         PRO           1         C         324         LEU           1         D         194         MET           1         D         234         ALA           1         D         234         ALA           1         D         234         ALA           1         D         234         ALA           1         B         9         SER           1         B         154         ALA           1         C         30         ASN           1         C         270         GLU           1         C         307         PHE           1         C         320         ALA           1         C         320         ALA           1         D         213         GLN           1         D         292         GLY           1         A         41         PRO           1         A         327         LEU           1         A         327         LEU           1         B         105         VAL           1         B         326	1	C	184	LYS
1         C         324         LEU           1         D         194         MET           1         D         234         ALA           1         A         8         HIS           1         B         9         SER           1         B         154         ALA           1         C         30         ASN           1         C         270         GLU           1         C         270         GLU           1         C         307         PHE           1         C         320         ALA           1         C         320         ALA           1         C         320         ALA           1         D         292         GLY           1         A         41         PRO           1         A         33         SER           1         A         327         LEU           1         A         327         LEU           1         B         105         VAL           1         B         322         GLN           1         C         529	1	C	228	PRO
1         D         194         MET           1         D         234         ALA           1         A         8         HIS           1         B         9         SER           1         B         154         ALA           1         B         154         ALA           1         C         30         ASN           1         C         270         GLU           1         C         290         GLN           1         C         307         PHE           1         C         320         ALA           1         C         320         ALA           1         D         213         GLN           1         D         292         GLY           1         A         41         PRO           1         A         327         LEU           1         A         327         LEU           1         B         105         VAL           1         B         322         GLN           1         C         62         GLU           1         C         326	1	C	324	LEU
1         D         234         ALA           1         A         8         HIS           1         B         9         SER           1         B         154         ALA           1         C         30         ASN           1         C         270         GLU           1         C         290         GLN           1         C         307         PHE           1         C         320         ALA           1         C         320         ALA           1         C         321         PRO           1         D         213         GLN           1         D         292         GLY           1         A         41         PRO           1         A         83         SER           1         A         286         TRP           1         A         327         LEU           1         B         322         GLN           1         C         62         GLU           1         C         326         TRP           1         D         108	1	D	194	MET
1         A         8         HIS           1         B         9         SER           1         B         154         ALA           1         C         30         ASN           1         C         270         GLU           1         C         290         GLN           1         C         307         PHE           1         C         307         PHE           1         C         320         ALA           1         C         321         PRO           1         D         213         GLN           1         D         292         GLY           1         A         41         PRO           1         A         41         PRO           1         A         327         LEU           1         B         105         VAL           1         B         322         GLN           1         C         62         GLU           1         C         326         TRP           1         D         108         LEU           1         D         236	1	D	234	ALA
1         B         9         SER           1         B         154         ALA           1         C         30         ASN           1         C         270         GLU           1         C         270         GLN           1         C         307         PHE           1         C         320         ALA           1         C         320         ALA           1         C         320         ALA           1         C         321         PRO           1         D         292         GLY           1         A         41         PRO           1         A         83         SER           1         A         83         SER           1         A         286         TRP           1         B         105         VAL           1         B         322         GLN           1         C         62         GLU           1         D         43         ASP           1         D         108         LEU           1         D         236	1	A	8	HIS
1         B         154         ALA           1         C         30         ASN           1         C         270         GLU           1         C         290         GLN           1         C         307         PHE           1         C         320         ALA           1         C         320         ALA           1         C         321         PRO           1         D         213         GLN           1         D         292         GLY           1         A         41         PRO           1         A         41         PRO           1         A         83         SER           1         A         83         SER           1         A         286         TRP           1         B         105         VAL           1         B         322         GLN           1         C         62         GLU           1         C         326         TRP           1         D         172         ASP           1         D         282	1	B	9	SER
1         D         101         HBA           1         C         30         ASN           1         C         270         GLU           1         C         290         GLN           1         C         307         PHE           1         C         320         ALA           1         C         321         PRO           1         D         213         GLN           1         D         292         GLY           1         A         41         PRO           1         A         41         PRO           1         A         41         PRO           1         A         83         SER           1         A         83         SER           1         A         327         LEU           1         B         105         VAL           1         B         322         GLN           1         C         259         ASP           1         D         43         ASP           1         D         172         ASP           1         D         236	1	B	154	ALA
1       C       270       GLU         1       C       290       GLN         1       C       307       PHE         1       C       320       ALA         1       C       321       PRO         1       D       213       GLN         1       D       292       GLY         1       A       41       PRO         1       A       41       PRO         1       A       41       PRO         1       A       43       SER         1       A       286       TRP         1       A       327       LEU         1       B       105       VAL         1       B       322       GLN         1       C       62       GLU         1       C       326       TRP         1       D       108       LEU         1       D       108       LEU         1       D       236       ARG         1       D       282       PHE         1       A       12       PHE         1       B	1	C	30	ASN
1         C         290         GLN           1         C         307         PHE           1         C         320         ALA           1         C         321         PRO           1         D         213         GLN           1         D         213         GLN           1         D         292         GLY           1         A         41         PRO           1         A         41         PRO           1         A         41         PRO           1         A         83         SER           1         A         286         TRP           1         A         327         LEU           1         B         322         GLN           1         C         62         GLU           1         C         326         TRP           1         D         108         LEU           1         D         172         ASP           1         D         236         ARG           1         D         282         PHE           1         A         12	1	C	270	GLU
1         C         307         PHE           1         C         320         ALA           1         C         321         PRO           1         D         213         GLN           1         D         292         GLY           1         A         41         PRO           1         A         41         PRO           1         A         43         SER           1         A         286         TRP           1         A         327         LEU           1         B         105         VAL           1         B         322         GLN           1         C         62         GLU           1         C         326         TRP           1         D         108         LEU           1         D         108         LEU           1         D         236         ARG           1         D         236         ARG           1         D         282         PHE           1         A         12         PHE           1         B         125	1	C	290	GLN
1         C         320         ALA           1         C         321         PRO           1         D         213         GLN           1         D         292         GLY           1         A         41         PRO           1         A         41         PRO           1         A         41         PRO           1         A         83         SER           1         A         286         TRP           1         A         327         LEU           1         B         105         VAL           1         B         322         GLN           1         C         62         GLU           1         C         326         TRP           1         D         108         LEU           1         D         108         LEU           1         D         108         LEU           1         D         236         ARG           1         D         282         PHE           1         B         125         PRO           1         C         162	1	C	307	PHE
1       C $321$ PRO         1       D $213$ GLN         1       D $292$ GLY         1       A       41       PRO         1       A       41       PRO         1       A       41       PRO         1       A       43       SER         1       A $327$ LEU         1       B $105$ VAL         1       B $322$ GLN         1       C $62$ GLU         1       C $62$ GLU         1       C $326$ TRP         1       D $43$ ASP         1       D $108$ LEU         1       D $172$ ASP         1       D $236$ ARG         1       D $282$ PHE         1       A $12$ PHE         1       B $125$ PRO         1       C $162$ CYS         1       C $171$ MET	1	C	320	ALA
1       D       213       GLN         1       D       292       GLY         1       A       41       PRO         1       A       41       PRO         1       A       83       SER         1       A       286       TRP         1       A       327       LEU         1       B       105       VAL         1       B       322       GLN         1       C       62       GLU         1       C       59       ASP         1       C       326       TRP         1       D       43       ASP         1       D       108       LEU         1       D       108       LEU         1       D       108       LEU         1       D       236       ARG         1       D       282       PHE         1       A       12       PHE         1       B       125       PRO         1       C       162       CYS         1       C       210       ASP         1       D<	1	C	321	PRO
1         D         292         GLY           1         A         41         PRO           1         A         83         SER           1         A         286         TRP           1         A         286         TRP           1         A         327         LEU           1         B         105         VAL           1         B         322         GLN           1         C         62         GLU           1         C         326         TRP           1         D         43         ASP           1         D         108         LEU           1         D         108         LEU           1         D         172         ASP           1         D         236         ARG           1         D         282         PHE           1         A         12         PHE           1         B         125         PRO           1         C         162         CYS           1         C         210         ASP           1         D         269	1	D	213	GLN
1       A       41       PRO         1       A       83       SER         1       A       286       TRP         1       A       286       TRP         1       A       327       LEU         1       B       105       VAL         1       B       322       GLN         1       C       62       GLU         1       C       326       TRP         1       C       326       TRP         1       D       43       ASP         1       D       108       LEU         1       D       108       LEU         1       D       108       LEU         1       D       108       LEU         1       D       236       ARG         1       D       282       PHE         1       A       12       PHE         1       B       125       PRO         1       C       162       CYS         1       C       171       MET         1       C       210       ASP         1	1	D	292	GLY
1       A       83       SER         1       A       286       TRP         1       A       327       LEU         1       B       105       VAL         1       B       322       GLN         1       B       322       GLN         1       C       62       GLU         1       C       326       TRP         1       D       43       ASP         1       D       108       LEU         1       D       108       LEU         1       D       236       ARG         1       D       282       PHE         1       D       282       PHE         1       A       12       PHE         1       B       125       PRO         1       C       162       CYS         1       C       171       MET         1       C       210       ASP         1       D       269       PRO         1       A       113       PRO         1       B       188       GLY         1 <td< th=""><th>1</th><th>A</th><th>41</th><th>PRO</th></td<>	1	A	41	PRO
1       A       286       TRP         1       A       327       LEU         1       B       105       VAL         1       B       322       GLN         1       B       322       GLN         1       C       62       GLU         1       C       326       TRP         1       C       326       TRP         1       D       43       ASP         1       D       108       LEU         1       D       108       LEU         1       D       108       LEU         1       D       236       ARG         1       D       236       ARG         1       D       282       PHE         1       A       12       PHE         1       B       125       PRO         1       C       162       CYS         1       C       171       MET         1       C       210       ASP         1       D       269       PRO         1       A       113       PRO         1 <t< th=""><th>1</th><th>A</th><th>83</th><th>SER</th></t<>	1	A	83	SER
1       A $327$ LEU         1       B $105$ VAL         1       B $322$ GLN         1       C $62$ GLU         1       C $259$ ASP         1       C $326$ TRP         1       D $43$ ASP         1       D $108$ LEU         1       D $108$ LEU         1       D $108$ LEU         1       D $126$ ASP         1       D $236$ ARG         1       D $236$ ARG         1       D $282$ PHE         1       A $12$ PHE         1       B $125$ PRO         1       C $162$ CYS         1       C $210$ ASP         1       D $269$ PRO         1       A $113$ PRO         1       B $188$ GLY         1       A $102$ ILE	1	A	286	TRP
1       B $105$ VAL         1       B $322$ GLN         1       C $62$ GLU         1       C $259$ ASP         1       C $326$ TRP         1       D $43$ ASP         1       D $43$ ASP         1       D $108$ LEU         1       D $172$ ASP         1       D $236$ ARG         1       D $236$ ARG         1       D $282$ PHE         1       A $12$ PHE         1       B $125$ PRO         1       C $162$ CYS         1       C $171$ MET         1       C $210$ ASP         1       D $269$ PRO         1       A $113$ PRO         1       B $188$ GLY         1       A $102$ ILE         1       D $153$ VAL	1	A	327	LEU
1       B $322$ GLN         1       C $62$ GLU         1       C $259$ ASP         1       C $326$ TRP         1       D $43$ ASP         1       D $108$ LEU         1       D $108$ LEU         1       D $172$ ASP         1       D $236$ ARG         1       D $236$ ARG         1       D $282$ PHE         1       A $12$ PHE         1       B $125$ PRO         1       C $162$ CYS         1       C $171$ MET         1       C $210$ ASP         1       D $269$ PRO         1       A $113$ PRO         1       B $188$ GLY         1       A $102$ ILE         1       D $153$ VAL	1	B	105	VAL
1       C $62$ $GLU$ 1       C $259$ $ASP$ 1       C $326$ $TRP$ 1       D $43$ $ASP$ 1       D $43$ $ASP$ 1       D $108$ $LEU$ 1       D $172$ $ASP$ 1       D $236$ $ARG$ 1       D $236$ $ARG$ 1       D $282$ $PHE$ 1       A $12$ $PHE$ 1       B $125$ $PRO$ 1       C $162$ $CYS$ 1       C $171$ $MET$ 1       C $210$ $ASP$ 1       D $269$ $PRO$ 1       A $113$ $PRO$ 1       B $188$ $GLY$ 1       A $102$ $ILE$ 1       D $153$ $VAL$	1	B	322	GLN
1       C $259$ ASP         1       C $326$ TRP         1       D $43$ ASP         1       D $108$ LEU         1       D $108$ LEU         1       D $108$ LEU         1       D $172$ ASP         1       D $236$ ARG         1       D $236$ ARG         1       D $282$ PHE         1       A $12$ PHE         1       B $125$ PRO         1       C $162$ CYS         1       C $210$ ASP         1       C $210$ ASP         1       D $269$ PRO         1       A $113$ PRO         1       B $188$ GLY         1       A $102$ ILE         1       D $153$ VAL	1	C	62	GLU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	C	259	ASP
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	C	326	TRP
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	D	43	ASP
1       D       172       ASP         1       D       236       ARG         1       D       282       PHE         1       A       12       PHE         1       A       12       PHE         1       B       125       PRO         1       C       162       CYS         1       C       171       MET         1       C       210       ASP         1       D       269       PRO         1       A       113       PRO         1       B       188       GLY         1       A       102       ILE         1       D       253       VAL	1	D	108	LEU
1       D       236       ARG         1       D       282       PHE         1       A       12       PHE         1       B       125       PRO         1       C       162       CYS         1       C       171       MET         1       C       210       ASP         1       D       269       PRO         1       A       113       PRO         1       B       188       GLY         1       A       102       ILE         1       D       153       VAL	1	D	172	ASP
1       D       282       PHE         1       A       12       PHE         1       B       125       PRO         1       C       162       CYS         1       C       171       MET         1       C       210       ASP         1       D       269       PRO         1       A       113       PRO         1       B       188       GLY         1       A       102       ILE         1       D       153       VAL	1	D	236	ARG
1       A       12       PHE         1       B       125       PRO         1       C       162       CYS         1       C       171       MET         1       C       210       ASP         1       D       269       PRO         1       A       113       PRO         1       B       188       GLY         1       A       102       ILE         1       D       153       VAL	1	D	282	PHE
1         B         125         PRO           1         C         162         CYS           1         C         171         MET           1         C         210         ASP           1         D         269         PRO           1         A         113         PRO           1         B         188         GLY           1         A         102         ILE           1         D         153         VAL	1	А	12	PHE
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	В	125	PRO
1         C         171         MET           1         C         210         ASP           1         D         269         PRO           1         A         113         PRO           1         B         188         GLY           1         A         102         ILE           1         D         153         VAL	1	С	162	CYS
1         C         210         ASP           1         D         269         PRO           1         A         113         PRO           1         B         188         GLY           1         A         102         ILE           1         D         153         VAL	1	С	171	MET
1         D         269         PRO           1         A         113         PRO           1         B         188         GLY           1         A         102         ILE           1         D         153         VAL	1	С	210	ASP
1         A         113         PRO           1         B         188         GLY           1         A         102         ILE           1         D         153         VAL	1	D	269	PRO
1         B         188         GLY           1         A         102         ILE           1         D         153         VAL	1	А	113	PRO
1 A 102 ILE 1 D 153 VAL	1	В	188	GLY
1 D 153 VAL	1	А	102	ILE
	1	D	153	VAL
1 B 242 ILE	1	В	242	ILE



Continued from previous page...

Mol	Chain	Res	Type
1	D	14	PRO
1	А	321	PRO
1	D	215	SER
1	С	253	PRO

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain outliers of the chain as a percentile score with respect to all 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	Outliers	Percentiles
1	А	235/267~(88%)	214 (91%)	21 (9%)	9 32
1	В	258/267~(97%)	235~(91%)	23 (9%)	9 32
1	С	233/267~(87%)	216~(93%)	17 (7%)	14 41
1	D	239/267~(90%)	219~(92%)	20 (8%)	11 35
All	All	965/1068~(90%)	884 (92%)	81 (8%)	11 35

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	11	TYR
1	А	35	ILE
1	А	56	TYR
1	А	62	GLU
1	А	64	MET
1	А	74	ARG
1	А	84	ARG
1	А	105	VAL
1	А	116	LEU
1	А	123	LEU
1	А	145	GLU
1	А	147	ARG
1	А	224	TYR
1	А	240	ARG
1	А	242	ILE
1	А	248	MET
1	А	260	MET



$\mathbf{Mol}$	Chain	Res	Type
1	A	265	LYS
1	А	276	TYR
1	А	314	ILE
1	А	324	LEU
1	В	11	TYR
1	В	16	LEU
1	В	39	ASP
1	В	42	ASP
1	В	62	GLU
1	В	64	MET
1	В	66	ARG
1	В	74	ARG
1	В	77	LEU
1	В	110	LYS
1	В	116	LEU
1	В	155	LEU
1	В	189	ASN
1	В	190	ARG
1	В	231	ARG
1	В	248	MET
1	В	255	LEU
1	В	260	MET
1	В	276	TYR
1	В	308	ARG
1	В	323	LEU
1	В	325	LYS
1	В	326	TRP
1	С	11	TYR
1	С	12	PHE
1	С	39	ASP
1	С	43	ASP
1	С	75	CYS
1	С	84	ARG
1	C	157	TYR
1	С	197	SER
1	C	$20\overline{0}$	PHE
1	С	210	ASP
1	С	224	TYR
1	$\mathbf{C}$	$24\overline{2}$	ILE
1	С	265	LYS
1	C	290	GLN
1	$\mathbf{C}$	308	ARG



Mol	Chain	Res	Type
1	С	314	ILE
1	С	322	GLN
1	D	35	ILE
1	D	39	ASP
1	D	42	ASP
1	D	56	TYR
1	D	79	PHE
1	D	110	LYS
1	D	119	CYS
1	D	120	ASP
1	D	157	TYR
1	D	220	ASP
1	D	242	ILE
1	D	248	MET
1	D	249	LEU
1	D	255	LEU
1	D	260	MET
1	D	269	PRO
1	D	273	LEU
1	D	282	PHE
1	D	308	ARG
1	D	325	LYS

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	30	ASN
1	А	60	GLN
1	А	277	GLN
1	В	8	HIS
1	В	30	ASN
1	В	45	GLN
1	В	59	ASN
1	В	60	GLN
1	В	131	HIS
1	С	60	GLN
1	С	277	GLN
1	D	59	ASN
1	D	60	GLN
1	D	148	GLN
1	D	185	HIS



#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

### 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	2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	290/330~(87%)	-0.09	2 (0%) 87 8	88	25, 54, 106, 134	0
1	В	320/330~(96%)	-0.08	4 (1%) 77	77	24,56,101,127	0
1	С	288/330~(87%)	0.19	17 (5%) 22	22	36, 80, 126, 148	0
1	D	296/330~(89%)	0.18	9 (3%) 50 4	49	34, 83, 130, 143	0
All	All	1194/1320~(90%)	0.05	32 (2%) 54	52	24, 66, 120, 148	0

All (32) RSRZ outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	С	96	SER	6.2
1	С	95	ASP	5.1
1	С	38	THR	4.5
1	В	131	HIS	3.9
1	С	169	ASP	3.8
1	D	42	ASP	3.6
1	С	61	LEU	3.6
1	А	96	SER	3.4
1	D	82	PRO	3.0
1	С	37	VAL	3.0
1	С	73	LEU	2.9
1	А	187	LEU	2.9
1	С	100	PRO	2.8
1	С	40	VAL	2.7
1	В	178	ILE	2.7
1	В	98	ASP	2.6
1	D	84	ARG	2.5
1	D	39	ASP	2.4
1	С	82	PRO	2.3
1	С	36	PHE	2.3
1	В	100	PRO	2.2



		1	1 0	
Mol	Chain	Res	Type	RSRZ
1	D	12	PHE	2.2
1	С	175	VAL	2.2
1	С	212	ALA	2.2
1	С	35	ILE	2.2
1	D	188	GLY	2.2
1	D	216	PRO	2.2
1	С	145	GLU	2.2
1	D	105	VAL	2.1
1	С	72	GLY	2.1
1	С	84	ARG	2.0
1	D	149	ARG	2.0

### 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)

There are no ligands in this entry.

### 6.5 Other polymers (i)

There are no such residues in this entry.

