

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

#### Sep 10, 2023 – 10:41 AM EDT

PDB ID	:	4KN4
Title	:	X-ray crystal structure of the Escherichia coli RNA polymerase in complex
		with Benzoxazinorifamycin-2b
Authors	:	Murakami, K.S.
Deposited on	:	2013-05-08
Resolution	:	3.96  Å(reported)

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

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

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.35.1
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

## 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 3.96 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	1025 (4.22-3.70)
Clashscore	141614	1085 (4.22-3.70)
Ramachandran outliers	138981	1047 (4.22-3.70)
Sidechain outliers	138945	1039 (4.22-3.70)
RSRZ outliers	127900	1013 (4.28-3.64)

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	Δ	329	3%		220/						
1	11	025	5%		2270	••					
1	В	329	47%	18% •	33%						
1	F	300	7%	150/	200/						
1	Ľ	529	54%	15% •	30%						
1	G	329	52%	13% •	34%						
	C	1949	4%								
2	C	1342	67%		29%	••					



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Mol	Chain	$\mathbf{Length}$	Quality of chair	n		
0	TT	1949	6%			
	п	1542	68%		27%	••
	-		3%			
3	D	1407	49% 30	0%	•	18%
			5%			
3	Ι	1407	51% 2	28%	•	18%
			% •			
4	E	91	76%		19%	• • •
			4%			
4	J	91	63%	18%	••	16%
			7%			
5	Х	613	60%	22%	•	16%
			6%			
5	Y	613	56% 1	.7% •	25%	ò

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	1RL	Н	1401	-	-	-	Х



## 2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 56333 atoms, of which 122 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		Ate	oms			ZeroOcc	AltConf	Trace
1	Δ	292	Total	С	Ν	0	$\mathbf{S}$	0	0	0
	A	3∠3	2514	1571	443	492	8	0	0	0
1	D	221	Total	С	Ν	0	S	0	0	0
	D	221	1706	1065	300	335	6	0	0	0
1	Б	220	Total	С	Ν	0	S	0	0	0
1	Г	229	1775	1106	313	350	6	0	0	0
1	С	217	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
	G	211	1671	1045	293	327	6	0	0	0

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

• Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	С	1335	Total 10523	C 6601	N 1836	O 2043	S 43	0	0	0
2	Н	1335	Total 10523	C 6601	N 1836	O 2043	S 43	0	0	0

• Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1160	Total 9060	C 5695	N 1621	O 1697	S 47	0	0	0
3	Ι	1160	Total 9060	C 5695	N 1621	O 1697	S 47	0	0	0

• Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Е	90	Total 708	C 430	N 136	0 141	S 1	0	0	0
4	J	76	Total 605	C 368	N 115	0 121	S 1	0	0	0





• Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
5	v	517	Total	С	Ν	0	S	0	0	0	
	Λ	011	4198	2621	745	806	26	0	0	0	
5	V	158	Total	С	Ν	0	S	0	0	0	
5	I	400	3732	2335	671	703	23	0	0	0	

• Molecule 6 is Benzoxazinorifamycin-2<br/>b (three-letter code: 1RL) (formula:  $\rm C_{49}H_{61}N_3O_{13}).$ 



Mol	Chain	Residues		At	oms		ZeroOcc	AltConf		
6	С	1	Total	С	Η	Ν	0	0	0	
0	U	1	126	49	61	3	13	0	0	
6	Ц	1	Total	С	Η	Ν	0	0	0	
0	11	1	126	49	61	3	13	0	0	

• Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	2	Total Zn 2 2	0	0
7	Ι	2	Total Zn 2 2	0	0

• Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total Mg 1 1	0	0
8	Ι	1	Total Mg 1 1	0	0



## 3 Residue-property plots (i)

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



• Molecule 1: DNA-directed RNA polymerase subunit alpha





VAL ARG PRO CGLU VAL LYSS GLU CLYSS GLU CLYSS GLU CLYSS CFU CGLU CLEU ARSP PRO GLU CLEU VAL CLEU VAL CLEU VAL CLEU LEU VAL CLEU VAL CLEU VAL CLEU VAL CLYSS CFU CLUSS CFU CLYSS CFU C C C C C C C C

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 $\bullet$  Molecule 1: DNA-directed RNA polymerase subunit alpha



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• Molecule 2: DNA-directed RNA polymerase subunit beta





























#### L261 V262 P263 K264 Q265 F266 K238 G239 R240 S241 H242 A243 T244 T244 E247 G308 T312 T311 5312 S312 5312 S312 5312 M315 7312 M315 7312 M315 7312 M315 7312 M315 7312 M315 7312 M315 7322 M325 7322 M325 7322 M325 7322 ASP ASP ASN SER 269 1273 1274 1288 289 290 V301 7302 1361 N362 R363 T351 C352 C352 L353 T354 T355 T355 1367 1368 E458 T459 L488 M489 P490 E491 E503 P504 1511 0512 0513 0514 0514 1513 0516 2517 1519 1518 N461 K462 L463 N464 R465 R468 Q469 M470 L471 Q472 L540 R541 **A542** A543 A543 T544 H545 E477



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	184.68Å 203.97Å 307.91Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{ascolution}}(\hat{\boldsymbol{\lambda}})$	29.77 - 3.96	Depositor
Resolution (A)	29.77 - 3.96	EDS
% Data completeness	94.5 (29.77-3.96)	Depositor
(in resolution range)	90.0 (29.77-3.96)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.49 (at 3.98Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
D D.	0.251 , $0.315$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.251 , $0.316$	DCC
$R_{free}$ test set	4761 reflections $(4.99%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	151.9	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.27, $52.2$	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.43, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	56333	wwPDB-VP
Average B, all atoms $(Å^2)$	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.

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



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

## 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN,  $1\mathrm{RL}$ 

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

Mol Chain		Bond lengths		Bond angles	
WIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.19	0/2548	0.37	0/3454
1	В	0.19	0/1725	0.40	0/2337
1	F	0.20	0/1797	0.40	0/2436
1	G	0.19	0/1690	0.40	1/2290~(0.0%)
2	С	0.20	0/10690	0.39	0/14423
2	Н	0.20	0/10690	0.39	0/14423
3	D	0.20	0/9198	0.40	0/12413
3	Ι	0.20	0/9198	0.40	0/12413
4	Е	0.19	0/710	0.36	0/956
4	J	0.19	0/607	0.36	0/817
5	Х	0.20	0/4253	0.37	0/5719
5	Y	0.20	0/3783	0.36	0/5083
All	All	0.20	0/56889	0.39	1/76764~(0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	G	228	LEU	CA-CB-CG	5.14	127.13	115.30

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	2514	0	2566	66	0
1	В	1706	0	1738	62	0
1	F	1775	0	1800	40	0
1	G	1671	0	1706	45	0
2	С	10523	0	10546	373	0
2	Н	10523	0	10546	344	0
3	D	9060	0	9256	382	0
3	Ι	9060	0	9255	346	0
4	Е	708	0	719	20	0
4	J	605	0	612	16	0
5	Х	4198	0	4250	109	0
5	Y	3732	0	3809	74	0
6	С	65	61	61	6	0
6	Н	65	61	61	10	0
7	D	2	0	0	0	0
7	Ι	2	0	0	0	0
8	D	1	0	0	0	0
8	Ι	1	0	0	0	0
All	All	56211	122	56925	1751	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 15.

All (1751) 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 $(\text{\AA})$	overlap (Å)
3:I:1173:ARG:HA	3:I:1174:ARG:HB2	1.32	1.10
2:H:1119:MET:HG2	2:H:1228:GLY:HA2	1.34	1.09
3:D:1173:ARG:HA	3:D:1174:ARG:HB2	1.30	1.06
3:D:310:GLY:HA3	3:D:311:ARG:HB2	1.34	1.04
2:C:42:ASP:HB3	2:C:43:PRO:HD2	1.35	1.03
2:C:55:SER:HB3	2:C:56:VAL:HG22	1.40	1.01
3:I:858:VAL:HB	3:I:859:PRO:HD3	1.45	0.98
3:D:858:VAL:HB	3:D:859:PRO:HD3	1.46	0.98
2:C:1119:MET:HG2	2:C:1228:GLY:HA2	1.46	0.97
4:J:5:THR:HA	4:J:6:VAL:HB	1.46	0.96
2:H:54:ARG:H	2:H:55:SER:HB2	1.28	0.95
4:E:5:THR:HA	4:E:6:VAL:HB	1.46	0.95
2:H:487:LEU:HB3	2:H:488:MET:HA	1.48	0.94
2:H:488:MET:HB2	2:H:490:GLN:H	1.29	0.94
6:H:1401:1RL:H322	6:H:1401:1RL:H313	1.48	0.93
2:C:163:LYS:H	2:C:163:LYS:HD3	1.32	0.92



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:H:55:SER:HB3	2:H:56:VAL:HG22	1.48	0.92
4:E:5:THR:HA	4:E:6:VAL:CB	2.00	0.90
6:C:1401:1RL:H322	6:C:1401:1RL:H313	1.53	0.90
2:H:13:LYS:HE3	2:H:1183:ALA:HB2	1.55	0.88
4:J:5:THR:HA	4:J:6:VAL:CB	2.02	0.87
3:D:1173:ARG:HA	3:D:1174:ARG:CB	2.03	0.87
2:H:488:MET:HB2	2:H:490:GLN:N	1.89	0.87
2:C:54:ARG:H	2:C:55:SER:HB2	1.38	0.87
3:I:749:LYS:HG3	3:I:750:PRO:HD2	1.55	0.86
3:D:749:LYS:HG3	3:D:750:PRO:HD2	1.57	0.86
2:C:13:LYS:HE3	2:C:1183:ALA:HB2	1.56	0.86
2:H:660:VAL:HG13	2:H:661:VAL:HG13	1.56	0.85
2:H:487:LEU:CB	2:H:488:MET:HA	2.06	0.84
3:D:310:GLY:CA	3:D:311:ARG:HB2	2.08	0.84
3:I:1173:ARG:HA	3:I:1174:ARG:CB	2.05	0.83
3:D:1263:LYS:HA	3:D:1279:GLN:HA	1.60	0.83
3:I:1263:LYS:HA	3:I:1279:GLN:HA	1.60	0.82
2:H:1073:LYS:HD3	3:I:462:ASP:HB3	1.62	0.82
4:J:5:THR:CA	4:J:6:VAL:HB	2.09	0.82
3:D:310:GLY:HA3	3:D:311:ARG:CB	2.08	0.81
2:H:908:GLU:HG2	2:H:909:LYS:H	1.43	0.81
4:E:38:LEU:HD13	4:E:58:LEU:HD23	1.63	0.80
2:C:303:ASP:HB2	2:C:310:ILE:HD11	1.61	0.80
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.62	0.79
3:D:643:ASP:O	3:D:720:ASN:ND2	2.16	0.79
3:I:850:LYS:HD2	3:I:851:PRO:HD2	1.63	0.78
2:C:49:LEU:HD11	2:C:464:PHE:HB3	1.64	0.78
2:C:55:SER:HB3	2:C:56:VAL:CG2	2.14	0.78
3:I:20:ILE:HD11	3:I:1320:ILE:HD11	1.63	0.78
2:H:487:LEU:HB3	2:H:488:MET:CA	2.13	0.77
2:C:54:ARG:HG2	2:C:55:SER:HB2	1.67	0.77
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.66	0.77
1:G:29:GLU:HB3	1:G:30:PRO:HD3	1.65	0.76
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.67	0.76
1:B:181:GLU:HG2	3:D:531:LYS:HD3	1.68	0.76
3:I:1149:ARG:HD3	3:I:1149:ARG:H	1.50	0.75
4:E:5:THR:CA	4:E:6:VAL:HB	2.15	0.75
5:X:59:ALA:HB3	5:X:60:PRO:HD3	1.69	0.75
1:G:45:ARG:O	3:I:538:ARG:NH2	2.20	0.75
3:I:423:LEU:HD21	3:I:447:ILE:HD11	1.66	0.75
2:C:1117:LEU:HD11	2:C:1182:ILE:HD13	1.68	0.75



	<b>A</b> + <b>O</b>	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:C:131:THR:HG21	2:C:135:THR:HG22	1.67	0.74
2:C:742:TYR:HB3	2:C:743:PRO:HD3	1.68	0.74
2:H:699:LEU:HD11	2:H:1179:GLY:HA3	1.69	0.74
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.68	0.74
2:H:55:SER:HB3	2:H:56:VAL:CG2	2.18	0.74
2:H:99:LYS:HD3	2:H:99:LYS:N	2.02	0.73
5:Y:262:VAL:HG13	5:Y:263:PRO:HD2	1.68	0.73
5:X:35:ILE:HG13	5:X:36:VAL:H	1.52	0.73
2:H:54:ARG:N	2:H:55:SER:HB2	2.01	0.73
2:H:142:GLU:HG2	2:H:515:MET:SD	2.27	0.73
3:I:850:LYS:O	3:I:852:GLY:N	2.21	0.73
5:X:108:VAL:HG23	5:X:109:GLU:H	1.54	0.73
2:C:131:THR:CG2	2:C:135:THR:HG22	2.19	0.72
5:X:262:VAL:HG13	5:X:263:PRO:HD2	1.71	0.72
3:D:120:LEU:CB	3:D:121:PRO:HD3	2.19	0.72
2:H:645:PHE:CE1	2:H:650:VAL:HB	2.25	0.72
5:X:12:LEU:CD2	5:X:27:VAL:HG21	2.19	0.72
3:I:1347:LEU:HD23	3:I:1358:PRO:HG2	1.70	0.72
3:D:850:LYS:HD2	3:D:851:PRO:HD2	1.71	0.72
1:B:29:GLU:HA	1:B:200:LYS:CB	2.18	0.72
3:D:822:MET:SD	3:D:838:ARG:NH1	2.63	0.72
3:I:925:GLU:HB3	3:I:926:PRO:HD3	1.72	0.72
2:H:1065:LYS:NZ	3:I:462:ASP:O	2.23	0.71
3:D:151:MET:SD	3:D:151:MET:N	2.63	0.71
1:G:65:LEU:HD23	1:G:65:LEU:H	1.55	0.71
2:H:1269:ARG:HG3	3:I:346:ARG:HG2	1.70	0.71
3:D:850:LYS:O	3:D:852:GLY:N	2.22	0.71
1:A:45:ARG:HG3	2:C:1083:GLU:HB2	1.72	0.71
2:C:13:LYS:CD	2:C:1181:PRO:HG2	2.21	0.71
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.72	0.71
2:H:516:ASP:HB2	6:H:1401:1RL:H201	1.73	0.71
2:C:55:SER:CB	2:C:56:VAL:HG22	2.17	0.71
3:I:426:ALA:HB3	3:I:427:PRO:HD3	1.72	0.71
2:H:131:THR:CG2	2:H:135:THR:HG22	2.21	0.70
3:D:1362:GLY:O	3:D:1364:ALA:N	2.24	0.70
2:C:134:GLY:O	2:C:527:LYS:NZ	2.24	0.70
2:C:519:ASN:HB2	2:C:520:PRO:HD2	1.74	0.70
3:I:1247:LYS:H	3:I:1247:LYS:HD3	1.55	0.70
1:A:231:PHE:CZ	1:B:39:LEU:HD13	2.27	0.70
2:H:54:ARG:HG2	2:H:55:SER:HB2	1.74	0.70
2:H:55:SER:CB	2:H:56:VAL:HG22	2.22	0.70



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:H:1239:VAL:HG12	2:H:1240:ASP:H	1.57	0.70
3:D:584:PRO:HG2	3:D:587:LEU:HD13	1.74	0.69
2:H:519:ASN:HB2	2:H:520:PRO:HD2	1.74	0.69
3:I:120:LEU:CB	3:I:121:PRO:HD3	2.22	0.69
5:Y:108:VAL:HG23	5:Y:109:GLU:H	1.56	0.69
2:C:634:VAL:HG22	2:C:645:PHE:HE2	1.58	0.69
2:C:302:ILE:HA	2:C:309:LEU:HA	1.75	0.69
3:D:1225:GLY:HA2	3:I:1294:ALA:HA	1.73	0.69
2:C:20:GLN:O	2:C:22:LEU:N	2.25	0.69
2:C:37:LYS:HA	2:C:37:LYS:HE3	1.75	0.69
2:H:49:LEU:HD11	2:H:464:PHE:HB3	1.74	0.69
1:B:192:VAL:HG21	1:B:198:LEU:HD12	1.73	0.69
2:H:742:TYR:HB3	2:H:743:PRO:HD3	1.76	0.69
2:C:1239:VAL:HG12	2:C:1240:ASP:H	1.57	0.68
3:D:1191:PRO:O	3:D:1193:TRP:N	2.26	0.68
3:D:1247:LYS:HD3	3:D:1247:LYS:H	1.57	0.68
2:H:55:SER:HB3	2:H:56:VAL:HG13	1.75	0.68
3:I:186:GLN:HB2	3:I:238:ILE:HD11	1.75	0.68
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.75	0.68
5:Y:511:ILE:HG23	5:Y:512:GLY:H	1.58	0.68
2:C:170:VAL:HG23	2:C:171:LEU:H	1.57	0.68
1:F:29:GLU:HB3	1:F:30:PRO:HD3	1.76	0.68
1:F:211:ILE:HD11	1:F:215:GLU:HG3	1.75	0.68
2:C:645:PHE:CE1	2:C:650:VAL:HB	2.28	0.68
3:D:378:LYS:HB3	3:D:379:PRO:HD3	1.76	0.68
2:H:489:PRO:HB2	2:H:492:MET:HB3	1.75	0.68
3:D:405:GLU:O	3:D:407:VAL:N	2.27	0.68
2:H:664:GLY:O	2:H:686:GLN:NE2	2.27	0.68
3:I:720:ASN:O	3:I:722:ILE:N	2.27	0.68
1:A:110:VAL:HB	1:A:131:CYS:HB2	1.76	0.67
2:C:487:LEU:HB2	2:C:489:PRO:HD3	1.76	0.67
3:D:746:LEU:HD13	3:D:758:PRO:HG3	1.77	0.67
4:J:38:LEU:HD13	4:J:58:LEU:HD23	1.76	0.67
2:C:43:PRO:HD3	2:C:47:TYR:CD2	2.29	0.67
3:I:1191:PRO:O	3:I:1193:TRP:N	2.27	0.67
5:Y:137:TYR:CE2	5:Y:139:GLU:HB2	2.29	0.67
1:A:323:PRO:CB	1:A:324:ALA:HB2	2.25	0.67
2:C:54:ARG:CG	2:C:55:SER:HB2	2.25	0.67
2:H:21:VAL:HG13	2:H:22:LEU:H	1.59	0.67
3:I:1171:GLY:HA3	3:I:1172:LYS:HB2	1.77	0.67
2:C:611:GLU:CG	2:C:616:ILE:HD11	2.25	0.66



A 4 1	<b>A t</b> and <b>D</b>	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:H:54:ARG:H	2:H:55:SER:CB	2.05	0.66
3:I:120:LEU:HB2	3:I:121:PRO:HD3	1.75	0.66
5:X:240:ARG:HD3	5:X:244:THR:HB	1.75	0.66
2:C:816:ILE:HG13	2:C:1098:LEU:HD22	1.76	0.66
3:D:245:LEU:O	3:D:250:ARG:NH1	2.29	0.66
3:D:1171:GLY:HA3	3:D:1172:LYS:HB2	1.77	0.66
3:D:1320:ILE:HG22	3:D:1352:ILE:HD11	1.77	0.66
5:X:511:ILE:HG23	5:X:512:GLY:H	1.58	0.66
2:H:1180:MET:HB3	2:H:1181:PRO:CA	2.25	0.66
2:C:529:ARG:CZ	6:C:1401:1RL:H171	2.25	0.66
3:I:139:LEU:HD13	3:I:140:TYR:N	2.11	0.66
2:C:49:LEU:HD11	2:C:464:PHE:CB	2.25	0.66
2:C:1180:MET:HB3	2:C:1181:PRO:CA	2.25	0.66
2:H:1042:LEU:HD13	2:H:1042:LEU:H	1.61	0.66
2:C:448:LEU:HB2	2:C:553:THR:HG21	1.77	0.66
3:D:610:ARG:HG2	3:D:864:LEU:HD22	1.78	0.66
3:D:711:GLY:O	3:D:712:GLN:HG2	1.95	0.66
5:X:152:GLU:OE2	5:X:218:ARG:NH1	2.29	0.66
2:C:11:ILE:HD13	2:C:697:LYS:NZ	2.11	0.66
3:D:139:LEU:HD13	3:D:140:TYR:N	2.11	0.65
2:H:487:LEU:HB3	2:H:488:MET:HG3	1.77	0.65
4:J:39:VAL:HG13	4:J:40:PRO:HD2	1.77	0.65
2:C:54:ARG:N	2:C:55:SER:HB2	2.09	0.65
2:C:634:VAL:HG22	2:C:645:PHE:CE2	2.31	0.65
3:D:932:MET:O	3:D:933:ARG:HG3	1.96	0.65
1:A:13:LEU:HD21	1:A:16:ILE:HD11	1.78	0.65
1:F:100:LEU:HD21	1:F:121:VAL:HG21	1.78	0.65
2:C:402:ARG:NH2	2:C:419:ILE:O	2.30	0.65
3:D:546:ALA:N	3:D:547:ARG:HA	2.11	0.65
3:I:378:LYS:HB3	3:I:379:PRO:HD3	1.77	0.65
3:I:643:ASP:O	3:I:720:ASN:ND2	2.21	0.65
2:C:845:LEU:HD13	2:C:845:LEU:H	1.60	0.65
2:H:13:LYS:CD	2:H:1181:PRO:HG2	2.25	0.65
2:H:1239:VAL:O	2:H:1241:ASP:N	2.30	0.65
3:D:1347:LEU:HD23	3:D:1358:PRO:HG2	1.77	0.65
1:A:323:PRO:HB2	1:A:324:ALA:HB2	1.78	0.65
1:B:12:ARG:H	1:B:30:PRO:HG2	1.60	0.65
1:B:49:SER:HA	1:B:151:GLY:HA2	1.78	0.65
2:C:1237:HIS:O	2:C:1238:LEU:HG	1.97	0.65
3:D:1301:THR:HG23	3:I:1301:THR:HG23	1.77	0.65
3:I:546:ALA:N	3:I:547:ARG:HA	2.11	0.65



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:C:736:VAL:HG11	2:C:740:GLU:HA	1.78	0.65
2:H:127:ILE:H	2:H:127:ILE:HD13	1.62	0.65
2:C:1042:LEU:HD13	2:C:1042:LEU:H	1.62	0.65
2:H:131:THR:HG21	2:H:135:THR:HG22	1.76	0.65
5:X:138:PRO:HD2	5:X:353:LEU:HD11	1.79	0.65
2:H:816:ILE:HG13	2:H:1098:LEU:HD22	1.78	0.65
3:I:1148:ARG:NH2	3:I:1149:ARG:O	2.30	0.65
3:D:546:ALA:H	3:D:547:ARG:HA	1.61	0.64
5:X:12:LEU:HD23	5:X:27:VAL:HG21	1.77	0.64
5:X:476:ARG:H	5:X:476:ARG:HD2	1.62	0.64
2:C:800:MET:HE2	2:C:800:MET:HA	1.78	0.64
3:D:1343:GLU:HA	3:D:1344:LEU:HB2	1.78	0.64
3:I:546:ALA:H	3:I:547:ARG:HA	1.62	0.64
2:H:845:LEU:HD13	2:H:845:LEU:H	1.62	0.64
2:C:105:TYR:CG	2:C:114:VAL:HG13	2.33	0.64
3:I:20:ILE:CD1	3:I:1320:ILE:HD11	2.27	0.64
3:I:151:MET:SD	3:I:151:MET:N	2.70	0.64
2:C:1065:LYS:NZ	3:D:462:ASP:O	2.27	0.64
1:G:192:VAL:HG21	1:G:198:LEU:HD12	1.78	0.64
3:I:450:HIS:NE2	3:I:625:MET:SD	2.71	0.64
3:I:822:MET:SD	3:I:838:ARG:NH1	2.71	0.64
3:D:720:ASN:O	3:D:722:ILE:N	2.31	0.64
2:C:700:VAL:HG11	2:C:1114:GLU:HG3	1.80	0.64
5:X:390:ILE:HD11	5:X:435:ILE:HG22	1.81	0.63
2:H:13:LYS:HD3	2:H:1181:PRO:HG2	1.80	0.63
2:H:1252:SER:OG	2:H:1255:THR:O	2.15	0.63
3:I:711:GLY:O	3:I:712:GLN:HG2	1.99	0.63
2:C:660:VAL:HG22	2:C:661:VAL:H	1.62	0.63
3:D:389:GLY:O	3:D:391:ALA:N	2.32	0.63
3:I:1362:GLY:O	3:I:1364:ALA:N	2.31	0.63
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.80	0.63
3:I:709:ARG:O	3:I:711:GLY:N	2.32	0.63
2:H:1237:HIS:O	2:H:1238:LEU:HG	1.98	0.63
5:Y:517:SER:O	5:Y:518:HIS:ND1	2.32	0.63
2:C:13:LYS:HD2	2:C:1181:PRO:HG2	1.81	0.63
1:B:29:GLU:HA	1:B:200:LYS:HB2	1.80	0.62
2:C:488:MET:N	2:C:489:PRO:HD3	2.15	0.62
2:C:794:LEU:HD21	2:C:796:LEU:HG	1.81	0.62
2:H:1335:ILE:HD11	3:I:22:ILE:HD11	1.81	0.62
2:C:1119:MET:HG2	2:C:1228:GLY:CA	2.25	0.62
2:C:1259:LEU:HD12	2:C:1260:GLY:N	2.14	0.62



	1 J	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:I:1343:GLU:HA	3:I:1344:LEU:HB2	1.81	0.62
3:D:1268:ASN:HB3	3:D:1300:ALA:HB1	1.80	0.62
2:C:1239:VAL:O	2:C:1241:ASP:N	2.32	0.62
3:D:450:HIS:CD2	3:D:451:PRO:HD2	2.34	0.62
5:X:136:GLU:OE2	5:X:364:ARG:NH2	2.32	0.62
2:H:1274:GLU:OE1	2:H:1274:GLU:N	2.32	0.62
3:I:533:ALA:HB2	3:I:578:ILE:HD13	1.81	0.62
1:A:318:LEU:O	1:A:320:ASN:N	2.33	0.62
2:C:54:ARG:H	2:C:55:SER:CB	2.12	0.62
1:G:49:SER:OG	3:I:538:ARG:NH2	2.33	0.62
2:H:459:MET:SD	2:H:511:LEU:HD22	2.40	0.62
3:I:584:PRO:HG2	3:I:587:LEU:HD13	1.81	0.62
3:I:1274:PHE:CD2	3:I:1275:LEU:HG	2.35	0.62
5:X:517:SER:O	5:X:518:HIS:ND1	2.32	0.62
2:H:504:GLU:O	2:H:508:SER:HB3	2.00	0.62
2:H:529:ARG:NE	6:H:1401:1RL:H171	2.15	0.62
4:E:39:VAL:HG13	4:E:40:PRO:HD2	1.80	0.62
5:X:457:ILE:O	5:X:461:ASN:ND2	2.33	0.62
3:I:768:ASN:O	3:I:771:GLN:NE2	2.33	0.61
2:C:15:PHE:CE2	2:C:1182:ILE:HD11	2.35	0.61
3:D:522:GLY:HA2	3:D:545:HIS:CG	2.35	0.61
1:B:29:GLU:HA	1:B:200:LYS:HB3	1.82	0.61
4:E:5:THR:HA	4:E:6:VAL:CG1	2.29	0.61
3:I:389:GLY:O	3:I:391:ALA:N	2.33	0.61
2:H:505:PHE:O	2:H:512:SER:OG	2.16	0.61
3:I:1297:LYS:HZ3	3:I:1297:LYS:HA	1.65	0.61
2:C:448:LEU:HB2	2:C:553:THR:CG2	2.30	0.61
1:G:29:GLU:HA	1:G:200:LYS:CB	2.30	0.61
2:H:590:PRO:O	2:H:659:GLN:NE2	2.33	0.61
3:I:422:LEU:HD11	3:I:469:HIS:HB2	1.83	0.61
3:D:848:VAL:HG11	3:D:880:VAL:HA	1.83	0.61
1:F:11:PRO:HB3	1:F:31:LEU:HD21	1.82	0.61
2:H:99:LYS:HD3	2:H:99:LYS:H	1.65	0.61
3:D:316:ILE:HG23	3:D:317:THR:H	1.66	0.61
5:X:139:GLU:HA	5:X:142:THR:HG22	1.82	0.61
2:H:908:GLU:HG2	2:H:909:LYS:N	2.15	0.61
2:C:768:MET:O	2:C:785:ASP:N	2.33	0.61
3:D:186:GLN:HB2	3:D:238:ILE:HD11	1.81	0.61
5:X:471:LEU:HB3	5:X:478:PRO:HD3	1.81	0.61
3:I:145:VAL:HG22	3:I:180:MET:SD	2.40	0.61
2:C:189:ASP:OD1	2:C:193:ASN:N	2.29	0.61



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:D:709:ARG:O	3:D:711:GLY:N	2.34	0.61
3:I:1297:LYS:HA	3:I:1297:LYS:NZ	2.16	0.61
2:C:13:LYS:HD3	2:C:1181:PRO:HG2	1.83	0.60
3:D:245:LEU:HD12	3:D:246:PRO:HD2	1.84	0.60
2:C:127:ILE:H	2:C:127:ILE:HD13	1.67	0.60
2:C:1200:LYS:O	2:C:1202:GLY:N	2.33	0.60
2:C:119:GLU:CD	2:C:489:PRO:HG2	2.22	0.60
2:C:1269:ARG:HG2	3:D:346:ARG:HG2	1.84	0.60
3:D:108:ALA:HB3	3:D:279:LEU:HD12	1.82	0.60
3:D:120:LEU:CB	3:D:121:PRO:CD	2.78	0.60
3:D:349:TYR:CD1	3:D:472:LEU:HD11	2.37	0.60
3:D:1149:ARG:HD3	3:D:1149:ARG:H	1.65	0.60
2:H:163:LYS:H	2:H:163:LYS:HD3	1.66	0.60
3:I:589:TYR:O	3:I:591:ILE:N	2.35	0.60
3:D:535:ARG:HB3	3:D:541:LEU:HD21	1.83	0.60
2:H:700:VAL:HG11	2:H:1114:GLU:HG3	1.84	0.60
2:C:1211:ARG:O	2:C:1211:ARG:NE	2.31	0.60
1:B:33:ARG:NH1	2:C:820:GLU:OE2	2.35	0.60
3:D:79:LYS:HE3	5:X:569:THR:N	2.17	0.60
1:G:227:GLN:C	1:G:228:LEU:HD23	2.21	0.60
5:Y:274:ARG:NH1	5:Y:369:GLU:OE2	2.35	0.60
1:A:163:GLU:HB3	1:A:166:ARG:HB3	1.84	0.60
3:D:664:ILE:HG21	3:D:681:LYS:HD2	1.82	0.60
2:C:1117:LEU:HD11	2:C:1182:ILE:CD1	2.32	0.60
2:H:660:VAL:HG22	2:H:661:VAL:H	1.65	0.60
2:H:768:MET:O	2:H:785:ASP:N	2.35	0.60
3:D:19:ALA:CB	3:D:1343:GLU:HB3	2.32	0.59
6:H:1401:1RL:O10	6:H:1401:1RL:O9	2.17	0.59
3:I:405:GLU:O	3:I:407:VAL:N	2.35	0.59
3:I:426:ALA:HB3	3:I:427:PRO:CD	2.32	0.59
2:H:933:VAL:HG12	2:H:948:ILE:HD11	1.84	0.59
2:C:669:PRO:HG2	2:C:1070:HIS:CE1	2.38	0.59
3:D:546:ALA:H	3:D:547:ARG:CA	2.14	0.59
5:X:562:ARG:NH1	5:X:591:GLU:OE2	2.36	0.59
2:H:454:ARG:HD3	2:H:459:MET:HG2	1.84	0.59
2:C:478:ARG:HD3	2:C:492:MET:HG3	1.84	0.59
3:D:589:TYR:O	3:D:591:ILE:N	2.33	0.59
5:Y:240:ARG:HD3	5:Y:244:THR:HB	1.83	0.59
2:C:372:PRO:HB2	5:X:34:ASP:HB3	1.85	0.59
2:C:618:GLN:OE1	2:C:637:ARG:NH1	2.35	0.59
1:F:66:HIS:CE1	1:F:69:SER:HB2	2.38	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:I:31:ARG:NH2	3:I:106:GLU:OE2	2.35	0.59
2:C:309:LEU:HD23	2:C:309:LEU:H	1.68	0.59
3:D:56:LEU:O	3:D:250:ARG:NH2	2.36	0.59
5:X:240:ARG:O	5:X:242:HIS:N	2.35	0.59
2:H:1186:VAL:HG13	2:H:1187:PHE:H	1.67	0.59
3:I:88:CYS:O	3:I:90:VAL:N	2.36	0.59
2:C:685:MET:HE3	2:C:1235:LEU:HD11	1.85	0.59
2:C:752:ASN:O	2:C:753:LEU:HG	2.03	0.59
2:C:1186:VAL:HG13	2:C:1187:PHE:H	1.67	0.59
2:H:1200:LYS:O	2:H:1202:GLY:N	2.36	0.59
3:I:120:LEU:HB2	3:I:121:PRO:CD	2.32	0.59
1:G:124:VAL:HG11	1:G:209:GLY:HA3	1.85	0.59
2:C:143:ARG:NH1	2:C:512:SER:O	2.36	0.58
2:H:20:GLN:O	2:H:22:LEU:N	2.36	0.58
2:H:309:LEU:HD23	2:H:309:LEU:H	1.68	0.58
3:I:57:PHE:CZ	3:I:252:LEU:HD22	2.38	0.58
3:I:514:THR:HG23	3:I:576:ARG:HE	1.68	0.58
3:I:828:GLY:HA2	3:I:832:LYS:N	2.18	0.58
3:I:1173:ARG:HB3	3:I:1174:ARG:O	2.02	0.58
2:H:55:SER:HB3	2:H:56:VAL:CB	2.33	0.58
3:I:450:HIS:CD2	3:I:451:PRO:HD2	2.38	0.58
3:D:316:ILE:HG13	3:D:317:THR:N	2.18	0.58
3:D:658:GLU:HA	3:D:661:VAL:HG12	1.85	0.58
3:I:1274:PHE:HD2	3:I:1275:LEU:HG	1.68	0.58
3:D:1237:VAL:O	3:D:1240:VAL:HG22	2.03	0.58
2:H:672:GLU:HG3	2:H:673:HIS:CD2	2.38	0.58
2:H:1185:PRO:HD2	2:H:1189:GLY:HA2	1.85	0.58
3:I:858:VAL:CB	3:I:859:PRO:HD3	2.28	0.58
2:C:1274:GLU:OE1	2:C:1274:GLU:N	2.36	0.58
3:D:120:LEU:HB2	3:D:121:PRO:CD	2.34	0.58
3:D:426:ALA:HB3	3:D:427:PRO:CD	2.33	0.58
5:Y:449:THR:OG1	5:Y:503:GLU:O	2.21	0.58
2:C:660:VAL:O	2:C:661:VAL:HG22	2.03	0.58
2:C:42:ASP:CB	2:C:43:PRO:HD2	2.16	0.58
3:D:932:MET:SD	3:D:932:MET:N	2.74	0.58
1:G:182:ARG:HG2	1:G:206:GLU:HB3	1.86	0.58
2:H:106:GLU:HB3	2:H:107:ARG:HA	1.85	0.58
2:H:660:VAL:O	2:H:661:VAL:HG22	2.04	0.58
3:I:423:LEU:CD2	3:I:447:ILE:HD11	2.34	0.58
2:C:142:GLU:HG2	2:C:515:MET:SD	2.43	0.58
2:C:618:GLN:OE1	3:D:770:LEU:HB2	2.03	0.58



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:D:1254:GLU:O	3:D:1257:VAL:HG12	2.04	0.58
5:X:560:ARG:HG2	5:X:565:ILE:HG23	1.86	0.58
5:X:584:ARG:O	5:X:587:ILE:HG22	2.04	0.58
2:H:1014:LEU:O	2:H:1017:GLN:NE2	2.37	0.58
3:I:827:GLU:O	3:I:831:VAL:HG12	2.03	0.58
2:C:1281:TYR:CZ	3:D:431:ARG:HG2	2.39	0.58
2:H:245:ARG:HB3	2:H:337:PHE:CZ	2.39	0.58
2:H:1211:ARG:O	2:H:1211:ARG:NE	2.36	0.58
3:I:707:ILE:HG22	3:I:708:ASN:H	1.69	0.58
2:C:106:GLU:N	2:C:107:ARG:HA	2.18	0.57
2:C:1180:MET:HB3	2:C:1181:PRO:C	2.23	0.57
3:D:120:LEU:HD22	3:D:1330:ARG:HD2	1.84	0.57
3:D:583:VAL:HG13	3:D:584:PRO:HD2	1.86	0.57
2:C:105:TYR:CD1	2:C:106:GLU:HB2	2.39	0.57
2:C:510:GLN:O	2:C:511:LEU:HB2	2.04	0.57
2:C:1141:LEU:CD1	2:C:1141:LEU:H	2.18	0.57
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.86	0.57
2:C:685:MET:CE	2:C:1235:LEU:HD11	2.34	0.57
3:D:708:ASN:OD1	3:D:712:GLN:HB2	2.04	0.57
1:F:234:LEU:HD22	1:G:214:GLU:OE2	2.03	0.57
1:A:50:SER:HB3	1:B:8:PHE:HZ	1.69	0.57
2:C:526:HIS:HA	2:C:529:ARG:NH1	2.19	0.57
3:D:1261:LEU:HD21	3:D:1306:LEU:HD22	1.85	0.57
5:X:17:LYS:N	5:X:18:GLU:HA	2.19	0.57
5:X:138:PRO:CD	5:X:353:LEU:HD11	2.34	0.57
2:H:106:GLU:N	2:H:107:ARG:HA	2.19	0.57
2:H:1254:VAL:HG23	2:H:1255:THR:H	1.70	0.57
3:D:316:ILE:HG23	3:D:317:THR:N	2.19	0.57
2:H:54:ARG:CG	2:H:55:SER:HB2	2.34	0.57
2:H:1142:ARG:NH2	2:H:1165:SER:O	2.38	0.57
3:I:828:GLY:HA2	3:I:832:LYS:H	1.69	0.57
2:C:1252:SER:OG	2:C:1255:THR:O	2.21	0.57
5:X:145:LEU:HD11	5:X:225:ARG:NH2	2.20	0.57
2:H:38:PHE:O	2:H:39:ILE:HB	2.05	0.57
1:A:207:THR:OG1	1:A:208:ASN:N	2.38	0.57
1:B:11:PRO:HA	1:B:30:PRO:HB2	1.86	0.57
5:X:137:TYR:CE2	5:X:139:GLU:HB2	2.40	0.57
4:J:5:THR:HA	4:J:6:VAL:CG1	2.35	0.57
2:H:531:SER:OG	6:H:1401:1RL:O2	2.20	0.57
3:I:546:ALA:H	3:I:547:ARG:CA	2.17	0.57
3:I:583:VAL:HG13	3:I:584:PRO:HD2	1.87	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:I:828:GLY:HA2	3:I:832:LYS:HA	1.86	0.57
1:B:227:GLN:O	1:B:228:LEU:HG	2.04	0.57
2:C:740:GLU:HB2	2:C:741:MET:SD	2.44	0.57
3:D:614:LEU:HG	4:E:7:GLN:HG3	1.85	0.57
2:C:568:ASN:HB3	2:C:572:ILE:CD1	2.35	0.56
2:C:660:VAL:HG13	2:C:661:VAL:CG1	2.34	0.56
3:D:573:THR:HG22	3:D:576:ARG:CD	2.34	0.56
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.69	0.56
3:I:197:GLU:O	3:I:201:LEU:HD23	2.05	0.56
1:B:65:LEU:HD23	1:B:65:LEU:H	1.69	0.56
3:D:546:ALA:HB3	3:D:547:ARG:O	2.05	0.56
1:F:41:ASN:OD1	2:H:1218:GLY:HA3	2.04	0.56
2:H:1141:LEU:CD1	2:H:1141:LEU:H	2.19	0.56
3:I:768:ASN:ND2	3:I:771:GLN:OE1	2.38	0.56
3:I:828:GLY:HA2	3:I:832:LYS:CA	2.35	0.56
2:C:741:MET:SD	2:C:741:MET:N	2.78	0.56
2:C:1255:THR:O	2:C:1257:GLN:N	2.36	0.56
3:D:858:VAL:CB	3:D:859:PRO:HD3	2.28	0.56
5:X:120:ALA:HB3	5:X:421:TYR:HB3	1.87	0.56
2:H:496:LYS:N	2:H:497:PRO:HD2	2.21	0.56
2:H:1105:SER:HB2	3:I:731:ARG:HD3	1.87	0.56
5:Y:556:ALA:O	5:Y:560:ARG:HB2	2.05	0.56
3:D:128:LEU:HA	3:D:192:MET:HE1	1.87	0.56
3:D:749:LYS:CG	3:D:750:PRO:HD2	2.33	0.56
3:D:768:ASN:ND2	3:D:771:GLN:OE1	2.37	0.56
3:D:1369:ARG:HB3	3:D:1369:ARG:NH1	2.20	0.56
1:G:29:GLU:HA	1:G:200:LYS:HB3	1.85	0.56
3:I:160:LEU:HA	3:I:164:GLN:NE2	2.21	0.56
3:I:422:LEU:CD1	3:I:469:HIS:HB2	2.36	0.56
3:I:545:HIS:HB2	3:I:546:ALA:HA	1.86	0.56
2:H:488:MET:HE3	2:H:489:PRO:HA	1.88	0.56
2:H:794:LEU:HD21	2:H:796:LEU:HG	1.86	0.56
2:C:1254:VAL:HG23	2:C:1255:THR:H	1.70	0.56
3:D:50:LYS:HG2	3:D:51:PRO:HD2	1.88	0.56
1:F:107:ILE:HD11	1:F:136:GLU:HG3	1.88	0.56
2:H:105:TYR:CD1	2:H:106:GLU:HB2	2.41	0.56
2:H:618:GLN:OE1	3:I:770:LEU:HB2	2.06	0.56
2:H:170:VAL:HG23	2:H:171:LEU:H	1.70	0.56
2:H:1180:MET:HB3	2:H:1181:PRO:C	2.26	0.56
3:I:708:ASN:OD1	3:I:712:GLN:HB2	2.05	0.56
3:I:1297:LYS:HA	3:I:1297:LYS:CE	2.36	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:D:120:LEU:HB2	3:D:121:PRO:HD3	1.88	0.56
5:X:16:GLY:HA2	5:X:19:GLN:HG3	1.88	0.56
3:I:120:LEU:CB	3:I:121:PRO:CD	2.83	0.56
3:I:903:LEU:HD11	3:I:909:ILE:HG22	1.88	0.56
5:Y:562:ARG:NH1	5:Y:591:GLU:OE2	2.39	0.56
1:A:42:ALA:O	1:A:46:ILE:HG12	2.06	0.56
2:H:55:SER:HB3	2:H:56:VAL:CG1	2.36	0.56
3:I:1283:SER:O	3:I:1287:ILE:HG23	2.06	0.56
1:A:239:GLN:HG3	1:A:240:PRO:HD2	1.87	0.55
2:C:1313:HIS:CG	4:E:31:GLN:HE22	2.24	0.55
3:D:600:ALA:HA	3:D:603:LYS:HB3	1.87	0.55
5:X:445:ASP:OD1	5:X:445:ASP:N	2.39	0.55
3:I:749:LYS:CG	3:I:750:PRO:HD2	2.31	0.55
3:I:803:VAL:HG22	3:I:1259:GLN:OE1	2.07	0.55
4:E:25:ARG:NH2	4:E:68:GLU:OE1	2.39	0.55
1:B:124:VAL:HG11	1:B:209:GLY:HA3	1.88	0.55
2:C:1141:LEU:H	2:C:1141:LEU:HD13	1.72	0.55
2:H:562:GLU:HG2	2:H:574:SER:HB2	1.89	0.55
1:B:83:LEU:HD21	3:D:551:ARG:HG3	1.89	0.55
5:Y:515:GLU:N	5:Y:516:ASP:HA	2.21	0.55
2:C:106:GLU:HB3	2:C:107:ARG:HA	1.88	0.55
3:D:697:MET:SD	3:D:741:ALA:HB3	2.47	0.55
2:H:42:ASP:HB2	2:H:47:TYR:CD2	2.42	0.55
2:H:660:VAL:HG13	2:H:661:VAL:CG1	2.31	0.55
2:C:178:PRO:HA	2:C:397:LEU:HD23	1.88	0.55
2:H:540:ARG:NH2	2:H:568:ASN:OD1	2.40	0.55
2:H:557:ARG:HB3	2:H:587:LEU:HD23	1.89	0.55
2:H:747:GLY:O	2:H:748:ILE:HG13	2.06	0.55
2:H:1176:LEU:HD22	2:H:1180:MET:O	2.06	0.55
3:D:205:LEU:HD22	3:D:217:LEU:HD22	1.88	0.55
5:X:363:ARG:O	5:X:367:ILE:HG12	2.07	0.55
3:I:918:ILE:HD13	3:I:919:ALA:N	2.22	0.55
5:Y:355:ILE:HD13	5:Y:355:ILE:O	2.07	0.55
3:D:1323:ALA:O	3:D:1328:THR:HG22	2.08	0.54
2:H:637:ARG:HE	3:I:770:LEU:HD23	1.72	0.54
3:I:245:LEU:HD12	3:I:246:PRO:HD2	1.89	0.54
3:I:394:ILE:CG2	5:Y:536:THR:HG22	2.37	0.54
3:D:1322:ALA:HB3	3:D:1331:VAL:HG21	1.89	0.54
1:F:9:LEU:O	1:G:227:GLN:NE2	2.40	0.54
3:D:1155:ILE:HG13	3:D:1210:ILE:HG23	1.88	0.54
3:D:1256:ILE:HG13	3:D:1257:VAL:N	2.23	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
3:I:205:LEU:HD13	3:I:217:LEU:HD22	1.89	0.54
5:Y:503:GLU:N	5:Y:504:PRO:HA	2.22	0.54
2:C:894:GLN:O	2:C:895:LEU:HB2	2.07	0.54
2:C:1108:ASN:ND2	2:C:1111:GLN:OE1	2.40	0.54
3:D:20:ILE:CD1	3:D:1320:ILE:HD11	2.37	0.54
3:D:422:LEU:HD11	3:D:469:HIS:HB2	1.89	0.54
5:X:564:GLY:HA3	5:X:570:ASP:HB3	1.89	0.54
1:F:11:PRO:HB3	1:F:31:LEU:CD2	2.38	0.54
2:H:49:LEU:HD11	2:H:464:PHE:CB	2.38	0.54
3:I:77:ARG:HG3	3:I:78:LEU:H	1.72	0.54
3:I:838:ARG:NH2	3:I:1250:ASP:OD2	2.41	0.54
3:I:1256:ILE:HG13	3:I:1257:VAL:N	2.21	0.54
5:Y:139:GLU:HA	5:Y:142:THR:HG22	1.90	0.54
1:A:91:ARG:NH2	1:A:209:GLY:O	2.40	0.54
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.90	0.54
3:D:1284:ARG:HA	3:D:1287:ILE:HG12	1.89	0.54
3:I:473:THR:HB	3:I:476:ALA:HB2	1.90	0.54
2:C:11:ILE:HD13	2:C:697:LYS:HZ1	1.73	0.54
2:C:681:MET:O	2:C:685:MET:HG2	2.07	0.54
3:D:858:VAL:HB	3:D:859:PRO:CD	2.29	0.54
3:I:108:ALA:HB3	3:I:279:LEU:HD12	1.90	0.54
2:C:496:LYS:N	2:C:497:PRO:HD2	2.21	0.54
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.40	0.54
3:D:105:ILE:HD13	3:D:273:ILE:HD11	1.89	0.54
5:Y:98:VAL:HB	5:Y:402:LEU:HD21	1.89	0.54
2:C:1180:MET:HB3	2:C:1181:PRO:O	2.08	0.54
3:D:316:ILE:HG13	3:D:317:THR:H	1.72	0.54
5:X:503:GLU:N	5:X:504:PRO:HA	2.22	0.54
2:H:488:MET:HB2	2:H:489:PRO:CA	2.38	0.54
2:H:926:GLY:HA3	2:H:1056:VAL:HG12	1.90	0.54
2:H:1223:ARG:HG3	2:H:1224:PRO:HD2	1.90	0.54
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.89	0.54
2:C:933:VAL:HG12	2:C:948:ILE:HD11	1.90	0.54
3:D:19:ALA:HB2	3:D:1343:GLU:HB3	1.88	0.54
1:A:219:ARG:O	1:A:223:ILE:HG13	2.08	0.54
3:D:610:ARG:HG3	3:D:864:LEU:HD13	1.89	0.54
2:H:143:ARG:NH1	2:H:512:SER:O	2.41	0.54
2:C:562:GLU:HG2	2:C:574:SER:CB	2.38	0.53
2:C:568:ASN:HB3	2:C:572:ILE:HD12	1.89	0.53
3:D:1225:GLY:CA	3:I:1294:ALA:HA	2.37	0.53
2:H:21:VAL:HG13	2:H:22:LEU:N	2.22	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:H:189:ASP:HB2	2:H:190:PRO:HD2	1.88	0.53
2:H:752:ASN:O	2:H:753:LEU:HG	2.08	0.53
2:H:800:MET:HE2	2:H:800:MET:HA	1.88	0.53
3:I:681:LYS:HB2	3:I:681:LYS:NZ	2.22	0.53
2:C:397:LEU:O	2:C:398:SER:OG	2.21	0.53
3:D:88:CYS:O	3:D:90:VAL:N	2.42	0.53
2:H:514:PHE:O	6:H:1401:1RL:H321	2.09	0.53
3:I:152:THR:O	3:I:154:LEU:N	2.40	0.53
5:Y:138:PRO:HG3	5:Y:353:LEU:HD21	1.90	0.53
2:C:9:LYS:N	2:C:9:LYS:HD3	2.23	0.53
2:C:1295:SER:HB2	3:D:347:VAL:HG12	1.90	0.53
3:D:85:CYS:HB3	3:D:88:CYS:O	2.08	0.53
3:D:422:LEU:HA	3:D:436:ALA:HA	1.89	0.53
3:I:227:PHE:O	3:I:230:SER:OG	2.18	0.53
3:I:824:PRO:O	3:I:826:ILE:HG13	2.08	0.53
1:B:64:VAL:HG13	1:B:69:SER:OG	2.08	0.53
2:C:840:SER:HB3	2:C:850:ILE:HD11	1.90	0.53
3:D:545:HIS:HB2	3:D:546:ALA:HA	1.91	0.53
3:D:1195:GLN:OE1	3:D:1195:GLN:N	2.42	0.53
3:D:1283:SER:O	3:D:1287:ILE:HG23	2.07	0.53
2:H:1043:ALA:HB1	2:H:1044:PRO:HD2	1.89	0.53
3:I:546:ALA:HB3	3:I:547:ARG:O	2.09	0.53
5:Y:457:ILE:O	5:Y:461:ASN:ND2	2.42	0.53
5:Y:600:HIS:H	5:Y:601:PRO:CD	2.20	0.53
2:H:562:GLU:HG2	2:H:574:SER:CB	2.38	0.53
3:I:57:PHE:CE1	3:I:252:LEU:HD22	2.42	0.53
3:I:610:ARG:HG3	3:I:864:LEU:HD13	1.89	0.53
2:C:21:VAL:HG13	2:C:22:LEU:H	1.73	0.53
2:H:1101:LEU:HD13	3:I:504:GLN:HB2	1.91	0.53
3:I:1254:GLU:O	3:I:1257:VAL:HG12	2.08	0.53
2:C:55:SER:HB3	2:C:56:VAL:CB	2.38	0.53
2:C:745:GLU:HB2	2:C:1017:GLN:HG3	1.90	0.53
5:X:580:PHE:O	5:X:582:VAL:N	2.42	0.53
2:H:1086:PRO:HG2	2:H:1094:VAL:HG21	1.90	0.53
5:Y:445:ASP:OD1	5:Y:445:ASP:N	2.41	0.53
2:C:454:ARG:HD3	2:C:459:MET:HG2	1.91	0.53
2:C:841:ARG:NH1	3:D:256:ASP:HB3	2.23	0.53
3:D:608:CYS:O	3:D:612:LEU:HB2	2.09	0.53
3:D:1173:ARG:HB3	3:D:1174:ARG:O	2.08	0.53
2:C:201:ARG:NH1	5:X:36:VAL:HG11	2.24	0.53
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	1.91	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:D:20:ILE:HD11	3:D:1320:ILE:HD11	1.90	0.53
3:D:1257:VAL:HA	3:D:1260:MET:HB3	1.90	0.53
5:Y:324:LYS:HB3	5:Y:325:PRO:HD2	1.90	0.53
1:B:151:GLY:O	1:B:177:TYR:HB2	2.09	0.53
5:X:28:ASN:ND2	5:X:29:ASP:OD2	2.41	0.53
5:X:35:ILE:HG23	5:X:36:VAL:N	2.24	0.53
5:X:355:ILE:O	5:X:355:ILE:HD13	2.08	0.53
2:H:303:ASP:HB2	2:H:310:ILE:HD11	1.90	0.53
2:H:1335:ILE:HD11	3:I:22:ILE:CD1	2.39	0.53
2:C:1233:LEU:O	2:C:1233:LEU:HD12	2.08	0.52
3:D:546:ALA:N	3:D:547:ARG:CA	2.70	0.52
3:D:768:ASN:O	3:D:771:GLN:NE2	2.42	0.52
5:X:515:GLU:N	5:X:516:ASP:HA	2.24	0.52
3:I:38:VAL:HG11	3:I:56:LEU:HD13	1.90	0.52
2:C:747:GLY:O	2:C:748:ILE:HG13	2.09	0.52
2:C:975:ILE:O	2:C:975:ILE:HD13	2.08	0.52
2:H:840:SER:OG	2:H:1048:LYS:O	2.27	0.52
2:H:1141:LEU:H	2:H:1141:LEU:HD13	1.74	0.52
1:B:83:LEU:HD11	3:D:527:LEU:HA	1.90	0.52
2:C:1127:LYS:HG2	2:C:1144:PHE:CZ	2.45	0.52
3:D:681:LYS:HB2	3:D:681:LYS:NZ	2.24	0.52
3:I:546:ALA:N	3:I:547:ARG:CA	2.71	0.52
2:C:245:ARG:HB3	2:C:337:PHE:CZ	2.44	0.52
2:C:660:VAL:HG22	2:C:661:VAL:N	2.25	0.52
2:C:690:VAL:HG11	2:C:830:THR:HG21	1.91	0.52
3:D:77:ARG:HG3	3:D:78:LEU:H	1.74	0.52
1:F:50:SER:HB3	1:G:8:PHE:CZ	2.44	0.52
2:H:9:LYS:HD3	2:H:9:LYS:N	2.24	0.52
3:I:508:LEU:O	3:I:508:LEU:HD23	2.09	0.52
3:I:614:LEU:HG	4:J:7:GLN:HG3	1.90	0.52
3:I:759:ILE:HG23	3:I:771:GLN:HG3	1.91	0.52
2:C:728:ASP:OD2	2:C:729:ALA:N	2.42	0.52
2:C:1251:TYR:O	5:X:525:ASP:N	2.42	0.52
3:D:227:PHE:O	3:D:230:SER:OG	2.19	0.52
1:F:11:PRO:HD3	1:G:227:GLN:HG3	1.91	0.52
2:H:185:ASP:HB2	2:H:197:ARG:HB2	1.90	0.52
2:H:1255:THR:O	2:H:1257:GLN:N	2.42	0.52
3:I:394:ILE:HG23	5:Y:536:THR:HG22	1.91	0.52
3:I:425:ARG:HD2	3:I:459:ALA:HB2	1.90	0.52
3:I:807:LEU:HD12	3:I:807:LEU:O	2.10	0.52
3:I:1280:VAL:HG11	3:I:1304:ARG:HE	1.74	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:65:LEU:HD23	1:B:65:LEU:N	2.25	0.52
2:C:672:GLU:HG3	2:C:673:HIS:CD2	2.45	0.52
3:D:1290:ARG:NH1	3:D:1296:GLY:O	2.43	0.52
5:X:600:HIS:H	5:X:601:PRO:CD	2.22	0.52
1:F:190:ALA:HB2	1:F:200:LYS:HB3	1.91	0.52
3:I:610:ARG:HG2	3:I:864:LEU:HD22	1.90	0.52
5:Y:152:GLU:OE2	5:Y:218:ARG:NH1	2.43	0.52
1:B:42:ALA:O	1:B:46:ILE:HG12	2.10	0.52
2:C:59:ILE:HG21	2:C:479:LEU:HD13	1.91	0.52
2:C:540:ARG:NH2	2:C:568:ASN:OD1	2.43	0.52
2:C:690:VAL:HG13	2:C:691:PRO:HD2	1.90	0.52
3:D:152:THR:O	3:D:154:LEU:N	2.42	0.52
4:E:44:ASP:HB2	4:E:49:ILE:HD11	1.92	0.52
5:X:112:THR:HG22	5:X:113:ARG:H	1.74	0.52
3:I:502:PRO:HB3	3:I:506:VAL:HG11	1.90	0.52
2:C:72:SER:O	2:C:98:VAL:HG23	2.10	0.52
2:C:590:PRO:O	2:C:659:GLN:NE2	2.41	0.52
2:C:816:ILE:HG13	2:C:1098:LEU:CD2	2.40	0.52
3:D:1145:PHE:HB3	3:D:1309:ILE:HD13	1.91	0.52
3:D:1280:VAL:HA	3:D:1283:SER:HB2	1.92	0.52
2:H:896:THR:HG23	2:H:897:PRO:HD2	1.91	0.52
2:C:528:ARG:NH2	2:C:576:SER:O	2.43	0.52
2:C:562:GLU:HG2	2:C:574:SER:HB2	1.91	0.52
2:C:926:GLY:HA3	2:C:1056:VAL:HG12	1.92	0.52
2:C:1042:LEU:HD13	2:C:1042:LEU:N	2.24	0.52
2:C:1212:LEU:HD12	2:C:1225:VAL:HG21	1.92	0.52
2:C:1223:ARG:HG3	2:C:1224:PRO:HD2	1.92	0.52
3:D:1171:GLY:N	3:D:1172:LYS:O	2.42	0.52
3:D:1193:TRP:O	3:D:1194:ARG:HB2	2.10	0.52
2:H:811:ASN:O	2:H:1099:ASN:ND2	2.43	0.52
3:I:615:LYS:HB3	3:I:616:PRO:HD3	1.91	0.52
3:I:1207:GLY:HA2	3:I:1223:LEU:HD21	1.92	0.52
2:C:452:ARG:NH2	2:C:458:GLU:OE1	2.43	0.52
2:C:539:THR:O	2:C:540:ARG:HG3	2.10	0.52
2:C:1070:HIS:CD2	2:C:1111:GLN:HA	2.45	0.52
5:X:600:HIS:H	5:X:601:PRO:HD2	1.74	0.51
2:H:105:TYR:HA	2:H:106:GLU:HB2	1.92	0.51
2:H:131:THR:HG22	2:H:135:THR:HG22	1.92	0.51
3:I:1195:GLN:OE1	3:I:1195:GLN:N	2.40	0.51
3:I:1257:VAL:HA	3:I:1260:MET:HB3	1.91	0.51
2:C:342:ASP:HA	2:C:437:ASN:HB3	1.92	0.51



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:C:1176:LEU:HD22	2:C:1180:MET:O	2.10	0.51
1:G:49:SER:HA	1:G:151:GLY:HA2	1.92	0.51
2:H:1268:GLN:O	3:I:346:ARG:HA	2.10	0.51
4:J:39:VAL:CG1	4:J:40:PRO:HD2	2.40	0.51
3:I:19:ALA:CB	3:I:1343:GLU:HB3	2.41	0.51
3:I:385:LEU:CD2	3:I:411:ILE:HG13	2.41	0.51
3:I:515:ARG:NH2	3:I:718:SER:O	2.44	0.51
3:I:1320:ILE:HG22	3:I:1352:ILE:HD11	1.91	0.51
5:Y:600:HIS:H	5:Y:601:PRO:HD2	1.76	0.51
2:C:840:SER:OG	2:C:1048:LYS:O	2.27	0.51
3:D:514:THR:HG21	3:D:595:ALA:O	2.10	0.51
3:D:1254:GLU:HA	3:D:1257:VAL:HG12	1.92	0.51
1:F:228:LEU:HD21	1:G:224:LEU:HD23	1.93	0.51
2:H:1331:ARG:NH2	2:H:1337:ILE:O	2.43	0.51
3:I:1266:ILE:HG13	3:I:1274:PHE:O	2.10	0.51
3:D:1311:LYS:NZ	5:X:50:ASP:O	2.44	0.51
2:H:13:LYS:CE	2:H:1183:ALA:HB2	2.34	0.51
2:H:208:ILE:HD11	2:H:365:GLU:HB3	1.92	0.51
2:H:519:ASN:ND2	2:H:689:ALA:O	2.44	0.51
2:C:694:ARG:NH2	2:C:768:MET:SD	2.84	0.51
2:C:936:ARG:NH1	5:X:495:ARG:HD3	2.25	0.51
3:D:828:GLY:HA2	3:D:832:LYS:H	1.74	0.51
4:E:5:THR:HA	4:E:6:VAL:HG12	1.92	0.51
2:H:403:MET:HG3	2:H:414:ILE:HB	1.93	0.51
1:B:19:VAL:O	1:B:20:SER:HB3	2.10	0.51
2:C:39:ILE:HG22	2:C:40:GLU:HG2	1.93	0.51
2:C:127:ILE:HD13	2:C:127:ILE:N	2.26	0.51
1:A:79:LEU:O	1:A:83:LEU:HD13	2.11	0.51
1:B:192:VAL:HG21	1:B:198:LEU:CD1	2.40	0.51
3:D:451:PRO:HG2	3:D:625:MET:SD	2.50	0.51
1:G:118:ASP:OD1	1:G:119:GLY:N	2.43	0.51
2:H:528:ARG:NH2	2:H:576:SER:O	2.44	0.51
3:I:166:LEU:HD12	3:I:167:ASP:N	2.26	0.51
3:D:422:LEU:CD1	3:D:469:HIS:HB2	2.40	0.51
2:H:728:ASP:OD2	2:H:729:ALA:N	2.43	0.51
2:C:189:ASP:HB2	2:C:190:PRO:HD2	1.92	0.51
2:C:197:ARG:NH1	5:X:29:ASP:OD1	2.41	0.51
3:D:120:LEU:CD2	5:X:46:GLN:HB2	2.41	0.51
3:D:828:GLY:HA2	3:D:832:LYS:HA	1.91	0.51
5:X:301:ASN:O	5:X:305:LEU:HD13	2.11	0.51
2:C:15:PHE:CD2	2:C:1182:ILE:HD11	2.46	0.50



A 4 1	A 4 D	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:C:714:VAL:CG2	2:C:787:PRO:HD2	2.41	0.50
2:C:1214:ASP:HA	2:C:1221:PHE:CZ	2.46	0.50
2:H:134:GLY:O	2:H:527:LYS:NZ	2.44	0.50
2:H:660:VAL:HG22	2:H:661:VAL:N	2.27	0.50
2:H:800:MET:HA	2:H:800:MET:CE	2.40	0.50
2:H:896:THR:CG2	2:H:897:PRO:HD2	2.40	0.50
3:D:125:GLY:O	3:D:129:ASP:N	2.43	0.50
3:D:1292:LEU:HD21	3:I:1284:ARG:HH22	1.75	0.50
2:H:801:ARG:NH1	2:H:1093:PRO:O	2.45	0.50
2:H:842:ASP:CB	2:H:1046:VAL:HG11	2.41	0.50
3:I:390:LEU:HD21	3:I:407:VAL:HG11	1.94	0.50
3:I:1290:ARG:NH1	3:I:1296:GLY:O	2.43	0.50
5:Y:113:ARG:O	5:Y:117:ILE:HD13	2.11	0.50
5:Y:148:TYR:OH	5:Y:218:ARG:HG2	2.12	0.50
2:C:38:PHE:HE2	2:C:49:LEU:HD12	1.77	0.50
2:C:814:ASP:O	2:C:1074:GLY:HA2	2.12	0.50
2:C:1186:VAL:HG13	2:C:1187:PHE:N	2.26	0.50
3:D:573:THR:HG22	3:D:576:ARG:HG3	1.93	0.50
5:X:525:ASP:OD1	5:X:527:THR:HG22	2.11	0.50
1:F:45:ARG:NH2	2:H:1216:ARG:O	2.45	0.50
1:G:192:VAL:HG12	1:G:194:GLN:HG2	1.92	0.50
2:C:55:SER:HB3	2:C:56:VAL:HG13	1.92	0.50
3:D:903:LEU:HD11	3:D:909:ILE:HG22	1.93	0.50
2:H:514:PHE:HB2	6:H:1401:1RL:O8	2.12	0.50
2:H:521:LEU:CD2	2:H:686:GLN:HB3	2.42	0.50
2:H:753:LEU:HD12	2:H:753:LEU:O	2.11	0.50
2:H:844:LYS:HB2	2:H:844:LYS:NZ	2.26	0.50
2:H:1298:VAL:HG23	2:H:1299:ASN:H	1.76	0.50
3:I:545:HIS:HB2	3:I:546:ALA:CA	2.42	0.50
4:J:3:ARG:O	4:J:4:VAL:HG13	2.11	0.50
2:C:1107:MET:SD	2:C:1107:MET:N	2.85	0.50
3:D:124:ILE:HG13	3:D:189:LEU:HD11	1.94	0.50
3:D:502:PRO:HB3	3:D:506:VAL:HG11	1.93	0.50
1:G:192:VAL:CG2	1:G:198:LEU:HD12	2.41	0.50
1:A:8:PHE:CE1	1:B:223:ILE:HG12	2.46	0.50
2:C:520:PRO:HB3	2:C:714:VAL:HG11	1.94	0.50
3:D:366:CYS:SG	3:D:437:PHE:HB2	2.51	0.50
3:D:518:VAL:HG23	3:D:716:GLN:OE1	2.12	0.50
5:X:384:LEU:O	5:X:384:LEU:HD13	2.12	0.50
5:X:600:HIS:HB2	5:X:601:PRO:HD3	1.92	0.50
3:I:19:ALA:HB1	3:I:1343:GLU:HB3	1.94	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:I:356:THR:O	3:I:448:GLN:HA	2.11	0.50
2:C:511:LEU:HD12	6:C:1401:1RL:H141	1.93	0.50
2:C:892:GLU:O	2:C:893:THR:OG1	2.24	0.50
3:D:1270:GLY:HA3	3:D:1299:GLY:HA2	1.92	0.50
1:G:181:GLU:HG2	3:I:531:LYS:HD3	1.93	0.50
2:H:105:TYR:CG	2:H:114:VAL:HG13	2.46	0.50
2:H:452:ARG:NH2	2:H:458:GLU:OE1	2.45	0.50
2:H:740:GLU:HB2	2:H:741:MET:SD	2.51	0.50
3:I:773:PHE:O	3:I:776:THR:HG22	2.12	0.50
1:A:41:ASN:OD1	2:C:1218:GLY:HA3	2.11	0.50
2:C:21:VAL:HG13	2:C:22:LEU:N	2.27	0.50
2:C:800:MET:HA	2:C:800:MET:CE	2.41	0.50
2:C:876:GLU:N	2:C:876:GLU:OE2	2.45	0.50
3:D:590:SER:O	3:D:594:GLN:N	2.44	0.50
3:D:810:THR:OG1	3:D:811:GLU:N	2.44	0.50
3:D:1322:ALA:HB1	3:D:1326:GLN:NE2	2.26	0.50
4:E:45:LYS:O	4:E:49:ILE:HG12	2.12	0.50
2:H:36:GLN:O	2:H:39:ILE:HG22	2.11	0.50
2:H:975:ILE:HD13	2:H:975:ILE:O	2.11	0.50
2:H:1210:ILE:HG23	2:H:1211:ARG:NH1	2.27	0.50
2:C:91:THR:HG21	2:C:503:LYS:HE3	1.94	0.50
2:C:933:VAL:HG12	2:C:948:ILE:CD1	2.42	0.50
3:D:573:THR:CG2	3:D:576:ARG:HG3	2.42	0.50
3:D:803:VAL:HG22	3:D:1259:GLN:OE1	2.12	0.50
3:D:1261:LEU:CD2	3:D:1306:LEU:HD22	2.42	0.50
2:H:1107:MET:N	2:H:1107:MET:SD	2.85	0.50
2:H:1186:VAL:HG13	2:H:1187:PHE:N	2.27	0.50
2:C:1292:THR:OG1	2:C:1293:VAL:N	2.44	0.49
3:D:356:THR:O	3:D:448:GLN:HA	2.12	0.49
3:D:388:ARG:NH2	3:D:414:GLU:OE2	2.45	0.49
2:H:487:LEU:HB3	2:H:488:MET:CG	2.40	0.49
3:D:546:ALA:H	3:D:547:ARG:C	2.15	0.49
3:D:349:TYR:CD2	3:D:472:LEU:HD21	2.47	0.49
1:G:107:ILE:HD11	1:G:136:GLU:HG2	1.94	0.49
3:D:213:LYS:O	3:D:217:LEU:HG	2.11	0.49
2:H:645:PHE:HE1	2:H:650:VAL:HB	1.73	0.49
2:H:816:ILE:HG13	2:H:1098:LEU:CD2	2.41	0.49
3:I:349:TYR:HE2	3:I:379:PRO:HG2	1.77	0.49
3:I:1270:GLY:HA3	3:I:1299:GLY:HA2	1.94	0.49
1:A:192:VAL:O	1:A:194:GLN:N	2.44	0.49
1:A:243:LYS:HD3	1:A:243:LYS:N	2.27	0.49



A 1 -1	At 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:C:105:TYR:HA	2:C:106:GLU:HB2	1.94	0.49
2:C:960:LEU:HD12	2:C:1032:LYS:HD3	1.95	0.49
3:D:57:PHE:HB3	3:D:98:ARG:NH1	2.27	0.49
1:F:11:PRO:CG	1:G:228:LEU:H	2.26	0.49
2:H:57:PHE:CE2	2:H:472:GLU:HG3	2.47	0.49
2:H:1042:LEU:HD13	2:H:1042:LEU:N	2.25	0.49
2:H:1127:LYS:HG2	2:H:1144:PHE:CZ	2.47	0.49
5:Y:112:THR:HG22	5:Y:113:ARG:H	1.76	0.49
1:A:158:ARG:HB2	1:A:158:ARG:NH2	2.28	0.49
1:A:167:PRO:HG2	1:A:170:ARG:HG3	1.94	0.49
1:A:310:ARG:HA	1:A:310:ARG:HE	1.76	0.49
3:D:1261:LEU:HD21	3:D:1306:LEU:CD2	2.42	0.49
1:G:227:GLN:O	1:G:229:GLU:N	2.45	0.49
3:I:125:GLY:O	3:I:129:ASP:N	2.45	0.49
2:C:400:VAL:HG12	2:C:404:LYS:CE	2.43	0.49
2:H:448:LEU:HB2	2:H:553:THR:HG21	1.94	0.49
2:H:697:LYS:HG3	2:H:698:PRO:HD2	1.94	0.49
3:I:543:SER:O	3:I:574:VAL:HB	2.12	0.49
2:C:18:ARG:HG3	2:C:19:PRO:HD2	1.94	0.49
3:D:85:CYS:SG	3:D:86:GLU:N	2.85	0.49
4:E:39:VAL:CG1	4:E:40:PRO:HD2	2.43	0.49
5:X:324:LYS:HB3	5:X:325:PRO:HD2	1.94	0.49
1:F:231:PHE:HZ	1:G:39:LEU:HD13	1.76	0.49
2:H:1239:VAL:HG12	2:H:1240:ASP:N	2.27	0.49
2:H:1251:TYR:O	5:Y:525:ASP:N	2.45	0.49
3:I:316:ILE:HD13	3:I:316:ILE:N	2.28	0.49
3:I:1145:PHE:HB3	3:I:1309:ILE:HD13	1.95	0.49
1:A:50:SER:HB3	1:B:8:PHE:CZ	2.47	0.49
1:A:134:THR:HG21	2:C:727:VAL:HG23	1.95	0.49
1:B:83:LEU:CD2	3:D:551:ARG:HG3	2.42	0.49
2:C:897:PRO:HB3	5:X:564:GLY:O	2.13	0.49
3:I:147:ILE:HG23	3:I:156:ARG:C	2.33	0.49
3:I:1295:ASN:O	3:I:1298:VAL:HG12	2.12	0.49
5:Y:240:ARG:O	5:Y:242:HIS:N	2.46	0.49
5:Y:477:GLU:OE1	5:Y:477:GLU:N	2.44	0.49
1:A:118:ASP:OD1	1:A:119:GLY:N	2.46	0.49
1:B:118:ASP:OD1	1:B:119:GLY:N	2.45	0.49
2:C:1105:SER:HB2	3:D:731:ARG:HD3	1.93	0.49
3:D:501:VAL:HG21	3:D:602:SER:HB2	1.95	0.49
3:D:822:MET:HG2	3:D:839:VAL:CG2	2.43	0.49
2:H:817:LEU:HB3	2:H:1097:VAL:CG1	2.43	0.49


		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:H:1180:MET:HB3	2:H:1181:PRO:HA	1.93	0.49
2:C:891:GLY:O	2:C:893:THR:HG23	2.13	0.48
3:D:545:HIS:HB2	3:D:546:ALA:CA	2.42	0.48
3:D:615:LYS:HB3	3:D:616:PRO:HD3	1.95	0.48
3:D:1347:LEU:CD2	3:D:1358:PRO:HG2	2.43	0.48
2:H:13:LYS:HD2	2:H:1181:PRO:HG2	1.93	0.48
3:D:1280:VAL:HG11	3:D:1304:ARG:NE	2.28	0.48
3:I:1322:ALA:HB3	3:I:1331:VAL:HG21	1.94	0.48
5:Y:264:LYS:N	5:Y:264:LYS:HD2	2.28	0.48
2:C:403:MET:HG3	2:C:414:ILE:HB	1.95	0.48
2:C:572:ILE:HD13	6:C:1401:1RL:O1	2.12	0.48
2:C:1276:TRP:HA	2:C:1276:TRP:HE3	1.79	0.48
3:D:807:LEU:HD12	3:D:807:LEU:O	2.12	0.48
3:I:392:THR:HB	5:Y:606:VAL:HG21	1.95	0.48
3:I:919:ALA:O	3:I:923:ILE:HG12	2.14	0.48
2:C:99:LYS:NZ	2:C:99:LYS:HB3	2.28	0.48
2:C:1276:TRP:HA	2:C:1276:TRP:CE3	2.49	0.48
2:C:1296:ASP:OD1	3:D:345:LYS:NZ	2.45	0.48
5:X:561:MET:SD	5:X:576:VAL:HG22	2.53	0.48
2:H:548:ARG:NH2	2:H:567:PRO:O	2.46	0.48
2:H:876:GLU:N	2:H:876:GLU:OE2	2.46	0.48
2:H:979:LEU:HD12	2:H:1002:LEU:HD23	1.95	0.48
3:I:239:LEU:HD12	3:I:239:LEU:O	2.13	0.48
1:A:100:LEU:HD21	1:A:121:VAL:HG21	1.95	0.48
2:C:57:PHE:CE1	2:C:475:VAL:HG11	2.48	0.48
2:C:119:GLU:HG2	2:C:120:GLN:N	2.29	0.48
3:D:50:LYS:HB3	3:D:50:LYS:NZ	2.28	0.48
3:D:368:LEU:HD12	3:D:369:PRO:HD2	1.95	0.48
3:D:1269:ALA:H	3:D:1300:ALA:HB2	1.79	0.48
2:H:127:ILE:HD13	2:H:127:ILE:N	2.27	0.48
2:H:514:PHE:HB2	6:H:1401:1RL:C35	2.44	0.48
3:I:1284:ARG:HA	3:I:1287:ILE:HG12	1.95	0.48
5:Y:301:ASN:O	5:Y:305:LEU:HD13	2.14	0.48
1:A:243:LYS:HB2	1:A:243:LYS:NZ	2.29	0.48
1:A:310:ARG:HA	1:A:310:ARG:NE	2.28	0.48
2:C:1192:GLU:O	2:C:1196:LYS:HD3	2.14	0.48
3:D:147:ILE:HG13	3:D:148:GLU:N	2.28	0.48
1:F:118:ASP:OD1	1:F:119:GLY:N	2.46	0.48
3:I:120:LEU:HB3	3:I:121:PRO:HD3	1.95	0.48
5:Y:541:ARG:O	5:Y:545:HIS:HB2	2.14	0.48
1:A:53:GLY:HA3	1:A:179:PRO:HG3	1.95	0.48



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:C:131:THR:HG22	2:C:135:THR:HG22	1.96	0.48
2:C:700:VAL:HG11	2:C:1114:GLU:CG	2.43	0.48
3:D:197:GLU:O	3:D:201:LEU:HD23	2.14	0.48
3:D:500:ILE:H	3:D:500:ILE:HD13	1.79	0.48
2:H:241:LEU:HD11	2:H:246:LEU:HD11	1.95	0.48
3:I:541:LEU:HB2	3:I:545:HIS:CE1	2.49	0.48
5:Y:138:PRO:HD2	5:Y:353:LEU:HD11	1.96	0.48
5:Y:363:ARG:O	5:Y:367:ILE:HG12	2.14	0.48
2:C:490:GLN:O	5:X:472:GLN:HG3	2.13	0.48
2:C:765:ILE:HG13	2:C:787:PRO:HG2	1.94	0.48
3:D:473:THR:HB	3:D:476:ALA:HB2	1.96	0.48
3:D:786:THR:O	3:D:790:THR:HG23	2.12	0.48
2:H:484:LEU:H	2:H:484:LEU:HD22	1.78	0.48
2:H:568:ASN:HB3	2:H:572:ILE:HD12	1.95	0.48
3:I:85:CYS:HB3	3:I:88:CYS:O	2.14	0.48
3:I:128:LEU:HD12	3:I:192:MET:CE	2.44	0.48
3:I:554:GLU:HA	3:I:589:TYR:CD2	2.49	0.48
2:C:989:LEU:HG	2:C:990:ASP:H	1.79	0.48
2:C:1341:ASP:HB2	2:C:1342:GLU:OE1	2.13	0.48
3:D:8:LEU:HD23	3:D:8:LEU:N	2.29	0.48
3:D:412:LEU:O	3:D:416:ILE:HD12	2.14	0.48
3:D:647:PRO:HG3	3:D:697:MET:HA	1.96	0.48
1:G:47:LEU:CD2	1:G:220:ALA:HB2	2.44	0.48
2:H:448:LEU:HB2	2:H:553:THR:CG2	2.44	0.48
3:I:213:LYS:O	3:I:217:LEU:HG	2.13	0.48
3:I:1291:GLU:HB2	3:I:1292:LEU:HD12	1.96	0.48
1:A:102:LEU:HD12	1:A:115:ILE:HG12	1.95	0.48
2:C:13:LYS:CE	2:C:1183:ALA:HB2	2.37	0.48
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.48	0.48
2:C:753:LEU:O	2:C:753:LEU:HD12	2.13	0.48
3:D:704:GLU:O	3:D:705:THR:OG1	2.25	0.48
1:F:45:ARG:NE	1:G:38:THR:OG1	2.45	0.48
2:H:106:GLU:CB	2:H:107:ARG:HA	2.43	0.48
2:H:741:MET:SD	2:H:741:MET:N	2.86	0.48
2:H:845:LEU:HD23	2:H:889:PRO:HG2	1.96	0.48
3:I:598:LYS:HG3	3:I:599:LYS:HG3	1.95	0.48
3:I:858:VAL:HB	3:I:859:PRO:CD	2.29	0.48
5:Y:503:GLU:HB3	5:Y:504:PRO:O	2.14	0.48
2:C:690:VAL:HG11	2:C:830:THR:CG2	2.44	0.47
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.47	0.47
3:D:1169:THR:HA	3:D:1173:ARG:HB3	1.96	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
5:X:560:ARG:CG	5:X:565:ILE:HG23	2.44	0.47
2:H:521:LEU:HD23	2:H:686:GLN:HB3	1.96	0.47
2:H:716:ALA:HB3	2:H:784:ALA:HB3	1.96	0.47
3:I:1194:ARG:N	3:I:1194:ARG:HD2	2.28	0.47
3:I:1247:LYS:HD3	3:I:1247:LYS:N	2.26	0.47
1:A:224:LEU:HD23	1:B:228:LEU:HD22	1.96	0.47
2:C:1335:ILE:HD11	3:D:22:ILE:HD11	1.96	0.47
3:D:423:LEU:HD21	3:D:447:ILE:HD11	1.96	0.47
3:I:8:LEU:HD23	3:I:8:LEU:N	2.29	0.47
3:I:24:LEU:HD11	3:I:116:PHE:CZ	2.50	0.47
3:I:1323:ALA:O	3:I:1328:THR:HG22	2.13	0.47
5:Y:455:HIS:O	5:Y:459:THR:HG23	2.14	0.47
1:A:158:ARG:NH2	1:A:162:GLU:HB3	2.30	0.47
2:C:119:GLU:OE1	2:C:490:GLN:HB3	2.15	0.47
2:C:149:LEU:HD12	2:C:452:ARG:O	2.14	0.47
2:C:660:VAL:C	2:C:661:VAL:HG13	2.34	0.47
2:C:842:ASP:N	2:C:1046:VAL:HG11	2.29	0.47
3:D:686:TRP:HB3	3:D:758:PRO:HG2	1.96	0.47
2:H:159:SER:OG	2:H:442:VAL:HG11	2.15	0.47
2:H:342:ASP:HA	2:H:437:ASN:HB3	1.96	0.47
2:H:434:ASP:HB3	2:H:439:LYS:HB2	1.97	0.47
3:I:385:LEU:HD21	3:I:411:ILE:HG13	1.97	0.47
3:I:786:THR:O	3:I:790:THR:HG23	2.14	0.47
3:I:810:THR:OG1	3:I:811:GLU:N	2.45	0.47
3:D:539:SER:OG	3:D:540:GLY:N	2.47	0.47
3:D:611:ILE:HG13	3:D:612:LEU:CD2	2.45	0.47
3:D:901:ARG:HB3	3:D:908:ILE:HA	1.95	0.47
3:D:914:ALA:O	3:D:918:ILE:HG22	2.14	0.47
5:X:113:ARG:O	5:X:117:ILE:HD13	2.14	0.47
1:G:192:VAL:HG21	1:G:198:LEU:CD1	2.44	0.47
2:H:204:LEU:HD11	2:H:369:MET:HG3	1.96	0.47
2:H:971:LEU:HD12	2:H:1018:TYR:HD1	1.78	0.47
3:I:37:GLU:HB2	3:I:104:HIS:CE1	2.49	0.47
2:C:748:ILE:HD12	2:C:748:ILE:O	2.14	0.47
3:D:19:ALA:HB2	3:D:1343:GLU:CB	2.45	0.47
3:D:828:GLY:HA2	3:D:832:LYS:N	2.29	0.47
5:X:262:VAL:HG12	5:X:264:LYS:H	1.78	0.47
5:X:503:GLU:HB3	5:X:504:PRO:O	2.13	0.47
5:X:532:LEU:O	5:X:536:THR:HG23	2.15	0.47
1:F:182:ARG:NH2	1:F:206:GLU:OE1	2.47	0.47
2:H:94:ALA:HB2	2:H:129:LEU:HD11	1.97	0.47



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:H:119:GLU:HG2	2:H:120:GLN:N	2.29	0.47
3:I:535:ARG:HB3	3:I:541:LEU:HD11	1.96	0.47
3:I:611:ILE:HG13	3:I:612:LEU:CD2	2.45	0.47
3:I:704:GLU:O	3:I:705:THR:OG1	2.26	0.47
3:I:800:LEU:HB3	3:I:920:ALA:HB1	1.96	0.47
5:Y:262:VAL:HG12	5:Y:264:LYS:H	1.80	0.47
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.80	0.47
2:C:205:PRO:O	2:C:208:ILE:HG22	2.15	0.47
5:X:264:LYS:HD2	5:X:264:LYS:N	2.29	0.47
5:X:357:GLN:NE2	5:X:360:ASP:OD2	2.47	0.47
2:H:960:LEU:HD12	2:H:1032:LYS:HD3	1.95	0.47
2:H:1289:GLU:HG3	2:H:1290:MET:N	2.30	0.47
3:I:832:LYS:HB2	3:I:832:LYS:HZ2	1.79	0.47
3:I:1171:GLY:N	3:I:1172:LYS:O	2.47	0.47
3:I:1347:LEU:O	3:I:1351:VAL:HG23	2.15	0.47
1:A:303:ILE:O	1:A:307:LEU:HD13	2.14	0.47
1:B:19:VAL:O	1:B:19:VAL:HG12	2.15	0.47
2:C:812:PHE:CD2	2:C:813:GLU:HG3	2.50	0.47
2:C:1180:MET:HB3	2:C:1181:PRO:HA	1.96	0.47
2:C:1254:VAL:HG23	2:C:1255:THR:N	2.29	0.47
2:C:1298:VAL:HG23	2:C:1299:ASN:H	1.79	0.47
3:D:139:LEU:O	3:D:139:LEU:HD22	2.15	0.47
3:D:166:LEU:HD12	3:D:167:ASP:N	2.30	0.47
3:D:294:ASN:ND2	3:D:298:MET:SD	2.87	0.47
3:D:355:ILE:HG12	3:D:464:ASP:O	2.14	0.47
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.95	0.47
4:E:5:THR:HB	4:E:7:GLN:HB2	1.97	0.47
5:X:138:PRO:HG3	5:X:353:LEU:HD21	1.97	0.47
5:X:333:VAL:HG22	5:X:336:GLU:HB2	1.96	0.47
5:X:551:LEU:HD22	5:X:597:LYS:HD2	1.97	0.47
1:G:42:ALA:O	1:G:46:ILE:HG12	2.15	0.47
2:H:73:TYR:O	2:H:74:ARG:HB2	2.14	0.47
2:H:127:ILE:O	2:H:127:ILE:HG12	2.14	0.47
2:H:813:GLU:HG2	3:I:504:GLN:NE2	2.30	0.47
3:I:50:LYS:HG2	3:I:51:PRO:HD2	1.95	0.47
3:I:112:ALA:HA	3:I:238:ILE:HG22	1.96	0.47
3:I:600:ALA:HA	3:I:603:LYS:HB3	1.95	0.47
3:I:886:VAL:CG1	3:I:1230:THR:HG21	2.44	0.47
3:I:1322:ALA:HB1	3:I:1326:GLN:NE2	2.30	0.47
5:Y:470:MET:HB2	5:Y:478:PRO:HB3	1.96	0.47
2:C:533:LEU:HG	6:C:1401:1RL:H142	1.97	0.47



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:D:423:LEU:HB3	3:D:466:MET:CE	2.44	0.47
3:D:554:GLU:HA	3:D:589:TYR:CD2	2.49	0.47
3:D:598:LYS:HG3	3:D:599:LYS:HG3	1.95	0.47
3:D:824:PRO:HB3	3:D:836:ARG:HD3	1.97	0.47
3:D:1268:ASN:HB3	3:D:1300:ALA:CB	2.45	0.47
2:H:156:PHE:CE2	2:H:177:ILE:HD13	2.50	0.47
2:H:1045:GLY:O	2:H:1046:VAL:HB	2.14	0.47
2:H:1180:MET:HB3	2:H:1181:PRO:O	2.13	0.47
1:B:19:VAL:O	1:B:20:SER:CB	2.63	0.47
3:D:120:LEU:HG	5:X:46:GLN:HB2	1.96	0.47
3:D:141:PHE:O	3:D:297:ARG:HD3	2.15	0.47
1:F:41:ASN:HD21	2:H:1218:GLY:HA3	1.80	0.47
2:H:106:GLU:HB3	2:H:107:ARG:CA	2.45	0.47
3:I:746:LEU:HD13	3:I:758:PRO:HG3	1.95	0.47
2:C:42:ASP:HB3	2:C:43:PRO:CD	2.26	0.47
2:C:71:VAL:O	2:C:72:SER:OG	2.30	0.47
2:C:519:ASN:ND2	2:C:689:ALA:O	2.47	0.47
3:D:120:LEU:CD2	3:D:1330:ARG:HD2	2.45	0.47
3:D:145:VAL:HG22	3:D:180:MET:SD	2.55	0.47
3:D:291:ILE:HD11	5:X:384:LEU:HD21	1.97	0.47
3:D:1198:VAL:HB	3:D:1210:ILE:CD1	2.45	0.47
2:H:989:LEU:HG	2:H:990:ASP:H	1.80	0.47
2:H:1101:LEU:HD21	3:I:508:LEU:CD1	2.45	0.47
2:H:1163:THR:HG22	2:H:1164:PHE:H	1.80	0.47
2:H:1254:VAL:HG23	2:H:1255:THR:N	2.29	0.47
3:I:147:ILE:HG13	3:I:148:GLU:N	2.29	0.47
2:C:92:TYR:CD1	2:C:129:LEU:HB2	2.50	0.46
2:C:542:ARG:O	2:C:544:GLY:N	2.41	0.46
3:D:138:VAL:O	3:D:143:SER:HB3	2.14	0.46
3:D:543:SER:O	3:D:574:VAL:HB	2.14	0.46
3:D:573:THR:HG22	3:D:576:ARG:CG	2.44	0.46
1:F:11:PRO:HG2	1:G:228:LEU:H	1.80	0.46
2:H:494:ASN:OD1	2:H:495:ALA:N	2.47	0.46
2:H:634:VAL:HG22	2:H:645:PHE:CE2	2.50	0.46
3:I:658:GLU:HA	3:I:661:VAL:HG12	1.96	0.46
3:I:678:ARG:O	3:I:681:LYS:HG3	2.15	0.46
2:C:105:TYR:CG	2:C:106:GLU:HB2	2.50	0.46
3:D:679:TYR:CZ	3:D:683:ILE:HD11	2.49	0.46
2:H:21:VAL:HG21	2:H:592:ARG:HD3	1.97	0.46
3:I:42:GLU:HG3	5:Y:451:ARG:NH2	2.31	0.46
5:Y:355:ILE:O	5:Y:358:VAL:HG22	2.14	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:134:THR:HG21	2:C:727:VAL:O	2.16	0.46
1:A:300:LEU:CD1	1:A:304:LYS:HE2	2.46	0.46
1:A:318:LEU:HD13	1:A:318:LEU:N	2.30	0.46
3:D:57:PHE:CZ	3:D:252:LEU:HD22	2.50	0.46
4:E:38:LEU:HD13	4:E:58:LEU:CD2	2.40	0.46
2:H:674:ASP:OD2	2:H:1070:HIS:ND1	2.49	0.46
1:B:37:HIS:CD2	2:C:1216:ARG:HB3	2.51	0.46
2:C:697:LYS:HG3	2:C:698:PRO:HD2	1.98	0.46
3:D:105:ILE:HD13	3:D:273:ILE:CD1	2.44	0.46
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.31	0.46
3:D:1198:VAL:HB	3:D:1210:ILE:HD13	1.98	0.46
1:F:158:ARG:HB2	1:F:158:ARG:NH2	2.30	0.46
3:I:66:LYS:HB2	3:I:69:GLU:HG2	1.98	0.46
2:C:1239:VAL:HG12	2:C:1240:ASP:N	2.27	0.46
2:C:1285:TYR:CG	3:D:475:GLU:HG3	2.50	0.46
1:G:227:GLN:C	1:G:229:GLU:H	2.19	0.46
2:H:1301:ARG:HG3	2:H:1302:THR:N	2.30	0.46
3:I:161:THR:HG22	3:I:162:GLU:N	2.30	0.46
1:A:69:SER:OG	1:A:70:THR:N	2.48	0.46
2:C:106:GLU:HG2	2:C:109:ALA:H	1.80	0.46
2:C:163:LYS:H	2:C:163:LYS:CD	2.12	0.46
2:C:1006:GLU:O	2:C:1006:GLU:HG2	2.16	0.46
3:D:583:VAL:CG1	3:D:584:PRO:HD2	2.46	0.46
3:D:1234:VAL:HG13	3:D:1235:ASN:N	2.31	0.46
2:H:1233:LEU:HD12	2:H:1233:LEU:O	2.15	0.46
3:I:403:ARG:O	3:I:405:GLU:N	2.49	0.46
2:C:850:ILE:HG23	2:C:885:GLY:O	2.16	0.46
3:D:22:ILE:HG12	3:D:1336:ALA:HA	1.98	0.46
3:D:1167:LYS:HE3	3:D:1173:ARG:HH12	1.81	0.46
3:D:1274:PHE:HD2	3:D:1275:LEU:HG	1.79	0.46
3:I:349:TYR:CE2	3:I:379:PRO:HG2	2.50	0.46
2:C:727:VAL:HG22	2:C:773:LEU:HB3	1.98	0.46
3:D:38:VAL:HG11	3:D:56:LEU:HD13	1.97	0.46
3:D:99:ARG:HA	3:D:248:ASP:HB2	1.98	0.46
3:D:235:GLU:OE1	3:D:235:GLU:N	2.48	0.46
2:H:453:ILE:O	2:H:453:ILE:HG23	2.16	0.46
3:I:366:CYS:SG	3:I:437:PHE:HB2	2.56	0.46
3:I:582:ILE:HG23	3:I:623:GLN:HB3	1.98	0.46
1:A:231:PHE:CD2	1:B:43:LEU:HD11	2.51	0.46
1:B:14:VAL:HG13	1:B:28:LEU:CD2	2.46	0.46
2:C:400:VAL:HG12	2:C:404:LYS:HE2	1.97	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:C:751:TYR:CE1	2:C:783:LEU:HD12	2.51	0.46
2:C:817:LEU:HB3	2:C:1097:VAL:HG13	1.98	0.46
3:D:395:LYS:HD3	5:X:607:LEU:HD13	1.98	0.46
3:D:535:ARG:HB3	3:D:541:LEU:HD11	1.98	0.46
3:D:678:ARG:O	3:D:681:LYS:HG3	2.16	0.46
1:F:223:ILE:HD13	1:G:8:PHE:CE1	2.50	0.46
2:H:72:SER:O	2:H:98:VAL:HG23	2.16	0.46
2:H:568:ASN:HB3	2:H:572:ILE:CD1	2.45	0.46
2:H:748:ILE:HD12	2:H:748:ILE:O	2.16	0.46
2:H:1272:GLU:HA	2:H:1275:VAL:HG22	1.97	0.46
3:I:824:PRO:HB3	3:I:836:ARG:HD3	1.98	0.46
3:I:1237:VAL:O	3:I:1240:VAL:HG22	2.16	0.46
2:C:202:ARG:NE	2:C:369:MET:HG2	2.31	0.46
2:C:1289:GLU:HG3	2:C:1290:MET:N	2.31	0.46
3:D:161:THR:HG22	3:D:162:GLU:N	2.31	0.46
3:D:1241:TYR:CD1	3:D:1248:ILE:HG21	2.51	0.46
5:X:115:GLY:O	5:X:119:ILE:HG12	2.16	0.46
1:F:79:LEU:O	1:F:83:LEU:HD13	2.16	0.46
2:H:55:SER:CB	2:H:56:VAL:HG13	2.43	0.46
3:I:608:CYS:O	3:I:612:LEU:HB2	2.16	0.46
3:I:1193:TRP:O	3:I:1194:ARG:HB2	2.15	0.46
4:J:5:THR:HA	4:J:6:VAL:HG12	1.98	0.46
2:C:592:ARG:HB2	2:C:653:MET:HB3	1.98	0.45
2:C:972:PHE:HA	2:C:975:ILE:HG22	1.98	0.45
3:D:120:LEU:HG	5:X:46:GLN:NE2	2.31	0.45
3:D:522:GLY:HA2	3:D:545:HIS:CD2	2.51	0.45
3:D:909:ILE:HD12	3:D:909:ILE:O	2.17	0.45
3:D:1138:LEU:HB3	3:D:1139:PRO:HD3	1.99	0.45
2:H:189:ASP:HB2	2:H:190:PRO:CD	2.47	0.45
2:H:1006:GLU:HG2	2:H:1006:GLU:O	2.16	0.45
5:Y:471:LEU:HD12	5:Y:472:GLN:N	2.31	0.45
2:C:742:TYR:CB	2:C:743:PRO:HD3	2.42	0.45
2:H:814:ASP:O	2:H:1074:GLY:HA2	2.17	0.45
2:H:1005:GLU:O	2:H:1007:LYS:N	2.49	0.45
6:H:1401:1RL:O2	6:H:1401:1RL:O1	2.35	0.45
3:I:147:ILE:HD12	3:I:178:ALA:CB	2.46	0.45
3:I:325:LYS:NZ	3:I:330:MET:HG2	2.31	0.45
3:I:1268:ASN:HB3	3:I:1300:ALA:HB1	1.98	0.45
1:B:22:THR:HG22	1:B:208:ASN:O	2.16	0.45
2:C:963:GLU:O	2:C:966:ILE:HG22	2.16	0.45
3:I:294:ASN:ND2	5:Y:406:GLN:OE1	2.49	0.45



A 4 1	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:I:546:ALA:H	3:I:547:ARG:C	2.20	0.45
1:B:192:VAL:HG12	1:B:194:GLN:HG2	1.98	0.45
2:C:105:TYR:CD1	2:C:114:VAL:HG13	2.51	0.45
2:C:185:ASP:HB2	2:C:197:ARG:HB2	1.99	0.45
2:C:901:LEU:O	2:C:905:ILE:HG13	2.17	0.45
2:C:1238:LEU:HD12	2:C:1239:VAL:O	2.16	0.45
3:D:245:LEU:CD1	3:D:246:PRO:HD2	2.45	0.45
3:D:515:ARG:NH2	3:D:718:SER:O	2.50	0.45
3:D:572:THR:HG22	3:D:594:GLN:HE22	1.82	0.45
3:D:773:PHE:O	3:D:776:THR:HG22	2.16	0.45
3:D:822:MET:HG2	3:D:839:VAL:HG22	1.98	0.45
3:D:1307:LEU:N	3:D:1307:LEU:HD23	2.32	0.45
1:F:86:LYS:HE2	1:F:173:VAL:HG23	1.98	0.45
2:H:488:MET:H	2:H:489:PRO:HA	1.81	0.45
2:H:1116:HIS:HE1	2:H:1226:THR:HG23	1.81	0.45
3:I:265:LEU:HD11	3:I:330:MET:SD	2.57	0.45
3:I:647:PRO:HG3	3:I:697:MET:HA	1.98	0.45
3:I:1306:LEU:HD13	3:I:1307:LEU:N	2.31	0.45
4:J:31:GLN:HB2	4:J:46:THR:HG21	1.98	0.45
5:Y:459:THR:O	5:Y:463:LEU:HD13	2.16	0.45
2:C:166:SER:O	2:C:167:SER:OG	2.30	0.45
3:D:162:GLU:HG2	3:D:163:GLU:N	2.31	0.45
3:D:316:ILE:O	3:D:317:THR:OG1	2.19	0.45
3:D:664:ILE:HG21	3:D:681:LYS:CD	2.47	0.45
3:D:664:ILE:HD12	3:D:681:LYS:HE3	1.99	0.45
3:D:759:ILE:HG23	3:D:771:GLN:HG3	1.99	0.45
1:F:41:ASN:HD21	2:H:1218:GLY:CA	2.29	0.45
2:H:576:SER:HB3	2:H:579:ALA:HB2	1.99	0.45
2:H:1086:PRO:HG2	2:H:1094:VAL:CG2	2.47	0.45
2:H:1105:SER:HB2	3:I:731:ARG:HB2	1.99	0.45
2:H:1276:TRP:HA	2:H:1276:TRP:HE3	1.82	0.45
3:I:58:CYS:SG	3:I:60:ARG:N	2.89	0.45
3:I:382:TYR:HB3	3:I:394:ILE:CD1	2.46	0.45
3:I:513:MET:O	3:I:575:GLY:HA3	2.16	0.45
3:I:583:VAL:CG1	3:I:584:PRO:HD2	2.46	0.45
3:I:733:SER:O	3:I:737:ILE:HG12	2.17	0.45
1:A:166:ARG:HA	1:A:167:PRO:HD2	1.82	0.45
1:A:178:SER:HA	1:A:179:PRO:HD3	1.77	0.45
2:C:845:LEU:HD13	2:C:845:LEU:N	2.28	0.45
3:D:128:LEU:HD12	3:D:192:MET:HE3	1.99	0.45
3:D:918:ILE:HD13	3:D:919:ALA:N	2.32	0.45



	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
5:X:459:THR:O	5:X:463:LEU:HD13	2.15	0.45
2:H:500:ALA:O	2:H:504:GLU:HB2	2.17	0.45
2:H:994:ARG:HD3	2:H:994:ARG:N	2.32	0.45
3:I:138:VAL:O	3:I:143:SER:HB3	2.17	0.45
3:I:179:LYS:HD3	3:I:179:LYS:N	2.32	0.45
3:I:422:LEU:HA	3:I:436:ALA:HA	1.99	0.45
2:C:44:GLU:HG3	2:C:45:GLY:N	2.32	0.45
2:C:88:ARG:NH2	2:C:1040:ASP:OD1	2.49	0.45
2:C:106:GLU:HB3	2:C:107:ARG:CA	2.46	0.45
3:D:395:LYS:NZ	5:X:607:LEU:O	2.36	0.45
3:D:611:ILE:HG13	3:D:612:LEU:HD23	1.99	0.45
3:D:1291:GLU:HB2	3:D:1292:LEU:HD12	1.99	0.45
5:X:379:MET:HE2	5:X:379:MET:HA	1.99	0.45
2:H:106:GLU:HG2	2:H:109:ALA:H	1.82	0.45
2:H:551:HIS:CG	2:H:552:PRO:HD2	2.52	0.45
3:I:579:LEU:O	3:I:579:LEU:HD13	2.16	0.45
3:I:744:ARG:HB2	3:I:759:ILE:HB	1.97	0.45
2:C:893:THR:O	2:C:894:GLN:HB2	2.17	0.45
3:D:502:PRO:HB3	3:D:506:VAL:CG1	2.47	0.45
2:H:31:GLN:HG3	2:H:130:MET:HE1	1.99	0.45
2:H:660:VAL:C	2:H:661:VAL:HG13	2.37	0.45
3:I:390:LEU:N	3:I:390:LEU:HD12	2.31	0.45
3:I:886:VAL:HG23	3:I:1254:GLU:HB3	1.99	0.45
3:I:1247:LYS:H	3:I:1247:LYS:CD	2.26	0.45
3:I:1256:ILE:O	3:I:1260:MET:HB2	2.17	0.45
1:B:18:GLN:C	1:B:20:SER:H	2.19	0.45
2:C:80:PHE:O	2:C:84:GLU:HB3	2.16	0.45
2:C:533:LEU:N	2:C:533:LEU:HD23	2.32	0.45
2:C:1336:ASN:HB2	3:D:25:ALA:HB2	1.99	0.45
3:D:1266:ILE:HG13	3:D:1274:PHE:O	2.17	0.45
5:X:23:THR:HG22	5:X:26:GLU:HG2	1.99	0.45
5:X:379:MET:HA	5:X:379:MET:CE	2.47	0.45
2:H:700:VAL:HG11	2:H:1114:GLU:CG	2.46	0.45
2:H:941:LYS:HD2	2:H:941:LYS:O	2.16	0.45
1:A:11:PRO:HB3	1:A:31:LEU:HD21	1.98	0.45
2:C:589:THR:HG23	2:C:591:TYR:CE2	2.52	0.45
2:C:1290:MET:SD	2:C:1294:LYS:HD3	2.57	0.45
3:D:841:GLY:CA	3:D:901:ARG:HD3	2.46	0.45
3:D:863:LEU:HB2	3:D:866:GLU:HB2	1.99	0.45
5:X:519:LEU:O	5:X:519:LEU:HD13	2.17	0.45
2:H:1276:TRP:HA	2:H:1276:TRP:CE3	2.52	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
5:Y:99:ARG:O	5:Y:99:ARG:HD3	2.17	0.45
1:A:279:GLY:HA3	1:A:321:TRP:CZ2	2.52	0.44
2:C:551:HIS:CD2	2:C:552:PRO:HD2	2.52	0.44
3:D:30:ILE:HG23	3:D:243:PRO:HB3	1.99	0.44
3:D:884:SER:OG	3:D:1254:GLU:OE1	2.25	0.44
1:G:149:GLY:HA3	1:G:177:TYR:CD2	2.52	0.44
1:A:33:ARG:NH1	1:A:199:ASP:OD2	2.50	0.44
1:A:321:TRP:HA	1:A:322:PRO:HA	1.71	0.44
2:C:403:MET:HE1	2:C:584:TYR:CD1	2.53	0.44
3:D:233:LYS:HD2	3:D:234:PRO:HD2	1.99	0.44
3:D:275:ARG:HD2	3:D:302:ALA:HB2	2.00	0.44
3:D:396:ALA:HB2	5:X:606:VAL:HG11	1.97	0.44
3:D:1295:ASN:O	3:D:1298:VAL:HG12	2.16	0.44
5:X:290:LEU:HB3	5:X:333:VAL:HG21	1.98	0.44
1:G:29:GLU:HA	1:G:200:LYS:HB2	1.99	0.44
2:H:732:ILE:HD11	2:H:769:PRO:HB3	1.98	0.44
2:H:843:THR:HB	2:H:845:LEU:CD2	2.47	0.44
3:I:205:LEU:HD22	3:I:217:LEU:HD22	1.98	0.44
3:I:482:ALA:C	3:I:483:LEU:HD12	2.38	0.44
2:C:542:ARG:HG2	2:C:543:ALA:N	2.32	0.44
2:C:1243:MET:SD	3:D:445:LYS:HB3	2.58	0.44
3:D:124:ILE:HA	3:D:237:MET:HE2	1.99	0.44
5:X:288:MET:HA	5:X:302:PHE:CZ	2.52	0.44
2:H:344:GLY:HA2	2:H:345:PRO:HD3	1.83	0.44
2:H:1325:VAL:O	2:H:1329:GLU:HG3	2.18	0.44
3:I:1168:GLU:O	3:I:1169:THR:OG1	2.35	0.44
3:I:1190:ILE:HD12	3:I:1190:ILE:N	2.32	0.44
2:C:17:LYS:HG2	2:C:1155:VAL:HG11	1.99	0.44
2:C:1148:ALA:HB1	2:C:1180:MET:CE	2.47	0.44
3:D:1306:LEU:HD13	3:D:1307:LEU:N	2.33	0.44
2:H:157:PHE:CD2	2:H:174:ALA:HB2	2.52	0.44
2:C:453:ILE:HG23	2:C:453:ILE:O	2.17	0.44
2:C:936:ARG:HH11	5:X:495:ARG:HD3	1.82	0.44
3:D:610:ARG:CG	3:D:864:LEU:HD22	2.45	0.44
2:H:105:TYR:CG	2:H:106:GLU:HB2	2.52	0.44
2:H:1129:ASN:OD1	2:H:1177:ARG:NH1	2.49	0.44
2:H:1212:LEU:HD12	2:H:1225:VAL:HG21	1.99	0.44
3:I:252:LEU:H	3:I:252:LEU:HD23	1.81	0.44
3:I:363:LEU:O	3:I:486:SER:OG	2.29	0.44
3:I:886:VAL:HG13	3:I:1230:THR:HG21	2.00	0.44
1:A:317:ARG:C	1:A:318:LEU:HD13	2.38	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:192:VAL:CG2	1:B:198:LEU:HD12	2.43	0.44
2:C:933:VAL:CG1	2:C:948:ILE:HD11	2.47	0.44
2:C:1140:LYS:HE2	2:C:1166:ASP:HB3	1.99	0.44
3:D:832:LYS:HB2	3:D:832:LYS:HZ2	1.83	0.44
2:H:62:TYR:CD2	2:H:480:SER:HB3	2.53	0.44
2:H:699:LEU:HD11	2:H:1179:GLY:CA	2.44	0.44
3:I:288:PRO:HB2	3:I:291:ILE:HG12	2.00	0.44
1:A:221:ALA:HB1	1:B:228:LEU:HD13	2.00	0.44
1:B:27:THR:HG22	1:B:202:VAL:HG22	1.98	0.44
2:C:1028:LYS:O	2:C:1032:LYS:HG2	2.18	0.44
2:C:1045:GLY:O	2:C:1046:VAL:HB	2.17	0.44
2:C:1158:LYS:HD2	2:C:1158:LYS:O	2.18	0.44
3:D:205:LEU:HB3	3:D:217:LEU:HD22	1.99	0.44
3:D:233:LYS:HG3	3:D:234:PRO:HD2	2.00	0.44
3:D:899:TYR:CD2	3:D:909:ILE:HG12	2.53	0.44
5:X:592:ALA:O	5:X:596:ARG:HG2	2.16	0.44
2:H:653:MET:HG2	2:H:654:ASP:N	2.33	0.44
2:H:1277:ALA:HB3	3:I:434:ILE:HD13	2.00	0.44
3:I:822:MET:HG2	3:I:839:VAL:CG2	2.48	0.44
1:A:29:GLU:O	1:A:31:LEU:N	2.50	0.44
2:C:42:ASP:O	2:C:44:GLU:HG2	2.17	0.44
2:C:1270:PHE:CE1	2:C:1290:MET:HG2	2.53	0.44
3:D:841:GLY:HA3	3:D:901:ARG:HD3	1.99	0.44
3:D:1255:VAL:O	3:D:1258:ARG:HB3	2.18	0.44
2:H:122:VAL:HG13	2:H:124:MET:HG3	2.00	0.44
2:H:488:MET:HB2	2:H:489:PRO:HA	1.99	0.44
2:H:551:HIS:CD2	2:H:552:PRO:HD2	2.52	0.44
2:H:1298:VAL:HG13	2:H:1321:GLU:HG3	1.99	0.44
3:I:242:LEU:HD12	3:I:243:PRO:HD2	2.00	0.44
3:I:412:LEU:O	3:I:415:VAL:HG22	2.17	0.44
3:I:515:ARG:NH2	3:I:717:VAL:HG12	2.32	0.44
3:I:610:ARG:CG	3:I:864:LEU:HD22	2.48	0.44
3:I:1307:LEU:N	3:I:1307:LEU:HD23	2.33	0.44
4:J:25:ARG:NH2	4:J:68:GLU:OE1	2.51	0.44
5:Y:139:GLU:HG3	5:Y:351:THR:HA	2.00	0.44
2:C:817:LEU:HB3	2:C:1097:VAL:CG1	2.48	0.44
2:C:841:ARG:HA	2:C:1046:VAL:HG13	2.00	0.44
2:C:1073:LYS:HD3	3:D:462:ASP:HB3	1.99	0.44
3:D:144:TYR:HB3	3:D:159:ILE:CG2	2.48	0.44
3:D:709:ARG:HD2	3:D:714:GLU:HB2	2.00	0.44
3:D:828:GLY:HA2	3:D:832:LYS:CA	2.47	0.44



A 4 a m 1		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:D:1238:GLN:O	3:D:1242:ARG:HG2	2.17	0.44
4:E:82:ALA:O	4:E:86:ILE:HG13	2.17	0.44
1:F:234:LEU:HD12	1:F:234:LEU:N	2.33	0.44
2:H:218:GLU:HG2	2:H:299:LYS:HA	2.00	0.44
2:H:549:ASP:OD1	2:H:550:VAL:N	2.50	0.44
2:H:747:GLY:C	2:H:748:ILE:HG13	2.38	0.44
2:H:843:THR:HB	2:H:845:LEU:HD22	1.99	0.44
3:I:108:ALA:CB	3:I:279:LEU:HD12	2.48	0.44
3:I:1234:VAL:HG13	3:I:1235:ASN:N	2.33	0.44
3:I:1258:ARG:HG3	3:I:1259:GLN:N	2.33	0.44
5:Y:96:ASP:CG	5:Y:97:PRO:HD2	2.37	0.44
2:C:1255:THR:HG22	2:C:1257:GLN:HG3	1.98	0.43
3:D:482:ALA:C	3:D:483:LEU:HD12	2.39	0.43
2:H:127:ILE:HA	2:H:128:PRO:HD3	1.90	0.43
3:I:162:GLU:HG2	3:I:163:GLU:N	2.33	0.43
3:I:413:ASP:HA	3:I:416:ILE:CD1	2.47	0.43
3:I:545:HIS:CB	3:I:546:ALA:HA	2.41	0.43
5:Y:395:THR:HA	5:Y:404:LEU:CD2	2.48	0.43
2:C:1103:VAL:N	2:C:1104:PRO:HD2	2.33	0.43
3:D:139:LEU:HD22	3:D:139:LEU:C	2.39	0.43
3:D:233:LYS:CD	3:D:234:PRO:HD2	2.48	0.43
3:D:390:LEU:N	3:D:390:LEU:HD12	2.33	0.43
3:D:579:LEU:O	3:D:579:LEU:HD13	2.17	0.43
3:D:915:ILE:O	3:D:918:ILE:HG23	2.17	0.43
3:D:1190:ILE:HD12	3:D:1190:ILE:N	2.32	0.43
5:X:47:MET:O	5:X:55:VAL:HG11	2.18	0.43
2:H:971:LEU:HD21	2:H:1017:GLN:NE2	2.33	0.43
2:H:1017:GLN:O	2:H:1020:GLU:HB3	2.18	0.43
3:I:155:GLU:CG	3:I:158:GLN:HB2	2.48	0.43
3:I:518:VAL:HG23	3:I:716:GLN:OE1	2.18	0.43
3:I:534:GLU:O	3:I:538:ARG:HB2	2.18	0.43
3:I:582:ILE:HG23	3:I:623:GLN:CB	2.48	0.43
5:Y:115:GLY:O	5:Y:119:ILE:HG12	2.18	0.43
1:B:232:VAL:O	1:B:233:ASP:HB2	2.18	0.43
2:C:122:VAL:HG22	2:C:123:TYR:N	2.33	0.43
2:C:994:ARG:HD3	2:C:994:ARG:N	2.33	0.43
2:C:1244:HIS:HB3	2:C:1265:PHE:CD2	2.53	0.43
2:C:1281:TYR:O	3:D:483:LEU:HD23	2.19	0.43
3:D:202:ARG:O	3:D:206:ASN:ND2	2.51	0.43
3:D:648:GLU:OE2	3:D:648:GLU:N	2.51	0.43
5:X:17:LYS:NZ	5:X:17:LYS:HB3	2.32	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:H:465:ARG:O	2:H:469:VAL:HG23	2.18	0.43
2:H:902:LEU:HD21	5:Y:608:ARG:HG3	2.00	0.43
2:H:1258:PRO:HG2	3:I:346:ARG:HB3	1.99	0.43
3:I:856:ILE:HG13	3:I:857:LEU:O	2.19	0.43
3:I:901:ARG:CB	3:I:908:ILE:HA	2.49	0.43
2:C:936:ARG:HB3	2:C:939:VAL:CG2	2.49	0.43
2:C:993:PRO:HB2	2:C:994:ARG:H	1.60	0.43
3:D:40:LYS:HA	3:D:41:PRO:HD3	1.80	0.43
3:D:63:GLY:O	3:D:98:ARG:NH2	2.50	0.43
5:X:105:MET:O	5:X:385:ARG:NH1	2.51	0.43
2:H:37:LYS:HA	2:H:37:LYS:HE3	2.00	0.43
2:H:397:LEU:O	2:H:398:SER:OG	2.23	0.43
2:H:705:GLU:HB2	2:H:794:LEU:HB3	2.01	0.43
3:I:1254:GLU:HA	3:I:1257:VAL:HG12	1.99	0.43
5:Y:465:ARG:O	5:Y:468:ARG:HG2	2.18	0.43
1:A:234:LEU:N	1:A:234:LEU:HD12	2.34	0.43
1:B:62:ASP:OD1	1:B:143:ARG:NH1	2.50	0.43
2:C:699:LEU:HD23	2:C:799:ASN:CG	2.38	0.43
2:H:898:GLU:HB2	5:Y:540:LEU:HD21	1.99	0.43
2:H:1103:VAL:N	2:H:1104:PRO:HD2	2.34	0.43
3:I:590:SER:O	3:I:594:GLN:N	2.51	0.43
3:I:909:ILE:HD12	3:I:909:ILE:O	2.18	0.43
3:I:1346:GLY:HA3	3:I:1349:GLU:OE2	2.18	0.43
5:Y:290:LEU:O	5:Y:294:GLN:HB3	2.18	0.43
1:B:27:THR:HG22	1:B:202:VAL:HG13	2.00	0.43
2:C:106:GLU:H	2:C:107:ARG:HA	1.83	0.43
3:D:19:ALA:HB1	3:D:1343:GLU:HB3	1.97	0.43
3:D:762:ASN:OD1	3:D:764:ARG:HB3	2.19	0.43
3:D:1320:ILE:HG22	3:D:1352:ILE:CD1	2.47	0.43
1:G:37:HIS:CD2	2:H:1216:ARG:HB3	2.54	0.43
2:H:333:ILE:N	2:H:333:ILE:HD12	2.34	0.43
2:H:529:ARG:CD	6:H:1401:1RL:H171	2.48	0.43
2:H:892:GLU:O	2:H:893:THR:OG1	2.22	0.43
3:I:27:PRO:HD3	3:I:236:TRP:CE3	2.53	0.43
3:I:572:THR:HB	3:I:576:ARG:HD2	2.01	0.43
1:B:47:LEU:HD13	1:B:205:MET:HE2	1.99	0.43
1:B:153:VAL:HA	1:B:154:PRO:HD3	1.83	0.43
2:C:170:VAL:O	2:C:171:LEU:HB2	2.18	0.43
2:C:189:ASP:HB2	2:C:190:PRO:CD	2.49	0.43
2:C:589:THR:OG1	2:C:590:PRO:HD2	2.19	0.43
3:D:240:THR:HG23	3:D:241:VAL:HG23	2.01	0.43



	A L	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:D:252:LEU:HD23	3:D:252:LEU:H	1.82	0.43
3:D:519:ASN:OD1	3:D:520:ALA:N	2.51	0.43
3:I:305:ALA:O	3:I:309:ASN:ND2	2.51	0.43
5:Y:264:LYS:HD2	5:Y:264:LYS:H	1.84	0.43
2:C:135:THR:OG1	2:C:143:ARG:O	2.35	0.43
2:C:747:GLY:C	2:C:748:ILE:HG13	2.39	0.43
2:C:844:LYS:HB2	2:C:844:LYS:NZ	2.33	0.43
3:D:27:PRO:O	3:D:31:ARG:HD3	2.19	0.43
3:D:50:LYS:HG2	3:D:51:PRO:CD	2.49	0.43
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	1.99	0.43
2:H:992:LEU:HD23	2:H:996:ARG:HG3	1.99	0.43
2:H:1014:LEU:HA	2:H:1017:GLN:OE1	2.19	0.43
2:H:1285:TYR:CG	3:I:475:GLU:HG3	2.54	0.43
3:I:799:ARG:NH1	3:I:1146:GLU:OE1	2.51	0.43
3:I:834:PRO:C	3:I:835:LEU:HD12	2.39	0.43
2:C:73:TYR:O	2:C:74:ARG:HB2	2.18	0.43
2:C:82:VAL:HG13	2:C:83:GLN:N	2.34	0.43
2:C:94:ALA:HB2	2:C:129:LEU:HD11	2.00	0.43
3:D:690:ASN:ND2	3:D:745:GLY:HA3	2.34	0.43
3:D:824:PRO:O	3:D:826:ILE:HG13	2.19	0.43
3:D:919:ALA:O	3:D:923:ILE:HG12	2.18	0.43
5:X:264:LYS:H	5:X:264:LYS:HD2	1.83	0.43
2:H:73:TYR:N	2:H:73:TYR:CD2	2.85	0.43
2:H:170:VAL:O	2:H:171:LEU:HB2	2.19	0.43
2:H:557:ARG:NH1	2:H:611:GLU:OE1	2.52	0.43
2:H:868:SER:OG	2:H:942:ASP:OD1	2.36	0.43
2:H:888:THR:O	2:H:914:LYS:N	2.51	0.43
2:H:1122:LYS:HG2	2:H:1229:TYR:CE2	2.54	0.43
3:I:367:GLY:HA3	3:I:448:GLN:HB2	2.00	0.43
3:I:848:VAL:HG11	3:I:880:VAL:HA	2.00	0.43
3:I:1347:LEU:CD2	3:I:1358:PRO:HG2	2.43	0.43
5:Y:408:GLY:HA2	5:Y:435:ILE:HG23	1.99	0.43
1:A:163:GLU:CB	1:A:166:ARG:HB3	2.48	0.43
2:C:736:VAL:HG11	2:C:740:GLU:CA	2.48	0.43
3:D:58:CYS:SG	3:D:60:ARG:N	2.92	0.43
3:D:124:ILE:CG1	3:D:189:LEU:HD11	2.49	0.43
3:D:403:ARG:O	3:D:405:GLU:N	2.52	0.43
3:D:701:LEU:CD2	3:D:723:TYR:HB2	2.48	0.43
3:D:834:PRO:C	3:D:835:LEU:HD12	2.39	0.43
3:D:1226:VAL:HG11	3:I:1292:LEU:HA	2.01	0.43
2:H:818:VAL:HG22	2:H:819:SER:N	2.34	0.43



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:I:77:ARG:HD2	3:I:77:ARG:HA	1.76	0.43
3:I:648:GLU:OE2	3:I:648:GLU:N	2.52	0.43
3:I:1238:GLN:O	3:I:1242:ARG:HG2	2.19	0.43
4:J:10:VAL:HG21	4:J:16:ARG:HG2	2.01	0.43
5:Y:108:VAL:HB	5:Y:110:LEU:HG	2.01	0.43
5:Y:476:ARG:H	5:Y:476:ARG:HD2	1.84	0.43
5:Y:600:HIS:N	5:Y:601:PRO:CD	2.82	0.43
1:A:300:LEU:O	1:A:300:LEU:HD13	2.19	0.42
2:C:52:ALA:O	2:C:53:PHE:HB2	2.19	0.42
2:C:1153:ALA:HB2	2:C:1194:GLU:HG2	2.01	0.42
2:C:1163:THR:HG22	2:C:1164:PHE:H	1.84	0.42
3:D:105:ILE:CD1	3:D:273:ILE:HD11	2.48	0.42
3:D:107:LEU:HD23	3:D:299:LEU:HD21	2.00	0.42
3:D:541:LEU:HB2	3:D:545:HIS:CE1	2.54	0.42
3:D:579:LEU:HD23	3:D:627:THR:HG21	2.00	0.42
3:D:1138:LEU:N	3:D:1139:PRO:CD	2.81	0.42
2:H:205:PRO:O	2:H:208:ILE:HG22	2.19	0.42
3:I:361:LEU:HD23	3:I:366:CYS:HA	2.00	0.42
3:I:519:ASN:OD1	3:I:520:ALA:N	2.52	0.42
3:I:701:LEU:CD2	3:I:723:TYR:HB2	2.49	0.42
1:A:226:GLU:HB3	1:B:10:LYS:NZ	2.34	0.42
1:A:244:GLU:HB2	1:A:246:LYS:NZ	2.33	0.42
2:C:10:ARG:NH1	2:C:775:GLU:OE2	2.52	0.42
2:C:494:ASN:OD1	2:C:495:ALA:N	2.52	0.42
2:C:759:SER:OG	2:C:760:ASN:N	2.52	0.42
3:D:423:LEU:HB3	3:D:466:MET:HE2	2.01	0.42
2:H:185:ASP:OD1	2:H:185:ASP:N	2.51	0.42
2:H:773:LEU:C	2:H:773:LEU:HD22	2.39	0.42
2:H:845:LEU:HD13	2:H:845:LEU:N	2.30	0.42
2:H:998:LEU:O	2:H:998:LEU:HD13	2.19	0.42
2:H:1294:LYS:HE2	3:I:348:ASP:O	2.19	0.42
3:I:139:LEU:O	3:I:139:LEU:HD22	2.19	0.42
3:I:686:TRP:HB3	3:I:758:PRO:HG2	2.00	0.42
1:A:45:ARG:HG2	2:C:1083:GLU:OE1	2.19	0.42
2:C:41:GLN:CD	2:C:42:ASP:H	2.23	0.42
2:C:622:ASN:OD1	2:C:623:LEU:N	2.52	0.42
2:C:705:GLU:HB2	2:C:794:LEU:HB3	2.00	0.42
2:C:748:ILE:HD12	2:C:748:ILE:C	2.40	0.42
2:H:59:ILE:HD13	2:H:479:LEU:HD12	2.01	0.42
2:H:337:PHE:O	2:H:338:THR:OG1	2.32	0.42
2:H:600:THR:HG22	2:H:601:ASP:H	1.84	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:H:1158:LYS:HD2	2:H:1158:LYS:O	2.19	0.42
3:I:796:LEU:O	3:I:800:LEU:HD23	2.19	0.42
1:B:65:LEU:HA	1:B:169:GLY:HA2	2.00	0.42
2:C:39:ILE:CG2	2:C:40:GLU:HG2	2.48	0.42
2:C:557:ARG:NH2	2:C:606:LEU:O	2.52	0.42
3:D:112:ALA:HA	3:D:238:ILE:HG22	2.00	0.42
3:D:124:ILE:HD11	3:D:189:LEU:HD11	2.01	0.42
3:D:154:LEU:HD21	3:D:160:LEU:HD21	2.01	0.42
5:X:565:ILE:HG12	5:X:566:ASP:N	2.34	0.42
5:X:582:VAL:HG11	5:X:586:ARG:HG2	2.01	0.42
1:G:149:GLY:HA3	1:G:177:TYR:CE2	2.54	0.42
2:H:691:PRO:HA	2:H:788:SER:OG	2.19	0.42
3:I:139:LEU:HD22	3:I:139:LEU:C	2.39	0.42
3:I:368:LEU:HD12	3:I:369:PRO:HD2	2.01	0.42
3:I:482:ALA:O	3:I:488:ASN:ND2	2.52	0.42
3:I:611:ILE:HG13	3:I:612:LEU:HD23	2.01	0.42
5:Y:143:TYR:CD1	5:Y:269:LEU:HD21	2.54	0.42
2:C:948:ILE:HG13	2:C:949:GLU:N	2.34	0.42
2:C:1002:LEU:CD1	2:C:1003:THR:H	2.32	0.42
3:D:369:PRO:HG3	3:D:446:ALA:O	2.19	0.42
4:E:5:THR:CA	4:E:6:VAL:CB	2.80	0.42
5:X:45:ILE:C	5:X:45:ILE:HD12	2.40	0.42
5:X:442:SER:OG	5:X:446:GLN:NE2	2.52	0.42
5:X:461:ASN:HB3	5:X:465:ARG:CZ	2.49	0.42
1:F:51:MET:HB2	1:F:179:PRO:HD2	2.01	0.42
2:H:10:ARG:NH1	2:H:775:GLU:OE2	2.51	0.42
2:H:759:SER:OG	2:H:760:ASN:N	2.53	0.42
2:H:948:ILE:HG13	2:H:949:GLU:N	2.34	0.42
2:H:1303:LYS:HE2	2:H:1303:LYS:HA	2.01	0.42
3:I:1261:LEU:HD21	3:I:1306:LEU:HD22	2.01	0.42
2:C:177:ILE:N	2:C:177:ILE:HD12	2.34	0.42
2:C:1331:ARG:HG3	3:D:33:TRP:CH2	2.54	0.42
3:D:242:LEU:HD12	3:D:243:PRO:HD2	2.01	0.42
3:D:313:GLY:O	3:D:314:ARG:HB2	2.20	0.42
3:D:606:ASN:OD1	3:D:610:ARG:NH1	2.53	0.42
3:D:886:VAL:HG23	3:D:1254:GLU:HB3	2.00	0.42
5:X:143:TYR:O	5:X:147:GLN:HG2	2.19	0.42
2:H:106:GLU:CB	2:H:107:ARG:CA	2.97	0.42
3:I:413:ASP:HA	3:I:416:ILE:HD12	2.01	0.42
3:I:526:VAL:HG12	3:I:549:LYS:HB2	2.00	0.42
3:I:901:ARG:HB3	3:I:908:ILE:HA	2.02	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:45:ARG:NE	1:B:38:THR:OG1	2.49	0.42
1:B:83:LEU:CD1	3:D:527:LEU:HA	2.50	0.42
2:C:127:ILE:O	2:C:127:ILE:HG12	2.19	0.42
2:C:603:ILE:HD12	2:C:603:ILE:O	2.19	0.42
2:C:1081:PRO:HB2	2:C:1083:GLU:HG2	2.02	0.42
3:D:596:LEU:N	3:D:596:LEU:HD23	2.34	0.42
3:D:605:LEU:O	3:D:605:LEU:HD13	2.20	0.42
3:D:901:ARG:CB	3:D:908:ILE:HA	2.49	0.42
3:D:1173:ARG:CZ	3:D:1176:VAL:HG21	2.50	0.42
5:X:108:VAL:HG23	5:X:109:GLU:N	2.30	0.42
1:F:42:ALA:O	1:F:46:ILE:HG12	2.20	0.42
2:H:24:VAL:HA	2:H:25:PRO:HD3	1.85	0.42
2:H:177:ILE:N	2:H:177:ILE:HD12	2.35	0.42
2:H:253:PHE:CZ	2:H:287:VAL:HG12	2.55	0.42
3:I:529:GLY:HA3	3:I:530:PRO:HD3	1.92	0.42
3:I:596:LEU:N	3:I:596:LEU:HD23	2.34	0.42
3:I:678:ARG:O	3:I:682:VAL:HG13	2.20	0.42
3:I:932:MET:O	3:I:933:ARG:HG3	2.19	0.42
3:I:1138:LEU:HB3	3:I:1139:PRO:HD3	2.01	0.42
3:I:1184:ASP:HA	3:I:1185:PRO:HD3	1.79	0.42
5:Y:543:ALA:O	5:Y:547:VAL:HG23	2.19	0.42
5:Y:582:VAL:HB	5:Y:586:ARG:HG2	2.01	0.42
1:A:44:ARG:HG3	1:A:183:ILE:HG22	2.02	0.42
3:D:1270:GLY:CA	3:D:1299:GLY:HA2	2.49	0.42
2:H:842:ASP:N	2:H:1046:VAL:HG11	2.35	0.42
2:H:894:GLN:O	2:H:895:LEU:HB2	2.20	0.42
2:H:1238:LEU:HD12	2:H:1239:VAL:O	2.19	0.42
3:I:72:CYS:SG	3:I:73:GLY:N	2.93	0.42
3:I:298:MET:HE3	5:Y:402:LEU:HB3	2.02	0.42
3:I:450:HIS:HE1	3:I:452:LEU:HD12	1.84	0.42
3:I:1297:LYS:HA	3:I:1297:LYS:HE2	2.00	0.42
5:Y:262:VAL:HG13	5:Y:263:PRO:CD	2.45	0.42
1:A:323:PRO:CA	1:A:324:ALA:HB2	2.50	0.42
2:C:73:TYR:CG	2:C:74:ARG:N	2.86	0.42
2:C:333:ILE:N	2:C:333:ILE:HD12	2.34	0.42
2:C:685:MET:HE2	2:C:1067:ALA:CB	2.49	0.42
3:D:136:GLU:HA	3:D:139:LEU:HD12	2.00	0.42
3:D:159:ILE:N	3:D:159:ILE:HD12	2.34	0.42
3:D:292:VAL:HG13	3:D:293:ARG:N	2.34	0.42
3:D:392:THR:CG2	5:X:603:ARG:HG2	2.49	0.42
3:D:517:CYS:N	3:D:544:LEU:O	2.47	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
5:X:12:LEU:HD21	5:X:27:VAL:HG21	1.98	0.42
5:X:24:TYR:O	5:X:26:GLU:N	2.52	0.42
1:G:86:LYS:NZ	3:I:526:VAL:O	2.52	0.42
1:G:207:THR:OG1	1:G:208:ASN:N	2.52	0.42
2:H:135:THR:OG1	2:H:143:ARG:O	2.30	0.42
2:H:634:VAL:HG22	2:H:645:PHE:HE2	1.85	0.42
3:I:189:LEU:HB3	3:I:234:PRO:HB2	2.02	0.42
3:I:369:PRO:HG3	3:I:446:ALA:O	2.20	0.42
3:I:771:GLN:HE21	3:I:772:TYR:N	2.18	0.42
1:A:42:ALA:HA	1:B:38:THR:HG23	2.02	0.42
1:B:154:PRO:O	1:B:157:THR:HG22	2.20	0.42
2:C:225:PHE:HB2	2:C:336:LEU:HD22	2.01	0.42
2:C:639:LYS:HE2	2:C:639:LYS:HA	2.02	0.42
2:C:818:VAL:HG22	2:C:819:SER:N	2.35	0.42
2:C:1101:LEU:HD23	3:D:725:MET:SD	2.60	0.42
3:D:320:ASN:HB3	3:D:322:ARG:HG2	2.01	0.42
3:D:392:THR:HG22	5:X:603:ARG:HG2	2.00	0.42
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.84	0.42
3:D:1161:GLY:HA2	3:D:1181:ASP:CB	2.49	0.42
2:H:11:ILE:HG21	2:H:697:LYS:NZ	2.35	0.42
2:H:59:ILE:HD11	2:H:63:SER:HB3	2.02	0.42
2:H:163:LYS:HG2	2:H:163:LYS:O	2.20	0.42
2:H:166:SER:O	2:H:167:SER:OG	2.32	0.42
2:H:484:LEU:HB3	2:H:486:THR:HG22	2.01	0.42
2:H:742:TYR:CB	2:H:743:PRO:HD3	2.48	0.42
3:I:292:VAL:HG13	3:I:293:ARG:N	2.35	0.42
3:I:502:PRO:HB3	3:I:506:VAL:CG1	2.50	0.42
3:I:644:MET:O	3:I:764:ARG:NH1	2.53	0.42
1:B:9:LEU:H	1:B:9:LEU:HD23	1.85	0.41
1:B:190:ALA:HB2	1:B:200:LYS:HB3	2.01	0.41
2:C:91:THR:HG22	2:C:138:ILE:HA	2.02	0.41
2:C:367:TYR:CE1	2:C:380:ALA:HB1	2.55	0.41
3:D:45:ASN:OD1	3:D:46:TYR:N	2.53	0.41
2:H:384:LEU:O	2:H:388:LEU:HG	2.20	0.41
2:H:600:THR:HG22	2:H:601:ASP:N	2.35	0.41
2:H:639:LYS:HA	2:H:639:LYS:HE2	2.00	0.41
2:H:714:VAL:CG2	2:H:787:PRO:HD2	2.50	0.41
2:H:893:THR:O	2:H:894:GLN:HB2	2.20	0.41
2:H:971:LEU:HD12	2:H:1018:TYR:CD1	2.54	0.41
3:I:240:THR:HG23	3:I:241:VAL:HG23	2.01	0.41
3:I:252:LEU:HG	3:I:252:LEU:O	2.20	0.41



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:I:1173:ARG:NH1	3:I:1176:VAL:HG21	2.34	0.41
1:B:207:THR:OG1	1:B:208:ASN:N	2.52	0.41
2:C:152:SER:HA	2:C:153:PRO:HD3	1.89	0.41
2:C:166:SER:O	2:C:168:GLY:N	2.45	0.41
2:C:773:LEU:C	2:C:773:LEU:HD22	2.40	0.41
2:C:873:ILE:HD11	2:C:931:VAL:HG22	2.02	0.41
2:C:896:THR:HG23	2:C:897:PRO:HD2	2.02	0.41
3:D:395:LYS:HG3	5:X:536:THR:HG21	2.02	0.41
4:E:3:ARG:O	4:E:4:VAL:HG13	2.20	0.41
5:X:511:ILE:HG23	5:X:512:GLY:N	2.32	0.41
1:F:54:CYS:SG	1:F:148:ARG:NH1	2.93	0.41
2:H:727:VAL:HG22	2:H:773:LEU:HB3	2.00	0.41
2:H:992:LEU:HD23	2:H:996:ARG:CG	2.50	0.41
3:I:233:LYS:HG3	3:I:234:PRO:HD2	2.01	0.41
3:I:508:LEU:HD12	3:I:725:MET:HG2	2.03	0.41
3:I:550:VAL:HG23	3:I:552:ILE:HD11	2.02	0.41
3:I:863:LEU:HB2	3:I:866:GLU:HB2	2.03	0.41
5:Y:519:LEU:HD13	5:Y:519:LEU:O	2.20	0.41
2:C:510:GLN:C	2:C:512:SER:H	2.24	0.41
2:C:516:ASP:O	2:C:522:SER:OG	2.29	0.41
2:C:519:ASN:CB	2:C:520:PRO:HD2	2.47	0.41
2:C:698:PRO:HB3	2:C:1231:TYR:CZ	2.55	0.41
3:D:394:ILE:HG21	5:X:536:THR:HA	2.03	0.41
3:D:412:LEU:O	3:D:416:ILE:HG23	2.19	0.41
5:X:52:GLY:O	5:X:53:ILE:HB	2.19	0.41
1:F:41:ASN:ND2	2:H:1218:GLY:HA3	2.35	0.41
2:H:1314:GLN:HG3	4:J:28:ARG:NH1	2.34	0.41
3:I:63:GLY:O	3:I:98:ARG:NH2	2.52	0.41
3:I:451:PRO:HG2	3:I:625:MET:SD	2.60	0.41
2:C:201:ARG:HD2	2:C:370:MET:SD	2.60	0.41
2:C:538:LEU:HD12	2:C:538:LEU:N	2.35	0.41
3:D:310:GLY:O	3:D:314:ARG:HG2	2.19	0.41
3:D:514:THR:HG23	3:D:576:ARG:HE	1.86	0.41
3:D:706:VAL:C	3:D:707:ILE:HG13	2.41	0.41
3:D:911:LYS:HG3	4:E:15:ASN:ND2	2.36	0.41
3:I:66:LYS:HG3	3:I:69:GLU:OE2	2.20	0.41
3:I:222:LYS:HE2	3:I:1273:ASP:CG	2.40	0.41
3:I:503:SER:O	3:I:507:VAL:HG23	2.20	0.41
3:I:573:THR:HG22	3:I:576:ARG:CD	2.50	0.41
3:I:1226:VAL:O	3:I:1230:THR:HG23	2.20	0.41
1:B:182:ARG:NH1	3:D:581:MET:SD	2.93	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.55	0.41
2:C:533:LEU:HD23	2:C:533:LEU:H	1.85	0.41
2:C:546:GLU:O	2:C:547:VAL:HB	2.20	0.41
2:C:936:ARG:HB3	2:C:939:VAL:HG21	2.02	0.41
3:D:252:LEU:HG	3:D:252:LEU:O	2.20	0.41
3:D:474:LEU:HD13	3:D:478:LEU:HD13	2.01	0.41
3:D:501:VAL:HA	3:D:502:PRO:HD3	1.97	0.41
3:D:825:VAL:CG2	3:D:835:LEU:HB2	2.50	0.41
3:D:909:ILE:H	3:D:909:ILE:HG13	1.62	0.41
2:H:54:ARG:CA	2:H:55:SER:HB2	2.51	0.41
2:H:870:ILE:HG22	2:H:944:ARG:NH1	2.35	0.41
2:H:1146:GLN:NE2	2:H:1160:ASP:HB2	2.35	0.41
3:I:19:ALA:HB2	3:I:1343:GLU:CB	2.50	0.41
3:I:221:ILE:HG13	3:I:222:LYS:N	2.36	0.41
3:I:527:LEU:HD13	3:I:531:LYS:HB3	2.02	0.41
3:I:583:VAL:HG13	3:I:587:LEU:HD22	2.01	0.41
5:Y:311:THR:HG23	5:Y:355:ILE:HG21	2.03	0.41
1:A:104:LYS:HD3	1:A:105:SER:N	2.35	0.41
1:A:104:LYS:HD2	1:A:110:VAL:HG22	2.02	0.41
2:C:49:LEU:HD11	2:C:464:PHE:CG	2.55	0.41
2:C:106:GLU:CB	2:C:107:ARG:HA	2.46	0.41
3:D:97:VAL:HG13	3:D:101:ARG:CZ	2.50	0.41
2:H:748:ILE:HD12	2:H:748:ILE:C	2.40	0.41
2:H:1332:SER:O	3:I:243:PRO:HG2	2.21	0.41
3:I:139:LEU:HD21	3:I:185:ILE:HD13	2.02	0.41
3:I:886:VAL:HG22	3:I:1257:VAL:CG1	2.51	0.41
3:I:910:ASN:HB3	4:J:15:ASN:OD1	2.20	0.41
3:I:1138:LEU:N	3:I:1139:PRO:CD	2.84	0.41
1:A:41:ASN:HD21	2:C:1218:GLY:CA	2.34	0.41
2:C:487:LEU:HD12	2:C:487:LEU:H	1.86	0.41
2:C:898:GLU:OE1	2:C:898:GLU:N	2.51	0.41
2:C:908:GLU:CG	2:C:909:LYS:H	2.33	0.41
2:C:1064:ASP:OD1	2:C:1239:VAL:HG23	2.21	0.41
3:D:133:ARG:HB2	3:D:133:ARG:NH2	2.36	0.41
3:D:269:TYR:HA	3:D:272:VAL:HG12	2.02	0.41
3:D:545:HIS:HB2	3:D:546:ALA:HB2	2.03	0.41
3:D:1161:GLY:HA2	3:D:1181:ASP:HB3	2.02	0.41
3:D:1256:ILE:HA	3:D:1259:GLN:HE21	1.85	0.41
5:X:112:THR:HG22	5:X:113:ARG:N	2.36	0.41
2:H:603:ILE:HD12	2:H:603:ILE:O	2.20	0.41
2:H:1156:ARG:O	2:H:1157:GLN:HB2	2.21	0.41



	••••••••••••••••••••••••••••••••••••••	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:H:1291:LEU:HD13	3:I:345:LYS:NZ	2.35	0.41
5:Y:511:ILE:HG23	5:Y:512:GLY:N	2.32	0.41
2:C:55:SER:HB3	2:C:56:VAL:CG1	2.50	0.41
6:C:1401:1RL:O9	6:C:1401:1RL:O10	2.18	0.41
1:G:52:PRO:HB2	1:G:53:GLY:H	1.59	0.41
2:H:106:GLU:H	2:H:107:ARG:HA	1.86	0.41
2:H:496:LYS:N	2:H:497:PRO:CD	2.84	0.41
3:I:313:GLY:O	3:I:314:ARG:HB2	2.21	0.41
3:I:660:GLU:O	3:I:664:ILE:HG12	2.20	0.41
3:I:1210:ILE:O	3:I:1210:ILE:HG13	2.21	0.41
3:I:1357:ILE:HD12	3:I:1357:ILE:N	2.36	0.41
2:C:169:LYS:HA	2:C:169:LYS:HD3	1.89	0.41
2:C:653:MET:HG2	2:C:654:ASP:N	2.35	0.41
2:C:667:LEU:O	2:C:1069:ARG:NH2	2.54	0.41
2:C:699:LEU:HD11	2:C:1179:GLY:HA3	2.03	0.41
2:C:988:LYS:O	2:C:991:LYS:HE3	2.20	0.41
2:C:1301:ARG:HG3	2:C:1302:THR:N	2.35	0.41
3:D:147:ILE:HG23	3:D:156:ARG:C	2.41	0.41
3:D:221:ILE:HG13	3:D:222:LYS:N	2.35	0.41
3:D:789:LYS:HB3	3:D:932:MET:SD	2.61	0.41
3:D:803:VAL:HB	3:D:1313:SER:HB3	2.03	0.41
3:D:1210:ILE:O	3:D:1210:ILE:HG13	2.21	0.41
3:D:1264:ALA:HB1	3:D:1303:SER:O	2.21	0.41
4:E:30:MET:O	4:E:35:LYS:HG2	2.20	0.41
5:X:54:GLN:CA	5:X:54:GLN:HE21	2.34	0.41
5:X:244:THR:O	5:X:247:GLU:HB2	2.21	0.41
5:X:494:ILE:O	5:X:498:LEU:HD23	2.21	0.41
1:F:10:LYS:HE3	1:G:226:GLU:HB3	2.03	0.41
1:F:45:ARG:NH2	1:G:37:HIS:HB3	2.36	0.41
1:F:150:ARG:HD2	1:G:8:PHE:CZ	2.55	0.41
1:G:81:ILE:HG23	1:G:131:CYS:SG	2.61	0.41
2:H:82:VAL:HG13	2:H:83:GLN:N	2.35	0.41
2:H:378:ARG:NE	2:H:382:GLU:OE2	2.54	0.41
2:H:589:THR:HG23	2:H:591:TYR:CE2	2.56	0.41
2:H:637:ARG:NE	3:I:770:LEU:HD23	2.36	0.41
2:H:645:PHE:CD1	2:H:650:VAL:HB	2.55	0.41
3:I:111:THR:HG23	3:I:300:GLN:NE2	2.36	0.41
3:I:316:ILE:HD13	3:I:316:ILE:H	1.86	0.41
3:I:501:VAL:HA	3:I:502:PRO:HD3	1.97	0.41
3:I:822:MET:HG2	3:I:839:VAL:HG22	2.02	0.41
3:I:884:SER:OG	3:I:1254:GLU:OE1	2.31	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
5:Y:243:ALA:O	5:Y:247:GLU:HG3	2.21	0.41
5:Y:333:VAL:HG22	5:Y:336:GLU:HB2	2.03	0.41
1:B:14:VAL:HG13	1:B:28:LEU:HD23	2.03	0.41
1:B:227:GLN:C	1:B:229:GLU:H	2.24	0.41
3:D:147:ILE:HA	3:D:178:ALA:CB	2.51	0.41
1:F:207:THR:OG1	1:F:208:ASN:N	2.54	0.41
1:G:181:GLU:HB2	1:G:206:GLU:O	2.21	0.41
2:H:146:VAL:HG13	2:H:513:GLN:HG3	2.03	0.41
2:H:524:ILE:HD12	2:H:708:VAL:HG13	2.03	0.41
2:H:681:MET:O	2:H:685:MET:HG2	2.21	0.41
2:H:1087:TYR:HE2	2:H:1215:GLY:HA2	1.86	0.41
3:I:1169:THR:HA	3:I:1173:ARG:HB3	2.02	0.41
1:A:45:ARG:NH2	2:C:1216:ARG:O	2.54	0.40
1:A:143:ARG:HD2	1:A:143:ARG:N	2.36	0.40
1:A:246:LYS:HD3	1:A:246:LYS:N	2.35	0.40
1:B:176:CYS:C	1:B:178:SER:H	2.25	0.40
1:B:232:VAL:HG12	1:B:233:ASP:O	2.21	0.40
2:C:821:ARG:HB2	2:C:1082:ILE:CD1	2.51	0.40
2:C:1283:ALA:HB1	2:C:1286:THR:HB	2.02	0.40
2:C:1331:ARG:NH2	2:C:1337:ILE:O	2.54	0.40
3:D:238:ILE:O	3:D:238:ILE:HG13	2.20	0.40
3:D:503:SER:O	3:D:507:VAL:HG23	2.21	0.40
3:D:573:THR:HG23	3:D:576:ARG:H	1.85	0.40
3:D:733:SER:O	3:D:737:ILE:HG12	2.22	0.40
5:X:361:ILE:HG13	5:X:362:ASN:N	2.36	0.40
1:F:102:LEU:HG	1:F:115:ILE:HG12	2.03	0.40
1:G:185:TYR:HA	1:G:202:VAL:O	2.21	0.40
2:H:1339:LEU:H	2:H:1339:LEU:HD12	1.86	0.40
3:I:532:GLU:O	3:I:535:ARG:HB2	2.21	0.40
3:I:1264:ALA:HB1	3:I:1303:SER:O	2.21	0.40
5:Y:290:LEU:HB3	5:Y:333:VAL:HG21	2.02	0.40
5:Y:361:ILE:HG13	5:Y:362:ASN:N	2.36	0.40
5:Y:540:LEU:HD13	5:Y:607:LEU:HD22	2.04	0.40
1:A:223:ILE:HD13	1:B:8:PHE:CE1	2.57	0.40
1:B:234:LEU:O	1:B:235:ARG:HB2	2.21	0.40
2:C:54:ARG:N	2:C:55:SER:C	2.75	0.40
2:C:98:VAL:HG11	2:C:124:MET:SD	2.60	0.40
2:C:103:VAL:HG22	2:C:104:ILE:N	2.36	0.40
2:C:106:GLU:CB	2:C:107:ARG:CA	2.98	0.40
2:C:185:ASP:N	2:C:185:ASP:OD1	2.55	0.40
2:C:342:ASP:O	2:C:437:ASN:ND2	2.54	0.40



A + a 1	1 J	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:C:1303:LYS:HE2	2:C:1303:LYS:HA	2.02	0.40
3:D:179:LYS:H	3:D:179:LYS:HD3	1.87	0.40
3:D:265:LEU:HD21	3:D:327:LEU:HD23	2.02	0.40
3:D:609:TYR:HA	3:D:617:THR:OG1	2.21	0.40
3:D:1284:ARG:NH2	3:I:1292:LEU:HD11	2.36	0.40
5:X:224:LEU:HB2	5:X:259:PHE:CZ	2.56	0.40
5:X:455:HIS:O	5:X:459:THR:HG23	2.21	0.40
1:G:219:ARG:O	1:G:222:THR:HG22	2.21	0.40
2:H:119:GLU:OE1	2:H:490:GLN:HB2	2.21	0.40
2:H:442:VAL:HG12	2:H:443:ASP:N	2.37	0.40
2:H:876:GLU:HG3	2:H:927:THR:HG22	2.03	0.40
2:H:1336:ASN:HB2	3:I:33:TRP:CH2	2.56	0.40
3:I:128:LEU:HD12	3:I:192:MET:HE3	2.02	0.40
3:I:598:LYS:HG3	3:I:599:LYS:N	2.36	0.40
4:J:5:THR:HB	4:J:7:GLN:HB2	2.03	0.40
2:C:56:VAL:HB	2:C:57:PHE:H	1.60	0.40
2:C:600:THR:HG22	2:C:601:ASP:H	1.87	0.40
2:C:1017:GLN:O	2:C:1020:GLU:HB3	2.20	0.40
2:C:1117:LEU:HD21	2:C:1182:ILE:HD13	2.02	0.40
3:D:558:ASP:OD1	3:D:559:ALA:N	2.54	0.40
3:D:610:ARG:N	3:D:610:ARG:HD2	2.36	0.40
3:D:1256:ILE:O	3:D:1260:MET:HB2	2.21	0.40
5:X:493:LYS:O	5:X:497:VAL:HG23	2.21	0.40
5:X:559:LEU:HD12	5:X:594:ALA:HB1	2.03	0.40
1:F:51:MET:HA	1:F:52:PRO:HD3	1.87	0.40
1:F:117:HIS:O	1:F:117:HIS:ND1	2.50	0.40
2:H:1341:ASP:HB2	2:H:1342:GLU:OE1	2.22	0.40
3:I:85:CYS:SG	3:I:86:GLU:N	2.93	0.40
3:I:165:TYR:CE1	3:I:169:LEU:HD23	2.56	0.40
3:I:238:ILE:O	3:I:238:ILE:HG13	2.20	0.40
3:I:435:GLN:HB2	3:I:457:TYR:OH	2.20	0.40
5:Y:288:MET:HA	5:Y:302:PHE:CZ	2.57	0.40
2:C:253:PHE:CZ	2:C:287:VAL:HG12	2.57	0.40
2:C:745:GLU:HA	2:C:1017:GLN:OE1	2.21	0.40
3:D:213:LYS:O	3:D:215:LYS:N	2.54	0.40
3:D:233:LYS:CG	3:D:234:PRO:HD2	2.51	0.40
2:H:698:PRO:HB3	2:H:1231:TYR:CZ	2.57	0.40
2:H:898:GLU:CB	5:Y:540:LEU:HD21	2.52	0.40
3:I:483:LEU:HD12	3:I:483:LEU:N	2.36	0.40
1:B:183:ILE:HD11	1:B:205:MET:HG3	2.04	0.40
1:B:218:ARG:NH1	1:B:222:THR:OG1	2.54	0.40



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:117:ILE:HD13	2:C:487:LEU:HB3	2.04	0.40
2:C:658:GLN:HB3	2:C:1186:VAL:HG11	2.03	0.40
3:D:43:THR:OG1	3:D:44:ILE:N	2.55	0.40
3:D:823:THR:OG1	3:D:824:PRO:HD2	2.21	0.40
3:D:1258:ARG:HG3	3:D:1259:GLN:N	2.37	0.40
3:D:1347:LEU:O	3:D:1351:VAL:HG23	2.21	0.40
3:D:1369:ARG:HB3	3:D:1369:ARG:HH11	1.86	0.40
1:F:190:ALA:HB2	1:F:200:LYS:CB	2.52	0.40
2:H:1255:THR:HG22	2:H:1257:GLN:HG3	2.03	0.40
2:H:1296:ASP:OD2	2:H:1320:PRO:HB2	2.21	0.40
3:I:40:LYS:HA	3:I:41:PRO:HD3	1.80	0.40
3:I:50:LYS:HB3	3:I:50:LYS:NZ	2.35	0.40
3:I:1145:PHE:CE2	3:I:1256:ILE:HD11	2.57	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	Pe	rce	entiles
1	А	321/329~(98%)	263 (82%)	42 (13%)	16 (5%)	·	2	22
1	В	217/329~(66%)	187 (86%)	25~(12%)	5 (2%)		6	37
1	F	227/329~(69%)	195 (86%)	27 (12%)	5 (2%)		6	37
1	G	213/329~(65%)	188 (88%)	22 (10%)	3 (1%)	1	1	45
2	С	1333/1342~(99%)	1087 (82%)	204 (15%)	42 (3%)	4	4	31
2	Н	1333/1342~(99%)	1091 (82%)	197 (15%)	45 (3%)		3	30
3	D	1154/1407~(82%)	933 (81%)	180 (16%)	41 (4%)		3	28
3	Ι	1154/1407~(82%)	934 (81%)	180 (16%)	40 (4%)		3	29
4	Е	$8\overline{8/91}\ (97\%)$	77~(88%)	$\overline{6(7\%)}$	5 (6%)		1	19
4	J	74/91 (81%)	64 (86%)	5 (7%)	5 (7%)		1	17



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	P	erc	entile	es
5	Х	511/613~(83%)	453 (89%)	44 (9%)	14 (3%)		5	34	
5	Y	454/613~(74%)	414 (91%)	30 (7%)	10 (2%)		6	37	
All	All	7079/8222 (86%)	5886 (83%)	962 (14%)	231 (3%)		4	30	

All (231) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	52	PRO
1	А	319	GLU
1	В	20	SER
2	С	21	VAL
2	С	39	ILE
2	С	43	PRO
2	С	53	PHE
2	С	110	PRO
2	С	114	VAL
2	С	170	VAL
2	С	661	VAL
2	С	669	PRO
2	С	686	GLN
2	С	748	ILE
2	С	753	LEU
2	С	993	PRO
2	С	1185	PRO
2	С	1186	VAL
2	С	1341	ASP
3	D	120	LEU
3	D	311	ARG
3	D	390	LEU
3	D	404	GLU
3	D	406	ALA
3	D	708	ASN
3	D	710	ASP
3	D	847	ASP
3	D	1268	ASN
3	D	1363	TYR
4	Е	6	VAL
5	Х	241	SER
1	F	52	PRO
1	G	52	PRO
2	Н	21	VAL



Mol	Chain	Res	Type
2	Н	39	ILE
2	Н	53	PHE
2	Н	110	PRO
2	Н	114	VAL
2	Н	661	VAL
2	Н	748	ILE
2	Н	993	PRO
2	Н	1185	PRO
2	Н	1341	ASP
3	Ι	120	LEU
3	Ι	390	LEU
3	Ι	404	GLU
3	Ι	406	ALA
3	Ι	542	ALA
3	Ι	710	ASP
3	Ι	847	ASP
3	Ι	851	PRO
4	J	4	VAL
4	J	6	VAL
4	J	35	LYS
5	Y	241	SER
1	А	193	GLU
1	А	201	LEU
1	А	232	VAL
1	В	19	VAL
1	В	52	PRO
2	С	437	ASN
2	С	812	PHE
2	C	1236	ASN
2	С	1239	VAL
2	С	1256	GLN
3	D	89	GLY
3	D	214	ARG
3	D	417	ARG
3	D	542	ALA
3	D	595	ALA
3	D	721	SER
3	D	728	SER
3	D	851	PRO
3	D	901	ARG
3	D	914	ALA
3	D	1192	LYS



Mol	Chain	Res	Type
4	Е	35	LYS
5	Х	20	GLY
5	Х	23	THR
5	Х	108	VAL
5	Х	490	PRO
5	Х	514	ASP
5	Х	581	ASP
1	G	188	GLU
1	G	228	LEU
2	Н	170	VAL
2	Н	437	ASN
2	Н	669	PRO
2	Н	753	LEU
2	Н	812	PHE
2	Н	1006	GLU
2	Н	1186	VAL
2	Н	1236	ASN
2	Н	1239	VAL
3	Ι	89	GLY
3	Ι	214	ARG
3	Ι	345	LYS
3	Ι	417	ARG
3	Ι	595	ALA
3	Ι	707	ILE
3	Ι	708	ASN
3	Ι	721	SER
3	Ι	901	ARG
3	Ι	914	ALA
3	Ι	1192	LYS
3	Ι	1195	GLN
3	Ι	1268	ASN
3	Ι	1363	TYR
5	Y	308	GLY
5	Y	490	PRO
1	А	93	GLN
1	А	196	THR
1	В	188	GLU
2	С	143	ARG
2	С	1240	ASP
3	D	53	ARG
3	D	210	SER
3	D	316	ILE



Mol	Chain	Res	Type
3	D	559	ALA
3	D	590	SER
3	D	672	LEU
3	D	703	THR
3	D	707	ILE
3	D	913	GLU
3	D	1195	GLN
4	Е	4	VAL
5	Х	308	GLY
5	Х	491	GLU
1	F	33	ARG
1	F	188	GLU
2	Н	44	GLU
2	Н	487	LEU
2	Н	543	ALA
2	Н	1046	VAL
2	Н	1137	GLU
2	Н	1240	ASP
2	Н	1256	GLN
3	Ι	53	ARG
3	Ι	153	ASN
3	Ι	210	SER
3	Ι	559	ALA
3	Ι	590	SER
3	Ι	728	SER
3	Ι	913	GLU
5	Y	108	VAL
5	Y	491	GLU
5	Y	514	ASP
1	A	166	ARG
1	А	188	GLU
1	В	235	ARG
2	C	44	GLU
2	C	487	LEU
2	С	1006	GLU
2	C	1080	ASN
2	C	1137	GLU
2	C	1139	ALA
3	D	153	ASN
3	D	832	LYS
3	D	888	CYS
4	E	5	THR



Mol	Chain	Res	Type
5	Х	600	HIS
1	F	153	VAL
1	F	166	ARG
2	Н	143	ARG
2	Н	488	MET
2	Н	535	PRO
2	Н	895	LEU
2	Н	1045	GLY
2	Н	1080	ASN
2	Н	1139	ALA
3	Ι	672	LEU
3	Ι	703	THR
3	Ι	832	LYS
3	Ι	888	CYS
3	Ι	1194	ARG
5	Y	107	THR
5	Y	581	ASP
1	А	14	VAL
1	А	322	PRO
1	А	324	ALA
2	С	699	LEU
2	С	746	ALA
2	С	1203	ASP
2	С	1315	MET
3	D	816	THR
5	Х	50	ASP
5	Х	107	THR
2	Н	1093	PRO
2	Н	1315	MET
3	Ι	1290	ARG
4	J	5	THR
5	Y	600	HIS
1	A	163	GLU
1	A	194	GLN
2	С	69	GLN
2	С	895	LEU
2	С	1045	GLY
2	С	1046	VAL
2	С	1093	PRO
2	C	1201	LEU
3	D	255	LEU
3	D	902	ASP



Mol	Chain	Res	Type
3	D	1173	ARG
3	D	1194	ARG
4	Е	59	ILE
2	Н	56	VAL
2	Н	739	ASP
2	Н	746	ALA
2	Н	1238	LEU
3	Ι	596	LEU
3	Ι	712	GLN
3	Ι	731	ARG
3	Ι	816	THR
5	Х	97	PRO
4	J	59	ILE
1	А	153	VAL
2	С	56	VAL
2	С	373	GLY
5	Х	35	ILE
2	С	59	ILE
2	Н	59	ILE
2	Н	373	GLY
3	Ι	850	LYS
5	Y	97	PRO
1	А	30	PRO
3	D	850	LYS
3	D	1185	PRO
2	Н	78	PRO
2	Н	134	GLY
2	Н	43	PRO
2	Н	489	PRO

## 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	281/286~(98%)	272~(97%)	9~(3%)	39 62
1	В	189/286~(66%)	183 (97%)	6 (3%)	39 62



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	F	197/286~(69%)	193~(98%)	4 (2%)	55	73
1	G	185/286~(65%)	184 (100%)	1 (0%)	88	93
2	С	1150/1157~(99%)	1090 (95%)	60 (5%)	23	51
2	Н	1150/1157~(99%)	1090 (95%)	60 (5%)	23	51
3	D	971/1168 (83%)	916 (94%)	55 (6%)	20	49
3	Ι	971/1168 (83%)	916 (94%)	55 (6%)	20	49
4	Е	74/75~(99%)	72 (97%)	2 (3%)	44	66
4	J	65/75~(87%)	64 (98%)	1 (2%)	65	79
5	Х	460/540~(85%)	443 (96%)	17 (4%)	34	59
5	Y	407/540~(75%)	392 (96%)	15 (4%)	34	59
All	All	6100/7024 (87%)	5815 (95%)	285 (5%)	26	53

All (285) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	А	33	ARG
1	А	79	LEU
1	А	88	LEU
1	А	117	HIS
1	А	158	ARG
1	А	243	LYS
1	А	246	LYS
1	А	262	LEU
1	А	318	LEU
1	В	13	LEU
1	В	37	HIS
1	В	65	LEU
1	В	182	ARG
1	В	196	THR
1	В	228	LEU
2	С	9	LYS
2	С	15	PHE
2	С	18	ARG
2	С	32	LEU
2	С	37	LYS
2	С	39	ILE
2	С	41	GLN
2	С	56	VAL



Mol	Chain	Res	Type
2	С	70	TYR
2	С	80	PHE
2	С	88	ARG
2	С	127	ILE
2	С	133	ASN
2	С	150	HIS
2	С	163	LYS
2	С	185	ASP
2	С	479	LEU
2	С	487	LEU
2	С	645	PHE
2	С	661	VAL
2	С	693	LEU
2	С	704	MET
2	С	711	ASP
2	C	773	LEU
2	С	800	MET
2	С	807	TRP
2	С	817	LEU
2	С	843	THR
2	С	845	LEU
2	С	941	LYS
2	С	944	ARG
2	С	953	LEU
2	С	955	GLN
2	С	964	LEU
2	С	975	ILE
2	С	994	ARG
2	С	1002	LEU
2	С	1010	GLN
2	С	1011	LEU
2	С	1017	GLN
2	С	1032	LYS
2	С	1042	LEU
2	С	1106	ARG
2	С	1119	MET
2	С	1141	LEU
2	С	1146	GLN
2	С	1158	LYS
2	С	1180	MET
2	С	1209	GLN
2	С	1211	ARG



Mol	Chain	Res	Type
2	С	1233	LEU
2	С	1248	THR
2	С	1259	LEU
2	С	1264	GLN
2	С	1265	PHE
2	С	1276	TRP
2	С	1288	GLN
2	С	1291	LEU
2	С	1326	LEU
2	С	1339	LEU
3	D	13	LYS
3	D	31	ARG
3	D	50	LYS
3	D	92	VAL
3	D	114	ILE
3	D	133	ARG
3	D	139	LEU
3	D	140	TYR
3	D	141	PHE
3	D	151	MET
3	D	169	LEU
3	D	175	GLU
3	D	179	LYS
3	D	207	GLU
3	D	239	LEU
3	D	248	ASP
3	D	250	ARG
3	D	416	ILE
3	D	430	HIS
3	D	500	ILE
3	D	505	ASP
3	D	508	LEU
3	D	527	LEU
3	D	532	GLU
3	D	538	ARG
3	D	541	LEU
3	D	571	ASP
3	D	590	SER
3	D	605	LEU
3	D	668	PHE
3	D	678	ARG
3	D	681	LYS



Mol	Chain	Res	Type
3	D	709	ARG
3	D	713	GLU
3	D	771	GLN
3	D	795	TYR
3	D	816	THR
3	D	832	LYS
3	D	847	ASP
3	D	864	LEU
3	D	867	GLN
3	D	873	GLU
3	D	911	LYS
3	D	918	ILE
3	D	932	MET
3	D	933	ARG
3	D	1134	ILE
3	D	1148	ARG
3	D	1149	ARG
3	D	1188	GLU
3	D	1227	HIS
3	D	1247	LYS
3	D	1306	LEU
3	D	1341	ARG
3	D	1366	HIS
4	Е	4	VAL
4	Ε	6	VAL
5	Х	21	TYR
5	Х	28	ASN
5	Х	54	GLN
5	X	99	ARG
5	Х	266	PHE
5	Х	355	ILE
5	X	379	MET
5	Х	384	LEU
5	X	400	GLN
5	Х	452	ILE
5	X	457	ILE
5	Х	471	LEU
5	X	476	ARG
5	Х	545	HIS
5	Х	562	ARG
5	Х	565	ILE
5	Х	607	LEU



Mol	Chain	Res	Type
1	F	158	ARG
1	F	160	HIS
1	F	163	GLU
1	F	181	GLU
1	G	37	HIS
2	Н	9	LYS
2	Н	15	PHE
2	Н	18	ARG
2	Н	37	LYS
2	Н	42	ASP
2	Н	46	GLN
2	Н	56	VAL
2	Н	70	TYR
2	Н	73	TYR
2	Н	80	PHE
2	Н	88	ARG
2	Н	99	LYS
2	Н	127	ILE
2	Н	150	HIS
2	Н	163	LYS
2	Н	185	ASP
2	Н	311	CYS
2	Н	464	PHE
2	Н	479	LEU
2	Н	488	MET
2	Н	513	GLN
2	Н	514	PHE
2	Н	645	PHE
2	Н	661	VAL
2	Н	704	MET
2	Н	711	ASP
2	Н	773	LEU
2	Η	800	MET
2	Н	807	TRP
2	Η	817	LEU
2	H	845	LEU
2	Н	941	LYS
2	Η	944	ARG
2	H	953	LEU
2	Н	955	GLN
2	Н	964	LEU
2	Н	971	LEU



Mol	Chain	Res	Type
2	Н	975	ILE
2	Н	994	ARG
2	Н	1002	LEU
2	Н	1005	GLU
2	Н	1010	GLN
2	Н	1011	LEU
2	Н	1017	GLN
2	Н	1032	LYS
2	Н	1042	LEU
2	Н	1106	ARG
2	Н	1119	MET
2	Н	1141	LEU
2	Н	1158	LYS
2	Н	1180	MET
2	Н	1209	GLN
2	Н	1211	ARG
2	Н	1233	LEU
2	Н	1264	GLN
2	Н	1276	TRP
2	Н	1288	GLN
2	Н	1291	LEU
2	Н	1326	LEU
2	Н	1339	LEU
3	Ι	31	ARG
3	Ι	50	LYS
3	Ι	92	VAL
3	Ι	114	ILE
3	Ι	133	ARG
3	Ι	139	LEU
3	Ι	140	TYR
3	Ι	141	PHE
3	Ι	151	MET
3	Ι	169	LEU
3	I	175	GLU
3	Ι	179	LYS
3	Ι	207	GLU
3	Ι	235	GLU
3	Ι	239	LEU
3	Ι	248	ASP
3	Ι	250	ARG
3	Ι	316	ILE
3	Ι	325	LYS


Mol	Chain	Res	Type
3	Ι	416	ILE
3	Ι	430	HIS
3	Ι	475	GLU
3	Ι	500	ILE
3	Ι	505	ASP
3	Ι	527	LEU
3	Ι	532	GLU
3	Ι	538	ARG
3	Ι	541	LEU
3	Ι	571	ASP
3	Ι	594	GLN
3	Ι	605	LEU
3	Ι	668	PHE
3	Ι	678	ARG
3	Ι	681	LYS
3	Ι	709	ARG
3	Ι	771	GLN
3	Ι	795	TYR
3	Ι	816	THR
3	Ι	832	LYS
3	Ι	847	ASP
3	Ι	864	LEU
3	Ι	867	GLN
3	Ι	873	GLU
3	Ι	911	LYS
3	Ι	918	ILE
3	Ι	932	MET
3	Ι	933	ARG
3	Ι	1134	ILE
3	Ι	1148	ARG
3	Ι	1149	ARG
3	Ι	1247	LYS
3	Ι	1297	LYS
3	Ι	1306	LEU
3	Ι	1341	ARG
3	Ι	1366	HIS
4	J	4	VAL
5	Y	136	GLU
5	Y	266	PHE
5	Y	355	ILE
5	Y	371	LYS
5	Y	379	MET



Mol	Chain	Res	Type
5	Y	384	LEU
5	Y	400	GLN
5	Y	452	ILE
5	Y	457	ILE
5	Y	476	ARG
5	Y	545	HIS
5	Y	562	ARG
5	Y	565	ILE
5	Y	589	GLN
5	Y	607	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	75	GLN
2	С	513	GLN
2	С	673	HIS
2	С	684	ASN
2	С	955	GLN
2	С	1010	GLN
2	С	1017	GLN
2	С	1134	GLN
2	С	1146	GLN
2	С	1264	GLN
2	С	1313	HIS
3	D	164	GLN
3	D	209	ASN
3	D	504	GLN
3	D	875	ASN
3	D	921	GLN
3	D	1197	ASN
3	D	1268	ASN
3	D	1326	GLN
4	Е	31	GLN
5	Х	8	GLN
5	Х	40	GLN
5	Х	54	GLN
5	Х	406	GLN
5	Х	446	GLN
1	F	66	HIS
2	Н	46	GLN
2	Н	510	GLN



Mol	Chain	Res	Type
2	Н	513	GLN
2	Н	526	HIS
2	Н	649	GLN
2	Н	684	ASN
2	Н	1010	GLN
2	Н	1108	ASN
2	Н	1111	GLN
2	Н	1116	HIS
2	Н	1134	GLN
2	Н	1220	GLN
2	Н	1264	GLN
3	Ι	164	GLN
3	Ι	274	ASN
3	Ι	309	ASN
3	Ι	504	GLN
3	Ι	1227	HIS

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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



Mal	Turne	Chain	Dec	Res Link	В	ond leng	gths	Bo	ond angl	es
	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	1RL	Н	1401	-	68,70,70	<mark>3.18</mark>	21 (30%)	91,104,104	2.31	31 (34%)
6	1RL	С	1401	-	68,70,70	<mark>3.18</mark>	20 (29%)	91,104,104	2.19	25 (27%)

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
6	1RL	Н	1401	-	-	29/65/84/84	0/5/6/6
6	1RL	С	1401	-	-	31/65/84/84	0/5/6/6

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
6	С	1401	1RL	O3-C6	12.06	1.60	1.37
6	Н	1401	1RL	O3-C6	12.06	1.60	1.37
6	С	1401	1RL	C6-C7	10.96	1.58	1.39
6	Н	1401	1RL	C6-C7	10.86	1.58	1.39
6	Н	1401	1RL	C5-C11	-7.25	1.27	1.46
6	С	1401	1RL	C5-C6	-7.21	1.29	1.39
6	Н	1401	1RL	C5-C6	-7.17	1.29	1.39
6	С	1401	1RL	C5-C11	-7.16	1.27	1.46
6	Н	1401	1RL	C17-C16	7.13	1.55	1.34
6	С	1401	1RL	C17-C16	6.83	1.54	1.34
6	Н	1401	1RL	C15-N1	5.45	1.47	1.37
6	С	1401	1RL	C15-N1	5.33	1.47	1.37
6	Н	1401	1RL	C12-C11	-5.26	1.33	1.54
6	С	1401	1RL	C12-C11	-5.25	1.33	1.54
6	С	1401	1RL	C10-C4	5.16	1.53	1.46
6	С	1401	1RL	C18-C19	5.11	1.53	1.33
6	Н	1401	1RL	C18-C19	5.05	1.53	1.33
6	Н	1401	1RL	C10-C5	4.97	1.52	1.41
6	Н	1401	1RL	C10-C4	4.95	1.52	1.46
6	С	1401	1RL	C10-C5	4.93	1.52	1.41
6	С	1401	1RL	C4-N3	4.88	1.38	1.30
6	Н	1401	1RL	C4-N3	4.68	1.38	1.30
6	С	1401	1RL	O-C06	3.87	1.45	1.37
6	Н	1401	1RL	O-C06	3.84	1.45	1.37
6	С	1401	1RL	O7-C35	3.61	1.43	1.35
6	Н	1401	1RL	07-C35	3.43	1.42	1.35



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Н	1401	1RL	C18-C17	3.33	1.53	1.43
6	С	1401	1RL	C18-C17	3.25	1.53	1.43
6	Н	1401	1RL	C34-C26	-2.83	1.47	1.53
6	С	1401	1RL	C34-C26	-2.73	1.47	1.53
6	С	1401	1RL	O2-C8	2.52	1.42	1.37
6	С	1401	1RL	C06-C02	2.47	1.44	1.40
6	Н	1401	1RL	C06-C02	2.35	1.44	1.40
6	С	1401	1RL	O01-C3	2.31	1.42	1.37
6	Н	1401	1RL	O01-C3	2.20	1.41	1.37
6	Н	1401	1RL	O2-C8	2.15	1.41	1.37
6	Н	1401	1RL	O7-C25	-2.14	1.41	1.44
6	Н	1401	1RL	O01-C01	2.06	1.41	1.38
6	С	1401	1RL	C8-C7	2.05	1.44	1.40
6	С	1401	1RL	O01-C01	2.05	1.41	1.38
6	Н	1401	1RL	C8-C7	2.03	1.44	1.40

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
6	Н	1401	1RL	C20-C19-C18	-8.21	108.88	126.16
6	Н	1401	1RL	C12-O3-C6	-7.62	94.83	107.68
6	С	1401	1RL	C12-O3-C6	-7.42	95.17	107.68
6	Н	1401	1RL	C8-C7-C6	-7.23	106.66	116.78
6	С	1401	1RL	C8-C7-C6	-6.84	107.20	116.78
6	С	1401	1RL	C20-C19-C18	-6.74	111.97	126.16
6	С	1401	1RL	C10-C4-N3	5.24	124.40	118.04
6	Н	1401	1RL	C10-C4-N3	5.08	124.20	118.04
6	С	1401	1RL	C3-C4-N3	-4.27	116.91	122.56
6	С	1401	1RL	O7-C35-C36	4.25	118.91	111.09
6	Н	1401	1RL	C3-C4-N3	-4.18	117.03	122.56
6	Н	1401	1RL	C9-C10-C5	-4.13	114.33	119.90
6	С	1401	1RL	C9-C10-C5	-4.09	114.38	119.90
6	Н	1401	1RL	C34-C26-C25	-3.85	104.50	111.40
6	Н	1401	1RL	O01-C3-C4	3.80	122.66	118.08
6	Н	1401	1RL	C17-C18-C19	-3.78	115.36	124.53
6	Н	1401	1RL	C16-C15-N1	3.75	121.89	114.52
6	С	1401	1RL	O01-C3-C4	3.75	122.60	118.08
6	Н	1401	1RL	O4-C11-C5	-3.72	122.06	130.66
6	С	1401	1RL	O4-C11-C5	-3.68	122.16	130.66
6	Н	1401	1RL	O7-C35-C36	3.56	117.65	111.09
6	С	1401	1RL	C16-C15-N1	3.37	121.13	114.52
6	Н	1401	1RL	C18-C17-C16	-3.13	117.41	126.61



Mol	Chain	$\mathbf{Res}$	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
6	С	1401	1RL	C17-C18-C19	-3.12	116.97	124.53
6	С	1401	1RL	C02-N3-C4	2.99	122.97	117.82
6	Н	1401	1RL	C02-N3-C4	2.91	122.83	117.82
6	Н	1401	1RL	O11-C15-N1	-2.91	117.80	122.86
6	Н	1401	1RL	C9-C8-C7	2.88	127.07	122.33
6	С	1401	1RL	C18-C17-C16	-2.79	118.42	126.61
6	С	1401	1RL	C10-C9-C8	2.75	123.64	119.68
6	С	1401	1RL	O11-C15-N1	-2.74	118.09	122.86
6	С	1401	1RL	O3-C6-C5	-2.72	112.50	114.36
6	С	1401	1RL	C34-C26-C25	-2.63	106.68	111.40
6	Н	1401	1RL	C10-C9-C8	2.39	123.11	119.68
6	Н	1401	1RL	C14-C7-C8	2.39	124.54	120.50
6	Н	1401	1RL	O3-C6-C5	-2.36	112.75	114.36
6	С	1401	1RL	C06-C02-C01	-2.32	116.11	119.45
6	С	1401	1RL	C9-C8-C7	2.30	126.10	122.33
6	С	1401	1RL	C03-C01-C02	2.28	123.74	120.12
6	Н	1401	1RL	C03-C01-C02	2.27	123.73	120.12
6	С	1401	1RL	C8-C9-C1	-2.25	116.66	120.76
6	С	1401	1RL	C14-C7-C8	2.24	124.30	120.50
6	Н	1401	1RL	C8-C9-C1	-2.23	116.70	120.76
6	С	1401	1RL	C26-C25-C24	-2.22	110.14	114.68
6	Н	1401	1RL	C06-C02-C01	-2.22	116.25	119.45
6	С	1401	1RL	O3-C12-C13	2.22	115.75	109.55
6	С	1401	1RL	C13-C12-C11	2.22	119.39	113.90
6	Н	1401	1RL	C13-C12-C11	2.17	119.28	113.90
6	Н	1401	1RL	O3-C12-C13	2.16	115.57	109.55
6	Н	1401	1RL	C31-C20-C21	2.16	115.82	111.31
6	Н	1401	1RL	C26-C25-C24	-2.15	110.29	114.68
6	Н	1401	1RL	O2-C8-C9	-2.12	116.25	120.98
6	Н	1401	1RL	C23-C22-C21	-2.12	108.28	112.54
6	Н	1401	1RL	C31-C20-C19	-2.06	105.00	109.99
6	Н	1401	1RL	O7-C25-C24	2.03	112.22	107.50
6	Н	1401	1RL	C14-C7-C6	2.01	124.38	121.30

Continued from previous page...

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	С	1401	1RL	C11-C12-O5-C29
6	С	1401	1RL	C13-C12-O5-C29
6	С	1401	1RL	C16-C17-C18-C19
6	С	1401	1RL	C19-C20-C21-O10



Mol	Chain	Res	Type	Atoms
6	С	1401	1RL	C31-C20-C21-C22
6	С	1401	1RL	C21-C22-C23-C24
6	С	1401	1RL	C32-C22-C23-C24
6	С	1401	1RL	C26-C27-C28-C29
6	Н	1401	1RL	C11-C12-O5-C29
6	Н	1401	1RL	C13-C12-O5-C29
6	Н	1401	1RL	C30-C16-C17-C18
6	Н	1401	1RL	C19-C20-C21-O10
6	Н	1401	1RL	C31-C20-C21-C22
6	Н	1401	1RL	C21-C22-C23-C24
6	Н	1401	1RL	C32-C22-C23-C24
6	Н	1401	1RL	C26-C27-C28-C29
6	Н	1401	1RL	O8-C35-O7-C25
6	С	1401	1RL	O8-C35-O7-C25
6	С	1401	1RL	C32-C22-C23-O9
6	Н	1401	1RL	C32-C22-C23-O9
6	С	1401	1RL	C21-C22-C23-O9
6	Н	1401	1RL	C21-C22-C23-O9
6	С	1401	1RL	C17-C18-C19-C20
6	Н	1401	1RL	C17-C18-C19-C20
6	С	1401	1RL	C33-C24-C25-C26
6	Н	1401	1RL	C33-C24-C25-C26
6	С	1401	1RL	C36-C35-O7-C25
6	С	1401	1RL	C23-C24-C25-C26
6	Н	1401	1RL	C36-C35-O7-C25
6	С	1401	1RL	C31-C20-C21-O10
6	Н	1401	1RL	C31-C20-C21-O10
6	С	1401	1RL	C30-C16-C17-C18
6	С	1401	1RL	C19-C20-C21-C22
6	Н	1401	1RL	C19-C20-C21-C22
6	С	1401	1RL	C33-C24-C25-O7
6	С	1401	1RL	C23-C24-C25-O7
6	Н	1401	1RL	C23-C24-C25-O7
6	Н	1401	1RL	C23-C24-C25-C26
6	Н	1401	1RL	C33-C24-C25-O7
6	С	1401	1RL	C-C39-N-C08
6	Н	1401	1RL	C-C39-N-C08
6	H	1401	1RL	C-C39-N-C09
6	C	1401	1RL	C15-C16-C17-C18
6	H	1401	1RL	C15-C16-C17-C18
6	C	1401	1RL	C-C39-N-C09
6	C	1401	1RL	O3-C12-O5-C29

Continued from previous page...



Mol	Chain	Res	Type	Atoms
6	Н	1401	1RL	O3-C12-O5-C29
6	Н	1401	1RL	C16-C17-C18-C19
6	С	1401	1RL	C28-C29-O5-C12
6	Н	1401	1RL	C28-C29-O5-C12
6	С	1401	1RL	N1-C15-C16-C17
6	Н	1401	1RL	N1-C15-C16-C17
6	Н	1401	1RL	O11-C15-C16-C17
6	С	1401	1RL	O7-C25-C26-C34
6	Н	1401	1RL	O7-C25-C26-C34
6	С	1401	1RL	O7-C25-C26-C27
6	С	1401	1RL	O11-C15-C16-C17
6	С	1401	1RL	O6-C27-C28-C29
6	Н	1401	1RL	O6-C27-C28-C29
6	С	1401	1RL	O11-C15-C16-C30

Continued from previous page...

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Н	1401	1RL	10	0
6	С	1401	1RL	6	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	$OWAB(Å^2)$	Q<0.9
1	А	323/329~(98%)	0.01	10 (3%) 49 38	0, 68, 172, 270	0
1	В	221/329~(67%)	0.33	15 (6%) 17 14	6, 90, 201, 277	0
1	F	229/329~(69%)	0.41	22 (9%) 8 7	9, 123, 209, 249	0
1	G	217/329~(65%)	0.40	21 (9%) 7 7	34, 112, 176, 230	0
2	С	1335/1342~(99%)	-0.06	47 (3%) 44 35	0, 43, 165, 367	0
2	Н	1335/1342~(99%)	0.10	81 (6%) 21 17	0, 81, 205, 388	0
3	D	1160/1407~(82%)	-0.03	38 (3%) 46 37	0, 34, 158, 313	0
3	Ι	1160/1407~(82%)	0.11	72 (6%) 20 16	0, 50, 190, 338	0
4	Е	90/91~(98%)	-0.35	1 (1%) 80 72	0, 34, 108, 170	0
4	J	76/91~(83%)	0.16	4 (5%) 26 23	3, 75, 160, 201	0
5	Х	517/613~(84%)	0.26	44 (8%) 10 9	1, 99, 236, 425	0
5	Y	458/613~(74%)	0.19	37 (8%) 12 10	1, 102, 234, 374	0
All	All	7121/8222 (86%)	0.09	392 (5%) 25 22	0, 66, 199, 425	0

All (392) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	Х	319	ALA	12.8
5	Х	36	VAL	11.2
5	Υ	239	GLY	9.5
5	Х	35	ILE	9.2
3	Ι	11	GLN	8.8
3	Ι	10	ALA	8.5
5	Х	24	TYR	8.1
2	С	251	ALA	7.5
2	Н	1002	LEU	7.5
2	С	231	GLU	7.4
5	Х	56	MET	7.2



Mol	Chain	Res	Type	RSRZ
5	Х	53	ILE	7.0
1	В	169	GLY	6.9
2	Н	334	GLU	6.8
2	С	232	ILE	6.7
3	Ι	212	THR	6.6
5	Х	318	ALA	6.5
5	Y	337	VAL	6.2
3	Ι	208	THR	6.2
5	Y	317	ASN	6.0
3	D	1199	PHE	5.7
3	D	1171	GLY	5.7
1	F	194	GLN	5.7
1	G	171	LEU	5.6
3	Ι	1161	GLY	5.6
3	Ι	13	LYS	5.5
5	Y	320	ILE	5.5
2	С	116	ASP	5.5
1	F	162	GLU	5.5
2	Н	1000	LEU	5.5
1	F	148	ARG	5.5
3	Ι	12	THR	5.4
2	Н	1001	GLY	5.4
3	D	1203	ARG	5.4
3	Ι	1203	ARG	5.3
2	С	332	ARG	5.2
1	А	193	GLU	5.2
5	Х	315	TRP	5.1
1	В	172	LEU	5.0
1	F	161	SER	5.0
2	Н	998	LEU	4.9
1	В	171	LEU	4.8
1	G	172	LEU	4.8
2	С	238	GLN	4.8
2	Н	981	ALA	4.7
2	С	305	SER	4.7
5	Y	241	SER	4.7
3	Ι	521	LYS	4.7
3	Ι	732	GLY	4.7
2	Н	1004	ASP	4.6
2	Н	1003	THR	4.6
3	Ι	830	ASP	4.6
2	Н	258	ASN	4.6



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Mol	Chain	$\operatorname{Res}$	Type	RSRZ
1	F	193	GLU	4.6
3	Ι	1375	ALA	4.6
2	С	233	ARG	4.5
2	Н	299	LYS	4.5
3	Ι	9	LYS	4.5
3	Ι	217	LEU	4.4
2	Н	996	ARG	4.4
2	Н	1007	LYS	4.4
5	Х	6	GLN	4.4
5	Х	54	GLN	4.3
2	Н	990	ASP	4.3
2	С	165	HIS	4.3
2	Н	332	ARG	4.2
3	D	210	SER	4.2
5	Х	239	GLY	4.2
3	D	80	HIS	4.2
3	Ι	213	LYS	4.2
5	Х	241	SER	4.1
3	D	1133	ASP	4.1
2	С	331	LYS	4.1
5	Y	212	ILE	4.0
5	Y	318	ALA	4.0
3	Ι	205	LEU	4.0
1	G	122	GLU	4.0
2	Н	264	GLU	4.0
5	Y	321	ALA	4.0
3	Ι	333	GLY	3.9
2	Н	483	ASP	3.9
3	Ι	1162	ILE	3.9
1	А	3	GLY	3.9
1	А	41	ASN	3.9
5	Y	305	LEU	3.9
1	F	164	ASP	3.8
2	С	266	GLY	3.8
5	Y	421	TYR	3.8
5	Y	489	MET	3.8
2	С	118	LYS	3.8
2	Н	972	PHE	3.8
5	Х	52	GLY	3.8
2	Н	999	GLU	3.8
5	Y	293	GLU	3.7
3	D	830	ASP	3.7



4KN4

Mol	Chain	Res	Type	RSRZ
1	В	41	ASN	3.7
5	Х	307	THR	3.7
5	Х	44	ILE	3.7
2	Н	305	SER	3.7
2	Н	265	LYS	3.6
3	Ι	712	GLN	3.6
2	Н	1008	GLN	3.6
5	Y	240	ARG	3.6
5	Х	340	ALA	3.6
3	Ι	477	GLN	3.6
2	Н	251	ALA	3.6
2	Н	1006	GLU	3.6
3	Ι	876	SER	3.6
3	Ι	564	VAL	3.6
3	Ι	563	LEU	3.6
5	Х	57	GLU	3.6
2	Н	983	GLY	3.5
5	Y	574	GLU	3.5
2	С	311	CYS	3.5
2	Н	744	GLY	3.5
1	G	18	GLN	3.5
3	D	211	GLU	3.5
1	G	96	ASP	3.5
1	G	13	LEU	3.4
5	Y	311	THR	3.4
2	Н	165	HIS	3.4
2	Н	970	GLY	3.4
3	D	212	THR	3.4
3	Ι	1376	GLY	3.4
2	С	172	TYR	3.4
3	D	1172	LYS	3.4
1	В	147	GLN	3.4
2	С	1000	LEU	3.4
1	В	73	GLY	3.4
2	Н	1152	GLY	3.4
2	Н	982	GLY	3.3
5	Y	340	ALA	3.3
3	D	878	ASP	3.3
5	Х	237	ALA	3.3
5	X	43	ASP	3.3
5	Y	319	ALA	3.3
3	D	932	MET	3.3

Continued from previous page...



Mol

1

5

2

3

2

2

3

3

1

3

Ι	831	VAL	3.2
F	110	VAL	3.2
Н	742	TYR	3.2
Н	969	ALA	3.2
С	77	GLU	3.2
Н	252	SER	3.2
Х	485	GLU	3.1
F	95	LYS	3.1
Н	1010	GLN	3.1
D	314	ARG	3.1
Н	374	GLU	3.1
D	528	THR	3.1
G	191	ARG	3.1
D	1198	VAL	3.1
Н	912	ASP	3.0
Ι	708	ASN	3.0
Х	240	ARG	3.0
Y	316	PHE	3.0
Ι	540	GLY	3.0
В	170	ARG	3.0
С	304	GLU	3.0
Ι	80	HIS	3.0

Continued from previous page...

 $\mathbf{Res}$ 

4

306

267

1179

334

250

204

477

121

Type

SER

PHE

ARG

PRO

GLU

THR

GLU

GLN

VAL

RSRZ

3.2

3.2

3.2

3.2

3.2

3.2

3.2

3.2

3.2

Chain

А

Х

С

D

С

С

Ι

D

В

F

Η

С

С

Η

Ι

G

D

Х

Ι

Η

2

2

2

2

3

1

3

5

3

2

192

1072

483

999

60

676

127

831

314

559

725

 $\operatorname{GLN}$ Continued on next page...

VAL

ASN

ASP

GLU

GLN

GLY

GLN

VAL

THR

ALA

2.9

2.9

2.9

2.9

2.9

2.9

2.9

2.9

2.9

2.9

2.9



4KN4

Mol	Chain	Res	Type	RSRZ
3	Ι	174	174 ASP	
5	Y	315	TRP	2.9
2	С	258	ASN 2.	
1	G	182	ARG	2.8
5	Х	322	MET	2.8
3	Ι	1172	LYS	2.8
5	Х	478	PRO	2.8
2	С	76	GLY	2.8
2	С	237	LEU	2.8
3	D	333	GLY	2.8
3	D	1170	LYS	2.8
5	Y	478	PRO	2.8
1	F	147	GLN	2.8
2	С	252	SER	2.8
1	G	51	MET	2.8
3	Ι	1374	ALA	2.8
5	Х	305	LEU	2.8
2	Н	995	ASP	2.8
2	Н	298	ALA	2.8
3	Ι	675	ALA	2.8
1	F	163	GLU	2.8
2	Н	975	ILE	2.8
5	Y	322	MET	2.7
3	Ι	1250	ASP	2.7
2	Н	1005	GLU	2.7
1	G	75	GLN	2.7
1	А	245	GLU	2.7
5	Y	309	ASN	2.7
2	С	265	LYS	2.7
3	Ι	837	ASP	2.7
2	Н	333	ILE	2.7
2	Η	107	ARG	2.7
1	G	23	HIS	2.7
2	Н	986	ALA	2.7
1	G	204	GLU	2.7
3	D	829	GLY	2.7
3	Ι	1168	GLU	2.7
3	D	931	THR	2.7
5	X	327	SER	2.6
2	С	236	LYS	2.6
2	Н	172	TYR	2.6
2	Н	974	ARG	2.6



4KN4

Mol	Chain	Res	Type	RSRZ
3	D	832 LYS		2.6
3	Ι	209 ASN		2.6
1	F	94	94 GLY	
2	Н	269	ILE	2.6
3	D	547	ARG	2.6
2	С	1001	GLY	2.6
5	Х	260	ARG	2.6
5	Y	336	GLU	2.6
1	F	234	LEU	2.6
1	G	107	ILE	2.6
2	Н	662	SER	2.6
2	Н	1070	HIS	2.6
2	Н	301	TYR	2.6
5	Y	310	GLU	2.6
2	Н	111	GLU	2.6
3	Ι	218	THR	2.6
2	Н	987	GLU	2.6
2	Н	108	GLU	2.5
2	Н	984	VAL	2.5
3	Ι	1273	ASP	2.5
2	Н	1009	ASN	2.5
2	Н	263	VAL	2.5
3	D	1200	GLU	2.5
5	Y	273	MET	2.5
5	Х	328	GLU	2.5
1	В	168	ILE	2.5
2	Н	727	VAL	2.5
3	Ι	674	THR	2.5
1	В	122	GLU	2.5
2	Н	908	GLU	2.5
5	X	8	GLN	2.5
5	Y	312	SER	2.5
5	Y	341	LEU	2.5
1	G	24	ALA	2.5
2	Н	169	LYS	2.5
1	В	57	THR	2.5
1	F	96	ASP	2.4
2	Н	234	ASP	2.4
5	Х	583	THR	2.4
3	D	344	GLY	2.4
3	D	445	LYS	2.4
3	Ι	709	ARG	2.4



Mol

5

 $\mathbf{2}$ 

3

3

2

2

1

2

2

5

 $\frac{5}{2}$ 

 $\frac{5}{3}$ 

5

 $\frac{1}{3}$ 

1

1

 $\frac{5}{2}$ 

2

1

3

Х	515	GLU	2.4
Н	1071	GLY	2.4
Υ	237	ALA	2.4
D	471	PRO	2.4
Х	422	ARG	2.4
G	157	THR	2.4
Ι	210	SER	2.4
А	241	GLU	2.3
G	123	ILE	2.3
Х	289	LYS	2.3
Н	106	GLU	2.3
Н	979	LEU	2.3
G	86	LYS	2.3
Ι	1204	VAL	2.3
D	875	ASN	2.3
Ι	847	ASP	2.3
F	131	CYS	2.3

Continued from previous page...

 $\mathbf{Res}$ 

34

230

1198

746

997

257

5

319

720

293

Type

ASP

PHE

VAL

LEU

TRP

ALA

VAL

LEU

ARG

GLU

RSRZ

2.4

2.4

2.4

2.4

2.4

2.4

2.4

2.4

2.4

2.4

Chain

Х

С

Ι

Ι

Η

С

А

С

Н

Х

D 3 3 Ι F 1 3 Ι 392 THR 2.31 А 162GLU 2.3PRO 3 D 11852.3GLU 2.3 3 D 69 2С 482 GLY 2.32 ALA 4 J 2.3VAL 2 С 2.3 978 2 Η 980 VAL 2.3238 LYS 5Y 2.33 Ι 747 MET 2.3ALA 3 Ι 5652.32 С ARG 2.3 996 Y 5578LYS 2.370 THR 2.3 В 1 3 Ι 586GLY 2.3Continued on next page...



Mol	Chain	Res	Type	RSRZ
3	D	473	THR	2.3
3	Ι	1167 LYS		2.3
3	Ι	587	587 LEU	
3	Ι	8	LEU	2.2
5	Х	310	GLU	2.2
5	Х	311	THR	2.2
1	В	59	VAL	2.2
2	Н	232	ILE	2.2
3	Ι	207	GLU	2.2
3	Ι	1295	ASN	2.2
3	Ι	154	LEU	2.2
2	С	1016	GLU	2.2
5	Y	490	PRO	2.2
1	G	173	VAL	2.2
3	Ι	1171	GLY	2.2
5	Y	333	VAL	2.2
3	D	1168	GLU	2.2
2	Н	254	ASP	2.2
2	Н	268	ARG	2.2
3	Ι	713	GLU	2.2
2	Н	1153	ALA	2.2
3	Ι	716	GLN	2.2
1	G	87	GLY	2.1
3	Ι	473	THR	2.1
2	С	310	ILE	2.1
1	F	73	GLY	2.1
4	Е	91	ARG	2.1
3	D	82	GLY	2.1
3	Ι	811	GLU	2.1
1	F	211	ILE	2.1
2	Н	1134	GLN	2.1
3	Ι	1373	ARG	2.1
3	Ι	211	GLU	2.1
2	С	1002	LEU	2.1
2	Н	1020	GLU	2.1
2	H	61	SER	2.1
3	D	670	SER	2.1
2	С	282	VAL	2.1
1	F	97	GLU	2.1
3	Ι	1213	GLY	2.1
1	A	133	LEU	2.1
2	С	1040	ASP	2.1



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 Mol
 Chain
 Res
 Type
 RSRZ

-			-51	
3	Ι	267	ASP	2.1
5	Х	482	GLU	2.1
1	В	146	VAL	2.1
1	А	243	243 LYS	
1	F	196	THR	2.1
1	В	178	SER	2.1
2	Н	1018	TYR	2.1
1	F	24	ALA	2.1
2	С	57	PHE	2.1
2	С	1023	HIS	2.1
3	D	1204	VAL	2.1
3	Ι	1202	GLU	2.1
4	J	36	ASP	2.1
4	J	37	PRO	2.1
2	Н	1264	GLN	2.1
5	Y	420	GLU	2.1
3	Ι	1249	ASN	2.1
2	С	268	ARG	2.0
1	F	41	ASN	2.0
2	Н	953	LEU	2.0
5	Y	483	LEU	2.0
2	С	375	PRO	2.0
3	Ι	19	ALA	2.0
5	Х	514	ASP	2.0
1	G	181	GLU	2.0
3	Ι	520	ALA	2.0
2	Н	601	ASP	2.0
5	Y	261	LEU	2.0
3	Ι	875	ASN	2.0
3	D	638	SER	2.0
5	Y	330	LEU	2.0
2	С	374	GLU	2.0
2	Н	718	ALA	2.0
1	F	128	HIS	2.0
2	С	574	SER	2.0
5	Х	9	LEU	2.0
5	X	32	PRO	2.0
2	Н	988	LYS	2.0
5	Y	488	LEU	2.0
3	D	207	GLU	2.0
5	Х	423	ARG	2.0
2	С	982	GLY	2.0



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Mol	Chain	Res	Type	RSRZ
2	Н	413	GLU	2.0
4	J	77	ALA	2.0
5	Х	325	PRO	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)

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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
6	1RL	Н	1401	65/65	0.79	0.42	20,20,20,20	0
6	1RL	С	1401	65/65	0.82	0.36	20,20,20,20	0
8	MG	Ι	1503	1/1	0.92	0.66	20,20,20,20	0
7	ZN	D	1501	1/1	0.94	0.05	54,54,54,54	0
7	ZN	Ι	1501	1/1	0.95	0.03	60,60,60,60	0
8	MG	D	1503	1/1	0.96	0.32	24,24,24,24	0
7	ZN	D	1502	1/1	0.96	0.19	8,8,8,8	0
7	ZN	Ι	1502	1/1	0.98	0.11	49,49,49,49	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.

