

Full wwPDB X-ray Structure Validation Report (i)

Feb 6, 2024 – 04:32 PM EST

:	2FWR
:	Structure of Archaeoglobus Fulgidis XPB
:	Fan, L.; Arvai, A.S.; Tainer, J.A.
:	2006-02-02
:	2.60 Å(reported)
	: : : :

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

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

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 Å.

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



Motria	Whole archive	Similar resolution
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length		Quality of chain	
1	А	472	39%	45%	8% 8%
1	В	472	43%	40%	6% 10%
1	С	472	33%	44%	10% 12%
1	D	472	31%	50%	10% 9%



2FWR

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14769 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	494	Total	С	Ν	Ο	S	0	0	0
	A	404	3513	2242	627	638	6	0	0	0
1	D	492	Total	С	Ν	0	S	0	0	0
	D	423	3419	2181	611	619	8	0	0	0
1	C	414	Total	С	Ν	0	S	0	0	0
	U	414	3317	2119	589	604	5	0	0	0
1	Л	198	Total	С	Ν	0	S	0	0	0
		420	3402	2169	604	623	6	0	U	0

• Molecule 1 is a protein called DNA repair protein RAD25.

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	MET	-	initiating methionine	UNP O29889
А	2	GLY	-	cloning artifact	UNP O29889
А	3	SER	-	cloning artifact	UNP O29889
А	4	SER	-	cloning artifact	UNP O29889
А	5	HIS	-	expression tag	UNP O29889
А	6	HIS	-	expression tag	UNP O29889
А	7	HIS	-	expression tag	UNP O29889
А	8	HIS	-	expression tag	UNP O29889
А	9	HIS	-	expression tag	UNP O29889
А	10	HIS	-	expression tag	UNP O29889
A	11	SER	-	cloning artifact	UNP O29889
А	12	SER	-	cloning artifact	UNP O29889
А	13	GLY	-	cloning artifact	UNP O29889
А	14	LEU	-	cloning artifact	UNP O29889
А	15	VAL	-	cloning artifact	UNP O29889
A	16	PRO	-	cloning artifact	UNP O29889
A	17	ARG	-	cloning artifact	UNP O29889
A	18	GLY	-	cloning artifact	UNP O29889
A	19	SER	-	cloning artifact	UNP O29889
А	20	HIS	-	cloning artifact	UNP O29889
В	1	MET	-	initiating methionine	UNP O29889



$0\mathbf{F}$	W	\mathbf{D}
$\Delta \Gamma$	vv	п

	Residue	Modelled	Actual	Comment	Reference
B			Actual	cloping artifact	UNP O20880
D B		GLI SED	-	eloning artifact	UNI 029889
B		SER	-	cloning artifact	UNI 029889
B	5	HIS	-		UNI 029889
B	5	HIS	-	expression tag	UNI 029889
B	7	HIS	-	expression tag	UNI 029889
D B	8		-	expression tag	UNI 029889
D B	0	HIS	-	expression tag	UNI 029889
B	9	HIS	-	expression tag	UNI 029889
B	10	SEB	-	cloping artifact	UNI 029889
D B	11	SER	-	eloning artifact	UNI 029889
D P	12	CIV	-	cloning artifact	UNF 029889
D	10		-	cloning artifact	$\frac{\text{UND}}{\text{UND}} \frac{\text{O29889}}{\text{O29889}}$
D	14		-	cloning artifact	$\frac{\text{UNF}}{\text{UND}} \frac{029889}{29889}$
D	10	VAL	-	cloning artifact	$\frac{\text{UNP} \text$
D	10	ADC	-		UNP 029889
	10	ARG	-	cloning artifact	$\frac{\text{UNP O}29889}{\text{UND O}29889}$
	18	GLY	-	cloning artifact	UNP 029889
	19	SER IIIC	-	cloning artifact	UNP 029889
B	20	HIS MET	-	cloning artifact	UNP 029889
C	1	MET	-	initiating methionine	UNP 029889
	2	GLY	-	cloning artifact	UNP 029889
C	3	SER	-	cloning artifact	UNP 029889
C	4	SER	-	cloning artifact	UNP 029889
	5	HIS	-	expression tag	UNP 029889
C	6	HIS	-	expression tag	UNP 029889
C	7	HIS	-	expression tag	UNP 029889
C	8	HIS	-	expression tag	UNP 029889
C	9	HIS	-	expression tag	UNP 029889
C	10	HIS	-	expression tag	UNP 029889
C	11	SER	-	cloning artifact	UNP 029889
C	12	SER	-	cloning artifact	UNP 029889
C	13	GLY	-	cloning artifact	UNP 029889
C	14	LEU	-	cloning artifact	UNP 029889
C	15	VAL	-	cloning artifact	UNP 029889
C	16	PRO	-	cloning artifact	UNP 029889
C	17	ARG	-	cloning artifact	UNP 029889
C	18	GLY	-	cloning artifact	UNP 029889
C	19	SER	-	cloning artifact	UNP 029889
C	20	HIS	-	cloning artifact	UNP 029889
D	1	MET	-	initiating methionine	UNP 029889
D	2	GLY	-	cloning artifact	UNP O29889
D	3	SER	-	cloning artifact	UNP O29889



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Chain	Residue	Modelled	Actual	Comment	Reference
D	4	SER	-	cloning artifact	UNP O29889
D	5	HIS	-	expression tag	UNP O29889
D	6	HIS	-	expression tag	UNP O29889
D	7	HIS	-	expression tag	UNP O29889
D	8	HIS	-	expression tag	UNP O29889
D	9	HIS	-	expression tag	UNP O29889
D	10	HIS	-	expression tag	UNP O29889
D	11	SER	-	cloning artifact	UNP O29889
D	12	SER	-	cloning artifact	UNP O29889
D	13	GLY	-	cloning artifact	UNP O29889
D	14	LEU	-	cloning artifact	UNP O29889
D	15	VAL	-	cloning artifact	UNP O29889
D	16	PRO	-	cloning artifact	UNP O29889
D	17	ARG	-	cloning artifact	UNP O29889
D	18	GLY	-	cloning artifact	UNP O29889
D	19	SER	-	cloning artifact	UNP O29889
D	20	HIS	-	cloning artifact	UNP O29889

• Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
2	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
2	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
2	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 3 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 3 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 3 & 1 \end{array}$	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	286	Total O 286 286	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	299	Total O 299 299	0	0
4	С	261	Total O 261 261	0	0
4	D	220	Total O 220 220	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 repair protein RAD25









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	49.09Å 97.96Å 113.73Å	Depositor
a, b, c, α , β , γ	79.03° 85.54° 89.69°	Depositor
Bosolution(Å)	29.35 - 2.60	Depositor
Resolution (A)	29.35 - 2.60	EDS
% Data completeness	84.8 (29.35-2.60)	Depositor
(in resolution range)	84.7 (29.35-2.60)	EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.44 (at 2.61 \text{\AA})$	Xtriage
Refinement program	CNS 1.1	Depositor
P. P.	0.237 , 0.300	Depositor
n, n_{free}	0.211 , 0.224	DCC
R_{free} test set	2888 reflections (5.05%)	wwPDB-VP
Wilson B-factor $(Å^2)$	47.5	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31 , 102.6	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14769	wwPDB-VP
Average B, all atoms $(Å^2)$	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: IPA, $\mathrm{PO4}$

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

Mal	Chain	Bond lengths		Bond angles	
		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.49	0/3583	0.69	0/4827
1	В	0.48	0/3484	0.68	1/4688~(0.0%)
1	С	0.44	0/3383	0.67	0/4562
1	D	0.43	0/3466	0.65	0/4673
All	All	0.46	0/13916	0.67	1/18750~(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	В	190	GLY	N-CA-C	5.20	126.10	113.10

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	3513	0	3546	303	0
1	В	3419	0	3446	243	0
1	С	3317	0	3324	302	0
1	D	3402	0	3401	310	0
2	А	5	0	0	0	0
2	В	15	0	0	1	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	С	5	0	0	0	0
2	D	15	0	0	0	0
3	А	12	0	24	6	0
4	А	286	0	0	14	1
4	В	299	0	0	10	3
4	С	261	0	0	12	0
4	D	220	0	0	12	1
All	All	14769	0	13741	1153	4

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 42.

All (1153) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:438:PRO:HB3	1:D:444:GLU:HA	1.31	1.08
1:A:333:SER:HB3	1:A:336:LYS:HG3	1.36	1.07
1:C:24:ILE:HD12	1:C:24:ILE:H	1.20	1.03
1:D:356:THR:HG23	1:D:362:VAL:HG22	1.38	1.01
1:A:377:ARG:HG3	1:A:378:THR:H	1.23	1.01
1:D:95:ARG:HB3	1:D:259:LEU:HD11	1.39	1.01
1:A:438:PRO:HB2	1:A:443:LYS:HA	1.42	1.00
1:A:398:ILE:HD13	1:A:399:VAL:N	1.76	0.98
1:A:285:VAL:HG23	1:A:286:TYR:H	1.29	0.98
1:A:386:ILE:H	1:A:386:ILE:HD12	1.29	0.97
1:A:391:ARG:HB2	1:A:411:PRO:HG3	1.44	0.97
1:C:375:THR:HG22	1:C:378:THR:HG23	1.46	0.97
1:D:306:ILE:HG23	1:D:307:VAL:H	1.31	0.96
1:A:100:LYS:HZ2	1:A:104:ARG:HH21	1.11	0.96
1:D:132:LEU:HD23	1:D:458:VAL:HG21	1.47	0.95
1:C:408:ILE:HG23	1:C:409:ASP:H	1.32	0.94
1:C:148:GLN:HE21	1:C:152:ARG:HH12	1.15	0.94
1:D:132:LEU:HA	1:D:458:VAL:HG21	1.49	0.93
1:D:407:GLY:O	1:D:410:VAL:HG13	1.68	0.93
1:D:408:ILE:HG22	1:D:409:ASP:H	1.31	0.92
1:A:100:LYS:NZ	1:A:104:ARG:HH21	1.68	0.92
1:C:334:LYS:O	1:C:338:ARG:HD3	1.69	0.91
1:B:290:LEU:HB3	1:B:296:THR:HA	1.52	0.90
1:A:134:THR:HG22	4:A:2827:HOH:O	1.71	0.89
1:A:285:VAL:HG21	1:A:322:ALA:CB	2.02	0.89
1:C:325:GLU:HG3	1:C:329:ILE:HD13	1.53	0.89



Interatomic Clash					
Atom-1	Atom-2	distance $(Å)$	overlan (Å)		
1.C.389.GLY.HA2	1·C·392·THB·HG22	1.52	0.89		
1:D:162:GLY:HA3	1:D:172:LYS:HD3	1.55	0.89		
1:C:42:VAL:HG12	1·C·44·HIS·H	1.38	0.88		
1:C:282:ARG:O	1:C:286:TYR:HB2	1.73	0.88		
1:A:398:ILE:HD13	1:A:399:VAL:H	1.36	0.88		
1:D:418:ILE:HD11	1:D:447:LEU:HD11	1.50	0.87		
1.B.288.GLN.O	1.B·292·ALA·HB2	1.75	0.86		
1:D:370:LEU:HD13	1:D:370:LEU:H	1.40	0.86		
1:C:30:GLU:O	1:C:33:THR:HG22	1.76	0.86		
1:A:405:ASP:HB2	1:A:435:ILE:HD11	1.56	0.86		
1.B.352.ILE.HG22	1:B:415:VAL:HB	1.56	0.86		
1:A:103:GLU:HG3	1:A:426:ARG:NH1	1.90	0.85		
1:D:329:ILE:HD12	1:D:330:ALA:N	1.92	0.85		
1:A:377:ARG:HG3	1:A:378:THR:N	1.90	0.84		
1:D:380:ARG:O	1:D:384:GLU:HG2	1.75	0.84		
1:D:405:ASP:HB3	1:D:435:ILE:HD11	1.59	0.84		
1:A:66:GLU:HA	1:A:297:LEU:HD12	1.61	0.82		
1:C:361:LEU:HD11	1:C:419:MET:HG3	1.61	0.82		
1:D:329:ILE:HD12	1:D:330:ALA:H	1.41	0.82		
1:C:27:ILE:O	1:C:27:ILE:HG13	1.79	0.82		
1:C:26:GLU:HG3	1:C:78:ASN:HD22	1.44	0.81		
1:C:403:VAL:HG21	1:C:431:ARG:NH2	1.94	0.81		
1:D:102:LEU:O	1:D:106:LEU:HD13	1.81	0.81		
1:C:383:ARG:HH22	1:C:402:GLN:NE2	1.79	0.81		
1:A:89:ASP:HB3	4:A:2548:HOH:O	1.78	0.81		
1:C:205:PRO:HB2	1:C:230:ARG:HH11	1.46	0.81		
1:C:354:ILE:HG12	1:C:399:VAL:HG23	1.62	0.81		
1:A:103:GLU:HG3	1:A:426:ARG:HH11	1.44	0.80		
1:C:115:LEU:HD23	1:C:249:LEU:HB3	1.60	0.80		
1:C:259:LEU:HD11	1:C:262:TYR:CE2	2.16	0.80		
1:C:62:ARG:O	1:C:66:GLU:HG3	1.82	0.79		
1:B:115:LEU:O	1:B:121:LYS:HE3	1.83	0.79		
1:A:259:LEU:HD13	1:A:260:ALA:N	1.98	0.79		
1:B:377:ARG:HD2	1:B:377:ARG:O	1.83	0.79		
1:D:132:LEU:HA	1:D:458:VAL:CG2	2.11	0.79		
1:A:207:GLU:HG2	3:A:6002:IPA:H12	1.62	0.79		
1:A:358:HIS:O	1:A:362:VAL:HG23	1.83	0.79		
1:D:352:ILE:HD12	1:D:353:ILE:N	1.98	0.79		
1:A:295:ILE:HB	1:A:299:ARG:H	1.48	0.78		
1:B:333:SER:HB3	1:B:336:LYS:HG2	1.64	0.78		
1:B:389:GLY:O	1:B:394:ARG:HB3	1.83	0.78		



	louis page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:356:THR:CG2	1:D:362:VAL:HG22	2.12	0.78
1:D:100:LYS:HD3	1:D:426:ARG:HH22	1.49	0.78
1:C:272:ALA:HB3	1:C:275:GLU:HG3	1.67	0.77
1:B:121:LYS:HG3	2:B:4002:PO4:O4	1.85	0.77
1:D:232:ASP:OD1	1:D:234:ARG:HG3	1.84	0.77
1:C:420:SER:HB3	1:C:450:LEU:O	1.84	0.77
1:D:379:SER:HB3	1:D:382:GLU:HB2	1.67	0.76
1:A:42:VAL:HG13	1:A:43:PRO:HD2	1.67	0.76
1:D:321:ARG:O	1:D:325:GLU:HB2	1.84	0.76
1:C:257:LYS:NZ	1:C:260:ALA:HB3	2.00	0.76
1:D:205:PRO:HA	1:D:237:ILE:HD11	1.68	0.76
1:A:285:VAL:HG21	1:A:322:ALA:HB3	1.64	0.76
1:A:122:THR:HG21	1:A:152:ARG:CD	2.15	0.76
1:B:99:GLU:O	1:B:103:GLU:HG2	1.86	0.75
1:C:205:PRO:HA	1:C:237:ILE:HD11	1.67	0.75
1:C:95:ARG:HB2	1:C:98:GLN:HG3	1.69	0.75
1:C:115:LEU:HD21	1:C:247:PHE:HE1	1.50	0.75
1:D:325:GLU:O	1:D:329:ILE:HG13	1.85	0.75
1:D:388:GLU:HA	1:D:391:ARG:CG	2.17	0.75
1:B:27:ILE:HG22	1:B:36:VAL:HG22	1.68	0.75
1:D:269:VAL:HG21	1:D:336:LYS:HG2	1.68	0.75
1:C:28:TYR:HA	1:C:79:ALA:HB2	1.68	0.75
1:C:412:ASP:HB2	1:C:437:ARG:HD2	1.68	0.74
1:B:351:LYS:H	1:B:351:LYS:HD2	1.52	0.74
1:B:325:GLU:O	1:B:329:ILE:HG13	1.87	0.74
1:C:57:LEU:H	1:C:57:LEU:HD22	1.52	0.74
1:D:45:ALA:HB1	1:D:54:TYR:HB3	1.70	0.74
1:D:201:VAL:HG12	1:D:225:THR:HB	1.70	0.74
1:D:361:LEU:O	1:D:365:ILE:HG13	1.87	0.74
1:D:440:LYS:HE3	1:D:440:LYS:HA	1.67	0.74
1:D:70:SER:HA	1:D:292:ALA:HB2	1.68	0.73
1:D:290:LEU:H	1:D:290:LEU:HD22	1.53	0.73
1:C:267:ILE:HG21	1:C:339:LYS:HE2	1.70	0.73
1:B:303:PHE:O	1:B:307:VAL:HG23	1.89	0.73
1:C:392:THR:HG23	1:C:393:GLY:N	2.03	0.73
1:C:374:ILE:HA	1:C:378:THR:HG21	1.71	0.72
1:D:305:LYS:NZ	1:D:305:LYS:HB3	2.04	0.72
1:A:386:ILE:H	1:A:386:ILE:CD1	2.02	0.72
1:D:424:SER:OG	1:D:429:ILE:HD11	1.88	0.72
1:C:148:GLN:HG2	1:C:152:ARG:NH1	2.04	0.72
1:D:165:SER:HB2	4:D:2598:HOH:O	1.89	0.72



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:23:MET:HB2	1:B:38:GLY:HA2	1.71	0.72
1:B:24:ILE:O	1:B:24:ILE:HG22	1.89	0.72
1:C:71:ASN:O	1:C:73:ILE:HG13	1.89	0.72
1:A:66:GLU:HG3	1:A:297:LEU:HD13	1.71	0.72
1:A:285:VAL:HG23	1:A:286:TYR:N	2.04	0.71
1:C:383:ARG:HH22	1:C:402:GLN:HE21	1.38	0.71
1:D:34:ILE:HG12	1:D:58:ALA:HA	1.72	0.71
1:B:366:SER:HB2	1:B:373:ALA:HB2	1.72	0.71
1:C:185:ASN:O	1:C:189:LEU:HG	1.90	0.71
1:A:241:VAL:HG23	1:A:242:VAL:HG23	1.73	0.71
1:A:295:ILE:HD13	1:A:300:ALA:HB3	1.73	0.71
1:A:333:SER:HB3	1:A:336:LYS:CG	2.19	0.71
1:C:263:THR:CG2	1:C:446:VAL:HG22	2.19	0.71
1:A:295:ILE:O	1:A:295:ILE:HG13	1.90	0.71
1:C:389:GLY:CA	1:C:392:THR:HG22	2.20	0.71
1:D:388:GLU:HA	1:D:391:ARG:HG2	1.73	0.71
1:B:405:ASP:HB3	1:B:435:ILE:HD11	1.71	0.70
1:D:60:ARG:HA	4:D:2516:HOH:O	1.91	0.70
1:D:323:TRP:HA	1:D:326:ALA:HB3	1.72	0.70
1:B:375:THR:HG23	1:B:377:ARG:H	1.57	0.70
1:B:404:LEU:N	1:B:404:LEU:HD22	2.07	0.70
1:C:126:MET:CE	1:C:152:ARG:HB3	2.21	0.70
1:A:304:ASN:HA	1:A:307:VAL:HG22	1.73	0.70
1:C:230:ARG:HG3	1:C:235:HIS:HB3	1.74	0.70
1:D:234:ARG:HG2	1:D:234:ARG:HH11	1.56	0.70
1:B:143:LEU:O	1:B:147:GLU:HG3	1.92	0.70
1:B:37:LYS:HG2	1:B:53:THR:HG22	1.74	0.70
1:B:320:LEU:O	1:B:324:GLU:HG3	1.92	0.70
1:D:172:LYS:HB3	1:D:173:PRO:HD2	1.73	0.70
1:A:314:GLU:HG2	1:A:316:ALA:H	1.55	0.70
1:B:332:ASN:CG	1:B:333:SER:H	1.93	0.70
1:B:273:GLU:O	1:B:277:VAL:HG23	1.92	0.69
1:D:149:TRP:HE3	1:D:153:LEU:HD11	1.56	0.69
1:A:282:ARG:HH21	1:A:322:ALA:HA	1.57	0.69
1:B:286:TYR:HA	1:B:289:PHE:HB2	1.74	0.69
1:A:45:ALA:C	1:A:46:LYS:HD2	2.13	0.69
1:A:69:GLU:HG2	1:A:297:LEU:HG	1.75	0.69
1:D:305:LYS:HB3	1:D:305:LYS:HZ2	1.56	0.69
1:D:425:ALA:O	1:D:429:ILE:HG13	1.92	0.69
1:D:333:SER:O	1:D:337:ILE:HG12	1.92	0.69
1:C:109:LYS:HD3	1:C:132:LEU:HD21	1.76	0.68



	louo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:418:ILE:HD12	1:D:447:LEU:HD21	1.73	0.68
1:D:43:PRO:O	1:D:44:HIS:HB2	1.92	0.68
1:D:95:ARG:HB3	1:D:259:LEU:CD1	2.21	0.68
1:A:259:LEU:O	1:A:261:LYS:HG3	1.93	0.68
1:B:340:LEU:HD21	1:B:354:ILE:HD13	1.73	0.68
1:C:336:LYS:HE3	1:C:452:SER:HB3	1.74	0.68
1:D:283:GLU:HB3	1:D:286:TYR:CZ	2.28	0.68
1:B:358:HIS:CE1	1:B:360:GLU:HB3	2.29	0.68
1:B:332:ASN:CG	1:B:333:SER:N	2.46	0.68
1:C:332:ASN:HD22	1:C:364:ARG:HD2	1.59	0.68
1:C:439:SER:HB2	1:C:442:LYS:HD2	1.76	0.68
1:D:432:LEU:O	1:D:432:LEU:HD23	1.94	0.68
1:A:274:ASP:O	1:A:277:VAL:HG12	1.93	0.68
1:B:34:ILE:HG12	1:B:58:ALA:HA	1.76	0.68
1:B:102:LEU:HG	1:B:106:LEU:HD22	1.75	0.68
1:C:443:LYS:HG3	1:C:444:GLU:H	1.58	0.68
1:D:91:GLU:HB3	1:D:265:LYS:HD3	1.76	0.68
1:A:296:THR:O	1:A:297:LEU:HB2	1.92	0.68
1:B:321:ARG:HA	1:B:324:GLU:OE1	1.94	0.68
1:D:404:LEU:N	1:D:404:LEU:HD22	2.08	0.68
1:C:394:ARG:HE	1:C:394:ARG:HA	1.60	0.67
1:B:384:GLU:O	1:B:388:GLU:HG2	1.94	0.67
1:C:341:ARG:O	1:C:345:GLU:HG3	1.94	0.67
1:C:26:GLU:HG3	1:C:78:ASN:ND2	2.09	0.67
1:D:273:GLU:O	1:D:274:ASP:HB3	1.95	0.67
1:D:369:PHE:CE1	1:D:370:LEU:HD22	2.30	0.67
1:A:234:ARG:HH22	3:A:6002:IPA:H2	1.59	0.67
1:B:62:ARG:HB2	4:B:2009:HOH:O	1.95	0.67
1:D:362:VAL:HG13	1:D:399:VAL:HG22	1.77	0.67
1:A:110:ARG:HD2	1:A:221:ARG:HG3	1.78	0.66
1:A:402:GLN:O	1:A:404:LEU:HD22	1.96	0.66
1:C:418:ILE:HG12	1:C:425:ALA:HB2	1.75	0.66
1:C:339:LYS:O	1:C:343:ILE:HG13	1.95	0.66
1:D:260:ALA:HB2	4:D:2799:HOH:O	1.94	0.66
1:C:333:SER:HB3	1:C:336:LYS:HG2	1.77	0.66
1:B:37:LYS:HG2	1:B:53:THR:CG2	2.26	0.66
1:C:68:PHE:O	1:C:70:SER:N	2.28	0.66
1:A:100:LYS:NZ	1:A:104:ARG:NH2	2.43	0.66
1:A:359:ASN:HA	1:A:362:VAL:HB	1.78	0.66
1:B:50:ARG:HH21	1:B:50:ARG:HG2	1.60	0.66
1:B:364:ARG:O	1:B:368:VAL:HG23	1.96	0.66



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:365:ILE:HD12	1:D:399:VAL:HG21	1.77	0.66
1:D:372:PRO:HB2	1:D:398:ILE:HG22	1.77	0.66
1:C:263:THR:HG22	1:C:445:ALA:O	1.95	0.66
1:D:368:VAL:HG12	1:D:368:VAL:O	1.95	0.66
1:B:122:THR:HG21	1:B:152:ARG:HD3	1.77	0.65
1:A:444:GLU:HB3	4:A:2628:HOH:O	1.96	0.65
1:C:375:THR:HG23	1:C:377:ARG:H	1.61	0.65
1:C:24:ILE:H	1:C:24:ILE:CD1	1.98	0.65
1:A:305:LYS:HG2	1:A:323:TRP:CD2	2.32	0.65
1:B:273:GLU:O	1:B:276:ARG:HG2	1.97	0.65
1:B:279:TYR:CE1	1:B:330:ALA:HB2	2.32	0.65
1:D:134:THR:HB	1:D:194:MET:HB2	1.79	0.65
1:D:158:GLU:HB3	4:D:2667:HOH:O	1.97	0.65
1:C:356:THR:HB	1:C:419:MET:HG2	1.79	0.65
1:A:413:ALA:CB	1:A:436:LEU:HD23	2.27	0.65
1:A:442:LYS:NZ	1:A:442:LYS:HA	2.12	0.65
1:B:372:PRO:HG2	1:B:395:PHE:CG	2.31	0.65
1:C:134:THR:HG21	4:C:2617:HOH:O	1.96	0.64
1:D:80:ALA:C	1:D:82:PRO:HD3	2.17	0.64
1:D:340:LEU:HA	1:D:343:ILE:CD1	2.27	0.64
1:D:213:ALA:O	1:D:221:ARG:NH2	2.29	0.64
1:A:46:LYS:HA	1:A:46:LYS:HE3	1.79	0.64
1:A:66:GLU:HA	1:A:297:LEU:CD1	2.27	0.64
1:D:418:ILE:CD1	1:D:429:ILE:HA	2.27	0.64
1:B:387:LEU:HD23	1:B:387:LEU:O	1.97	0.64
1:C:126:MET:HE3	1:C:152:ARG:HB3	1.79	0.64
1:D:350:ASP:HB3	1:D:414:ASN:HB3	1.78	0.64
1:B:434:ARG:NH2	1:B:434:ARG:HB2	2.12	0.64
1:A:391:ARG:HG3	1:A:391:ARG:HH11	1.60	0.64
1:B:165:SER:O	1:B:169:LYS:HD2	1.98	0.64
1:D:33:THR:HG23	1:D:56:ALA:O	1.98	0.64
1:D:149:TRP:O	1:D:153:LEU:HD13	1.98	0.64
1:A:93:SER:HA	1:A:265:LYS:HG2	1.80	0.64
1:A:334:LYS:O	1:A:338:ARG:HG2	1.98	0.64
1:A:438:PRO:HB2	1:A:443:LYS:CA	2.25	0.63
1:D:340:LEU:O	1:D:343:ILE:HG12	1.97	0.63
1:A:357:ARG:HD3	1:A:428:TYR:OH	1.97	0.63
1:C:148:GLN:HG2	1:C:152:ARG:CZ	2.27	0.63
1:C:69:GLU:HG3	1:C:75:PHE:CZ	2.33	0.63
1:A:425:ALA:O	1:A:429:ILE:HG12	1.97	0.63
1:B:351:LYS:HB2	1:B:390:PHE:CZ	2.34	0.63



	lo ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:37:LYS:HA	1:D:53:THR:HG22	1.81	0.63
1:D:45:ALA:CB	1:D:54:TYR:HB3	2.27	0.63
1:D:340:LEU:HG	1:D:343:ILE:HD11	1.79	0.63
1:D:336:LYS:O	1:D:340:LEU:HB2	1.98	0.63
1:D:36:VAL:HG11	1:D:42:VAL:HG21	1.81	0.63
1:A:69:GLU:OE1	1:A:297:LEU:HD11	1.99	0.63
1:A:386:ILE:HD12	1:A:386:ILE:N	2.08	0.63
1:C:334:LYS:HG2	1:C:338:ARG:HE	1.62	0.63
1:D:369:PHE:CD1	1:D:371:ILE:HB	2.34	0.63
1:A:65:ILE:HG22	1:A:297:LEU:HD11	1.81	0.62
1:C:389:GLY:HA2	1:C:392:THR:CG2	2.28	0.62
1:B:234:ARG:O	1:B:237:ILE:HG23	1.99	0.62
1:A:285:VAL:HG21	1:A:322:ALA:HB1	1.81	0.62
1:C:148:GLN:NE2	1:C:152:ARG:HH12	1.94	0.62
1:C:257:LYS:HZ2	1:C:260:ALA:HB3	1.64	0.62
1:B:289:PHE:O	1:B:292:ALA:HB3	1.99	0.62
1:C:143:LEU:HD13	1:C:167:ARG:HD2	1.82	0.62
1:D:408:ILE:HG22	1:D:409:ASP:N	2.08	0.62
1:C:161:VAL:O	1:C:172:LYS:HG2	2.00	0.62
1:D:394:ARG:HD3	1:D:394:ARG:N	2.15	0.62
1:B:122:THR:HG21	1:B:152:ARG:CD	2.30	0.62
1:B:149:TRP:O	1:B:153:LEU:HD22	1.99	0.61
1:B:374:ILE:HG22	1:B:374:ILE:O	1.99	0.61
1:B:433:GLY:HA2	1:B:436:LEU:HD12	1.81	0.61
1:A:357:ARG:HD3	1:A:428:TYR:CZ	2.35	0.61
1:B:352:ILE:CG2	1:B:415:VAL:HB	2.29	0.61
1:C:408:ILE:HG23	1:C:409:ASP:N	2.10	0.61
1:D:289:PHE:C	1:D:291:ARG:H	2.04	0.61
1:C:254:LEU:O	1:C:255:ALA:HB2	2.00	0.61
1:C:148:GLN:O	1:C:152:ARG:HG3	2.00	0.61
1:C:378:THR:O	1:C:379:SER:O	2.19	0.61
1:A:408:ILE:O	1:A:408:ILE:HG22	2.01	0.61
1:A:413:ALA:HB3	1:A:436:LEU:HD23	1.82	0.61
1:A:382:GLU:O	1:A:383:ARG:HG2	2.01	0.61
1:C:100:LYS:HE2	1:C:104:ARG:HE	1.65	0.61
1:B:301:GLU:O	1:B:303:PHE:N	2.29	0.61
1:D:96:ASP:OD2	1:D:259:LEU:HD13	2.01	0.61
1:A:351:LYS:HD3	1:A:412:ASP:O	1.99	0.60
1:B:126:MET:HE3	1:B:152:ARG:HG2	1.83	0.60
1:A:109:LYS:HD3	1:A:132:LEU:HD21	1.82	0.60
1:A:340:LEU:HA	1:A:343:ILE:HD12	1.83	0.60



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:229:GLU:OE2	1:C:229:GLU:HA	2.02	0.60
1:A:307:VAL:HG23	1:A:308:MET:H	1.66	0.60
1:C:205:PRO:HB2	1:C:230:ARG:NH1	2.15	0.60
1:D:191:ASN:OD1	1:D:192:ARG:HD2	2.02	0.60
1:D:269:VAL:HG21	1:D:336:LYS:CG	2.30	0.60
1:A:125:ALA:O	1:A:129:ILE:HG13	2.01	0.60
1:A:377:ARG:NH1	1:A:378:THR:HA	2.16	0.60
1:B:333:SER:HB3	1:B:336:LYS:CG	2.29	0.60
1:A:393:GLY:C	1:A:395:PHE:H	2.03	0.60
1:C:418:ILE:HG12	1:C:425:ALA:CB	2.32	0.60
1:D:305:LYS:HZ3	1:D:305:LYS:N	1.97	0.60
1:A:387:LEU:O	1:A:411:PRO:HG2	2.02	0.60
1:D:37:LYS:HA	1:D:53:THR:CG2	2.32	0.60
1:D:210:VAL:HG21	1:D:237:ILE:HD12	1.82	0.60
1:A:191:ASN:HD22	1:A:191:ASN:H	1.50	0.60
1:B:110:ARG:HH12	1:B:219:PRO:HA	1.67	0.60
1:D:160:TYR:O	1:D:172:LYS:HB3	2.01	0.59
1:D:368:VAL:O	1:D:369:PHE:HB2	2.01	0.59
1:A:391:ARG:HB2	1:A:411:PRO:CG	2.26	0.59
1:B:415:VAL:HG12	1:B:416:GLY:N	2.17	0.59
1:C:116:PRO:HG2	1:C:251:PRO:HA	1.84	0.59
1:C:379:SER:OG	1:C:382:GLU:HG3	2.02	0.59
1:B:23:MET:C	1:B:25:ALA:H	2.06	0.59
1:B:283:GLU:C	1:B:285:VAL:H	2.05	0.59
1:A:295:ILE:HB	1:A:299:ARG:N	2.16	0.59
1:C:322:ALA:HA	1:C:324:GLU:HG2	1.82	0.59
1:B:450:LEU:N	1:B:450:LEU:HD22	2.17	0.59
1:D:109:LYS:HD3	1:D:132:LEU:HD21	1.85	0.59
1:D:366:SER:O	1:D:369:PHE:O	2.20	0.59
1:C:69:GLU:HG3	1:C:75:PHE:HZ	1.67	0.59
1:D:418:ILE:HD11	1:D:429:ILE:HA	1.85	0.59
1:A:269:VAL:HG21	1:A:336:LYS:HG2	1.84	0.59
1:C:393:GLY:O	1:C:394:ARG:O	2.21	0.59
1:D:325:GLU:C	1:D:327:ARG:H	2.05	0.59
1:A:372:PRO:HG3	1:A:395:PHE:HE2	1.68	0.59
1:B:442:LYS:HE3	4:B:3002:HOH:O	2.01	0.59
1:C:87:TYR:HE2	4:C:2561:HOH:O	1.85	0.59
1:B:115:LEU:HB3	1:B:119:SER:OG	2.02	0.58
1:C:110:ARG:HG3	1:C:242:VAL:O	2.03	0.58
1:C:231:GLU:HB2	4:C:2883:HOH:O	2.02	0.58
1:A:122:THR:HG22	1:A:126:MET:CE	2.33	0.58



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:267:ILE:CG2	1:C:339:LYS:HE2	2.33	0.58
1:C:340:LEU:HD11	1:C:354:ILE:HD13	1.85	0.58
1:A:432:LEU:HD13	1:A:432:LEU:O	2.03	0.58
1:A:361:LEU:O	1:A:361:LEU:HD23	2.04	0.58
1:B:290:LEU:HB3	1:B:296:THR:CA	2.27	0.58
1:C:194:MET:HA	1:C:219:PRO:HD2	1.85	0.58
1:D:84:PRO:HG2	4:D:2119:HOH:O	2.03	0.58
1:C:134:THR:HB	1:C:194:MET:HB2	1.85	0.58
1:C:323:TRP:CE2	1:C:327:ARG:HB2	2.38	0.58
1:D:149:TRP:CE3	1:D:153:LEU:HD11	2.38	0.58
1:D:346:ARG:HG3	1:D:347:HIS:CD2	2.38	0.58
1:C:160:TYR:O	1:C:172:LYS:HB3	2.03	0.58
1:A:143:LEU:O	1:A:147:GLU:HG3	2.03	0.58
1:B:273:GLU:HA	1:B:276:ARG:HG2	1.85	0.58
1:D:305:LYS:N	1:D:305:LYS:HD2	2.18	0.58
1:A:295:ILE:CB	1:A:299:ARG:HB3	2.34	0.58
1:A:404:LEU:HB3	1:A:410:VAL:HG11	1.86	0.58
1:B:103:GLU:HG3	1:B:426:ARG:NH1	2.19	0.58
1:C:375:THR:HG23	1:C:377:ARG:N	2.17	0.58
1:D:77:ASP:OD2	1:D:80:ALA:HB3	2.03	0.58
1:A:278:GLU:O	1:A:282:ARG:HG2	2.03	0.58
1:B:122:THR:CG2	1:B:152:ARG:HD3	2.34	0.58
1:A:230:ARG:NH2	3:A:6001:IPA:H2	2.18	0.58
1:C:211:GLN:HG2	1:C:215:MET:SD	2.44	0.58
1:C:432:LEU:O	1:C:436:LEU:HG	2.04	0.58
1:A:375:THR:OG1	1:A:376:HIS:N	2.35	0.57
1:D:239:LYS:O	1:D:243:GLY:HA2	2.04	0.57
1:D:404:LEU:HD22	1:D:404:LEU:H	1.69	0.57
1:B:372:PRO:HB2	1:B:398:ILE:HG22	1.86	0.57
1:C:68:PHE:HB3	1:C:75:PHE:CD2	2.39	0.57
1:A:31:ARG:HH11	1:A:31:ARG:HB2	1.68	0.57
1:A:115:LEU:HD12	1:A:121:LYS:HG2	1.87	0.57
1:B:62:ARG:O	1:B:66:GLU:HG3	2.04	0.57
1:D:132:LEU:CD2	1:D:458:VAL:HG11	2.35	0.57
1:A:259:LEU:HD21	1:A:262:TYR:HD2	1.69	0.57
1:D:238:LEU:O	1:D:243:GLY:N	2.37	0.57
1:A:318:GLU:OE1	1:A:318:GLU:HA	2.04	0.57
1:A:374:ILE:HD11	1:A:386:ILE:HG21	1.85	0.57
1:D:45:ALA:HB3	1:D:54:TYR:HD2	1.70	0.57
1:D:306:ILE:HG23	1:D:307:VAL:N	2.12	0.57
1:D:376:HIS:CD2	1:D:377:ARG:HG2	2.40	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:202:HIS:O	1:B:230:ARG:HD2	2.05	0.57
1:A:114:VAL:HA	1:A:225:THR:O	2.05	0.57
1:A:301:GLU:O	1:A:302:ASP:HB2	2.05	0.57
1:B:340:LEU:HD21	1:B:354:ILE:CD1	2.35	0.57
1:C:126:MET:HE1	1:C:152:ARG:HB3	1.87	0.57
1:A:393:GLY:C	1:A:395:PHE:N	2.59	0.57
1:B:414:ASN:O	1:B:445:ALA:HB1	2.05	0.57
1:C:352:ILE:O	1:C:397:ALA:HA	2.04	0.57
1:A:295:ILE:HG22	1:A:299:ARG:HB3	1.87	0.56
1:B:362:VAL:HG23	1:B:363:TYR:H	1.69	0.56
1:C:263:THR:HG21	1:C:446:VAL:HG22	1.86	0.56
1:D:278:GLU:O	1:D:282:ARG:HG2	2.05	0.56
1:B:103:GLU:HG3	1:B:426:ARG:CZ	2.34	0.56
1:C:49:SER:HB3	1:C:53:THR:OG1	2.05	0.56
1:B:432:LEU:HD12	1:B:436:LEU:HG	1.87	0.56
1:C:333:SER:HB3	1:C:336:LYS:CG	2.34	0.56
1:C:418:ILE:HD12	1:C:419:MET:N	2.21	0.56
1:B:354:ILE:HG22	1:B:355:PHE:N	2.19	0.56
1:C:24:ILE:HD12	1:C:24:ILE:N	2.05	0.56
1:C:93:SER:HA	1:C:265:LYS:HG2	1.86	0.56
1:D:369:PHE:HD1	1:D:371:ILE:HB	1.71	0.56
1:B:450:LEU:HD22	1:B:450:LEU:H	1.71	0.56
1:D:172:LYS:HE2	4:D:2211:HOH:O	2.04	0.56
1:A:285:VAL:O	1:A:290:LEU:HD23	2.04	0.56
1:A:393:GLY:O	1:A:395:PHE:N	2.39	0.56
1:B:23:MET:HB2	1:B:38:GLY:CA	2.35	0.56
1:A:283:GLU:O	1:A:287:LYS:HG2	2.05	0.56
1:B:268:PHE:HA	1:B:451:ILE:O	2.05	0.56
1:B:322:ALA:C	1:B:324:GLU:H	2.09	0.56
1:B:400:SER:HB3	1:B:404:LEU:HD21	1.87	0.56
1:C:361:LEU:HD22	1:C:361:LEU:O	2.05	0.56
1:C:425:ALA:O	1:C:427:GLU:N	2.37	0.56
1:D:24:ILE:O	1:D:24:ILE:HG22	2.06	0.56
1:D:234:ARG:HG2	1:D:234:ARG:NH1	2.21	0.56
1:D:256:GLY:C	1:D:258:HIS:H	2.09	0.56
1:A:113:ILE:HG22	1:A:113:ILE:O	2.06	0.56
1:A:205:PRO:HB2	1:A:230:ARG:NH1	2.21	0.56
1:A:320:LEU:HD23	1:A:320:LEU:C	2.26	0.56
1:A:330:ALA:O	1:A:331:PHE:C	2.44	0.56
1:C:103:GLU:HB3	1:C:426:ARG:NH2	2.21	0.56
1:C:250:PHE:HD1	1:C:251:PRO:HD2	1.71	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:358:HIS:HD2	1:C:361:LEU:H	1.52	0.56
1:D:95:ARG:HB2	1:D:98:GLN:HG3	1.88	0.56
1:C:42:VAL:HB	1:C:45:ALA:HB2	1.88	0.55
1:D:93:SER:HA	1:D:264:ILE:O	2.06	0.55
1:D:379:SER:HB3	1:D:382:GLU:CB	2.35	0.55
1:C:148:GLN:NE2	1:C:152:ARG:HH22	2.04	0.55
1:C:257:LYS:HZ3	1:C:260:ALA:HB3	1.69	0.55
1:A:282:ARG:HG3	1:A:329:ILE:HD11	1.86	0.55
1:D:180:ASP:O	1:D:184:VAL:HG23	2.06	0.55
1:D:306:ILE:HG13	1:D:307:VAL:N	2.20	0.55
1:A:391:ARG:HG3	1:A:391:ARG:NH1	2.21	0.55
1:B:290:LEU:CB	1:B:296:THR:HA	2.33	0.55
1:B:374:ILE:HG12	1:B:386:ILE:HD12	1.88	0.55
1:C:261:LYS:O	1:C:444:GLU:HB3	2.06	0.55
1:C:263:THR:HG22	1:C:446:VAL:HA	1.87	0.55
1:C:332:ASN:O	1:C:333:SER:C	2.44	0.55
1:A:442:LYS:HA	1:A:442:LYS:HZ3	1.70	0.55
1:B:126:MET:CE	1:B:152:ARG:HG2	2.36	0.55
1:C:136:THR:HB	1:C:174:LEU:HD23	1.88	0.55
1:C:406:GLU:HG2	1:C:406:GLU:O	2.06	0.55
1:D:372:PRO:HD3	1:D:395:PHE:CE1	2.41	0.55
1:A:334:LYS:O	1:A:338:ARG:CG	2.54	0.55
1:C:361:LEU:O	1:C:365:ILE:HG13	2.07	0.55
1:B:291:ARG:N	1:B:296:THR:HG22	2.22	0.55
1:A:350:ASP:HB3	1:A:414:ASN:HB3	1.89	0.55
1:C:36:VAL:O	1:C:54:TYR:HB2	2.07	0.55
1:C:85:THR:HG23	1:C:86:PRO:HD2	1.88	0.55
1:C:395:PHE:CD1	1:C:395:PHE:O	2.60	0.55
1:B:69:GLU:HG2	1:B:291:ARG:HH11	1.71	0.55
1:B:120:GLY:HA2	4:B:2256:HOH:O	2.07	0.55
1:D:360:GLU:O	1:D:363:TYR:HB3	2.06	0.55
1:B:382:GLU:O	1:B:386:ILE:HG13	2.07	0.54
1:B:88:PHE:HB3	1:B:156:PHE:CD1	2.43	0.54
1:B:264:ILE:HD12	1:B:264:ILE:N	2.22	0.54
1:C:50:ARG:O	1:C:51:SER:HB2	2.06	0.54
1:C:96:ASP:N	1:C:96:ASP:OD2	2.40	0.54
1:D:62:ARG:NH1	1:D:219:PRO:O	2.37	0.54
1:D:373:ALA:O	1:D:374:ILE:HG13	2.07	0.54
1:C:228:PHE:CD1	1:C:245:LYS:HE2	2.43	0.54
1:D:378:THR:HG22	1:D:379:SER:N	2.22	0.54
1:A:230:ARG:HH22	3:A:6001:IPA:H2	1.72	0.54



	i agein	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:321:ARG:O	1:A:321:ARG:HD3	2.06	0.54
1:D:336:LYS:HZ1	1:D:420:SER:CB	2.21	0.54
1:A:122:THR:HG21	1:A:152:ARG:HD3	1.89	0.54
1:A:314:GLU:HG2	1:A:315:ARG:N	2.23	0.54
1:A:338:ARG:O	1:A:341:ARG:HB3	2.07	0.54
1:A:356:THR:HG23	1:A:362:VAL:HG22	1.89	0.54
1:B:351:LYS:HB2	1:B:390:PHE:CE1	2.43	0.54
1:C:50:ARG:HG2	1:C:50:ARG:HH11	1.73	0.54
1:C:63:ASP:HA	1:C:66:GLU:OE2	2.08	0.54
1:D:227:THR:HG23	4:D:2756:HOH:O	2.08	0.54
1:A:295:ILE:HB	1:A:299:ARG:HB3	1.90	0.54
1:B:110:ARG:NH1	1:B:219:PRO:HA	2.22	0.54
1:C:451:ILE:HG22	1:C:452:SER:N	2.22	0.54
1:C:272:ALA:HB3	1:C:275:GLU:CG	2.35	0.54
1:D:328:ARG:HG3	1:D:328:ARG:HH11	1.73	0.54
1:A:74:GLU:OE2	1:A:74:GLU:HA	2.08	0.54
1:B:31:ARG:CG	1:B:187:GLU:HB3	2.38	0.54
1:B:62:ARG:N	4:B:2009:HOH:O	2.21	0.54
1:B:122:THR:HG21	1:B:152:ARG:CZ	2.38	0.54
1:B:334:LYS:O	1:B:338:ARG:HG3	2.08	0.54
1:B:344:LEU:CD2	1:B:352:ILE:HD11	2.38	0.54
1:D:261:LYS:HE3	1:D:438:PRO:HG3	1.89	0.54
1:D:418:ILE:HG12	1:D:432:LEU:HD13	1.89	0.54
1:A:24:ILE:HG22	1:A:25:ALA:N	2.22	0.54
1:A:99:GLU:HG3	1:A:426:ARG:NH2	2.23	0.54
1:A:283:GLU:C	1:A:285:VAL:N	2.61	0.54
1:D:409:ASP:O	1:D:410:VAL:O	2.25	0.54
1:A:44:HIS:CG	1:A:60:ARG:HD2	2.43	0.53
1:B:441:GLY:O	1:B:442:LYS:C	2.45	0.53
1:A:180:ASP:OD2	4:A:2475:HOH:O	2.19	0.53
1:C:381:GLU:HG3	1:C:382:GLU:H	1.73	0.53
1:D:105:TRP:CD1	1:D:222:LEU:HD13	2.44	0.53
1:D:388:GLU:OE2	1:D:391:ARG:NE	2.42	0.53
1:B:50:ARG:HG2	1:B:50:ARG:NH2	2.23	0.53
1:C:149:TRP:O	1:C:153:LEU:HD22	2.08	0.53
1:C:325:GLU:OE2	1:C:328:ARG:HD3	2.09	0.53
1:D:351:LYS:HB2	1:D:413:ALA:HA	1.91	0.53
1:C:140:VAL:O	1:C:178:THR:HA	2.08	0.53
1:D:162:GLY:O	1:D:175:THR:HA	2.09	0.53
1:A:46:LYS:HD2	1:A:46:LYS:N	2.24	0.53
1:A:62:ARG:HH11	1:A:110:ARG:HD3	1.73	0.53



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:205:PRO:O	1:A:206:ALA:C	2.46	0.53
1:A:323:TRP:O	1:A:327:ARG:HG2	2.09	0.53
1:A:427:GLU:HB2	1:A:431:ARG:HH21	1.74	0.53
1:D:389:GLY:O	1:D:395:PHE:HB2	2.08	0.53
1:A:309:ALA:O	1:A:310:SER:CB	2.55	0.53
1:A:409:ASP:O	1:A:410:VAL:HB	2.09	0.53
1:A:426:ARG:HH11	1:A:426:ARG:HG3	1.74	0.53
1:D:340:LEU:CG	1:D:343:ILE:HD11	2.39	0.53
1:D:356:THR:O	1:D:401:SER:HA	2.09	0.52
1:D:387:LEU:O	1:D:391:ARG:HG2	2.10	0.52
1:A:122:THR:HG22	1:A:126:MET:HE2	1.90	0.52
1:B:254:LEU:N	1:B:254:LEU:HD22	2.24	0.52
1:C:259:LEU:O	1:C:261:LYS:N	2.36	0.52
1:D:33:THR:HG21	1:D:55:ARG:HG2	1.92	0.52
1:B:24:ILE:O	1:B:24:ILE:CG2	2.58	0.52
1:C:201:VAL:O	1:C:205:PRO:HD3	2.09	0.52
1:C:263:THR:HG22	1:C:446:VAL:HG22	1.90	0.52
1:D:336:LYS:NZ	1:D:420:SER:HB2	2.24	0.52
1:D:163:GLU:O	1:D:170:GLU:HB2	2.10	0.52
1:C:389:GLY:O	1:C:392:THR:HG22	2.08	0.52
1:A:30:GLU:OE2	1:A:31:ARG:NH1	2.42	0.52
1:A:172:LYS:HD3	1:B:50:ARG:NE	2.25	0.52
1:A:344:LEU:HD12	1:A:369:PHE:CD2	2.45	0.52
1:B:187:GLU:CD	1:B:187:GLU:H	2.13	0.52
1:B:449:GLU:O	1:B:451:ILE:HG13	2.10	0.52
1:C:259:LEU:C	1:C:261:LYS:H	2.13	0.52
1:D:95:ARG:CB	1:D:259:LEU:HD11	2.27	0.52
1:B:248:GLU:HG3	1:B:249:LEU:N	2.24	0.52
1:C:35:VAL:HA	1:C:54:TYR:O	2.09	0.52
1:D:150:LYS:HD3	1:D:163:GLU:HB2	1.91	0.52
1:D:441:GLY:O	1:D:442:LYS:HB2	2.09	0.52
1:A:102:LEU:O	1:A:106:LEU:HD22	2.09	0.52
1:C:356:THR:HG23	1:C:362:VAL:HG22	1.91	0.52
1:D:81:ASP:N	1:D:82:PRO:HD3	2.25	0.52
1:D:378:THR:HG22	1:D:382:GLU:HB3	1.92	0.52
1:A:359:ASN:HA	1:A:362:VAL:CG2	2.40	0.52
1:A:416:GLY:HA3	1:A:436:LEU:HD11	1.91	0.52
1:B:122:THR:HG21	1:B:152:ARG:NH2	2.24	0.52
1:C:426:ARG:HG3	1:C:426:ARG:HH11	1.75	0.52
1:C:329:ILE:HD11	4:C:2804:HOH:O	2.10	0.52
1:C:334:LYS:CG	1:C:338:ARG:HE	2.23	0.52



	lo ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:252:ASP:HB3	4:A:2835:HOH:O	2.11	0.51
1:A:269:VAL:HG22	1:A:336:LYS:HE3	1.91	0.51
1:C:356:THR:CG2	1:C:362:VAL:HG22	2.40	0.51
1:D:194:MET:HA	1:D:219:PRO:HD2	1.91	0.51
1:A:45:ALA:HB3	4:A:2010:HOH:O	2.10	0.51
1:B:248:GLU:HG3	1:B:249:LEU:H	1.74	0.51
1:C:232:ASP:HB2	4:C:2589:HOH:O	2.11	0.51
1:C:347:HIS:O	1:C:349:LYS:N	2.44	0.51
1:A:290:LEU:O	1:A:291:ARG:CB	2.58	0.51
1:B:378:THR:HB	1:B:382:GLU:HB2	1.92	0.51
1:A:280:GLU:C	1:A:282:ARG:H	2.13	0.51
1:C:69:GLU:H	1:C:75:PHE:HE2	1.58	0.51
1:C:394:ARG:HA	1:C:394:ARG:NE	2.24	0.51
1:B:350:ASP:O	1:B:352:ILE:HG23	2.10	0.51
1:B:366:SER:CB	1:B:373:ALA:HB2	2.40	0.51
1:D:230:ARG:HH21	1:D:234:ARG:HD3	1.75	0.51
1:A:42:VAL:HG22	1:A:67:TYR:CE1	2.46	0.51
1:A:388:GLU:O	1:A:392:THR:HG23	2.10	0.51
1:C:33:THR:HG21	1:C:55:ARG:HE	1.76	0.51
1:D:318:GLU:O	1:D:319:ALA:HB2	2.11	0.51
1:A:295:ILE:CG2	1:A:299:ARG:HB3	2.41	0.51
1:B:391:ARG:HG3	4:B:2869:HOH:O	2.10	0.51
1:C:57:LEU:HD22	1:C:57:LEU:N	2.23	0.51
1:D:67:TYR:HA	1:D:70:SER:OG	2.09	0.51
1:D:249:LEU:HB3	1:D:254:LEU:HD21	1.93	0.51
1:D:450:LEU:N	1:D:450:LEU:HD23	2.24	0.51
1:A:34:ILE:HG12	1:A:58:ALA:HA	1.92	0.51
1:A:62:ARG:HB3	4:A:2002:HOH:O	2.10	0.51
1:A:172:LYS:HD3	1:B:50:ARG:HE	1.76	0.51
1:C:286:TYR:C	1:C:288:GLN:H	2.14	0.51
1:C:349:LYS:O	1:C:349:LYS:HG2	2.11	0.51
1:D:361:LEU:CD1	1:D:365:ILE:HD11	2.40	0.51
1:A:110:ARG:HG3	1:A:242:VAL:O	2.11	0.51
1:A:327:ARG:HH21	1:A:422:SER:HB3	1.76	0.51
1:B:130:ASN:ND2	1:B:268:PHE:HE1	2.09	0.51
1:B:434:ARG:NH2	1:B:434:ARG:CB	2.73	0.51
1:B:438:PRO:HA	1:B:445:ALA:HB2	1.93	0.51
1:A:234:ARG:C	1:A:236:GLU:H	2.15	0.50
1:C:371:ILE:CG2	1:C:399:VAL:HG12	2.41	0.50
1:D:59:PHE:HA	1:D:216:SER:O	2.11	0.50
1:A:267:ILE:HB	1:A:450:LEU:HD22	1.92	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:283:GLU:C	1:A:285:VAL:H	2.13	0.50
1:B:369:PHE:HB2	1:B:371:ILE:CD1	2.41	0.50
1:C:57:LEU:O	1:C:60:ARG:HG2	2.12	0.50
1:D:136:THR:N	1:D:173:PRO:O	2.42	0.50
1:D:259:LEU:C	1:D:261:LYS:H	2.13	0.50
1:B:63:ASP:OD1	4:B:2110:HOH:O	2.18	0.50
1:C:259:LEU:O	1:C:259:LEU:HD23	2.11	0.50
1:D:44:HIS:ND1	1:D:60:ARG:HD2	2.26	0.50
1:D:152:ARG:HH11	1:D:152:ARG:CG	2.25	0.50
1:A:42:VAL:CG1	1:A:43:PRO:HD2	2.37	0.50
1:C:343:ILE:HD11	1:C:450:LEU:HD21	1.93	0.50
1:A:327:ARG:O	1:A:330:ALA:HB3	2.12	0.50
1:C:57:LEU:H	1:C:57:LEU:CD2	2.22	0.50
1:C:331:PHE:CE2	1:C:421:GLY:HA2	2.47	0.50
1:C:426:ARG:HA	1:C:429:ILE:HD12	1.94	0.50
1:D:257:LYS:HG2	4:D:2604:HOH:O	2.11	0.50
1:D:305:LYS:NZ	1:D:305:LYS:CB	2.73	0.50
1:A:351:LYS:NZ	1:A:351:LYS:HB3	2.27	0.50
1:A:377:ARG:HG3	1:A:377:ARG:HH11	1.76	0.50
1:C:418:ILE:CG1	1:C:425:ALA:HB2	2.40	0.50
1:A:364:ARG:O	1:A:368:VAL:HG23	2.12	0.50
1:B:301:GLU:C	1:B:303:PHE:H	2.14	0.50
1:C:221:ARG:NH2	1:C:241:VAL:O	2.45	0.50
1:D:336:LYS:NZ	1:D:452:SER:HB2	2.27	0.50
1:D:340:LEU:O	1:D:344:LEU:HG	2.11	0.50
1:A:430:GLN:O	1:A:433:GLY:N	2.43	0.50
1:A:140:VAL:O	1:A:178:THR:HA	2.12	0.49
1:A:400:SER:OG	1:A:401:SER:N	2.45	0.49
1:C:126:MET:SD	1:C:153:LEU:HD13	2.52	0.49
1:C:237:ILE:HG13	1:C:238:LEU:N	2.27	0.49
1:C:390:PHE:CE2	1:C:398:ILE:HG12	2.48	0.49
1:D:112:CYS:O	1:D:246:VAL:HG22	2.12	0.49
1:A:357:ARG:HD3	1:A:428:TYR:CE2	2.47	0.49
1:A:414:ASN:OD1	1:A:439:SER:HB2	2.12	0.49
1:A:115:LEU:O	1:A:121:LYS:HE3	2.12	0.49
1:A:259:LEU:HD21	1:A:262:TYR:CD2	2.47	0.49
1:B:88:PHE:CD2	1:B:133:SER:HA	2.47	0.49
1:B:110:ARG:HD2	1:B:221:ARG:HG3	1.94	0.49
1:B:134:THR:HB	1:B:194:MET:HB2	1.95	0.49
1:C:229:GLU:OE2	1:C:235:HIS:NE2	2.45	0.49
1:A:141:PRO:HD2	1:A:145:LEU:HD12	1.92	0.49



	lo ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:99:GLU:OE1	1:B:99:GLU:HA	2.12	0.49
1:B:251:PRO:O	1:B:254:LEU:HD23	2.11	0.49
1:B:290:LEU:C	1:B:296:THR:HG22	2.33	0.49
1:A:39:ASP:HB3	1:A:42:VAL:HG23	1.94	0.49
1:B:336:LYS:HE3	1:B:452:SER:OG	2.13	0.49
1:B:450:LEU:H	1:B:450:LEU:CD2	2.25	0.49
1:A:180:ASP:OD1	1:D:143:LEU:HB2	2.13	0.49
1:A:330:ALA:O	1:A:332:ASN:N	2.45	0.49
1:B:253:SER:C	1:B:254:LEU:HD22	2.33	0.49
1:C:262:TYR:CE2	1:C:433:GLY:HA3	2.48	0.49
1:C:364:ARG:O	1:C:368:VAL:HG23	2.13	0.49
1:D:441:GLY:O	1:D:442:LYS:CB	2.61	0.49
1:A:256:GLY:O	1:A:258:HIS:N	2.42	0.49
1:B:247:PHE:C	1:B:247:PHE:CD1	2.86	0.49
1:C:348:ARG:HG3	1:C:349:LYS:H	1.77	0.49
1:A:191:ASN:H	1:A:191:ASN:ND2	2.11	0.49
1:A:379:SER:HB2	1:A:382:GLU:HB2	1.94	0.49
1:B:433:GLY:O	1:B:436:LEU:HB2	2.12	0.49
1:C:61:TYR:O	1:C:65:ILE:HG12	2.13	0.49
1:C:196:LEU:HG	1:C:218:ALA:HB3	1.94	0.49
1:D:27:ILE:O	1:D:27:ILE:HG13	2.13	0.49
1:C:291:ARG:O	1:C:292:ALA:HB3	2.13	0.49
1:A:304:ASN:HD22	1:A:307:VAL:CG2	2.26	0.49
1:B:382:GLU:HA	1:B:385:GLU:HB3	1.94	0.49
1:C:28:TYR:CA	1:C:79:ALA:HB2	2.40	0.49
1:C:375:THR:OG1	1:C:376:HIS:N	2.43	0.49
1:A:389:GLY:O	1:A:395:PHE:HB2	2.12	0.48
1:B:210:VAL:HG21	1:B:237:ILE:HD12	1.94	0.48
1:B:350:ASP:HB3	1:B:414:ASN:OD1	2.13	0.48
1:B:434:ARG:CB	1:B:434:ARG:HH21	2.25	0.48
1:C:42:VAL:HG12	1:C:45:ALA:H	1.77	0.48
1:C:431:ARG:O	1:C:435:ILE:HG13	2.13	0.48
1:D:383:ARG:O	1:D:387:LEU:HG	2.13	0.48
1:C:333:SER:O	1:C:337:ILE:HG12	2.13	0.48
1:D:340:LEU:CD2	1:D:343:ILE:HD11	2.43	0.48
1:D:352:ILE:HD12	1:D:353:ILE:H	1.78	0.48
1:C:34:ILE:HG12	1:C:58:ALA:HA	1.95	0.48
1:C:152:ARG:C	1:C:154:GLY:H	2.15	0.48
1:D:96:ASP:H	1:D:259:LEU:CD1	2.26	0.48
1:D:259:LEU:C	1:D:261:LYS:N	2.67	0.48
1:D:267:ILE:O	1:D:451:ILE:N	2.36	0.48



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:196:LEU:HG	1:C:218:ALA:CB	2.44	0.48
1:A:136:THR:N	1:A:173:PRO:O	2.32	0.48
1:A:259:LEU:HD22	1:A:261:LYS:HG3	1.95	0.48
1:B:105:TRP:HE3	1:B:106:LEU:HD13	1.78	0.48
1:C:159:GLU:OE2	1:C:159:GLU:N	2.39	0.48
1:C:204:LEU:N	1:C:205:PRO:CD	2.77	0.48
1:D:449:GLU:HG2	1:D:451:ILE:CG1	2.43	0.48
1:C:418:ILE:CD1	1:C:425:ALA:HB2	2.44	0.48
1:A:259:LEU:HD22	1:A:259:LEU:C	2.34	0.48
1:C:115:LEU:HB3	1:C:119:SER:HB2	1.94	0.48
1:D:369:PHE:O	1:D:371:ILE:N	2.41	0.48
1:D:391:ARG:HG3	1:D:392:THR:H	1.79	0.48
1:B:304:ASN:HA	1:B:307:VAL:HB	1.96	0.48
1:C:217:ILE:O	1:C:218:ALA:C	2.51	0.48
1:C:361:LEU:HD22	1:C:365:ILE:HG13	1.96	0.48
1:C:440:LYS:HG2	1:C:441:GLY:N	2.27	0.48
1:D:65:ILE:O	1:D:68:PHE:HB2	2.13	0.48
1:D:352:ILE:HA	1:D:415:VAL:O	2.14	0.48
1:A:102:LEU:HG	1:A:106:LEU:CD2	2.44	0.48
1:A:439:SER:O	1:A:441:GLY:N	2.46	0.48
1:C:132:LEU:O	1:C:133:SER:HB2	2.14	0.48
1:C:338:ARG:O	1:C:341:ARG:HB3	2.14	0.48
1:C:356:THR:HB	1:C:419:MET:CG	2.44	0.48
1:D:339:LYS:O	1:D:343:ILE:HG23	2.14	0.48
1:A:295:ILE:HB	1:A:299:ARG:CB	2.44	0.47
1:C:272:ALA:O	1:C:274:ASP:N	2.45	0.47
1:D:116:PRO:CG	1:D:251:PRO:HG3	2.44	0.47
1:A:234:ARG:NH2	3:A:6002:IPA:H2	2.29	0.47
1:A:277:VAL:HG13	1:A:278:GLU:N	2.29	0.47
1:A:304:ASN:C	1:A:306:ILE:H	2.18	0.47
1:B:110:ARG:NH1	1:B:219:PRO:O	2.44	0.47
1:B:282:ARG:O	1:B:322:ALA:HB1	2.14	0.47
1:D:27:ILE:C	1:D:27:ILE:HD12	2.34	0.47
1:A:259:LEU:HD22	1:A:261:LYS:H	1.79	0.47
1:B:105:TRP:CE3	1:B:106:LEU:HD13	2.49	0.47
1:C:71:ASN:O	1:C:73:ILE:N	2.42	0.47
1:C:254:LEU:O	1:C:255:ALA:CB	2.62	0.47
1:C:361:LEU:CD1	1:C:419:MET:HG3	2.40	0.47
1:D:266:ARG:HB3	1:D:451:ILE:HD12	1.95	0.47
1:A:261:LYS:NZ	1:A:261:LYS:HB3	2.29	0.47
1:A:426:ARG:NH2	4:A:2471:HOH:O	2.46	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:102:LEU:CD1	1:B:106:LEU:HD22	2.44	0.47
1:D:84:PRO:HB3	4:D:2177:HOH:O	2.14	0.47
1:D:140:VAL:O	1:D:178:THR:HA	2.14	0.47
1:D:149:TRP:HE3	1:D:153:LEU:CD1	2.24	0.47
1:D:361:LEU:HD13	1:D:365:ILE:HG13	1.95	0.47
1:A:355:PHE:CD2	1:A:356:THR:N	2.83	0.47
1:B:333:SER:CB	1:B:336:LYS:HG2	2.40	0.47
1:B:412:ASP:OD2	1:B:437:ARG:HG2	2.15	0.47
1:C:68:PHE:O	1:C:69:GLU:C	2.53	0.47
1:D:74:GLU:OE1	1:D:74:GLU:HA	2.14	0.47
1:D:460:THR:O	1:D:461:ALA:HB2	2.15	0.47
1:B:67:TYR:CD1	1:B:67:TYR:C	2.87	0.47
1:B:350:ASP:HB2	1:B:414:ASN:HB3	1.95	0.47
1:C:105:TRP:O	1:C:109:LYS:N	2.46	0.47
1:C:125:ALA:O	1:C:129:ILE:HG13	2.13	0.47
1:C:426:ARG:HA	1:C:429:ILE:CD1	2.44	0.47
1:D:344:LEU:O	1:D:346:ARG:N	2.48	0.47
1:A:352:ILE:HD11	1:A:354:ILE:HD11	1.97	0.47
1:A:389:GLY:HA2	1:A:392:THR:OG1	2.14	0.47
1:A:390:PHE:HA	1:A:395:PHE:CB	2.44	0.47
1:B:28:TYR:HE1	1:B:37:LYS:HD2	1.79	0.47
1:B:405:ASP:CB	1:B:435:ILE:HD11	2.41	0.47
1:C:348:ARG:HG3	1:C:349:LYS:N	2.29	0.47
1:C:363:TYR:O	1:C:367:LYS:HG2	2.15	0.47
1:D:250:PHE:O	1:D:253:SER:HB2	2.15	0.47
1:A:122:THR:O	1:A:126:MET:HE2	2.15	0.47
1:A:295:ILE:HD13	1:A:300:ALA:CB	2.43	0.47
1:A:404:LEU:O	1:A:410:VAL:HG11	2.15	0.47
1:B:31:ARG:HG2	1:B:187:GLU:HB3	1.95	0.47
1:C:26:GLU:HG2	1:C:27:ILE:N	2.29	0.47
1:D:132:LEU:HD23	1:D:458:VAL:CG2	2.32	0.47
1:A:307:VAL:HG23	1:A:308:MET:N	2.29	0.47
1:B:279:TYR:OH	1:B:422:SER:HB3	2.15	0.47
1:D:327:ARG:NH2	1:D:358:HIS:NE2	2.63	0.47
1:D:418:ILE:CG1	1:D:432:LEU:HD13	2.45	0.47
1:B:60:ARG:NH1	4:B:2110:HOH:O	2.43	0.47
1:B:81:ASP:O	1:B:192:ARG:HA	2.14	0.47
1:B:283:GLU:C	1:B:285:VAL:N	2.68	0.47
1:B:405:ASP:HB3	1:B:435:ILE:CD1	2.43	0.47
1:C:290:LEU:HD23	1:C:290:LEU:H	1.80	0.47
1:D:115:LEU:O	1:D:121:LYS:NZ	2.41	0.47



	1	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:359:ASN:HA	1:A:362:VAL:CB	2.44	0.46
1:A:403:VAL:HG23	1:A:403:VAL:O	2.15	0.46
1:B:375:THR:HG23	1:B:377:ARG:N	2.28	0.46
1:A:121:LYS:HE2	1:A:225:THR:C	2.36	0.46
1:A:122:THR:HG21	1:A:152:ARG:NE	2.30	0.46
1:B:205:PRO:HA	1:B:237:ILE:HD11	1.97	0.46
1:B:403:VAL:HG21	1:B:431:ARG:HE	1.80	0.46
1:C:168:ILE:HG12	1:C:170:GLU:HG3	1.97	0.46
1:D:32:GLY:HA3	1:D:215:MET:HE2	1.97	0.46
1:A:374:ILE:HD11	1:A:386:ILE:CG2	2.45	0.46
1:B:369:PHE:HB2	1:B:371:ILE:HG13	1.98	0.46
1:C:152:ARG:C	1:C:154:GLY:N	2.69	0.46
1:C:267:ILE:HD11	1:C:448:TYR:HD2	1.79	0.46
1:A:191:ASN:ND2	4:A:2501:HOH:O	2.47	0.46
1:A:365:ILE:O	1:A:369:PHE:HD1	1.99	0.46
1:D:43:PRO:HG3	1:D:67:TYR:CD2	2.50	0.46
1:D:100:LYS:HD3	1:D:426:ARG:NH2	2.25	0.46
1:D:403:VAL:HG11	1:D:431:ARG:HD3	1.96	0.46
1:A:205:PRO:HA	1:A:237:ILE:HD11	1.96	0.46
1:A:259:LEU:CD1	1:A:260:ALA:N	2.77	0.46
1:B:102:LEU:CG	1:B:106:LEU:HD22	2.43	0.46
1:B:299:ARG:C	1:B:301:GLU:H	2.17	0.46
1:C:27:ILE:HG22	1:C:36:VAL:HG13	1.96	0.46
1:D:66:GLU:O	1:D:68:PHE:N	2.48	0.46
1:D:376:HIS:HB3	1:D:402:GLN:HE22	1.80	0.46
1:B:367:LYS:C	1:B:369:PHE:N	2.67	0.46
1:D:198:PHE:CE1	1:D:204:LEU:HD13	2.50	0.46
1:D:333:SER:HB3	1:D:336:LYS:HG3	1.97	0.46
1:D:404:LEU:O	1:D:411:PRO:HD2	2.15	0.46
1:B:45:ALA:HB1	1:B:54:TYR:HB3	1.97	0.46
1:C:164:PHE:HE1	1:C:185:ASN:CG	2.18	0.46
1:C:423:GLY:O	1:C:424:SER:HB2	2.16	0.46
1:D:420:SER:OG	1:D:421:GLY:N	2.47	0.46
1:D:443:LYS:O	1:D:444:GLU:HG3	2.15	0.46
1:A:191:ASN:HD22	1:A:191:ASN:N	2.10	0.46
1:B:371:ILE:HA	1:B:372:PRO:HD3	1.68	0.46
1:C:259:LEU:C	1:C:261:LYS:N	2.69	0.46
1:B:434:ARG:HB2	1:B:434:ARG:CZ	2.44	0.46
1:C:284:LYS:C	1:C:286:TYR:N	2.66	0.46
1:D:274:ASP:HA	1:D:277:VAL:CG2	2.46	0.46
1:D:424:SER:HA	1:D:449:GLU:OE2	2.16	0.46



	i a pageini	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:254:LEU:N	1:A:254:LEU:HD12	2.31	0.46
1:A:304:ASN:HA	1:A:307:VAL:CG2	2.44	0.46
1:A:377:ARG:O	1:A:378:THR:C	2.53	0.46
1:A:451:ILE:HG22	1:A:452:SER:N	2.31	0.46
1:C:162:GLY:HA3	1:C:172:LYS:HB2	1.98	0.46
1:C:347:HIS:O	1:C:348:ARG:C	2.55	0.46
1:D:268:PHE:HA	1:D:451:ILE:O	2.16	0.46
1:A:282:ARG:HG3	1:A:329:ILE:CD1	2.46	0.45
1:A:340:LEU:O	1:A:344:LEU:HG	2.16	0.45
1:C:149:TRP:O	1:C:152:ARG:N	2.50	0.45
1:A:390:PHE:HA	1:A:395:PHE:HB3	1.98	0.45
1:B:344:LEU:O	1:B:348:ARG:HG3	2.15	0.45
1:D:110:ARG:HE	1:D:221:ARG:HG3	1.81	0.45
1:A:149:TRP:HA	1:A:152:ARG:HH11	1.81	0.45
1:A:388:GLU:O	1:A:392:THR:N	2.48	0.45
1:B:378:THR:O	1:B:379:SER:HB2	2.17	0.45
1:C:116:PRO:HD2	1:C:119:SER:OG	2.16	0.45
1:C:263:THR:HG23	1:C:446:VAL:HG13	1.99	0.45
1:C:407:GLY:O	1:C:408:ILE:HB	2.17	0.45
1:D:172:LYS:HB3	1:D:173:PRO:CD	2.44	0.45
1:D:256:GLY:O	1:D:258:HIS:N	2.40	0.45
1:D:258:HIS:C	1:D:260:ALA:H	2.20	0.45
1:D:336:LYS:HZ1	1:D:420:SER:HB2	1.82	0.45
1:A:271:LEU:HD21	1:A:452:SER:HB3	1.99	0.45
1:C:60:ARG:O	1:C:61:TYR:C	2.54	0.45
1:C:94:LEU:N	1:C:264:ILE:O	2.39	0.45
1:C:239:LYS:HA	1:C:243:GLY:C	2.36	0.45
1:D:357:ARG:HE	1:D:428:TYR:HE2	1.65	0.45
1:B:199:ASP:O	1:B:200:GLU:C	2.53	0.45
1:B:276:ARG:HG3	1:B:277:VAL:N	2.32	0.45
1:B:390:PHE:CE2	1:B:398:ILE:HG12	2.51	0.45
1:B:415:VAL:CG1	1:B:416:GLY:N	2.79	0.45
1:C:322:ALA:C	1:C:324:GLU:N	2.70	0.45
1:C:412:ASP:HB2	1:C:437:ARG:NH1	2.32	0.45
1:D:457:GLU:O	1:D:458:VAL:HB	2.16	0.45
1:A:62:ARG:NH1	1:A:110:ARG:HD3	2.31	0.45
1:A:372:PRO:HG3	1:A:395:PHE:CE2	2.49	0.45
1:A:443:LYS:O	1:A:444:GLU:HG3	2.17	0.45
1:B:26:GLU:HG2	1:B:27:ILE:N	2.31	0.45
1:B:427:GLU:HG2	1:B:428:TYR:CD2	2.52	0.45
1:D:43:PRO:O	1:D:44:HIS:CB	2.63	0.45



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:196:LEU:HG	1:A:218:ALA:CB	2.47	0.45
1:B:31:ARG:HG2	1:B:187:GLU:CG	2.46	0.45
1:B:375:THR:O	1:B:383:ARG:NH2	2.49	0.45
1:C:101:ALA:HB2	1:C:247:PHE:CE1	2.52	0.45
1:C:358:HIS:HB3	1:C:361:LEU:HB3	1.99	0.45
1:D:195:LEU:HD23	1:D:220:PHE:HB2	1.99	0.45
1:A:431:ARG:HD3	1:A:431:ARG:N	2.32	0.45
1:B:347:HIS:ND1	1:B:415:VAL:HG21	2.32	0.45
1:C:271:LEU:HD12	1:C:271:LEU:HA	1.81	0.45
1:C:389:GLY:C	1:C:392:THR:HG22	2.36	0.45
1:D:261:LYS:HA	1:D:444:GLU:HG2	1.99	0.45
1:A:241:VAL:HG23	1:A:242:VAL:N	2.32	0.45
1:A:398:ILE:CD1	1:A:399:VAL:N	2.66	0.45
1:B:339:LYS:O	1:B:342:GLU:HB2	2.17	0.45
1:C:232:ASP:OD1	1:C:234:ARG:HB2	2.16	0.45
1:C:234:ARG:HG3	1:C:234:ARG:HH11	1.81	0.45
1:D:116:PRO:HG3	1:D:251:PRO:HG3	1.99	0.45
1:A:266:ARG:HH21	1:A:266:ARG:HG2	1.82	0.45
1:A:339:LYS:O	1:A:343:ILE:HG13	2.17	0.45
1:B:329:ILE:O	1:B:332:ASN:OD1	2.35	0.45
1:B:430:GLN:HE21	1:B:430:GLN:HB2	1.53	0.45
1:D:42:VAL:HB	1:D:54:TYR:CD2	2.51	0.45
1:D:394:ARG:O	1:D:394:ARG:HG2	2.17	0.45
1:C:325:GLU:HG3	1:C:329:ILE:CD1	2.36	0.44
1:D:29:TYR:H	1:D:79:ALA:HA	1.82	0.44
1:D:328:ARG:HG3	1:D:328:ARG:NH1	2.32	0.44
1:D:352:ILE:HD11	1:D:354:ILE:HG12	1.99	0.44
1:B:322:ALA:C	1:B:324:GLU:N	2.71	0.44
1:C:103:GLU:OE2	1:C:103:GLU:HA	2.16	0.44
1:D:26:GLU:HG2	1:D:27:ILE:N	2.32	0.44
1:D:172:LYS:CB	1:D:173:PRO:HD2	2.43	0.44
1:A:81:ASP:O	1:A:192:ARG:HA	2.17	0.44
1:A:85:THR:HG23	1:A:86:PRO:HD2	1.99	0.44
4:A:2006:HOH:O	1:D:142:THR:HG22	2.16	0.44
1:B:429:ILE:HD11	1:B:449:GLU:OE2	2.18	0.44
1:C:190:GLY:O	1:C:217:ILE:HG23	2.17	0.44
1:D:109:LYS:O	1:D:220:PHE:HA	2.17	0.44
1:A:432:LEU:HD13	1:A:432:LEU:C	2.38	0.44
1:B:404:LEU:N	1:B:404:LEU:CD2	2.77	0.44
1:C:327:ARG:O	1:C:331:PHE:HB2	2.16	0.44
1:D:372:PRO:CB	1:D:398:ILE:HG22	2.45	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:204:LEU:HB3	1:A:205:PRO:HD3	1.98	0.44
1:A:259:LEU:HD13	1:A:261:LYS:H	1.83	0.44
1:A:288:GLN:HB2	1:A:290:LEU:HD22	1.99	0.44
1:A:320:LEU:HD23	1:A:320:LEU:O	2.17	0.44
1:A:377:ARG:HG3	1:A:377:ARG:NH1	2.32	0.44
1:B:31:ARG:HG2	1:B:187:GLU:HG2	1.99	0.44
1:C:202:HIS:O	1:C:205:PRO:HD2	2.17	0.44
1:C:250:PHE:CD1	1:C:251:PRO:HD2	2.50	0.44
1:C:266:ARG:HB2	4:C:2247:HOH:O	2.17	0.44
1:A:201:VAL:HG22	1:A:201:VAL:O	2.17	0.44
1:A:288:GLN:C	1:A:290:LEU:H	2.21	0.44
1:B:399:VAL:O	1:B:399:VAL:HG13	2.18	0.44
1:C:247:PHE:CE1	1:C:249:LEU:HB2	2.53	0.44
1:A:269:VAL:HG23	4:A:2285:HOH:O	2.17	0.44
1:A:326:ALA:O	1:A:329:ILE:HB	2.17	0.44
1:A:359:ASN:O	1:A:362:VAL:N	2.51	0.44
1:B:207:GLU:HG2	1:B:234:ARG:NH1	2.32	0.44
1:B:248:GLU:CG	1:B:249:LEU:N	2.80	0.44
1:C:356:THR:O	1:C:401:SER:HA	2.18	0.44
1:D:305:LYS:N	1:D:305:LYS:CD	2.81	0.44
1:D:361:LEU:HD22	1:D:364:ARG:HD2	1.99	0.44
1:A:116:PRO:O	1:A:119:SER:OG	2.33	0.44
1:A:431:ARG:HD3	1:A:431:ARG:H	1.81	0.44
1:C:96:ASP:CG	1:C:259:LEU:HD22	2.38	0.44
1:A:66:GLU:CG	1:A:297:LEU:HD13	2.44	0.44
1:A:134:THR:HB	1:A:135:PRO:HD2	2.00	0.44
1:A:300:ALA:HB1	1:A:304:ASN:HB2	1.99	0.44
1:B:354:ILE:HG22	1:B:355:PHE:H	1.81	0.44
1:B:366:SER:HA	1:B:371:ILE:HB	2.00	0.44
1:D:83:ILE:HD13	1:D:171:LEU:O	2.18	0.44
1:D:290:LEU:N	1:D:290:LEU:HD13	2.33	0.44
1:D:325:GLU:C	1:D:327:ARG:N	2.71	0.44
1:D:449:GLU:O	1:D:451:ILE:HG13	2.17	0.44
1:A:205:PRO:HB2	1:A:230:ARG:HH11	1.81	0.43
1:B:22:GLN:O	1:B:24:ILE:HG13	2.17	0.43
1:B:425:ALA:O	1:B:429:ILE:HG13	2.18	0.43
1:C:92:ILE:HG21	1:C:127:ALA:HB2	1.99	0.43
1:C:95:ARG:O	1:C:98:GLN:N	2.51	0.43
1:C:405:ASP:HA	1:C:410:VAL:HG22	1.99	0.43
1:C:426:ARG:HG3	1:C:426:ARG:NH1	2.33	0.43
1:A:29:TYR:H	1:A:79:ALA:HA	1.82	0.43



	louis page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:62:ARG:HH11	1:B:110:ARG:HD3	1.83	0.43
1:C:340:LEU:HD11	1:C:354:ILE:CD1	2.48	0.43
1:D:280:GLU:O	1:D:282:ARG:N	2.37	0.43
1:D:405:ASP:HB3	1:D:435:ILE:CD1	2.39	0.43
1:D:456:GLY:O	1:D:457:GLU:HB2	2.18	0.43
1:A:85:THR:HG22	1:A:86:PRO:O	2.18	0.43
1:A:103:GLU:HG3	1:A:426:ARG:HD3	2.00	0.43
1:A:180:ASP:OD1	1:A:209:TYR:OH	2.28	0.43
1:A:286:TYR:CE2	1:A:323:TRP:HA	2.53	0.43
1:A:418:ILE:HD12	1:A:429:ILE:HD13	1.99	0.43
1:A:430:GLN:HG3	4:A:2471:HOH:O	2.18	0.43
1:B:391:ARG:HD2	1:B:391:ARG:O	2.18	0.43
1:C:283:GLU:O	1:C:284:LYS:CB	2.66	0.43
1:C:361:LEU:O	1:C:365:ILE:CG1	2.67	0.43
1:C:392:THR:HG23	1:C:393:GLY:H	1.82	0.43
1:D:404:LEU:N	1:D:404:LEU:CD2	2.78	0.43
1:A:270:PRO:O	1:A:335:ASN:ND2	2.52	0.43
1:A:385:GLU:O	1:A:388:GLU:N	2.47	0.43
1:A:425:ALA:HB1	1:A:428:TYR:HD2	1.83	0.43
1:C:323:TRP:CZ2	1:C:327:ARG:HB2	2.53	0.43
1:C:331:PHE:CE1	1:C:358:HIS:HB2	2.54	0.43
1:C:403:VAL:HG21	1:C:431:ARG:CZ	2.48	0.43
1:D:417:VAL:HG12	1:D:419:MET:CE	2.49	0.43
1:D:458:VAL:HG12	1:D:459:ASN:N	2.33	0.43
1:A:305:LYS:C	1:A:306:ILE:HG13	2.39	0.43
1:A:351:LYS:NZ	1:A:390:PHE:CE1	2.87	0.43
1:A:425:ALA:HB1	1:A:428:TYR:CD2	2.53	0.43
1:B:299:ARG:C	1:B:301:GLU:N	2.72	0.43
1:D:73:ILE:HG22	1:D:74:GLU:N	2.33	0.43
1:D:261:LYS:CA	1:D:444:GLU:HG2	2.49	0.43
1:D:269:VAL:HG23	1:D:269:VAL:O	2.17	0.43
1:D:289:PHE:C	1:D:291:ARG:N	2.71	0.43
1:D:376:HIS:HB3	1:D:402:GLN:NE2	2.34	0.43
1:A:285:VAL:CG2	1:A:286:TYR:H	2.12	0.43
1:B:357:ARG:O	1:B:357:ARG:HG3	2.18	0.43
1:C:421:GLY:O	1:C:422:SER:CB	2.66	0.43
1:D:110:ARG:NE	1:D:221:ARG:HG3	2.33	0.43
1:D:132:LEU:HD23	1:D:458:VAL:HG11	2.00	0.43
1:D:356:THR:HB	1:D:419:MET:CG	2.49	0.43
1:A:169:LYS:NZ	1:A:185:ASN:HD21	2.16	0.43
1:A:228:PHE:CD1	1:A:245:LYS:HD3	2.54	0.43



	i agem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:428:TYR:O	1:A:432:LEU:HB3	2.19	0.43
1:B:103:GLU:OE1	1:B:426:ARG:HD2	2.19	0.43
1:C:229:GLU:HG3	4:C:2633:HOH:O	2.18	0.43
1:B:201:VAL:O	1:B:201:VAL:HG22	2.18	0.43
1:B:357:ARG:HD3	1:B:428:TYR:OH	2.18	0.43
1:B:437:ARG:O	1:B:438:PRO:O	2.36	0.43
1:C:361:LEU:O	1:C:361:LEU:HD13	2.18	0.43
1:D:371:ILE:HD12	1:D:371:ILE:HA	1.92	0.43
1:D:388:GLU:OE2	1:D:391:ARG:CZ	2.67	0.43
1:A:103:GLU:HA	1:A:106:LEU:HD23	2.01	0.43
1:A:122:THR:HG22	1:A:126:MET:HE1	2.00	0.43
1:A:141:PRO:HD2	1:A:145:LEU:CD1	2.49	0.43
1:A:336:LYS:O	1:A:340:LEU:HB2	2.19	0.43
1:B:187:GLU:HG3	1:B:215:MET:CE	2.49	0.43
1:B:273:GLU:HG3	1:B:276:ARG:HD3	2.00	0.43
1:B:400:SER:CB	1:B:404:LEU:HD11	2.49	0.43
1:C:96:ASP:OD1	1:C:259:LEU:HB2	2.19	0.43
1:C:171:LEU:C	1:C:172:LYS:HE2	2.39	0.43
1:A:202:HIS:O	1:A:205:PRO:HD2	2.19	0.43
1:B:231:GLU:OE2	1:B:232:ASP:N	2.52	0.43
1:B:332:ASN:O	1:B:333:SER:O	2.36	0.43
1:C:72:GLY:O	1:C:73:ILE:C	2.56	0.43
1:C:354:ILE:HD11	1:C:419:MET:SD	2.58	0.43
1:D:68:PHE:C	1:D:70:SER:H	2.22	0.43
1:D:329:ILE:CD1	1:D:330:ALA:N	2.72	0.43
1:D:340:LEU:HD23	1:D:343:ILE:HD11	1.99	0.43
1:C:269:VAL:HG21	1:C:336:LYS:HD3	2.01	0.42
1:D:34:ILE:HD13	1:D:34:ILE:HA	1.85	0.42
1:D:52:GLY:O	1:D:53:THR:HG23	2.18	0.42
1:D:62:ARG:HD3	1:D:110:ARG:NH1	2.33	0.42
1:D:421:GLY:C	1:D:423:GLY:N	2.72	0.42
1:A:46:LYS:HE2	4:A:2260:HOH:O	2.18	0.42
1:A:231:GLU:HG3	1:D:118:GLY:HA2	2.00	0.42
1:B:48:ASP:OD1	1:B:50:ARG:HB3	2.19	0.42
1:B:209:TYR:OH	1:C:142:THR:HB	2.18	0.42
1:B:329:ILE:O	1:B:329:ILE:HG22	2.18	0.42
1:C:375:THR:CG2	1:C:378:THR:HG23	2.31	0.42
1:D:115:LEU:HD12	1:D:121:LYS:HG2	2.00	0.42
1:B:80:ALA:C	1:B:82:PRO:HD3	2.39	0.42
1:B:295:ILE:O	1:B:295:ILE:HG23	2.19	0.42
1:B:435:ILE:O	1:B:437:ARG:HD2	2.18	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:357:ARG:NH1	4:C:2340:HOH:O	2.52	0.42
1:D:26:GLU:CG	1:D:27:ILE:N	2.82	0.42
1:D:413:ALA:HB3	1:D:436:LEU:HD23	2.01	0.42
1:B:102:LEU:HG	1:B:106:LEU:CD2	2.46	0.42
1:B:122:THR:O	1:B:122:THR:HG22	2.18	0.42
1:C:148:GLN:HE21	1:C:152:ARG:NH1	1.97	0.42
1:C:196:LEU:HD13	1:C:198:PHE:CZ	2.54	0.42
1:C:269:VAL:HG22	1:C:452:SER:HB3	2.01	0.42
1:C:358:HIS:O	1:C:362:VAL:HG23	2.19	0.42
1:D:191:ASN:OD1	1:D:192:ARG:CD	2.65	0.42
1:D:453:ARG:HB2	1:D:454:GLY:H	1.69	0.42
1:A:65:ILE:HG22	1:A:297:LEU:CD1	2.47	0.42
1:A:258:HIS:O	1:A:259:LEU:C	2.58	0.42
1:A:325:GLU:O	1:A:326:ALA:C	2.56	0.42
1:A:335:ASN:O	1:A:339:LYS:HB2	2.19	0.42
1:B:68:PHE:HB3	1:B:75:PHE:CE2	2.54	0.42
1:B:93:SER:HA	1:B:264:ILE:O	2.20	0.42
1:B:290:LEU:HD22	1:B:296:THR:C	2.40	0.42
1:B:372:PRO:HG2	1:B:395:PHE:CD1	2.54	0.42
1:C:100:LYS:HD2	1:C:247:PHE:HE2	1.84	0.42
1:D:309:ALA:O	1:D:311:GLY:N	2.52	0.42
1:D:336:LYS:NZ	1:D:420:SER:CB	2.82	0.42
1:A:59:PHE:HA	1:A:216:SER:O	2.20	0.42
1:A:92:ILE:N	1:A:92:ILE:HD12	2.34	0.42
1:A:269:VAL:CG2	1:A:336:LYS:HE3	2.50	0.42
1:D:33:THR:HG21	1:D:55:ARG:CG	2.50	0.42
1:D:44:HIS:HE1	1:D:63:ASP:OD1	2.01	0.42
1:D:68:PHE:CD1	1:D:75:PHE:CD2	3.06	0.42
1:A:239:LYS:HA	1:A:243:GLY:C	2.39	0.42
1:B:163:GLU:OE1	1:B:168:ILE:HG22	2.19	0.42
1:B:196:LEU:HG	1:B:218:ALA:HB3	2.01	0.42
1:B:356:THR:OG1	1:B:361:LEU:HD13	2.20	0.42
1:C:24:ILE:HG13	4:C:2709:HOH:O	2.18	0.42
1:C:254:LEU:C	1:C:254:LEU:HD23	2.40	0.42
1:C:267:ILE:CD1	1:C:448:TYR:HD2	2.32	0.42
1:C:372:PRO:HD2	1:C:398:ILE:HG22	2.01	0.42
1:D:109:LYS:HE2	1:D:458:VAL:CG1	2.50	0.42
1:D:138:ILE:N	1:D:138:ILE:HD12	2.35	0.42
1:D:152:ARG:HH11	1:D:152:ARG:HB2	1.85	0.42
1:D:167:ARG:C	1:D:168:ILE:CG1	2.88	0.42
1:A:301:GLU:O	1:A:302:ASP:CB	2.68	0.42



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:168:ILE:HG13	4:B:2122:HOH:O	2.18	0.42
1:B:382:GLU:O	1:B:385:GLU:HB3	2.20	0.42
1:C:65:ILE:O	1:C:69:GLU:HB2	2.20	0.42
1:C:418:ILE:HD12	1:C:419:MET:H	1.85	0.42
1:D:337:ILE:HD11	1:D:361:LEU:HD21	2.01	0.42
1:A:81:ASP:N	1:A:82:PRO:HD3	2.35	0.42
1:B:263:THR:HG23	1:B:444:GLU:HB3	2.02	0.42
1:B:367:LYS:O	1:B:369:PHE:N	2.53	0.42
1:C:50:ARG:HG2	1:C:50:ARG:NH1	2.34	0.42
1:C:62:ARG:NH1	1:C:219:PRO:O	2.51	0.42
1:C:325:GLU:HA	1:C:328:ARG:HB3	2.02	0.42
1:C:340:LEU:HD22	1:C:344:LEU:HG	2.02	0.42
1:C:396:ARG:HG2	1:C:396:ARG:HH11	1.83	0.42
1:D:276:ARG:O	1:D:279:TYR:HB3	2.20	0.42
1:D:403:VAL:HG21	1:D:431:ARG:NH1	2.34	0.42
1:B:43:PRO:C	1:B:45:ALA:H	2.24	0.42
1:B:99:GLU:OE1	1:B:99:GLU:CA	2.68	0.42
1:B:115:LEU:HD21	1:B:247:PHE:HE1	1.85	0.42
1:B:338:ARG:O	1:B:342:GLU:HG3	2.20	0.42
1:C:355:PHE:CD2	1:C:418:ILE:HD13	2.54	0.42
1:C:415:VAL:CG1	1:C:416:GLY:N	2.83	0.42
1:D:57:LEU:HD22	4:D:2560:HOH:O	2.19	0.42
1:D:152:ARG:HH11	1:D:152:ARG:CB	2.33	0.42
1:D:164:PHE:O	1:D:164:PHE:HD1	2.03	0.42
1:D:395:PHE:O	1:D:397:ALA:N	2.53	0.42
1:A:340:LEU:HD22	1:A:344:LEU:HD11	2.02	0.41
1:B:360:GLU:N	1:B:362:VAL:HG22	2.35	0.41
1:B:436:LEU:HD11	1:B:447:LEU:HB2	2.02	0.41
1:C:399:VAL:O	1:C:399:VAL:HG13	2.20	0.41
1:D:312:TYR:O	1:D:317:TYR:HB2	2.19	0.41
1:D:368:VAL:O	1:D:368:VAL:CG1	2.67	0.41
1:A:52:GLY:HA3	4:A:2818:HOH:O	2.19	0.41
1:A:234:ARG:HG2	1:A:234:ARG:HH11	1.85	0.41
1:A:303:PHE:O	1:A:303:PHE:CD1	2.73	0.41
1:B:405:ASP:HA	1:B:410:VAL:HG12	2.01	0.41
1:B:450:LEU:N	1:B:450:LEU:CD2	2.81	0.41
1:C:220:PHE:C	1:C:221:ARG:HG3	2.40	0.41
1:C:415:VAL:HG12	1:C:416:GLY:N	2.34	0.41
1:D:105:TRP:HE3	1:D:106:LEU:HD12	1.85	0.41
1:D:364:ARG:HG3	1:D:368:VAL:HG21	2.01	0.41
1:D:390:PHE:CE2	1:D:398:ILE:HG12	2.55	0.41



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:449:GLU:HG2	1:D:451:ILE:HD11	2.02	0.41
1:A:220:PHE:C	1:A:221:ARG:HG2	2.39	0.41
1:A:230:ARG:HH22	3:A:6001:IPA:C3	2.33	0.41
1:A:266:ARG:HD3	1:A:451:ILE:HD12	2.02	0.41
1:A:267:ILE:HG21	1:A:339:LYS:HE2	2.03	0.41
1:A:373:ALA:O	1:A:374:ILE:HG13	2.20	0.41
1:B:31:ARG:HG3	1:B:187:GLU:HB3	2.03	0.41
1:B:137:LEU:HB2	1:B:193:PHE:CD2	2.56	0.41
1:D:261:LYS:C	1:D:444:GLU:HB3	2.41	0.41
1:B:101:ALA:HA	1:B:247:PHE:CD2	2.55	0.41
1:B:205:PRO:O	1:B:206:ALA:C	2.57	0.41
1:B:207:GLU:HG3	4:B:2032:HOH:O	2.20	0.41
1:B:327:ARG:NH1	1:B:423:GLY:H	2.17	0.41
1:C:153:LEU:O	1:C:156:PHE:HB2	2.19	0.41
1:D:283:GLU:HB3	1:D:286:TYR:CE1	2.56	0.41
1:D:418:ILE:CD1	1:D:447:LEU:HD21	2.47	0.41
1:A:60:ARG:HH21	1:A:60:ARG:HG3	1.85	0.41
1:B:67:TYR:CD1	1:B:68:PHE:N	2.89	0.41
1:B:88:PHE:HB3	1:B:156:PHE:CE1	2.55	0.41
1:B:232:ASP:OD1	1:B:234:ARG:HB2	2.20	0.41
1:B:257:LYS:HD3	1:B:257:LYS:HA	1.82	0.41
1:C:141:PRO:HD2	1:C:145:LEU:HD13	2.02	0.41
1:D:28:TYR:N	1:D:28:TYR:CD1	2.88	0.41
1:D:305:LYS:HE3	1:D:320:LEU:HD11	2.02	0.41
1:D:355:PHE:CG	1:D:356:THR:N	2.89	0.41
1:A:434:ARG:H	1:A:434:ARG:HG2	1.75	0.41
1:C:102:LEU:O	1:C:106:LEU:HB2	2.20	0.41
1:A:24:ILE:HG22	1:A:25:ALA:H	1.86	0.41
1:B:152:ARG:NH1	4:B:2621:HOH:O	2.53	0.41
1:C:24:ILE:HB	1:C:25:ALA:H	1.66	0.41
1:C:194:MET:CE	1:C:219:PRO:HG3	2.50	0.41
1:D:27:ILE:HD12	1:D:79:ALA:HB2	2.03	0.41
1:D:432:LEU:HD23	1:D:432:LEU:C	2.41	0.41
1:A:305:LYS:HG2	1:A:323:TRP:CE3	2.56	0.41
1:A:305:LYS:HE2	1:A:320:LEU:HG	2.02	0.41
1:C:337:ILE:HG21	1:C:364:ARG:HH12	1.85	0.41
1:C:405:ASP:OD1	1:C:405:ASP:N	2.54	0.41
1:C:421:GLY:O	1:C:422:SER:HB2	2.21	0.41
1:D:438:PRO:HB3	1:D:444:GLU:CA	2.22	0.41
1:A:59:PHE:CD2	1:A:214:GLN:HA	2.56	0.41
1:A:100:LYS:HZ1	1:A:104:ARG:NH2	2.16	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:259:LEU:HD11	1:A:262:TYR:CD2	2.56	0.41
1:A:358:HIS:C	1:A:362:VAL:HG23	2.39	0.41
1:A:426:ARG:HA	1:A:429:ILE:CG1	2.51	0.41
1:B:102:LEU:O	1:B:106:LEU:HD22	2.20	0.41
1:B:344:LEU:HD23	1:B:352:ILE:HD11	2.03	0.41
1:B:414:ASN:HA	1:B:437:ARG:O	2.20	0.41
1:C:114:VAL:HA	1:C:225:THR:O	2.21	0.41
1:C:143:LEU:CD1	1:C:167:ARG:HD2	2.48	0.41
1:C:224:LEU:O	1:C:225:THR:HB	2.21	0.41
1:C:284:LYS:HG2	4:C:2887:HOH:O	2.20	0.41
1:C:337:ILE:HG21	1:C:364:ARG:NH1	2.36	0.41
1:C:358:HIS:CD2	1:C:361:LEU:H	2.36	0.41
1:C:361:LEU:HD13	1:C:365:ILE:HD12	2.02	0.41
1:D:46:LYS:HE3	1:D:55:ARG:O	2.20	0.41
1:D:68:PHE:HD2	1:D:68:PHE:HA	1.72	0.41
1:D:217:ILE:O	1:D:218:ALA:C	2.59	0.41
1:D:282:ARG:NH1	1:D:322:ALA:HA	2.35	0.41
1:A:74:GLU:OE2	1:A:74:GLU:CA	2.66	0.41
1:A:204:LEU:HD23	1:A:242:VAL:HG21	2.03	0.41
1:B:427:GLU:HG2	1:B:428:TYR:N	2.36	0.41
1:C:165:SER:HB2	4:C:2529:HOH:O	2.21	0.41
1:C:331:PHE:CD1	1:C:358:HIS:HB2	2.56	0.41
1:C:340:LEU:HD22	1:C:344:LEU:HD11	2.03	0.41
1:C:409:ASP:O	1:C:410:VAL:HB	2.21	0.41
1:D:29:TYR:HB2	1:D:79:ALA:HB1	2.01	0.41
1:D:67:TYR:CD1	1:D:67:TYR:O	2.74	0.41
1:D:167:ARG:O	1:D:168:ILE:HG12	2.21	0.41
1:D:264:ILE:HG22	1:D:265:LYS:N	2.35	0.41
1:A:29:TYR:N	1:A:79:ALA:HA	2.36	0.40
1:A:344:LEU:HD12	1:A:369:PHE:CE2	2.56	0.40
1:B:71:ASN:O	1:B:72:GLY:C	2.59	0.40
1:B:285:VAL:HG11	1:B:322:ALA:HB2	2.03	0.40
1:C:354:ILE:HG23	1:C:399:VAL:HA	2.03	0.40
1:C:412:ASP:HB2	1:C:437:ARG:CD	2.47	0.40
1:D:226:ALA:HB2	4:D:2283:HOH:O	2.20	0.40
1:A:140:VAL:HG21	1:A:146:ALA:HB2	2.03	0.40
1:C:258:HIS:C	1:C:260:ALA:H	2.24	0.40
1:C:340:LEU:HD22	1:C:344:LEU:CD1	2.51	0.40
1:C:389:GLY:HA3	1:C:395:PHE:CZ	2.57	0.40
1:D:227:THR:CG2	4:D:2756:HOH:O	2.69	0.40
1:B:92:ILE:N	1:B:92:ILE:HD12	2.35	0.40



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:68:PHE:HB3	1:C:75:PHE:CE2	2.56	0.40
1:C:95:ARG:O	1:C:96:ASP:C	2.60	0.40
1:D:66:GLU:C	1:D:68:PHE:N	2.75	0.40
1:D:264:ILE:HG23	1:D:447:LEU:HD22	2.03	0.40
1:D:340:LEU:HA	1:D:343:ILE:HD11	2.01	0.40
1:D:361:LEU:HD13	1:D:365:ILE:CG1	2.51	0.40
1:A:303:PHE:O	1:A:303:PHE:HD1	2.04	0.40
1:B:122:THR:HG21	1:B:152:ARG:NE	2.36	0.40
1:C:441:GLY:HA3	4:C:3007:HOH:O	2.22	0.40
1:D:250:PHE:HA	1:D:251:PRO:HD3	1.91	0.40
1:D:372:PRO:CG	1:D:398:ILE:HG22	2.51	0.40
1:A:65:ILE:HD13	1:A:65:ILE:HA	1.93	0.40
1:A:312:TYR:O	1:A:313:ASP:C	2.60	0.40
1:A:430:GLN:O	1:A:431:ARG:C	2.60	0.40
1:C:262:TYR:HE1	1:C:264:ILE:HD11	1.86	0.40
1:D:35:VAL:HG22	1:D:55:ARG:HG3	2.03	0.40
1:D:97:TYR:HE1	1:D:259:LEU:HD21	1.86	0.40
1:D:140:VAL:HG22	1:D:177:SER:O	2.22	0.40
1:D:371:ILE:HA	1:D:372:PRO:HD3	1.94	0.40
1:D:430:GLN:O	1:D:431:ARG:C	2.60	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom_1	Atom-2	Interatomic	Clash
	Atom-2	distance (Å)	overlap (Å)
4:A:2319:HOH:O	4:B:2932:HOH:O[1_455]	1.98	0.22
4:B:2454:HOH:O	4:B:2522:HOH:O[1_655]	2.16	0.04
4:B:2433:HOH:O	4:B:2745:HOH:O[1_455]	2.18	0.02
4:D:2465:HOH:O	4:D:2580:HOH:O[1_655]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	432/472~(92%)	343 (79%)	67~(16%)	22~(5%)	2	2
1	В	415/472~(88%)	341 (82%)	57 (14%)	17 (4%)	3	3
1	С	410/472 (87%)	304 (74%)	64 (16%)	42 (10%)	0	0
1	D	422/472~(89%)	313 (74%)	77 (18%)	32 (8%)	1	1
All	All	1679/1888~(89%)	1301 (78%)	265 (16%)	113 (7%)	1	1

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	259	LEU
1	А	297	LEU
1	А	307	VAL
1	А	313	ASP
1	А	331	PHE
1	А	440	LYS
1	А	455	THR
1	В	23	MET
1	В	302	ASP
1	В	333	SER
1	В	375	THR
1	В	438	PRO
1	В	443	LYS
1	С	24	ILE
1	С	47	PHE
1	С	61	TYR
1	С	69	GLU
1	С	73	ILE
1	С	255	ALA
1	С	258	HIS
1	С	274	ASP
1	С	284	LYS
1	С	295	ILE
1	С	348	ARG
1	С	379	SER
1	С	394	ARG
1	С	395	PHE
1	С	406	GLU
1	С	408	ILE
1	D	39	ASP
1	D	48	ASP
1	D	346	ARG
1	D	372	PRO



Mol	Chain	Res	Type
1	D	396	ARG
1	D	410	VAL
1	D	442	LYS
1	А	291	ARG
1	А	294	GLY
1	А	314	GLU
1	А	374	ILE
1	А	378	THR
1	А	379	SER
1	А	394	ARG
1	А	411	PRO
1	В	25	ALA
1	В	360	GLU
1	В	409	ASP
1	В	412	ASP
1	С	25	ALA
1	С	51	SER
1	С	68	PHE
1	С	273	GLU
1	С	282	ARG
1	С	368	VAL
1	С	393	GLY
1	С	419	MET
1	С	420	SER
1	С	426	ARG
1	D	52	GLY
1	D	67	TYR
1	D	72	GLY
1	D	281	LYS
1	D	293	ARG
1	D	310	SER
1	D	319	ALA
1	D	374	ILE
1	D	408	ILE
1	D	458	VAL
1	A	290	LEU
1	A	330	ALA
1	A	444	GLU
1	B	380	ARG
1	C	96	ASP
1	С	131	GLU
1	С	291	ARG



Continued from previous page				
Mol	Chain	Res	Type	
1	С	367	LYS	
1	С	443	LYS	
1	D	86	PRO	
1	D	257	LYS	
1	D	426	ARG	
1	А	273	GLU	
1	А	410	VAL	
1	В	397	ALA	
1	С	42	VAL	
1	С	45	ALA	
1	С	53	THR	
1	С	333	SER	
1	С	371	ILE	
1	С	410	VAL	
1	D	41	HIS	
1	D	46	LYS	
1	D	49	SER	
1	В	379	SER	
1	В	442	LYS	
1	С	440	LYS	
1	D	259	LEU	
1	D	307	VAL	
1	D	369	PHE	
1	D	407	GLY	
1	D	457	GLU	
1	А	383	ARG	
1	В	374	ILE	
1	С	287	LYS	
1	С	370	LEU	
1	С	403	VAL	
1	В	24	ILE	
1	D	242	VAL	
1	D	306	ILE	
1	В	362	VAL	
1	А	306	ILE	
1	С	417	VAL	
1	D	251	PRO	
1	D	368	VAL	



5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	366/398~(92%)	333~(91%)	33~(9%)	9 18
1	В	357/398~(90%)	332~(93%)	25~(7%)	15 30
1	С	343/398~(86%)	323 (94%)	20~(6%)	20 40
1	D	349/398~(88%)	314 (90%)	35 (10%)	7 14
All	All	1415/1592 (89%)	1302 (92%)	113 (8%)	12 24

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	31	ARG
1	А	69	GLU
1	А	74	GLU
1	А	87	TYR
1	А	106	LEU
1	А	113	ILE
1	А	133	SER
1	А	137	LEU
1	А	153	LEU
1	А	191	ASN
1	А	195	LEU
1	А	221	ARG
1	А	227	THR
1	А	229	GLU
1	А	231	GLU
1	А	293	ARG
1	А	296	THR
1	А	302	ASP
1	А	304	ASN
1	А	308	MET
1	А	314	GLU
1	А	321	ARG
1	A	340	LEU
1	А	346	ARG



1 A 351 LYS 1 A 352 ILE 1 A 358 HIS 1 A 367 LYS 1 A 367 LYS 1 A 398 ILE 1 A 398 ILE 1 A 411 PRO 1 A 414 ASN 1 A 414 ASN 1 A 442 LYS 1 A 442 LYS 1 B 31 ARG 1 B 67 TYR 1 B 106 LEU 1 B 134 THR 1 B 135 LEU 1 B 237 ILE 1 B 237 ILE 1 B 249 LEU 1 B 286 <th>Mol</th> <th>Chain</th> <th>Res</th> <th>Type</th>	Mol	Chain	Res	Type
1 A 352 ILE 1 A 358 HIS 1 A 367 LYS 1 A 398 ILE 1 A 398 ILE 1 A 411 PRO 1 A 411 PRO 1 A 414 ASN 1 A 431 ARG 1 A 442 LYS 1 B 31 ARG 1 B 67 TYR 1 B 106 LEU 1 B 134 THR 1 B 153 LEU 1 B 227 THR 1 B 237 ILE 1 B 237 ILEU 1 B 249 LEU 1 B 286 TYR 1 B 318 GLU 1 B 318 GLU <td>1</td> <td>A</td> <td>351</td> <td>LYS</td>	1	A	351	LYS
1 A 358 HIS 1 A 367 LYS 1 A 398 ILE 1 A 411 PRO 1 A 411 PRO 1 A 414 ASN 1 A 414 ASN 1 A 431 ARG 1 A 442 LYS 1 B 31 ARG 1 B 67 TYR 1 B 106 LEU 1 B 134 THR 1 B 135 LEU 1 B 127 THR 1 B 232 ASP 1 B 237 ILE 1 B 237 ILEU 1 B 249 LEU 1 B 273 GLU 1 B 286 TYR 1 B 289 PHE 1 <	1	А	352	ILE
1 A 367 LYS 1 A 398 ILE 1 A 411 PRO 1 A 414 ASN 1 A 414 ASN 1 A 414 ASN 1 A 431 ARG 1 A 442 LYS 1 B 31 ARG 1 B 67 TYR 1 B 106 LEU 1 B 134 THR 1 B 153 LEU 1 B 153 LEU 1 B 227 THR 1 B 232 ASP 1 B 237 ILE 1 B 237 ILE 1 B 249 LEU 1 B 273 GLU 1 B 286 TYR 1 B 289 PHE 1 <t< td=""><td>1</td><td>A</td><td>358</td><td>HIS</td></t<>	1	A	358	HIS
1 A 398 ILE 1 A 411 PRO 1 A 411 PRO 1 A 414 ASN 1 A 431 ARG 1 A 431 ARG 1 A 442 LYS 1 B 31 ARG 1 B 67 TYR 1 B 106 LEU 1 B 134 THR 1 B 153 LEU 1 B 153 LEU 1 B 227 THR 1 B 232 ASP 1 B 237 ILE 1 B 237 ILE 1 B 249 LEU 1 B 273 GLU 1 B 286 TYR 1 B 289 PHE 1 B 331 PHE 1 <t< td=""><td>1</td><td>A</td><td>367</td><td>LYS</td></t<>	1	A	367	LYS
1 A 411 PRO 1 A 414 ASN 1 A 431 ARG 1 A 431 ARG 1 A 442 LYS 1 B 31 ARG 1 B 67 TYR 1 B 106 LEU 1 B 134 THR 1 B 153 LEU 1 B 153 LEU 1 B 127 THR 1 B 232 ASP 1 B 237 ILE 1 B 237 ILEU 1 B 237 ILEU 1 B 237 GLU 1 B 249 LEU 1 B 273 GLU 1 B 286 TYR 1 B 318 GLU 1 B 331 PHE 1	1	A	398	ILE
1 A 414 ASN 1 A 431 ARG 1 A 442 LYS 1 B 31 ARG 1 B 31 ARG 1 B 67 TYR 1 B 106 LEU 1 B 134 THR 1 B 153 LEU 1 B 195 LEU 1 B 227 THR 1 B 232 ASP 1 B 237 ILE 1 B 237 ILE 1 B 237 ILE 1 B 249 LEU 1 B 273 GLU 1 B 286 TYR 1 B 289 PHE 1 B 331 PHE 1 B 345 GLU 1 B 350 ASP 1 <t< td=""><td>1</td><td>А</td><td>411</td><td>PRO</td></t<>	1	А	411	PRO
1 A 431 ARG 1 A 442 LYS 1 B 31 ARG 1 B 31 ARG 1 B 67 TYR 1 B 106 LEU 1 B 134 THR 1 B 153 LEU 1 B 195 LEU 1 B 227 THR 1 B 232 ASP 1 B 237 ILE 1 B 237 ILE 1 B 249 LEU 1 B 252 ASP 1 B 273 GLU 1 B 286 TYR 1 B 289 PHE 1 B 331 PHE 1 B 350 ASP 1 B 350 ASP 1 B 351 LYS 1 <td< td=""><td>1</td><td>А</td><td>414</td><td>ASN</td></td<>	1	А	414	ASN
1 A 442 LYS 1 B 31 ARG 1 B 67 TYR 1 B 106 LEU 1 B 134 THR 1 B 134 THR 1 B 153 LEU 1 B 195 LEU 1 B 227 THR 1 B 232 ASP 1 B 237 ILE 1 B 237 ILE 1 B 249 LEU 1 B 252 ASP 1 B 252 ASP 1 B 286 TYR 1 B 289 PHE 1 B 318 GLU 1 B 331 PHE 1 B 350 ASP 1 B 350 ASP 1 B 351 LYS 1 <t< td=""><td>1</td><td>А</td><td>431</td><td>ARG</td></t<>	1	А	431	ARG
1 B 31 ARG 1 B 67 TYR 1 B 106 LEU 1 B 134 THR 1 B 153 LEU 1 B 195 LEU 1 B 227 THR 1 B 232 ASP 1 B 237 ILE 1 B 237 ILE 1 B 237 ILE 1 B 237 GLU 1 B 249 LEU 1 B 252 ASP 1 B 273 GLU 1 B 286 TYR 1 B 286 TYR 1 B 331 PHE 1 B 331 PHE 1 B 350 ASP 1 B 350 ASP 1 B 351 LYS 1 <t< td=""><td>1</td><td>А</td><td>442</td><td>LYS</td></t<>	1	А	442	LYS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	В	31	ARG
1 B 106 LEU 1 B 134 THR 1 B 153 LEU 1 B 195 LEU 1 B 227 THR 1 B 232 ASP 1 B 237 ILE 1 B 249 LEU 1 B 252 ASP 1 B 273 GLU 1 B 286 TYR 1 B 289 PHE 1 B 318 GLU 1 B 331 PHE 1 B 350 ASP 1 B 350 ASP 1 B 351 LYS 1 B 362 VAL	1	В	67	TYR
1 B 134 THR 1 B 153 LEU 1 B 195 LEU 1 B 227 THR 1 B 232 ASP 1 B 232 ASP 1 B 237 ILE 1 B 237 ILE 1 B 237 ILE 1 B 249 LEU 1 B 252 ASP 1 B 252 ASP 1 B 252 ASP 1 B 286 TYR 1 B 286 TYR 1 B 318 GLU 1 B 331 PHE 1 B 345 GLU 1 B 350 ASP 1 B 351 LYS 1 B 362 VAL	1	В	106	LEU
1 B 153 LEU 1 B 195 LEU 1 B 227 THR 1 B 232 ASP 1 B 237 ILE 1 B 249 LEU 1 B 252 ASP 1 B 252 ASP 1 B 286 TYR 1 B 286 TYR 1 B 318 GLU 1 B 331 PHE 1 B 345 GLU 1 B 350 ASP 1 B 351 LYS 1 B 362 VAL	1	В	134	THR
1 B 195 LEU 1 B 227 THR 1 B 232 ASP 1 B 237 ILE 1 B 237 ILE 1 B 237 ILE 1 B 237 ILE 1 B 249 LEU 1 B 252 ASP 1 B 252 ASP 1 B 252 ASP 1 B 252 ASP 1 B 286 TYR 1 B 286 TYR 1 B 318 GLU 1 B 331 PHE 1 B 345 GLU 1 B 350 ASP 1 B 351 LYS 1 B 362 VAL	1	В	153	LEU
1 B 227 THR 1 B 232 ASP 1 B 237 ILE 1 B 249 LEU 1 B 252 ASP 1 B 252 ASP 1 B 252 ASP 1 B 252 ASP 1 B 286 TYR 1 B 286 TYR 1 B 318 GLU 1 B 318 GLU 1 B 331 PHE 1 B 350 ASP 1 B 350 ASP 1 B 351 LYS 1 B 362 VAL	1	В	195	LEU
1 B 232 ASP 1 B 237 ILE 1 B 249 LEU 1 B 252 ASP 1 B 252 ASP 1 B 252 ASP 1 B 286 TYR 1 B 289 PHE 1 B 318 GLU 1 B 331 PHE 1 B 331 PHE 1 B 350 ASP 1 B 350 ASP 1 B 351 LYS 1 B 362 VAL	1	В	227	THR
1 B 237 ILE 1 B 249 LEU 1 B 252 ASP 1 B 273 GLU 1 B 286 TYR 1 B 289 PHE 1 B 318 GLU 1 B 331 PHE 1 B 350 ASP 1 B 350 ASP 1 B 351 LYS 1 B 362 VAL	1	В	232	ASP
1 B 249 LEU 1 B 252 ASP 1 B 273 GLU 1 B 286 TYR 1 B 289 PHE 1 B 318 GLU 1 B 331 PHE 1 B 331 PHE 1 B 350 ASP 1 B 350 ASP 1 B 351 LYS 1 B 362 VAL	1	В	237	ILE
1 B 252 ASP 1 B 273 GLU 1 B 286 TYR 1 B 289 PHE 1 B 318 GLU 1 B 318 GLU 1 B 331 PHE 1 B 345 GLU 1 B 350 ASP 1 B 351 LYS 1 B 362 VAL	1	В	249	LEU
1 B 273 GLU 1 B 286 TYR 1 B 289 PHE 1 B 318 GLU 1 B 331 PHE 1 B 331 PHE 1 B 350 ASP 1 B 351 LYS 1 B 362 VAL	1	В	252	ASP
1 B 286 TYR 1 B 289 PHE 1 B 318 GLU 1 B 331 PHE 1 B 345 GLU 1 B 350 ASP 1 B 351 LYS 1 B 362 VAL	1	В	273	GLU
1 B 289 PHE 1 B 318 GLU 1 B 331 PHE 1 B 345 GLU 1 B 350 ASP 1 B 351 LYS 1 B 362 VAL	1	В	286	TYR
1 B 318 GLU 1 B 331 PHE 1 B 345 GLU 1 B 350 ASP 1 B 351 LYS 1 B 362 VAL	1	В	289	PHE
1 B 331 PHE 1 B 345 GLU 1 B 350 ASP 1 B 351 LYS 1 B 362 VAL	1	В	318	GLU
1 B 345 GLU 1 B 350 ASP 1 B 351 LYS 1 B 362 VAL	1	В	331	PHE
1 B 350 ASP 1 B 351 LYS 1 B 362 VAL	1	В	345	GLU
1 B 351 LYS 1 B 362 VAL	1	В	350	ASP
1 B 362 VAL	1	В	351	LYS
	1	В	362	VAL
1 B 391 ARG	1	В	391	ARG
1 B 414 ASN	1	В	414	ASN
1 B 430 GLN	1	В	430	GLN
1 B 432 LEU	1	В	432	LEU
1 B 437 ARG	1	В	437	ARG
1 C 24 ILE	1	С	24	ILE
1 C 54 TYR	1	С	54	TYR
1 C 87 TYR	1	С	87	TYR
1 C 93 SER	1	С	93	SER
1 C 106 LEU	1	С	106	LEU
1 C 134 THR	1	С	134	THR
1 C 195 LEU	1	С	195	LEU
1 C 234 ARG	1	С	234	ARG



Mol	Chain	Res	Type
1	С	259	LEU
1	С	323	TRP
1	С	331	PHE
1	С	338	ARG
1	C	340	LEU
1	С	354	ILE
1	С	356	THR
1	С	369	PHE
1	С	381	GLU
1	С	418	ILE
1	С	426	ARG
1	С	432	LEU
1	D	27	ILE
1	D	57	LEU
1	D	68	PHE
1	D	96	ASP
1	D	114	VAL
1	D	152	ARG
1	D	155	ILE
1	D	195	LEU
1	D	221	ARG
1	D	229	GLU
1	D	232	ASP
1	D	258	HIS
1	D	274	ASP
1	D	284	LYS
1	D	290	LEU
1	D	305	LYS
1	D	306	ILE
1	D	328	ARG
1	D	331	PHE
1	D	346	ARG
1	D	352	ILE
1	D	356	THR
1	D	357	ARG
1	D	358	HIS
1	D	367	LYS
1	D	370	LEU
1	D	392	THR
1	D	394	ARG
1	D	395	PHE
1	D	403	VAL



 $Continued \ from \ previous \ page...$

Mol	Chain	Res	Type
1	D	404	LEU
1	D	405	ASP
1	D	409	ASP
1	D	440	LYS
1	D	453	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	44	HIS
1	А	78	ASN
1	А	185	ASN
1	А	191	ASN
1	А	304	ASN
1	А	335	ASN
1	В	44	HIS
1	В	71	ASN
1	В	130	ASN
1	В	203	HIS
1	В	214	GLN
1	В	359	ASN
1	В	430	GLN
1	С	71	ASN
1	С	78	ASN
1	С	148	GLN
1	С	185	ASN
1	С	332	ASN
1	С	402	GLN
1	D	44	HIS
1	D	78	ASN
1	D	98	GLN
1	D	211	GLN
1	D	359	ASN
1	D	402	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.



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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

11 ligands are modelled in this entry.

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

Mol Type		Chain	Chain	Dec	Timle	Bond lengths			Bond angles		
	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2	
2	PO4	D	4006	-	4,4,4	1.61	0	$6,\!6,\!6$	0.48	0	
3	IPA	А	6003	-	3,3,3	0.38	0	3,3,3	0.33	0	
2	PO4	С	4003	-	4,4,4	1.75	0	$6,\!6,\!6$	0.42	0	
2	PO4	А	4001	-	4,4,4	1.66	1 (25%)	$6,\!6,\!6$	0.43	0	
2	PO4	D	4004	-	4,4,4	1.81	2 (50%)	$6,\!6,\!6$	0.43	0	
2	PO4	В	4007	-	4,4,4	1.71	0	$6,\!6,\!6$	0.42	0	
2	PO4	D	4005	-	4,4,4	1.64	0	$6,\!6,\!6$	0.43	0	
3	IPA	А	6002	-	$3,\!3,\!3$	0.42	0	$3,\!3,\!3$	0.37	0	
2	PO4	В	4008	-	4,4,4	1.65	1 (25%)	6,6,6	0.40	0	
3	IPA	А	6001	-	3,3,3	0.42	0	3, 3, 3	0.38	0	
2	PO4	В	4002	-	4,4,4	1.68	0	$6,\!6,\!6$	0.42	0	

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
2	D	4004	PO4	P-O4	-2.07	1.48	1.54
2	В	4008	PO4	P-O3	-2.05	1.48	1.54
2	А	4001	PO4	P-O2	-2.05	1.48	1.54
2	D	4004	PO4	P-O2	-2.02	1.48	1.54

There are no bond angle outliers.



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	6002	IPA	3	0
3	А	6001	IPA	3	0
2	В	4002	PO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	434/472~(91%)	0.06	31 (7%) 16 11	12, 46, 121, 131	0
1	В	423/472~(89%)	-0.03	23 (5%) 25 20	11, 47, 122, 129	0
1	С	414/472~(87%)	0.19	17 (4%) 37 30	19, 68, 120, 132	0
1	D	428/472~(90%)	0.27	37 (8%) 10 7	18, 70, 123, 131	0
All	All	1699/1888 (89%)	0.12	108 (6%) 19 14	11, 58, 122, 132	0

All (108) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	А	290	LEU	7.2
1	А	291	ARG	6.4
1	С	285	VAL	5.4
1	С	279	TYR	5.4
1	D	52	GLY	5.3
1	D	307	VAL	4.9
1	D	51	SER	4.8
1	D	260	ALA	4.6
1	D	323	TRP	4.6
1	D	308	MET	4.5
1	В	308	MET	4.4
1	С	288	GLN	4.0
1	D	309	ALA	4.0
1	С	286	TYR	3.9
1	А	320	LEU	3.9
1	D	293	ARG	3.9
1	В	287	LYS	3.9
1	В	23	MET	3.8
1	D	288	GLN	3.7
1	А	303	PHE	3.5
1	А	313	ASP	3.5



Mol	Chain	Res	5 Type RSR2	
1	А	272	ALA	3.4
1	D	316	ALA	3.4
1	С	320	LEU	3.4
1	А	390	PHE	3.4
1	В	286	TYR	3.4
1	В	302	ASP	3.3
1	D	296	THR	3.3
1	D	50	ARG	3.2
1	А	323	TRP	3.2
1	D	320	LEU	3.2
1	В	306	ILE	3.2
1	D	294	GLY	3.1
1	D	441	GLY	3.1
1	В	307	VAL	3.1
1	D	281	LYS	3.1
1	В	285	VAL	3.1
1	В	441	GLY	3.1
1	D	256	GLY	3.0
1	В	303	PHE	3.0
1	В	277	VAL	3.0
1	D	319	ALA	3.0
1	В	443	LYS	3.0
1	В	284	LYS	2.9
1	А	298	ARG	2.9
1	D	38	GLY	2.9
1	D	322	ALA	2.9
1	D	279	TYR	2.9
1	А	441	GLY	2.9
1	А	456	GLY	2.9
1	А	317	TYR	2.8
1	D	285	VAL	2.8
1	А	406	GLU	2.8
1	A	301	GLU	2.8
1	А	405	ASP	2.7
1	D	310	SER	2.7
1	D	295	ILE	2.7
1	D	329	ILE	2.7
1	С	23	MET	2.7
1	А	286	TYR	2.7
1	D	286	TYR	2.7
1	С	283	GLU	2.6
1	С	395	PHE	2.6



Mol	Chain	Res	Type	RSRZ
1	А	295	ILE	2.6
1	А	443	LYS	2.6
1	А	396	ARG	2.6
1	D	326	ALA	2.5
1	А	282	ARG	2.5
1	В	439	SER	2.5
1	D	461	ALA	2.5
1	В	390	PHE	2.5
1	А	277	VAL	2.4
1	D	53	THR	2.4
1	А	287	LYS	2.4
1	А	304	ASN	2.4
1	С	281	LYS	2.4
1	В	258	HIS	2.4
1	D	257	LYS	2.4
1	С	408	ILE	2.4
1	D	278	GLU	2.4
1	В	301	GLU	2.3
1	А	297	LEU	2.3
1	С	330	ALA	2.3
1	А	309	ALA	2.3
1	С	325	GLU	2.3
1	А	314	GLU	2.2
1	С	321	ARG	2.2
1	А	279	TYR	2.2
1	А	274	ASP	2.2
1	D	459	ASN	2.2
1	С	318	GLU	2.2
1	D	458	VAL	2.2
1	В	319	ALA	2.2
1	D	395	PHE	2.2
1	В	317	TYR	2.1
1	С	284	LYS	2.1
1	C	254	LEU	2.1
1	A	305	LYS	2.1
1	A	316	ALA	2.1
1	В	395	PHE	2.1
1	D	261	LYS	2.0
1	В	304	ASN	2.0
1	D	284	LYS	2.0
1	A	407	GLY	2.0
1	D	49	SER	2.0



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Mol	Chain	Res	Type	RSRZ
1	В	21	MET	2.0
1	В	289	PHE	2.0
1	С	289	PHE	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	$B-factors(Å^2)$	Q<0.9
2	PO4	А	4001	5/5	0.89	0.16	85,86,87,87	0
2	PO4	D	4005	5/5	0.89	0.23	113,114,114,114	0
2	PO4	В	4007	5/5	0.90	0.20	88,89,90,90	0
2	PO4	D	4006	5/5	0.91	0.16	75,75,76,77	0
2	PO4	В	4008	5/5	0.92	0.17	82,83,84,84	0
3	IPA	А	6003	4/4	0.94	0.19	58,59,59,60	0
3	IPA	А	6001	4/4	0.95	0.15	44,44,45,45	0
2	PO4	В	4002	5/5	0.96	0.12	64,67,67,68	0
3	IPA	А	6002	4/4	0.96	0.10	40,41,41,41	0
2	PO4	D	4004	5/5	0.96	0.15	65,65,66,67	0
2	PO4	С	4003	5/5	0.97	0.12	89,89,90,90	0

6.5 Other polymers (i)

There are no such residues in this entry.

