



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2024 – 04:09 PM EST

PDB ID : 4NSC  
Title : Crystal Structure of CBARA1 in the Apo-form  
Authors : Wang, L.; Yang, X.; Li, S.; Shen, Y.  
Deposited on : 2013-11-28  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
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

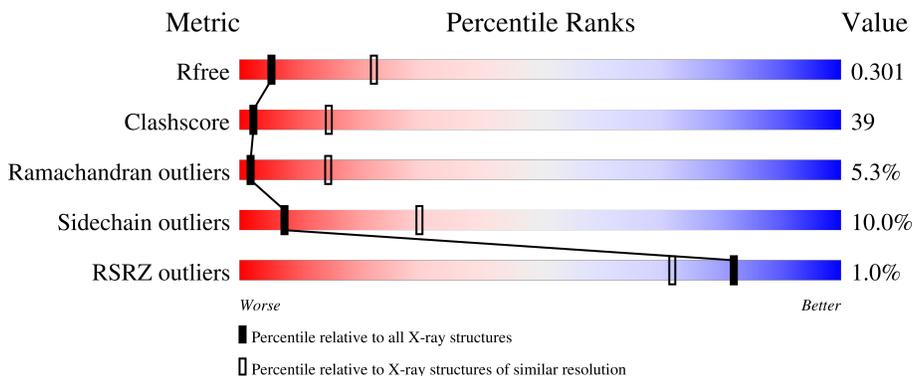
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



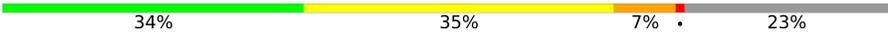
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	A	401	
1	B	401	
1	C	401	
1	D	401	
1	E	401	

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Mol	Chain	Length	Quality of chain
1	F	401	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into four segments: a green segment on the left labeled '34%', a yellow segment labeled '35%', a small red segment labeled '7%', and a grey segment on the right labeled '23%'. The segments are separated by thin white lines.</p>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 15349 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.

- Molecule 1 is a protein called Calcium uptake protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	310	Total 2472	C 1583	N 419	O 454	S 16	0	0	0
1	B	316	Total 2539	C 1622	N 426	O 473	S 18	0	0	0
1	C	330	Total 2619	C 1673	N 442	O 486	S 18	0	0	0
1	D	326	Total 2604	C 1662	N 438	O 487	S 17	0	0	0
1	E	330	Total 2598	C 1657	N 439	O 487	S 15	0	0	0
1	F	310	Total 2504	C 1601	N 422	O 468	S 13	0	0	0

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	MET	-	expression tag	UNP Q9BPX6
A	77	HIS	-	expression tag	UNP Q9BPX6
A	78	HIS	-	expression tag	UNP Q9BPX6
A	79	HIS	-	expression tag	UNP Q9BPX6
A	80	HIS	-	expression tag	UNP Q9BPX6
A	81	HIS	-	expression tag	UNP Q9BPX6
A	82	HIS	-	expression tag	UNP Q9BPX6
A	83	SER	-	expression tag	UNP Q9BPX6
A	84	SER	-	expression tag	UNP Q9BPX6
A	85	GLY	-	expression tag	UNP Q9BPX6
A	86	LEU	-	expression tag	UNP Q9BPX6
A	87	GLU	-	expression tag	UNP Q9BPX6
A	88	VAL	-	expression tag	UNP Q9BPX6
A	89	LEU	-	expression tag	UNP Q9BPX6
A	90	PHE	-	expression tag	UNP Q9BPX6
A	91	GLN	-	expression tag	UNP Q9BPX6
A	92	GLY	-	expression tag	UNP Q9BPX6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	93	PRO	-	expression tag	UNP Q9BPX6
A	94	GLY	-	expression tag	UNP Q9BPX6
A	95	SER	-	expression tag	UNP Q9BPX6
A	96	MET	-	expression tag	UNP Q9BPX6
B	76	MET	-	expression tag	UNP Q9BPX6
B	77	HIS	-	expression tag	UNP Q9BPX6
B	78	HIS	-	expression tag	UNP Q9BPX6
B	79	HIS	-	expression tag	UNP Q9BPX6
B	80	HIS	-	expression tag	UNP Q9BPX6
B	81	HIS	-	expression tag	UNP Q9BPX6
B	82	HIS	-	expression tag	UNP Q9BPX6
B	83	SER	-	expression tag	UNP Q9BPX6
B	84	SER	-	expression tag	UNP Q9BPX6
B	85	GLY	-	expression tag	UNP Q9BPX6
B	86	LEU	-	expression tag	UNP Q9BPX6
B	87	GLU	-	expression tag	UNP Q9BPX6
B	88	VAL	-	expression tag	UNP Q9BPX6
B	89	LEU	-	expression tag	UNP Q9BPX6
B	90	PHE	-	expression tag	UNP Q9BPX6
B	91	GLN	-	expression tag	UNP Q9BPX6
B	92	GLY	-	expression tag	UNP Q9BPX6
B	93	PRO	-	expression tag	UNP Q9BPX6
B	94	GLY	-	expression tag	UNP Q9BPX6
B	95	SER	-	expression tag	UNP Q9BPX6
B	96	MET	-	expression tag	UNP Q9BPX6
C	76	MET	-	expression tag	UNP Q9BPX6
C	77	HIS	-	expression tag	UNP Q9BPX6
C	78	HIS	-	expression tag	UNP Q9BPX6
C	79	HIS	-	expression tag	UNP Q9BPX6
C	80	HIS	-	expression tag	UNP Q9BPX6
C	81	HIS	-	expression tag	UNP Q9BPX6
C	82	HIS	-	expression tag	UNP Q9BPX6
C	83	SER	-	expression tag	UNP Q9BPX6
C	84	SER	-	expression tag	UNP Q9BPX6
C	85	GLY	-	expression tag	UNP Q9BPX6
C	86	LEU	-	expression tag	UNP Q9BPX6
C	87	GLU	-	expression tag	UNP Q9BPX6
C	88	VAL	-	expression tag	UNP Q9BPX6
C	89	LEU	-	expression tag	UNP Q9BPX6
C	90	PHE	-	expression tag	UNP Q9BPX6
C	91	GLN	-	expression tag	UNP Q9BPX6
C	92	GLY	-	expression tag	UNP Q9BPX6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	93	PRO	-	expression tag	UNP Q9BPX6
C	94	GLY	-	expression tag	UNP Q9BPX6
C	95	SER	-	expression tag	UNP Q9BPX6
C	96	MET	-	expression tag	UNP Q9BPX6
D	76	MET	-	expression tag	UNP Q9BPX6
D	77	HIS	-	expression tag	UNP Q9BPX6
D	78	HIS	-	expression tag	UNP Q9BPX6
D	79	HIS	-	expression tag	UNP Q9BPX6
D	80	HIS	-	expression tag	UNP Q9BPX6
D	81	HIS	-	expression tag	UNP Q9BPX6
D	82	HIS	-	expression tag	UNP Q9BPX6
D	83	SER	-	expression tag	UNP Q9BPX6
D	84	SER	-	expression tag	UNP Q9BPX6
D	85	GLY	-	expression tag	UNP Q9BPX6
D	86	LEU	-	expression tag	UNP Q9BPX6
D	87	GLU	-	expression tag	UNP Q9BPX6
D	88	VAL	-	expression tag	UNP Q9BPX6
D	89	LEU	-	expression tag	UNP Q9BPX6
D	90	PHE	-	expression tag	UNP Q9BPX6
D	91	GLN	-	expression tag	UNP Q9BPX6
D	92	GLY	-	expression tag	UNP Q9BPX6
D	93	PRO	-	expression tag	UNP Q9BPX6
D	94	GLY	-	expression tag	UNP Q9BPX6
D	95	SER	-	expression tag	UNP Q9BPX6
D	96	MET	-	expression tag	UNP Q9BPX6
E	76	MET	-	expression tag	UNP Q9BPX6
E	77	HIS	-	expression tag	UNP Q9BPX6
E	78	HIS	-	expression tag	UNP Q9BPX6
E	79	HIS	-	expression tag	UNP Q9BPX6
E	80	HIS	-	expression tag	UNP Q9BPX6
E	81	HIS	-	expression tag	UNP Q9BPX6
E	82	HIS	-	expression tag	UNP Q9BPX6
E	83	SER	-	expression tag	UNP Q9BPX6
E	84	SER	-	expression tag	UNP Q9BPX6
E	85	GLY	-	expression tag	UNP Q9BPX6
E	86	LEU	-	expression tag	UNP Q9BPX6
E	87	GLU	-	expression tag	UNP Q9BPX6
E	88	VAL	-	expression tag	UNP Q9BPX6
E	89	LEU	-	expression tag	UNP Q9BPX6
E	90	PHE	-	expression tag	UNP Q9BPX6
E	91	GLN	-	expression tag	UNP Q9BPX6
E	92	GLY	-	expression tag	UNP Q9BPX6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	93	PRO	-	expression tag	UNP Q9BPX6
E	94	GLY	-	expression tag	UNP Q9BPX6
E	95	SER	-	expression tag	UNP Q9BPX6
E	96	MET	-	expression tag	UNP Q9BPX6
F	76	MET	-	expression tag	UNP Q9BPX6
F	77	HIS	-	expression tag	UNP Q9BPX6
F	78	HIS	-	expression tag	UNP Q9BPX6
F	79	HIS	-	expression tag	UNP Q9BPX6
F	80	HIS	-	expression tag	UNP Q9BPX6
F	81	HIS	-	expression tag	UNP Q9BPX6
F	82	HIS	-	expression tag	UNP Q9BPX6
F	83	SER	-	expression tag	UNP Q9BPX6
F	84	SER	-	expression tag	UNP Q9BPX6
F	85	GLY	-	expression tag	UNP Q9BPX6
F	86	LEU	-	expression tag	UNP Q9BPX6
F	87	GLU	-	expression tag	UNP Q9BPX6
F	88	VAL	-	expression tag	UNP Q9BPX6
F	89	LEU	-	expression tag	UNP Q9BPX6
F	90	PHE	-	expression tag	UNP Q9BPX6
F	91	GLN	-	expression tag	UNP Q9BPX6
F	92	GLY	-	expression tag	UNP Q9BPX6
F	93	PRO	-	expression tag	UNP Q9BPX6
F	94	GLY	-	expression tag	UNP Q9BPX6
F	95	SER	-	expression tag	UNP Q9BPX6
F	96	MET	-	expression tag	UNP Q9BPX6

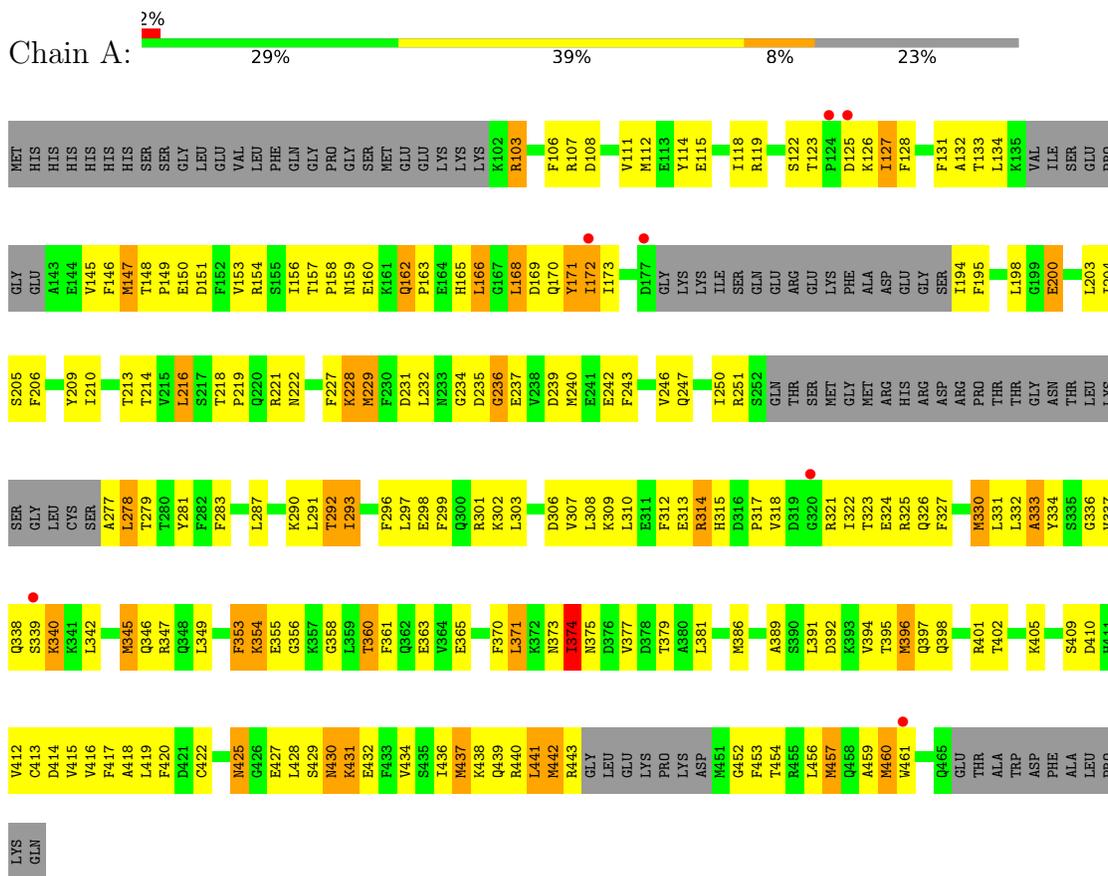
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total O 4 4	0	0
2	B	3	Total O 3 3	0	0
2	C	1	Total O 1 1	0	0
2	D	1	Total O 1 1	0	0
2	F	4	Total O 4 4	0	0

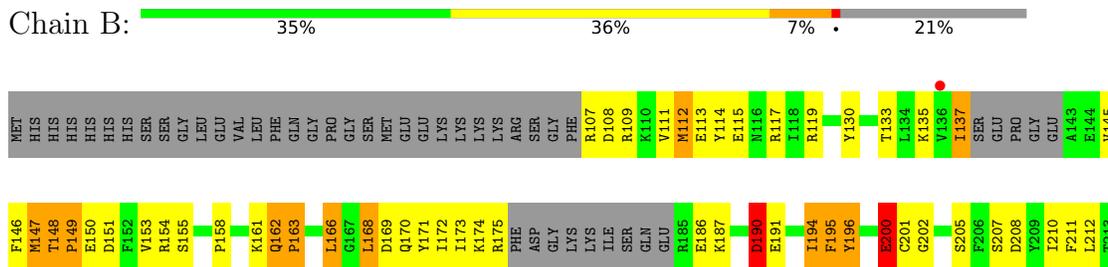
### 3 Residue-property plots

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.

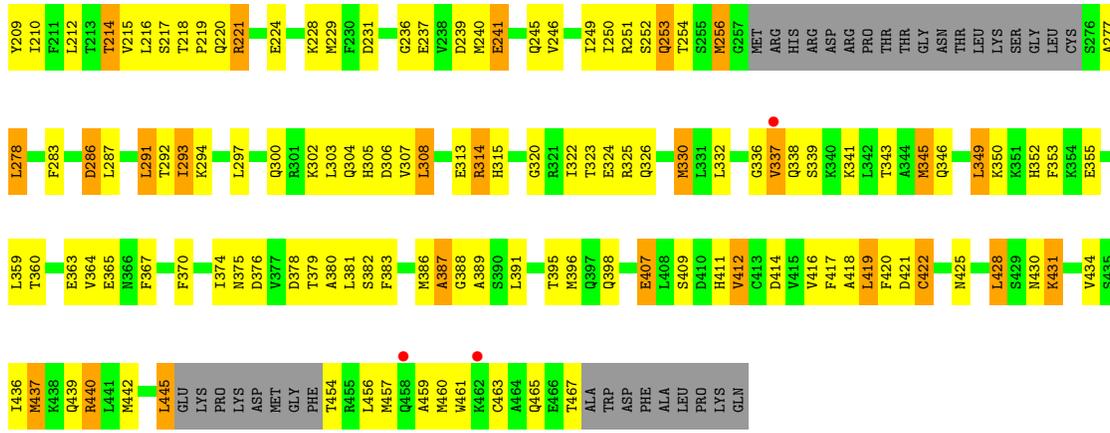
- Molecule 1: Calcium uptake protein 1, mitochondrial



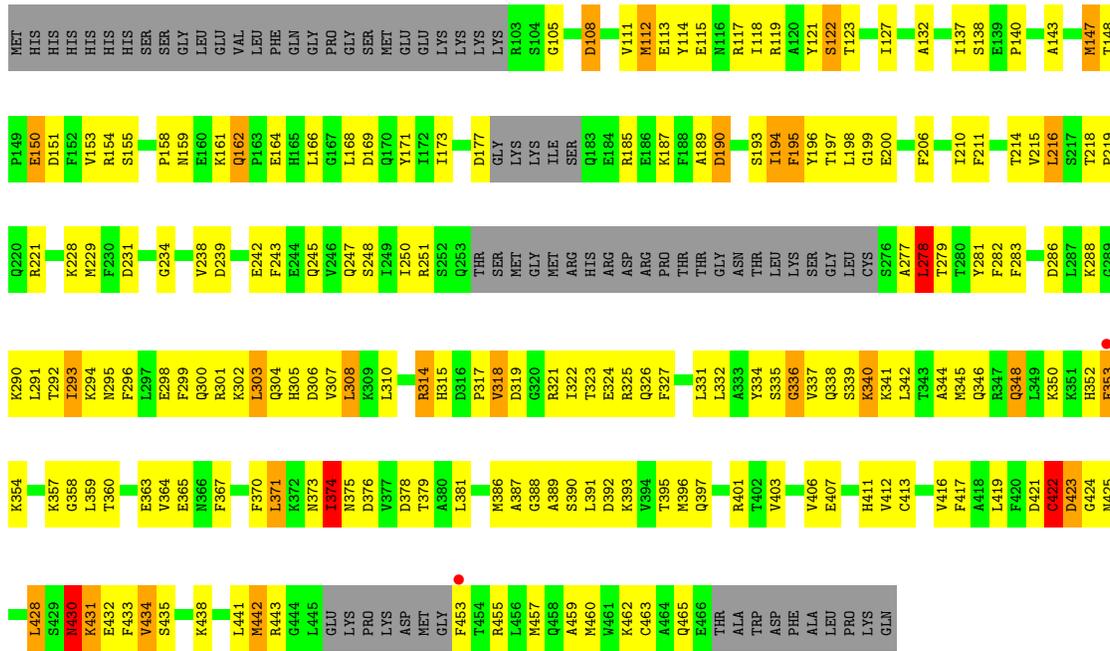
- Molecule 1: Calcium uptake protein 1, mitochondrial



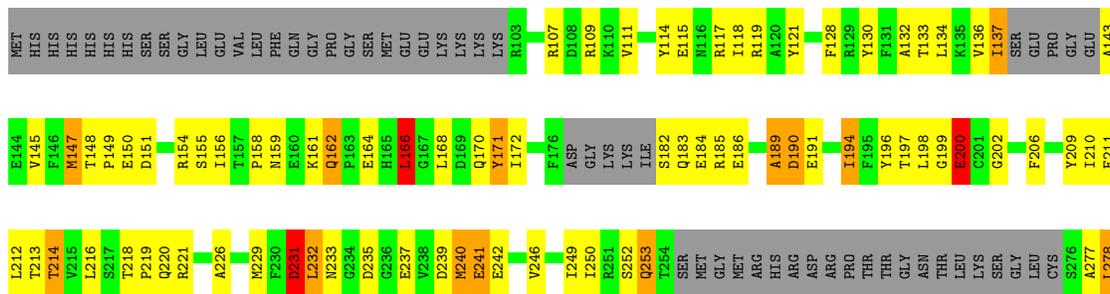




• Molecule 1: Calcium uptake protein 1, mitochondrial



• Molecule 1: Calcium uptake protein 1, mitochondrial



T379	T360	E432	GLY
T280	F361	F433	LEU
Y281	E365	V434	GLU
F283	N366	S435	LYS
D286	F367	I436	PRO
L287	F368	M437	LYS
L291	T369	K438	LYS
T292	F370	Q439	ASP
I293	F371	R440	MET
K294	K372	L441	GLY
L297	N373	M442	PHE
L303	I374	R443	THR
D306	N375	LEU	ARG
V307	D376	MET	LEU
L308	V377	GLN	MET
K309	D378	ALA	ALA
L310	T379	V394	GLN
E313	F383	T395	MET
R314	M386	M396	TRP
H315	S390	V399	LYS
V318	K393	T402	CYS
D319	V394	V403	ALA
G320	T395	A404	GLN
R321	M396	K405	GLU
I322	V399	L408	THR
T323	T402	S409	ALA
E324	V403	D410	TRP
R325	A404	H411	ASP
Q326	K405	V412	PHE
F327	L408	C413	ALA
M330	S409	D414	LEU
G336	H411	V415	PRO
V337	V412	F417	LYS
Q338	C413	A418	GLN
S339	D414	V419	
K340	V415	F420	
M345	F417	A419	
Q346	A418	D420	
Q346	L419	D421	
L349	F420	C422	
K350	D421	D423	
K351	C422	G424	
H352	D423	N425	
F353	G424	G426	
K354	N425	E427	
E355	G426	L428	
G356	E427	K431	
K357	L428		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.88Å 146.82Å 115.87Å 90.00° 111.08° 90.00°	Depositor
Resolution (Å)	36.72 – 3.20 36.71 – 3.20	Depositor EDS
% Data completeness (in resolution range)	92.3 (36.72-3.20) 92.4 (36.71-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 3.18Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.254 , 0.307 0.254 , 0.301	Depositor DCC
$R_{free}$ test set	2007 reflections (4.31%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.1	Xtrriage
Anisotropy	0.235	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 50.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	15349	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 5 Model quality i

### 5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.61	10/2517 (0.4%)	0.66	1/3379 (0.0%)
1	B	0.67	10/2581 (0.4%)	0.68	0/3456
1	C	0.65	9/2665 (0.3%)	0.68	1/3577 (0.0%)
1	D	0.69	8/2649 (0.3%)	0.73	0/3551
1	E	0.62	4/2644 (0.2%)	0.73	1/3550 (0.0%)
1	F	0.64	5/2549 (0.2%)	0.74	2/3418 (0.1%)
All	All	0.65	46/15605 (0.3%)	0.71	5/20931 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	147	MET	CG-SD	9.03	2.04	1.81
1	D	147	MET	CG-SD	8.10	2.02	1.81
1	D	229	MET	CG-SD	7.68	2.01	1.81
1	F	442	MET	CG-SD	7.67	2.01	1.81
1	D	256	MET	CG-SD	7.62	2.00	1.81
1	B	442	MET	CG-SD	7.54	2.00	1.81
1	F	147	MET	CG-SD	7.50	2.00	1.81
1	A	460	MET	CG-SD	7.38	2.00	1.81
1	A	147	MET	CG-SD	7.31	2.00	1.81
1	B	258	MET	CG-SD	7.04	1.99	1.81
1	E	147	MET	CG-SD	6.79	1.98	1.81
1	D	396	MET	CG-SD	6.74	1.98	1.81
1	E	229	MET	CG-SD	6.73	1.98	1.81
1	B	457	MET	CG-SD	6.71	1.98	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	457	MET	CG-SD	6.69	1.98	1.81
1	A	442	MET	CG-SD	6.50	1.98	1.81
1	C	330	MET	CG-SD	6.44	1.97	1.81
1	B	147	MET	CG-SD	6.26	1.97	1.81
1	F	396	MET	CG-SD	6.07	1.97	1.81
1	D	437	MET	CG-SD	6.04	1.96	1.81
1	F	386	MET	CG-SD	6.00	1.96	1.81
1	F	229	MET	CG-SD	5.95	1.96	1.81
1	C	229	MET	CG-SD	5.88	1.96	1.81
1	C	442	MET	CG-SD	5.87	1.96	1.81
1	E	396	MET	CG-SD	5.78	1.96	1.81
1	C	457	MET	CG-SD	5.74	1.96	1.81
1	B	345	MET	CG-SD	5.70	1.96	1.81
1	B	256	MET	CG-SD	5.68	1.96	1.81
1	C	396	MET	CG-SD	5.62	1.95	1.81
1	D	345	MET	CG-SD	5.59	1.95	1.81
1	D	330	MET	CG-SD	5.59	1.95	1.81
1	B	229	MET	CG-SD	5.52	1.95	1.81
1	A	330	MET	CG-SD	5.50	1.95	1.81
1	A	345	MET	CG-SD	5.43	1.95	1.81
1	A	112	MET	CG-SD	5.41	1.95	1.81
1	B	112	MET	CG-SD	5.41	1.95	1.81
1	A	229	MET	CG-SD	5.37	1.95	1.81
1	C	258	MET	CG-SD	5.35	1.95	1.81
1	A	437	MET	CG-SD	5.28	1.94	1.81
1	D	442	MET	CG-SD	5.22	1.94	1.81
1	B	330	MET	CG-SD	5.13	1.94	1.81
1	B	437	MET	CG-SD	5.13	1.94	1.81
1	C	112	MET	CG-SD	5.12	1.94	1.81
1	A	386	MET	CG-SD	5.09	1.94	1.81
1	C	460	MET	CG-SD	5.04	1.94	1.81
1	E	442	MET	CG-SD	5.02	1.94	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	448	PRO	N-CA-CB	6.02	110.52	103.30
1	F	356	GLY	N-CA-C	5.90	127.85	113.10
1	E	278	LEU	CA-CB-CG	5.53	128.02	115.30
1	F	166	LEU	CA-CB-CG	-5.36	102.97	115.30
1	A	441	LEU	CA-CB-CG	5.26	127.39	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	196	TYR	Sidechain

## 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	A	2472	0	2397	221	0
1	B	2539	0	2496	197	0
1	C	2619	0	2542	230	0
1	D	2604	0	2547	208	0
1	E	2598	0	2494	184	1
1	F	2504	0	2458	197	1
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	F	4	0	0	0	0
All	All	15349	0	14934	1171	1

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 39.

All (1171) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:MET:SD	1:D:147:MET:CG	2.02	1.48
1:C:147:MET:CG	1:C:147:MET:SD	2.04	1.44
1:C:323:THR:HB	1:C:326:GLN:HG3	1.23	1.14
1:F:323:THR:HB	1:F:326:GLN:HG3	1.23	1.14
1:E:323:THR:HB	1:E:326:GLN:HG3	1.28	1.14
1:F:422:CYS:HB2	1:F:425:ASN:HD22	1.13	1.12
1:B:323:THR:HB	1:B:326:GLN:HG3	1.11	1.08
1:E:390:SER:HB2	1:F:337:VAL:HG11	1.30	1.07
1:D:323:THR:HG22	1:D:325:ARG:H	1.20	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:THR:HG22	1:C:325:ARG:H	1.18	1.04
1:C:454:THR:HG21	1:E:460:MET:HB3	1.36	1.03
1:C:346:GLN:HE22	1:C:355:GLU:HG3	1.20	1.02
1:A:459:ALA:HB1	1:D:456:LEU:HD22	1.35	1.02
1:D:431:LYS:H	1:D:431:LYS:HD3	1.25	1.01
1:F:323:THR:HG22	1:F:325:ARG:H	1.25	1.00
1:E:194:ILE:HD12	1:E:195:PHE:H	1.23	0.99
1:C:154:ARG:HH21	1:C:162:GLN:NE2	1.59	0.99
1:C:174:LYS:HD2	1:C:186:GLU:OE1	1.66	0.96
1:A:460:MET:HG3	1:B:460:MET:HE1	1.47	0.96
1:C:293:ILE:HD12	1:C:293:ILE:H	1.28	0.96
1:B:323:THR:CB	1:B:326:GLN:HG3	1.96	0.94
1:F:422:CYS:HB2	1:F:425:ASN:ND2	1.82	0.93
1:F:323:THR:H	1:F:326:GLN:NE2	1.67	0.93
1:D:154:ARG:HE	1:D:162:GLN:HE21	1.09	0.93
1:E:390:SER:CB	1:F:337:VAL:HG11	1.99	0.92
1:E:315:HIS:HB3	1:E:326:GLN:OE1	1.70	0.92
1:C:154:ARG:HH21	1:C:162:GLN:HE22	1.12	0.91
1:E:194:ILE:HD12	1:E:195:PHE:N	1.84	0.91
1:A:172:ILE:HG22	1:A:173:ILE:H	1.36	0.90
1:B:149:PRO:HB3	1:B:310:LEU:HD21	1.54	0.90
1:E:303:LEU:O	1:E:307:VAL:HG23	1.72	0.89
1:F:323:THR:H	1:F:326:GLN:HE21	0.99	0.89
1:D:210:ILE:O	1:D:214:THR:HG23	1.70	0.89
1:C:454:THR:CG2	1:E:460:MET:HB3	2.01	0.89
1:B:323:THR:HG22	1:B:325:ARG:H	1.38	0.89
1:C:357:LYS:HB2	1:C:411:HIS:CE1	2.10	0.87
1:A:107:ARG:O	1:A:111:VAL:HG23	1.74	0.86
1:A:457:MET:HE3	1:A:461:TRP:HE1	1.37	0.86
1:C:119:ARG:HD3	1:C:155:SER:O	1.76	0.86
1:F:154:ARG:HD3	1:F:314:ARG:HH21	1.38	0.86
1:E:154:ARG:HH11	1:E:314:ARG:HH21	1.24	0.86
1:C:292:THR:HG22	1:C:294:LYS:H	1.41	0.86
1:D:194:ILE:HD12	1:D:195:PHE:N	1.90	0.85
1:B:293:ILE:HD12	1:B:294:LYS:H	1.42	0.85
1:B:190:ASP:O	1:B:196:TYR:HE2	1.58	0.85
1:C:323:THR:HG22	1:C:325:ARG:N	1.91	0.85
1:F:323:THR:CB	1:F:326:GLN:HG3	2.06	0.85
1:A:133:THR:O	1:A:134:LEU:HD23	1.76	0.85
1:A:360:THR:HG23	1:A:363:GLU:HG3	1.59	0.85
1:F:346:GLN:O	1:F:350:LYS:HG3	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ARG:HD3	1:A:358:GLY:HA3	1.59	0.85
1:B:292:THR:HG22	1:B:293:ILE:HD12	1.59	0.85
1:B:436:ILE:HD12	1:B:436:ILE:H	1.42	0.84
1:F:154:ARG:HE	1:F:162:GLN:HE21	1.19	0.84
1:C:335:SER:HA	1:C:439:GLN:OE1	1.78	0.84
1:A:119:ARG:HH21	1:A:158:PRO:HA	1.42	0.84
1:D:218:THR:HG21	1:D:250:ILE:CG2	2.07	0.84
1:A:218:THR:HG21	1:A:250:ILE:CG2	2.08	0.83
1:B:323:THR:HB	1:B:326:GLN:CG	2.05	0.83
1:D:217:SER:HB2	1:D:445:LEU:HD23	1.61	0.82
1:E:388:GLY:O	1:F:337:VAL:HG23	1.80	0.82
1:C:412:VAL:O	1:C:416:VAL:HG23	1.78	0.81
1:A:163:PRO:HB2	1:A:166:LEU:HD12	1.62	0.81
1:E:148:THR:OG1	1:E:150:GLU:HG2	1.80	0.81
1:F:323:THR:N	1:F:326:GLN:HE21	1.78	0.81
1:C:431:LYS:HG2	1:C:432:GLU:H	1.45	0.81
1:F:412:VAL:O	1:F:416:VAL:HG23	1.80	0.80
1:D:117:ARG:HD2	1:D:461:TRP:CH2	2.16	0.80
1:D:231:ASP:HB2	1:D:237:GLU:H	1.45	0.80
1:D:160:GLU:HB3	1:D:314:ARG:HH12	1.45	0.80
1:C:346:GLN:NE2	1:C:355:GLU:HG3	1.97	0.80
1:D:374:ILE:HD12	1:D:375:ASN:H	1.46	0.80
1:F:252:SER:O	1:F:253:GLN:HG3	1.82	0.79
1:E:173:ILE:N	1:E:173:ILE:HD12	1.97	0.79
1:A:293:ILE:HD12	1:A:293:ILE:H	1.48	0.79
1:B:292:THR:HG22	1:B:294:LYS:H	1.46	0.79
1:B:350:LYS:HG2	1:B:355:GLU:OE1	1.82	0.78
1:C:154:ARG:HD3	1:C:314:ARG:HH21	1.47	0.78
1:B:166:LEU:HD21	1:B:172:ILE:HG13	1.66	0.78
1:B:221:ARG:HB2	1:B:221:ARG:HH11	1.46	0.78
1:C:374:ILE:HD13	1:C:438:LYS:HE2	1.64	0.78
1:E:153:VAL:HG22	1:E:307:VAL:HG13	1.64	0.78
1:B:187:LYS:HA	1:B:201:CYS:HB3	1.65	0.78
1:C:154:ARG:NH2	1:C:162:GLN:NE2	2.32	0.78
1:A:103:ARG:HE	1:D:241:GLU:HG3	1.49	0.77
1:C:392:ASP:OD2	1:C:395:THR:HG23	1.83	0.77
1:D:154:ARG:NE	1:D:162:GLN:HE21	1.81	0.77
1:C:210:ILE:O	1:C:214:THR:HG23	1.85	0.77
1:C:220:GLN:HG3	1:C:297:LEU:HD22	1.67	0.77
1:D:206:PHE:O	1:D:210:ILE:HD13	1.83	0.77
1:F:367:PHE:O	1:F:370:PHE:HB3	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ARG:HD3	1:B:314:ARG:NH2	1.99	0.76
1:C:194:ILE:HD12	1:C:195:PHE:H	1.49	0.76
1:D:166:LEU:HD21	1:D:172:ILE:HG13	1.68	0.76
1:F:337:VAL:HG12	1:F:337:VAL:O	1.84	0.76
1:C:357:LYS:HB2	1:C:411:HIS:HE1	1.51	0.76
1:A:292:THR:HG22	1:A:293:ILE:HD12	1.68	0.76
1:F:409:SER:HB3	1:F:412:VAL:HG23	1.67	0.76
1:B:154:ARG:HH11	1:B:314:ARG:HH21	1.32	0.76
1:B:430:ASN:N	1:B:430:ASN:HD22	1.83	0.75
1:F:345:MET:CE	1:F:419:LEU:HG	2.16	0.75
1:A:222:ASN:HD22	1:B:383:PHE:HZ	1.34	0.75
1:B:315:HIS:O	1:B:316:ASP:HB2	1.86	0.75
1:B:366:ASN:ND2	1:B:406:VAL:HG23	2.02	0.74
1:E:238:VAL:HG13	1:E:242:GLU:HB2	1.69	0.74
1:A:278:LEU:O	1:A:281:TYR:HB3	1.86	0.74
1:B:325:ARG:HA	1:B:345:MET:HE1	1.70	0.74
1:C:315:HIS:HB3	1:C:322:ILE:HD11	1.70	0.74
1:D:454:THR:C	1:D:456:LEU:H	1.91	0.74
1:F:132:ALA:HB2	1:F:147:MET:HB3	1.67	0.74
1:C:315:HIS:CB	1:C:322:ILE:HD11	2.17	0.74
1:C:137:ILE:CD1	1:C:175:ARG:HA	2.17	0.74
1:B:107:ARG:O	1:B:111:VAL:HG23	1.87	0.73
1:D:240:MET:HG3	1:D:283:PHE:CD2	2.24	0.73
1:C:376:ASP:OD1	1:E:221:ARG:HD3	1.88	0.73
1:D:338:GLN:HE21	1:D:341:LYS:HE2	1.54	0.73
1:C:436:ILE:O	1:C:439:GLN:HG2	1.89	0.73
1:F:194:ILE:HG12	1:F:303:LEU:HA	1.70	0.73
1:E:210:ILE:O	1:E:214:THR:HG23	1.87	0.73
1:F:154:ARG:HD3	1:F:314:ARG:NH2	2.05	0.72
1:F:210:ILE:O	1:F:214:THR:HG23	1.90	0.72
1:A:103:ARG:HG2	1:A:103:ARG:HH11	1.54	0.72
1:D:431:LYS:H	1:D:431:LYS:CD	2.02	0.72
1:E:357:LYS:HB2	1:E:411:HIS:CE1	2.24	0.72
1:B:154:ARG:HH11	1:B:314:ARG:NH2	1.86	0.72
1:A:115:GLU:HA	1:A:118:ILE:HD12	1.71	0.72
1:A:166:LEU:O	1:A:170:GLN:HB2	1.90	0.72
1:A:153:VAL:HG21	1:A:310:LEU:HB3	1.70	0.72
1:B:435:SER:O	1:B:438:LYS:HB2	1.90	0.71
1:D:336:GLY:C	1:D:338:GLN:H	1.91	0.71
1:B:429:SER:HB2	1:B:431:LYS:HE2	1.71	0.71
1:C:137:ILE:HD11	1:C:175:ARG:HA	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:PHE:HE2	1:C:436:ILE:HD12	1.56	0.71
1:A:409:SER:OG	1:A:412:VAL:HG23	1.89	0.71
1:F:189:ALA:HB2	1:F:202:GLY:HA3	1.70	0.71
1:D:323:THR:H	1:D:326:GLN:NE2	1.87	0.71
1:E:247:GLN:HE21	1:E:251:ARG:HH12	1.36	0.71
1:F:189:ALA:HB3	1:F:196:TYR:CZ	2.26	0.71
1:A:293:ILE:HD12	1:A:293:ILE:N	2.05	0.71
1:B:367:PHE:O	1:B:370:PHE:HB3	1.91	0.71
1:B:315:HIS:HB3	1:B:322:ILE:HD11	1.73	0.70
1:C:303:LEU:O	1:C:307:VAL:HG23	1.91	0.70
1:B:366:ASN:HD22	1:B:406:VAL:CG2	2.05	0.70
1:A:456:LEU:HB2	1:D:463:CYS:SG	2.31	0.70
1:F:422:CYS:CB	1:F:425:ASN:HD22	1.99	0.70
1:A:194:ILE:HG23	1:A:306:ASP:OD1	1.92	0.70
1:E:323:THR:CB	1:E:326:GLN:HG3	2.17	0.70
1:C:154:ARG:NH2	1:C:162:GLN:HE22	1.88	0.70
1:B:366:ASN:HD22	1:B:406:VAL:HG23	1.54	0.70
1:E:293:ILE:HD12	1:E:293:ILE:H	1.56	0.69
1:F:315:HIS:HB2	1:F:322:ILE:HD11	1.74	0.69
1:B:373:ASN:O	1:B:375:ASN:N	2.24	0.69
1:C:239:ASP:CG	1:C:242:GLU:HG3	2.13	0.69
1:C:420:PHE:CE2	1:C:436:ILE:HD12	2.27	0.69
1:E:412:VAL:O	1:E:416:VAL:HG23	1.91	0.69
1:A:459:ALA:CB	1:D:456:LEU:HD22	2.18	0.69
1:F:182:SER:C	1:F:184:GLU:H	1.95	0.69
1:D:117:ARG:HD2	1:D:461:TRP:HH2	1.56	0.69
1:F:111:VAL:O	1:F:115:GLU:HG3	1.93	0.69
1:B:113:GLU:O	1:B:117:ARG:HG2	1.93	0.69
1:C:166:LEU:HD21	1:C:172:ILE:HD11	1.74	0.69
1:A:237:GLU:HB3	1:A:290:LYS:HE3	1.75	0.68
1:D:386:MET:C	1:D:388:GLY:H	1.95	0.68
1:F:431:LYS:HG2	1:F:432:GLU:H	1.59	0.68
1:A:198:LEU:HD13	1:A:204:ILE:HG12	1.74	0.68
1:B:323:THR:H	1:B:326:GLN:HE21	1.41	0.68
1:E:323:THR:HG22	1:E:324:GLU:N	2.07	0.68
1:E:453:PHE:O	1:E:457:MET:HB2	1.94	0.68
1:B:360:THR:HG23	1:B:363:GLU:HG3	1.76	0.68
1:D:338:GLN:HE21	1:D:341:LYS:CE	2.06	0.68
1:A:431:LYS:H	1:A:431:LYS:HD3	1.57	0.68
1:A:414:ASP:O	1:A:418:ALA:HB2	1.93	0.68
1:E:193:SER:O	1:E:195:PHE:N	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:317:PRO:HG3	1:E:322:ILE:CD1	2.24	0.68
1:B:278:LEU:O	1:B:281:TYR:HB3	1.95	0.67
1:A:149:PRO:HB3	1:A:310:LEU:HD11	1.76	0.67
1:C:292:THR:HG22	1:C:294:LYS:N	2.09	0.67
1:C:436:ILE:HA	1:C:439:GLN:HE21	1.60	0.67
1:C:327:PHE:CE1	1:C:364:VAL:HG22	2.29	0.67
1:B:242:GLU:O	1:B:246:VAL:HG12	1.94	0.67
1:B:431:LYS:H	1:B:431:LYS:HD3	1.59	0.67
1:F:115:GLU:OE2	1:F:162:GLN:HB2	1.95	0.67
1:D:293:ILE:HD12	1:D:293:ILE:H	1.58	0.67
1:D:374:ILE:HD12	1:D:375:ASN:N	2.09	0.67
1:E:293:ILE:HD12	1:E:293:ILE:N	2.08	0.67
1:A:119:ARG:NH2	1:A:158:PRO:HA	2.11	0.66
1:C:130:TYR:CE2	1:C:162:GLN:HG3	2.30	0.66
1:F:431:LYS:H	1:F:431:LYS:HD3	1.59	0.66
1:A:323:THR:HB	1:A:326:GLN:HG3	1.76	0.66
1:B:442:MET:O	1:B:443:ARG:HB2	1.95	0.66
1:E:323:THR:HG22	1:E:325:ARG:H	1.61	0.66
1:D:313:GLU:C	1:D:315:HIS:H	1.99	0.66
1:C:402:THR:HB	1:E:228:LYS:HG2	1.78	0.66
1:D:111:VAL:O	1:D:114:TYR:HB3	1.95	0.66
1:D:154:ARG:HH21	1:D:162:GLN:NE2	1.94	0.66
1:F:154:ARG:HE	1:F:162:GLN:NE2	1.92	0.65
1:A:436:ILE:O	1:A:439:GLN:HG2	1.96	0.65
1:D:386:MET:O	1:D:388:GLY:N	2.30	0.65
1:A:373:ASN:C	1:A:377:VAL:HG23	2.17	0.65
1:A:456:LEU:HD13	1:D:460:MET:HA	1.77	0.65
1:B:190:ASP:CG	1:B:191:GLU:N	2.50	0.65
1:F:345:MET:HE2	1:F:419:LEU:HG	1.76	0.65
1:F:437:MET:HA	1:F:437:MET:CE	2.27	0.65
1:A:412:VAL:O	1:A:416:VAL:HG23	1.97	0.65
1:A:456:LEU:HD11	1:D:460:MET:HE2	1.78	0.65
1:F:107:ARG:O	1:F:111:VAL:HG23	1.96	0.65
1:D:350:LYS:HD3	1:D:355:GLU:OE1	1.96	0.65
1:B:346:GLN:HE21	1:B:346:GLN:CA	2.09	0.65
1:B:153:VAL:HG22	1:B:307:VAL:HG13	1.79	0.65
1:D:445:LEU:HD13	1:D:445:LEU:O	1.96	0.65
1:D:215:VAL:HG12	1:D:215:VAL:O	1.97	0.65
1:A:398:GLN:HE22	1:B:232:LEU:HD21	1.61	0.65
1:D:115:GLU:OE1	1:D:161:LYS:HA	1.97	0.65
1:F:189:ALA:HB2	1:F:202:GLY:CA	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:ASN:O	1:D:379:THR:HG22	1.97	0.64
1:E:367:PHE:O	1:E:370:PHE:HB3	1.97	0.64
1:A:323:THR:HG22	1:A:325:ARG:H	1.63	0.64
1:C:220:GLN:HG3	1:C:297:LEU:CD2	2.27	0.64
1:E:194:ILE:O	1:E:196:TYR:N	2.30	0.64
1:B:190:ASP:O	1:B:196:TYR:CE2	2.47	0.64
1:F:417:PHE:HE1	1:F:426:GLY:O	1.80	0.64
1:D:338:GLN:HE21	1:D:341:LYS:NZ	1.95	0.64
1:F:350:LYS:HG2	1:F:355:GLU:CD	2.18	0.64
1:A:441:LEU:HD13	1:A:441:LEU:O	1.98	0.64
1:A:460:MET:HG3	1:B:460:MET:CE	2.27	0.64
1:F:171:TYR:CD1	1:F:171:TYR:N	2.65	0.64
1:A:149:PRO:CB	1:A:310:LEU:HD11	2.28	0.64
1:A:240:MET:HG3	1:A:283:PHE:CD2	2.33	0.64
1:A:438:LYS:O	1:A:442:MET:HG2	1.97	0.64
1:F:132:ALA:CB	1:F:147:MET:HB3	2.28	0.64
1:A:394:VAL:O	1:A:397:GLN:HB2	1.98	0.64
1:B:377:VAL:O	1:B:381:LEU:HG	1.97	0.63
1:D:253:GLN:HE22	1:F:383:PHE:HE1	1.44	0.63
1:C:154:ARG:HE	1:C:162:GLN:HE21	1.46	0.63
1:D:300:GLN:O	1:D:304:GLN:HG3	1.99	0.63
1:D:363:GLU:HG2	1:D:409:SER:HB2	1.80	0.63
1:E:187:LYS:HB3	1:E:196:TYR:OH	1.97	0.63
1:B:436:ILE:HD12	1:B:436:ILE:N	2.13	0.63
1:C:353:PHE:N	1:C:353:PHE:CD2	2.66	0.63
1:D:166:LEU:HD21	1:D:172:ILE:CG1	2.28	0.63
1:E:359:LEU:HD23	1:E:363:GLU:OE1	1.98	0.63
1:F:137:ILE:HG22	1:F:143:ALA:HB2	1.80	0.63
1:A:227:PHE:C	1:A:229:MET:H	2.01	0.63
1:A:103:ARG:NE	1:D:241:GLU:HG3	2.14	0.63
1:A:154:ARG:HH11	1:A:314:ARG:NH2	1.96	0.63
1:C:332:LEU:H	1:C:332:LEU:HD12	1.62	0.63
1:C:431:LYS:H	1:C:431:LYS:HD3	1.64	0.63
1:E:306:ASP:O	1:E:310:LEU:HD23	1.99	0.63
1:F:166:LEU:HD21	1:F:172:ILE:HG13	1.81	0.63
1:C:295:ASN:O	1:C:298:GLU:HB3	1.98	0.63
1:C:457:MET:SD	1:E:460:MET:HE1	2.39	0.63
1:A:172:ILE:O	1:A:173:ILE:HG13	1.98	0.62
1:C:237:GLU:O	1:C:238:VAL:HG23	1.99	0.62
1:D:199:GLY:HA3	1:D:277:ALA:HB1	1.80	0.62
1:A:231:ASP:HB2	1:A:237:GLU:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:ASP:O	1:D:196:TYR:HE2	1.82	0.62
1:C:252:SER:HB2	1:E:386:MET:HE3	1.80	0.62
1:C:462:LYS:O	1:C:462:LYS:HG2	2.00	0.62
1:D:194:ILE:HD12	1:D:194:ILE:C	2.20	0.62
1:E:218:THR:HG21	1:E:250:ILE:CG2	2.29	0.62
1:C:215:VAL:HG13	1:C:300:GLN:HG3	1.81	0.62
1:C:318:VAL:O	1:C:319:ASP:HB2	2.00	0.62
1:D:146:PHE:HD1	1:D:203:LEU:HB3	1.64	0.62
1:E:214:THR:HG21	1:E:251:ARG:HD3	1.80	0.62
1:E:390:SER:HB2	1:F:337:VAL:CG1	2.19	0.62
1:C:293:ILE:HD12	1:C:293:ILE:N	2.09	0.62
1:D:293:ILE:HD12	1:D:293:ILE:N	2.14	0.62
1:F:293:ILE:HD12	1:F:293:ILE:H	1.63	0.62
1:A:347:ARG:NH1	1:F:425:ASN:HA	2.15	0.61
1:D:119:ARG:NH1	1:D:154:ARG:O	2.33	0.61
1:C:332:LEU:HD11	1:C:419:LEU:HD22	1.81	0.61
1:A:153:VAL:HG23	1:A:310:LEU:HD13	1.83	0.61
1:A:195:PHE:O	1:A:198:LEU:HD12	2.01	0.61
1:C:327:PHE:CD2	1:C:359:LEU:HD22	2.35	0.61
1:A:147:MET:HE2	1:A:151:ASP:HB3	1.82	0.61
1:C:303:LEU:O	1:C:303:LEU:HD23	2.01	0.61
1:C:380:ALA:HB2	1:C:403:VAL:HG21	1.81	0.61
1:A:148:THR:OG1	1:A:150:GLU:HG2	1.99	0.61
1:A:214:THR:HG21	1:A:251:ARG:HG2	1.81	0.61
1:B:324:GLU:OE1	1:B:411:HIS:NE2	2.33	0.61
1:C:353:PHE:N	1:C:353:PHE:HD2	1.98	0.61
1:F:345:MET:HG3	1:F:418:ALA:CB	2.30	0.61
1:A:210:ILE:HD12	1:A:210:ILE:N	2.15	0.61
1:C:292:THR:HG22	1:C:293:ILE:N	2.16	0.61
1:B:346:GLN:HE21	1:B:346:GLN:HA	1.65	0.61
1:C:113:GLU:HB3	1:C:117:ARG:HH21	1.65	0.61
1:C:337:VAL:O	1:C:339:SER:N	2.32	0.61
1:F:206:PHE:O	1:F:209:TYR:HB3	2.01	0.61
1:D:386:MET:C	1:D:388:GLY:N	2.53	0.61
1:F:148:THR:HG22	1:F:151:ASP:CG	2.20	0.61
1:A:428:LEU:HD13	1:A:429:SER:N	2.16	0.60
1:D:214:THR:HG21	1:D:251:ARG:HG2	1.83	0.60
1:F:345:MET:HG3	1:F:418:ALA:HB3	1.82	0.60
1:A:231:ASP:CB	1:A:237:GLU:H	2.15	0.60
1:E:431:LYS:HD3	1:E:431:LYS:H	1.65	0.60
1:F:375:ASN:O	1:F:379:THR:HG23	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:GLU:HB3	1:C:117:ARG:NH2	2.16	0.60
1:D:286:ASP:O	1:D:287:LEU:HB2	2.00	0.60
1:A:148:THR:HG22	1:A:203:LEU:HD22	1.83	0.60
1:A:342:LEU:N	1:A:342:LEU:HD12	2.17	0.60
1:A:122:SER:HB3	1:A:126:LYS:HB3	1.82	0.60
1:C:359:LEU:HA	1:C:363:GLU:OE1	2.02	0.60
1:B:111:VAL:O	1:B:114:TYR:HB3	2.01	0.60
1:B:163:PRO:HB2	1:B:166:LEU:HD12	1.83	0.60
1:F:351:LYS:HD2	1:F:352:HIS:CE1	2.37	0.60
1:A:322:ILE:HG12	1:A:326:GLN:HE21	1.67	0.59
1:B:162:GLN:NE2	1:B:163:PRO:HD2	2.16	0.59
1:F:324:GLU:OE1	1:F:411:HIS:CE1	2.55	0.59
1:A:123:THR:O	1:A:127:ILE:HG13	2.02	0.59
1:A:210:ILE:H	1:A:210:ILE:CD1	2.15	0.59
1:B:346:GLN:HA	1:B:346:GLN:NE2	2.17	0.59
1:C:119:ARG:CD	1:C:155:SER:O	2.50	0.59
1:E:173:ILE:HD12	1:E:173:ILE:H	1.67	0.59
1:A:373:ASN:O	1:A:377:VAL:HG23	2.02	0.59
1:E:318:VAL:O	1:E:319:ASP:HB2	2.01	0.59
1:F:286:ASP:O	1:F:287:LEU:HB2	2.02	0.59
1:C:148:THR:O	1:C:151:ASP:N	2.35	0.59
1:C:337:VAL:C	1:C:339:SER:H	2.06	0.59
1:F:390:SER:O	1:F:395:THR:HG21	2.02	0.59
1:B:112:MET:HG2	1:B:161:LYS:HG2	1.85	0.59
1:F:136:VAL:O	1:F:143:ALA:HA	2.02	0.59
1:A:322:ILE:CG1	1:A:326:GLN:HE21	2.16	0.59
1:C:419:LEU:HD12	1:C:419:LEU:H	1.67	0.59
1:C:332:LEU:HD12	1:C:332:LEU:N	2.17	0.59
1:D:214:THR:HB	1:D:254:THR:HG21	1.82	0.59
1:D:221:ARG:HE	1:D:221:ARG:HA	1.68	0.59
1:E:293:ILE:H	1:E:293:ILE:CD1	2.14	0.59
1:B:371:LEU:CD2	1:B:437:MET:HB3	2.33	0.59
1:C:316:ASP:N	1:C:317:PRO:HD3	2.18	0.59
1:F:374:ILE:O	1:F:378:ASP:N	2.31	0.59
1:B:437:MET:O	1:B:441:LEU:HB2	2.02	0.58
1:B:461:TRP:O	1:B:465:GLN:HG3	2.02	0.58
1:C:168:LEU:HD13	1:C:168:LEU:H	1.66	0.58
1:A:420:PHE:CE2	1:A:436:ILE:HD12	2.37	0.58
1:E:392:ASP:OD2	1:E:395:THR:HG23	2.02	0.58
1:B:149:PRO:CB	1:B:310:LEU:HD21	2.30	0.58
1:C:163:PRO:HB3	1:C:165:HIS:CE1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:460:MET:C	1:E:462:LYS:H	2.07	0.58
1:F:431:LYS:HG2	1:F:432:GLU:N	2.17	0.58
1:A:128:PHE:CD2	1:A:206:PHE:HD2	2.22	0.58
1:D:305:HIS:CD2	1:D:365:GLU:OE2	2.57	0.58
1:F:399:VAL:O	1:F:403:VAL:HB	2.03	0.58
1:B:220:GLN:HG2	1:B:297:LEU:HD22	1.85	0.58
1:B:323:THR:HG22	1:B:325:ARG:N	2.12	0.58
1:E:194:ILE:O	1:E:197:THR:N	2.36	0.58
1:F:189:ALA:O	1:F:190:ASP:HB2	2.02	0.58
1:A:156:ILE:HD12	1:A:443:ARG:HD3	1.86	0.58
1:A:375:ASN:O	1:A:379:THR:HG23	2.04	0.58
1:B:430:ASN:N	1:B:430:ASN:ND2	2.51	0.58
1:E:231:ASP:OD2	1:E:234:GLY:HA3	2.04	0.58
1:E:321:ARG:HG2	1:E:359:LEU:N	2.19	0.58
1:A:401:ARG:HD2	1:B:232:LEU:CD2	2.33	0.58
1:E:340:LYS:HD2	1:E:340:LYS:N	2.19	0.58
1:F:395:THR:O	1:F:399:VAL:HG23	2.03	0.58
1:A:243:PHE:O	1:A:247:GLN:HG3	2.04	0.57
1:A:456:LEU:HD21	1:D:460:MET:HE2	1.87	0.57
1:B:190:ASP:OD1	1:B:191:GLU:N	2.37	0.57
1:C:154:ARG:CD	1:C:314:ARG:HH21	2.15	0.57
1:B:148:THR:OG1	1:B:150:GLU:HG2	2.03	0.57
1:B:154:ARG:NH1	1:B:314:ARG:HH21	2.02	0.57
1:E:388:GLY:O	1:F:337:VAL:CG2	2.52	0.57
1:A:195:PHE:CD1	1:A:204:ILE:HD11	2.40	0.57
1:A:119:ARG:NH1	1:A:131:PHE:CE1	2.73	0.57
1:A:340:LYS:HD2	1:A:340:LYS:N	2.19	0.57
1:D:313:GLU:O	1:D:315:HIS:N	2.37	0.57
1:F:434:VAL:O	1:F:438:LYS:HG3	2.05	0.57
1:A:103:ARG:HD2	1:A:107:ARG:NE	2.20	0.57
1:A:134:LEU:O	1:A:145:VAL:HG13	2.05	0.57
1:C:154:ARG:NE	1:C:162:GLN:HE21	2.03	0.57
1:C:346:GLN:HE22	1:C:355:GLU:CG	2.06	0.57
1:F:199:GLY:O	1:F:200:GLU:O	2.23	0.57
1:A:246:VAL:O	1:A:250:ILE:HG12	2.05	0.57
1:A:434:VAL:O	1:A:438:LYS:HG3	2.04	0.57
1:B:133:THR:HG22	1:B:166:LEU:HD13	1.85	0.57
1:B:293:ILE:HD12	1:B:294:LYS:N	2.16	0.57
1:B:313:GLU:C	1:B:315:HIS:H	2.08	0.57
1:B:442:MET:O	1:B:443:ARG:CB	2.52	0.57
1:D:252:SER:O	1:D:253:GLN:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:395:THR:HG22	1:F:109:ARG:NH2	2.20	0.57
1:A:168:LEU:HD22	1:A:169:ASP:OD2	2.04	0.57
1:C:286:ASP:OD2	1:C:288:LYS:HB2	2.04	0.57
1:C:315:HIS:HB2	1:C:322:ILE:HD11	1.85	0.57
1:C:346:GLN:CA	1:C:346:GLN:HE21	2.17	0.57
1:F:323:THR:HG22	1:F:324:GLU:N	2.19	0.57
1:A:148:THR:HB	1:A:149:PRO:CD	2.35	0.56
1:A:172:ILE:HG22	1:A:173:ILE:N	2.14	0.56
1:A:210:ILE:N	1:A:210:ILE:CD1	2.68	0.56
1:A:309:LYS:HA	1:A:361:PHE:HE1	1.70	0.56
1:B:210:ILE:O	1:B:214:THR:HG23	2.05	0.56
1:C:416:VAL:O	1:C:420:PHE:HB2	2.04	0.56
1:D:323:THR:H	1:D:326:GLN:HE21	1.49	0.56
1:A:327:PHE:HA	1:A:330:MET:HE2	1.87	0.56
1:B:119:ARG:HD3	1:B:155:SER:O	2.05	0.56
1:D:228:LYS:HE3	1:F:402:THR:O	2.05	0.56
1:F:293:ILE:HD12	1:F:293:ILE:N	2.20	0.56
1:A:278:LEU:HD12	1:A:278:LEU:H	1.71	0.56
1:B:293:ILE:CD1	1:B:294:LYS:H	2.17	0.56
1:A:416:VAL:O	1:A:420:PHE:HB2	2.06	0.56
1:D:194:ILE:HG23	1:D:302:LYS:HG2	1.88	0.56
1:E:194:ILE:HG23	1:E:302:LYS:HD3	1.87	0.56
1:E:292:THR:CG2	1:E:293:ILE:HD12	2.35	0.56
1:F:345:MET:HE3	1:F:419:LEU:HG	1.86	0.56
1:F:371:LEU:HG	1:F:437:MET:HG3	1.88	0.56
1:A:132:ALA:O	1:A:171:TYR:HD2	1.89	0.56
1:C:119:ARG:NH1	1:C:154:ARG:O	2.39	0.56
1:C:166:LEU:HD21	1:C:172:ILE:CD1	2.35	0.56
1:E:158:PRO:O	1:E:159:ASN:HB2	2.06	0.56
1:A:323:THR:HB	1:A:326:GLN:CG	2.36	0.56
1:D:332:LEU:HD11	1:D:419:LEU:HD22	1.87	0.56
1:E:395:THR:HG22	1:F:109:ARG:HH21	1.71	0.56
1:F:425:ASN:HB3	1:F:427:GLU:HB2	1.88	0.56
1:A:396:MET:O	1:A:396:MET:HG3	2.06	0.56
1:A:457:MET:CE	1:B:463:CYS:HB3	2.36	0.56
1:D:218:THR:HG21	1:D:250:ILE:HG23	1.87	0.56
1:C:152:PHE:HE1	1:C:213:THR:HG22	1.70	0.55
1:F:197:THR:O	1:F:278:LEU:HB3	2.05	0.55
1:D:122:SER:HB3	1:D:126:LYS:HB3	1.89	0.55
1:F:194:ILE:HD12	1:F:194:ILE:N	2.22	0.55
1:F:306:ASP:O	1:F:310:LEU:HD13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:PHE:O	1:A:210:ILE:HD13	2.05	0.55
1:B:276:SER:OG	1:B:278:LEU:HB2	2.07	0.55
1:B:293:ILE:HD12	1:B:293:ILE:N	2.21	0.55
1:D:378:ASP:HB2	1:D:434:VAL:HG11	1.87	0.55
1:D:411:HIS:HD2	1:D:414:ASP:OD2	1.89	0.55
1:E:342:LEU:O	1:E:345:MET:HB3	2.06	0.55
1:F:431:LYS:H	1:F:431:LYS:CD	2.19	0.55
1:E:292:THR:HG23	1:E:293:ILE:HD12	1.88	0.55
1:C:124:PRO:HD3	1:C:259:ARG:HB2	1.88	0.55
1:E:431:LYS:HG2	1:E:432:GLU:H	1.72	0.55
1:F:149:PRO:HD3	1:F:202:GLY:O	2.06	0.55
1:D:337:VAL:C	1:D:339:SER:H	2.09	0.55
1:B:317:PRO:HG3	1:B:322:ILE:HD13	1.88	0.55
1:B:436:ILE:H	1:B:436:ILE:CD1	2.16	0.55
1:D:345:MET:O	1:D:349:LEU:HB2	2.07	0.55
1:E:305:HIS:HD2	1:E:365:GLU:OE2	1.90	0.55
1:B:166:LEU:O	1:B:170:GLN:NE2	2.37	0.55
1:E:147:MET:HB2	1:E:151:ASP:HB2	1.88	0.55
1:D:456:LEU:HB2	1:D:457:MET:HE3	1.88	0.54
1:E:198:LEU:O	1:E:277:ALA:HB3	2.07	0.54
1:E:421:ASP:OD1	1:E:424:GLY:HA2	2.07	0.54
1:A:377:VAL:O	1:A:381:LEU:HD12	2.08	0.54
1:C:238:VAL:HG13	1:C:242:GLU:HB2	1.88	0.54
1:E:393:LYS:HA	1:E:417:PHE:CE2	2.42	0.54
1:F:151:ASP:OD1	1:F:154:ARG:NH2	2.39	0.54
1:F:337:VAL:C	1:F:339:SER:H	2.11	0.54
1:E:460:MET:HA	1:E:463:CYS:CB	2.37	0.54
1:C:314:ARG:HG2	1:C:314:ARG:HH11	1.72	0.54
1:A:456:LEU:HD11	1:D:460:MET:CE	2.36	0.54
1:C:235:ASP:HB2	1:C:293:ILE:HD11	1.89	0.54
1:E:353:PHE:N	1:E:353:PHE:CD2	2.73	0.54
1:E:111:VAL:O	1:E:115:GLU:HG3	2.07	0.54
1:E:194:ILE:CD1	1:E:195:PHE:N	2.66	0.54
1:E:374:ILE:HD12	1:E:375:ASN:H	1.73	0.54
1:E:442:MET:O	1:E:443:ARG:HB2	2.08	0.54
1:A:360:THR:HG23	1:A:363:GLU:CG	2.36	0.54
1:C:232:LEU:HD12	1:C:232:LEU:N	2.22	0.54
1:E:390:SER:O	1:E:395:THR:HG21	2.08	0.54
1:B:286:ASP:OD2	1:B:288:LYS:HB2	2.06	0.54
1:B:306:ASP:O	1:B:310:LEU:HD13	2.08	0.54
1:C:154:ARG:HE	1:C:162:GLN:NE2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:ASP:O	1:C:287:LEU:HB2	2.07	0.54
1:E:118:ILE:O	1:E:122:SER:HB2	2.08	0.54
1:E:401:ARG:HD3	1:E:407:GLU:OE2	2.07	0.54
1:A:166:LEU:HA	1:A:170:GLN:O	2.08	0.54
1:A:297:LEU:O	1:A:301:ARG:HB2	2.07	0.54
1:F:374:ILE:HD12	1:F:375:ASN:H	1.72	0.54
1:A:103:ARG:HG2	1:A:103:ARG:NH1	2.21	0.54
1:B:133:THR:HG23	1:B:151:ASP:OD2	2.08	0.54
1:C:360:THR:OG1	1:C:363:GLU:HG3	2.08	0.54
1:D:411:HIS:HA	1:D:414:ASP:OD2	2.08	0.54
1:F:313:GLU:C	1:F:315:HIS:H	2.10	0.54
1:A:309:LYS:HA	1:A:361:PHE:CE1	2.42	0.53
1:B:374:ILE:HA	1:B:377:VAL:HB	1.90	0.53
1:B:456:LEU:HD12	1:C:461:TRP:CH2	2.44	0.53
1:D:119:ARG:HG2	1:D:155:SER:O	2.08	0.53
1:F:130:TYR:CE2	1:F:162:GLN:HG3	2.43	0.53
1:F:246:VAL:O	1:F:250:ILE:HG12	2.07	0.53
1:B:371:LEU:C	1:B:373:ASN:H	2.11	0.53
1:C:293:ILE:H	1:C:293:ILE:CD1	2.03	0.53
1:E:193:SER:O	1:E:194:ILE:C	2.45	0.53
1:C:296:PHE:O	1:C:299:PHE:N	2.42	0.53
1:C:303:LEU:HD23	1:C:303:LEU:C	2.29	0.53
1:A:457:MET:HE2	1:B:463:CYS:HB3	1.90	0.53
1:D:338:GLN:NE2	1:D:341:LYS:NZ	2.56	0.53
1:D:436:ILE:O	1:D:439:GLN:HG2	2.08	0.53
1:A:430:ASN:O	1:A:434:VAL:HG23	2.08	0.53
1:D:292:THR:HG22	1:D:294:LYS:H	1.73	0.53
1:E:423:ASP:OD2	1:E:423:ASP:N	2.41	0.53
1:F:252:SER:O	1:F:253:GLN:CG	2.55	0.53
1:A:371:LEU:HD21	1:A:437:MET:SD	2.49	0.53
1:B:145:VAL:HG11	1:B:171:TYR:CE2	2.44	0.53
1:E:381:LEU:HD22	1:E:391:LEU:HD22	1.90	0.53
1:A:334:TYR:CZ	1:A:443:ARG:HG2	2.43	0.53
1:B:415:VAL:O	1:B:418:ALA:HB3	2.09	0.53
1:C:431:LYS:HG2	1:C:432:GLU:N	2.20	0.53
1:D:112:MET:O	1:D:114:TYR:N	2.42	0.53
1:D:454:THR:C	1:D:456:LEU:N	2.59	0.53
1:A:119:ARG:HH22	1:A:160:GLU:H	1.56	0.53
1:E:168:LEU:O	1:E:169:ASP:HB2	2.09	0.53
1:E:378:ASP:HB2	1:E:434:VAL:HG21	1.90	0.53
1:A:422:CYS:HB2	1:A:425:ASN:OD1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:LEU:O	1:D:445:LEU:CD1	2.56	0.53
1:E:278:LEU:HD22	1:E:282:PHE:HE2	1.73	0.53
1:F:318:VAL:HG23	1:F:318:VAL:O	2.09	0.53
1:F:337:VAL:O	1:F:337:VAL:CG1	2.57	0.53
1:B:409:SER:OG	1:B:412:VAL:HG23	2.09	0.52
1:F:283:PHE:CE1	1:F:291:LEU:HB2	2.44	0.52
1:F:396:MET:HE3	1:F:428:LEU:HG	1.91	0.52
1:B:453:PHE:CB	1:C:461:TRP:NE1	2.72	0.52
1:C:134:LEU:HD12	1:C:203:LEU:HD11	1.90	0.52
1:C:425:ASN:C	1:C:427:GLU:H	2.13	0.52
1:C:461:TRP:C	1:C:463:CYS:H	2.12	0.52
1:D:430:ASN:O	1:D:434:VAL:HG23	2.10	0.52
1:F:283:PHE:HE1	1:F:291:LEU:HB2	1.73	0.52
1:A:317:PRO:HB3	1:A:321:ARG:O	2.09	0.52
1:D:409:SER:HB3	1:D:412:VAL:HB	1.90	0.52
1:D:245:GLN:O	1:D:249:ILE:HG13	2.10	0.52
1:E:194:ILE:C	1:E:196:TYR:N	2.62	0.52
1:E:194:ILE:C	1:E:196:TYR:H	2.12	0.52
1:F:278:LEU:O	1:F:281:TYR:N	2.41	0.52
1:F:115:GLU:OE1	1:F:161:LYS:HA	2.09	0.52
1:A:318:VAL:HG23	1:A:318:VAL:O	2.10	0.52
1:B:133:THR:CG2	1:B:166:LEU:HD13	2.39	0.52
1:D:313:GLU:C	1:D:315:HIS:N	2.63	0.52
1:D:350:LYS:HB2	1:D:355:GLU:CD	2.30	0.52
1:D:382:SER:O	1:D:386:MET:HG3	2.09	0.52
1:E:393:LYS:HG3	1:E:413:CYS:HB3	1.91	0.52
1:F:409:SER:HB3	1:F:412:VAL:CG2	2.35	0.52
1:C:136:VAL:HG22	1:C:174:LYS:HE2	1.92	0.52
1:C:148:THR:HG23	1:C:151:ASP:OD2	2.10	0.52
1:A:429:SER:OG	1:A:431:LYS:HE2	2.10	0.52
1:A:460:MET:HE1	1:E:460:MET:SD	2.50	0.52
1:C:193:SER:HA	1:C:306:ASP:OD2	2.10	0.52
1:C:194:ILE:HD12	1:C:195:PHE:N	2.20	0.52
1:D:154:ARG:HE	1:D:162:GLN:NE2	1.92	0.52
1:F:137:ILE:HD13	1:F:137:ILE:H	1.75	0.52
1:F:349:LEU:HD22	1:F:354:LYS:HB2	1.92	0.52
1:A:296:PHE:O	1:A:299:PHE:HB3	2.10	0.52
1:B:346:GLN:O	1:B:350:LYS:HG3	2.10	0.52
1:B:371:LEU:O	1:B:374:ILE:HG13	2.10	0.52
1:D:134:LEU:HD11	1:D:188:PHE:CE1	2.44	0.52
1:D:454:THR:O	1:D:457:MET:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:LEU:O	1:B:170:GLN:HG3	2.10	0.52
1:B:433:PHE:CE1	1:B:437:MET:HG3	2.44	0.52
1:F:214:THR:O	1:F:218:THR:HG23	2.08	0.52
1:B:395:THR:O	1:B:399:VAL:HG23	2.10	0.51
1:C:428:LEU:HD23	1:C:429:SER:H	1.74	0.51
1:F:137:ILE:HD13	1:F:137:ILE:N	2.25	0.51
1:F:182:SER:C	1:F:184:GLU:N	2.64	0.51
1:F:190:ASP:O	1:F:196:TYR:HE2	1.92	0.51
1:F:322:ILE:HD13	1:F:330:MET:HE1	1.91	0.51
1:A:315:HIS:HB3	1:A:326:GLN:NE2	2.25	0.51
1:B:292:THR:HG22	1:B:294:LYS:N	2.22	0.51
1:D:336:GLY:C	1:D:338:GLN:N	2.61	0.51
1:A:119:ARG:NH1	1:A:131:PHE:HE1	2.09	0.51
1:A:154:ARG:HE	1:A:162:GLN:HE21	1.58	0.51
1:A:218:THR:HG21	1:A:250:ILE:HG22	1.89	0.51
1:C:306:ASP:O	1:C:310:LEU:HD13	2.10	0.51
1:D:151:ASP:OD1	1:D:154:ARG:NH2	2.43	0.51
1:E:119:ARG:NH1	1:E:154:ARG:O	2.43	0.51
1:C:194:ILE:HG23	1:C:302:LYS:HG2	1.91	0.51
1:F:422:CYS:CB	1:F:425:ASN:ND2	2.66	0.51
1:A:401:ARG:O	1:A:405:LYS:HA	2.10	0.51
1:D:163:PRO:HB3	1:D:165:HIS:CE1	2.46	0.51
1:E:441:LEU:HD13	1:E:441:LEU:O	2.11	0.51
1:A:293:ILE:H	1:A:293:ILE:CD1	2.07	0.51
1:C:317:PRO:HG3	1:C:322:ILE:HD13	1.92	0.51
1:D:349:LEU:HB3	1:D:355:GLU:CG	2.41	0.51
1:E:323:THR:HG22	1:E:324:GLU:H	1.75	0.51
1:A:154:ARG:NH1	1:A:314:ARG:NH2	2.59	0.51
1:A:287:LEU:N	1:A:287:LEU:HD22	2.25	0.51
1:B:233:ASN:N	1:B:233:ASN:HD22	2.08	0.51
1:D:387:ALA:HB2	1:F:249:ILE:CD1	2.41	0.51
1:E:279:THR:O	1:E:283:PHE:CD2	2.62	0.51
1:F:313:GLU:O	1:F:315:HIS:N	2.36	0.51
1:A:195:PHE:HZ	1:A:307:VAL:HG22	1.75	0.51
1:C:300:GLN:O	1:C:304:GLN:HG3	2.11	0.51
1:E:430:ASN:O	1:E:434:VAL:HG13	2.11	0.51
1:B:291:LEU:HD23	1:B:292:THR:H	1.75	0.51
1:C:371:LEU:C	1:C:373:ASN:H	2.14	0.51
1:D:246:VAL:O	1:D:250:ILE:HG12	2.10	0.51
1:E:242:GLU:O	1:E:245:GLN:HB2	2.11	0.51
1:F:156:ILE:O	1:F:158:PRO:HD3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:417:PHE:CZ	1:E:428:LEU:HD23	2.46	0.51
1:A:401:ARG:HD2	1:B:232:LEU:HD22	1.92	0.50
1:C:136:VAL:O	1:C:143:ALA:HA	2.10	0.50
1:D:115:GLU:HG2	1:D:130:TYR:OH	2.12	0.50
1:D:456:LEU:O	1:D:460:MET:N	2.44	0.50
1:F:416:VAL:O	1:F:420:PHE:HB2	2.11	0.50
1:A:154:ARG:NH1	1:A:314:ARG:HH21	2.09	0.50
1:A:158:PRO:O	1:A:159:ASN:HB2	2.11	0.50
1:B:214:THR:HB	1:B:254:THR:HG21	1.93	0.50
1:C:351:LYS:HG3	1:C:352:HIS:ND1	2.27	0.50
1:E:238:VAL:HG12	1:E:239:ASP:O	2.11	0.50
1:E:314:ARG:HG2	1:E:314:ARG:O	2.11	0.50
1:E:317:PRO:HG3	1:E:322:ILE:HD13	1.93	0.50
1:F:421:ASP:HB2	1:F:426:GLY:H	1.75	0.50
1:B:194:ILE:HD12	1:B:195:PHE:H	1.77	0.50
1:C:147:MET:HB2	1:C:151:ASP:HB2	1.93	0.50
1:B:245:GLN:HG3	1:E:121:TYR:CZ	2.45	0.50
1:C:137:ILE:HD12	1:C:175:ARG:HA	1.92	0.50
1:D:123:THR:O	1:D:127:ILE:HG13	2.12	0.50
1:E:323:THR:CG2	1:E:324:GLU:N	2.73	0.50
1:D:170:GLN:HE21	1:D:170:GLN:HA	1.76	0.50
1:E:322:ILE:HG22	1:E:359:LEU:HB2	1.94	0.50
1:C:375:ASN:O	1:C:379:THR:HG23	2.11	0.50
1:D:224:GLU:HA	1:D:293:ILE:HG21	1.94	0.50
1:D:454:THR:O	1:D:456:LEU:N	2.43	0.50
1:F:315:HIS:CB	1:F:322:ILE:HD11	2.41	0.50
1:C:168:LEU:HD13	1:C:168:LEU:N	2.27	0.50
1:C:314:ARG:HG2	1:C:314:ARG:O	2.11	0.50
1:C:359:LEU:N	1:C:359:LEU:HD12	2.26	0.50
1:D:381:LEU:HD22	1:D:391:LEU:HD22	1.94	0.50
1:A:242:GLU:O	1:A:246:VAL:HG23	2.11	0.50
1:C:239:ASP:OD1	1:C:241:GLU:HG2	2.11	0.50
1:D:283:PHE:HE1	1:D:291:LEU:HB2	1.77	0.50
1:E:216:LEU:HD23	1:E:304:GLN:HG2	1.93	0.50
1:E:300:GLN:O	1:E:304:GLN:HG3	2.12	0.50
1:C:119:ARG:NH1	1:C:157:THR:O	2.45	0.49
1:D:436:ILE:HG22	1:D:437:MET:CE	2.42	0.49
1:E:314:ARG:O	1:E:315:HIS:HD2	1.94	0.49
1:A:227:PHE:C	1:A:229:MET:N	2.65	0.49
1:A:398:GLN:NE2	1:B:232:LEU:HD21	2.27	0.49
1:B:115:GLU:HG2	1:B:130:TYR:OH	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ASP:OD2	1:C:242:GLU:HG3	2.12	0.49
1:C:238:VAL:HG12	1:C:239:ASP:O	2.11	0.49
1:C:425:ASN:HD22	1:C:427:GLU:HG2	1.77	0.49
1:D:323:THR:HG22	1:D:325:ARG:N	2.05	0.49
1:C:148:THR:O	1:C:149:PRO:C	2.50	0.49
1:C:460:MET:O	1:C:463:CYS:HB2	2.13	0.49
1:F:293:ILE:H	1:F:293:ILE:CD1	2.20	0.49
1:B:292:THR:CG2	1:B:293:ILE:HD12	2.37	0.49
1:C:132:ALA:HB1	1:C:146:PHE:O	2.12	0.49
1:A:145:VAL:HG11	1:A:171:TYR:CE2	2.48	0.49
1:A:336:GLY:C	1:A:338:GLN:H	2.15	0.49
1:B:315:HIS:CB	1:B:322:ILE:HD11	2.42	0.49
1:F:374:ILE:HD12	1:F:374:ILE:N	2.28	0.49
1:A:431:LYS:HG2	1:A:432:GLU:N	2.27	0.49
1:E:321:ARG:HD2	1:E:358:GLY:HA3	1.94	0.49
1:F:148:THR:HG22	1:F:151:ASP:OD2	2.13	0.49
1:F:399:VAL:O	1:F:399:VAL:HG12	2.11	0.49
1:A:114:TYR:O	1:A:118:ILE:HG13	2.12	0.49
1:A:324:GLU:HG3	1:A:355:GLU:O	2.13	0.49
1:B:227:PHE:CD1	1:B:293:ILE:HG23	2.47	0.49
1:B:346:GLN:CA	1:B:346:GLN:NE2	2.75	0.49
1:C:303:LEU:HD23	1:C:307:VAL:CG2	2.43	0.49
1:D:421:ASP:HA	1:D:428:LEU:HA	1.94	0.49
1:A:420:PHE:HE2	1:A:436:ILE:HD12	1.76	0.49
1:B:221:ARG:HH11	1:B:221:ARG:CB	2.21	0.49
1:C:428:LEU:HD23	1:C:429:SER:N	2.27	0.49
1:D:337:VAL:C	1:D:339:SER:N	2.64	0.49
1:E:337:VAL:C	1:E:339:SER:H	2.16	0.49
1:E:360:THR:O	1:E:364:VAL:HG23	2.13	0.49
1:E:432:GLU:O	1:E:432:GLU:HG2	2.12	0.49
1:B:245:GLN:O	1:B:249:ILE:HG13	2.13	0.49
1:F:416:VAL:O	1:F:416:VAL:HG12	2.12	0.49
1:A:459:ALA:HB1	1:D:456:LEU:CD2	2.24	0.48
1:B:174:LYS:HG3	1:B:175:ARG:N	2.28	0.48
1:C:291:LEU:HD23	1:C:292:THR:N	2.28	0.48
1:C:327:PHE:CD1	1:C:364:VAL:HG22	2.48	0.48
1:F:239:ASP:OD1	1:F:242:GLU:HG3	2.13	0.48
1:A:309:LYS:O	1:A:312:PHE:N	2.45	0.48
1:E:286:ASP:O	1:E:288:LYS:HG3	2.13	0.48
1:E:298:GLU:OE1	1:E:301:ARG:NH2	2.46	0.48
1:A:442:MET:O	1:A:443:ARG:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:THR:O	1:B:149:PRO:C	2.50	0.48
1:B:220:GLN:HG2	1:B:297:LEU:CD2	2.43	0.48
1:C:134:LEU:HD12	1:C:203:LEU:CD1	2.42	0.48
1:E:371:LEU:O	1:E:374:ILE:HG13	2.13	0.48
1:F:148:THR:OG1	1:F:149:PRO:HD2	2.13	0.48
1:D:166:LEU:CD2	1:D:172:ILE:HG13	2.40	0.48
1:A:153:VAL:CG2	1:A:310:LEU:HD13	2.43	0.48
1:E:460:MET:C	1:E:462:LYS:N	2.66	0.48
1:B:154:ARG:HD3	1:B:314:ARG:HH22	1.75	0.48
1:B:194:ILE:C	1:B:196:TYR:H	2.17	0.48
1:E:123:THR:O	1:E:127:ILE:HG13	2.12	0.48
1:E:296:PHE:O	1:E:299:PHE:HB3	2.13	0.48
1:A:452:GLY:O	1:A:454:THR:N	2.41	0.48
1:C:333:ALA:HB3	1:C:440:ARG:HH11	1.78	0.48
1:F:119:ARG:HG2	1:F:155:SER:O	2.12	0.48
1:F:437:MET:HE2	1:F:440:ARG:HG2	1.96	0.48
1:A:214:THR:HG21	1:A:251:ARG:CG	2.44	0.48
1:B:371:LEU:HB3	1:B:441:LEU:HD23	1.94	0.48
1:B:393:LYS:HG3	1:B:413:CYS:CB	2.44	0.48
1:D:346:GLN:O	1:D:355:GLU:OE2	2.31	0.48
1:B:371:LEU:HD21	1:B:437:MET:SD	2.54	0.48
1:D:206:PHE:CE2	1:D:210:ILE:HD11	2.48	0.48
1:D:330:MET:O	1:D:440:ARG:NH1	2.43	0.48
1:E:115:GLU:OE1	1:E:161:LYS:HA	2.14	0.48
1:C:124:PRO:HG2	1:C:260:HIS:CB	2.44	0.48
1:C:303:LEU:HD23	1:C:307:VAL:HG23	1.96	0.48
1:D:320:GLY:O	1:D:360:THR:HA	2.13	0.48
1:B:366:ASN:ND2	1:B:406:VAL:CG2	2.71	0.47
1:A:374:ILE:HD12	1:A:374:ILE:N	2.29	0.47
1:C:371:LEU:CD2	1:C:437:MET:HB3	2.44	0.47
1:A:349:LEU:HD22	1:A:354:LYS:O	2.14	0.47
1:B:368:PHE:HA	1:B:371:LEU:HB2	1.96	0.47
1:C:278:LEU:O	1:C:281:TYR:N	2.45	0.47
1:E:211:PHE:O	1:E:215:VAL:HG23	2.14	0.47
1:F:318:VAL:O	1:F:319:ASP:HB2	2.14	0.47
1:A:194:ILE:HD11	1:A:303:LEU:HD23	1.96	0.47
1:A:315:HIS:CD2	1:A:322:ILE:HD11	2.49	0.47
1:D:149:PRO:HG2	1:D:189:ALA:HB2	1.94	0.47
1:D:194:ILE:HG13	1:D:306:ASP:OD1	2.14	0.47
1:E:374:ILE:O	1:E:378:ASP:N	2.46	0.47
1:F:340:LYS:N	1:F:340:LYS:HD2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:GLN:NE2	1:E:117:ARG:HD3	2.28	0.47
1:C:174:LYS:NZ	1:C:188:PHE:HE2	2.13	0.47
1:C:238:VAL:CG1	1:C:243:PHE:HB2	2.45	0.47
1:D:206:PHE:CZ	1:D:210:ILE:HD11	2.49	0.47
1:D:456:LEU:O	1:D:459:ALA:N	2.48	0.47
1:E:334:TYR:CE2	1:E:443:ARG:HG2	2.49	0.47
1:A:431:LYS:HD3	1:A:431:LYS:N	2.28	0.47
1:B:462:LYS:O	1:B:463:CYS:C	2.53	0.47
1:C:128:PHE:CE2	1:C:206:PHE:HB2	2.49	0.47
1:C:335:SER:OG	1:C:336:GLY:N	2.47	0.47
1:F:324:GLU:OE1	1:F:411:HIS:HE1	1.96	0.47
1:A:119:ARG:CZ	1:A:157:THR:O	2.62	0.47
1:D:147:MET:HB2	1:D:151:ASP:HB2	1.96	0.47
1:D:196:TYR:C	1:D:198:LEU:N	2.68	0.47
1:F:365:GLU:O	1:F:369:THR:HG23	2.14	0.47
1:B:340:LYS:HD2	1:B:340:LYS:N	2.30	0.47
1:C:321:ARG:HA	1:C:359:LEU:O	2.15	0.47
1:E:137:ILE:HG12	1:E:143:ALA:CB	2.45	0.47
1:E:177:ASP:C	1:E:185:ARG:HD3	2.35	0.47
1:E:278:LEU:O	1:E:281:TYR:HB3	2.14	0.47
1:E:376:ASP:HB3	1:E:403:VAL:HG13	1.96	0.47
1:A:216:LEU:O	1:A:216:LEU:CD2	2.63	0.47
1:D:292:THR:HG22	1:D:293:ILE:HD12	1.97	0.47
1:E:132:ALA:HA	1:E:147:MET:HB3	1.97	0.47
1:B:162:GLN:CD	1:B:163:PRO:HD2	2.35	0.47
1:B:431:LYS:HG2	1:B:432:GLU:H	1.79	0.47
1:C:292:THR:CG2	1:C:293:ILE:N	2.78	0.47
1:D:194:ILE:C	1:D:194:ILE:CD1	2.83	0.47
1:B:371:LEU:O	1:B:373:ASN:N	2.46	0.46
1:D:231:ASP:CB	1:D:237:GLU:H	2.21	0.46
1:D:239:ASP:OD1	1:D:239:ASP:C	2.54	0.46
1:D:346:GLN:NE2	1:D:355:GLU:OE1	2.48	0.46
1:E:393:LYS:O	1:E:397:GLN:HG3	2.15	0.46
1:A:194:ILE:HG21	1:A:302:LYS:HD3	1.96	0.46
1:D:210:ILE:HD12	1:D:210:ILE:N	2.30	0.46
1:D:220:GLN:HG2	1:D:297:LEU:HD22	1.96	0.46
1:D:293:ILE:H	1:D:293:ILE:CD1	2.17	0.46
1:E:430:ASN:O	1:E:434:VAL:CG1	2.63	0.46
1:F:436:ILE:HG22	1:F:437:MET:N	2.29	0.46
1:A:303:LEU:O	1:A:307:VAL:HG23	2.15	0.46
1:B:228:LYS:O	1:B:228:LYS:HG2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:PHE:O	1:B:371:LEU:HB2	2.15	0.46
1:E:218:THR:HA	1:E:219:PRO:HD3	1.65	0.46
1:B:153:VAL:HG21	1:B:310:LEU:HB3	1.97	0.46
1:B:293:ILE:CD1	1:B:294:LYS:N	2.78	0.46
1:B:371:LEU:HD22	1:B:437:MET:HB3	1.97	0.46
1:F:345:MET:HE3	1:F:419:LEU:CG	2.45	0.46
1:C:232:LEU:N	1:C:232:LEU:CD1	2.79	0.46
1:B:431:LYS:H	1:B:431:LYS:CD	2.29	0.46
1:C:148:THR:OG1	1:C:150:GLU:HG2	2.16	0.46
1:C:232:LEU:CD1	1:C:232:LEU:H	2.28	0.46
1:F:308:LEU:HD13	1:F:361:PHE:HE1	1.80	0.46
1:F:390:SER:O	1:F:395:THR:CG2	2.64	0.46
1:F:417:PHE:CE1	1:F:426:GLY:O	2.65	0.46
1:A:148:THR:CB	1:A:149:PRO:CD	2.94	0.46
1:B:208:ASP:O	1:B:212:LEU:HG	2.15	0.46
1:C:249:ILE:CD1	1:E:387:ALA:HB2	2.46	0.46
1:C:436:ILE:HG22	1:C:437:MET:HE2	1.98	0.46
1:D:252:SER:HB2	1:F:386:MET:HG2	1.97	0.46
1:D:364:VAL:O	1:D:365:GLU:C	2.53	0.46
1:F:185:ARG:HG2	1:F:186:GLU:N	2.31	0.46
1:F:327:PHE:HD2	1:F:415:VAL:HG11	1.79	0.46
1:B:453:PHE:CB	1:C:461:TRP:CZ2	2.99	0.46
1:D:112:MET:C	1:D:114:TYR:N	2.67	0.46
1:A:227:PHE:HB3	1:A:236:GLY:HA3	1.98	0.46
1:B:200:GLU:N	1:B:200:GLU:OE1	2.49	0.46
1:C:249:ILE:HD11	1:E:387:ALA:HB2	1.98	0.46
1:C:451:MET:HA	1:C:454:THR:CG2	2.46	0.46
1:E:433:PHE:C	1:E:435:SER:N	2.69	0.46
1:F:419:LEU:HD13	1:F:420:PHE:CD1	2.51	0.46
1:B:109:ARG:O	1:B:113:GLU:HG3	2.16	0.46
1:C:239:ASP:OD1	1:C:239:ASP:C	2.53	0.46
1:C:323:THR:CG2	1:C:325:ARG:H	2.08	0.46
1:D:398:GLN:NE2	1:F:232:LEU:HD22	2.31	0.46
1:D:416:VAL:O	1:D:420:PHE:HB2	2.16	0.46
1:F:147:MET:HB2	1:F:151:ASP:HB2	1.97	0.46
1:F:337:VAL:C	1:F:339:SER:N	2.69	0.46
1:A:115:GLU:O	1:A:119:ARG:HG3	2.15	0.45
1:A:115:GLU:OE2	1:A:162:GLN:HB2	2.16	0.45
1:B:373:ASN:O	1:B:374:ILE:C	2.55	0.45
1:B:462:LYS:O	1:B:466:GLU:HG3	2.16	0.45
1:C:324:GLU:OE2	1:C:358:GLY:N	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:GLN:NE2	1:C:346:GLN:CA	2.79	0.45
1:C:346:GLN:NE2	1:C:346:GLN:HA	2.31	0.45
1:D:417:PHE:CE1	1:D:428:LEU:HB2	2.51	0.45
1:E:314:ARG:O	1:E:314:ARG:CG	2.64	0.45
1:F:166:LEU:O	1:F:170:GLN:HB2	2.16	0.45
1:F:431:LYS:HD3	1:F:431:LYS:N	2.27	0.45
1:A:147:MET:HB2	1:A:151:ASP:CB	2.47	0.45
1:B:334:TYR:CE2	1:B:443:ARG:HG2	2.50	0.45
1:F:231:ASP:O	1:F:233:ASN:N	2.49	0.45
1:D:203:LEU:HD23	1:D:203:LEU:HA	1.76	0.45
1:E:243:PHE:O	1:E:247:GLN:HG3	2.15	0.45
1:E:278:LEU:HD22	1:E:282:PHE:CE2	2.50	0.45
1:E:421:ASP:CG	1:E:424:GLY:HA2	2.36	0.45
1:E:434:VAL:O	1:E:438:LYS:HG2	2.17	0.45
1:F:114:TYR:CE2	1:F:118:ILE:HD11	2.51	0.45
1:A:194:ILE:N	1:A:306:ASP:OD1	2.49	0.45
1:B:218:THR:HG21	1:B:250:ILE:HG23	1.98	0.45
1:C:314:ARG:HG2	1:C:314:ARG:NH1	2.31	0.45
1:C:350:LYS:HA	1:C:355:GLU:OE2	2.16	0.45
1:C:461:TRP:O	1:C:463:CYS:N	2.43	0.45
1:D:322:ILE:HG22	1:D:359:LEU:HB2	1.97	0.45
1:F:190:ASP:OD1	1:F:191:GLU:HG2	2.16	0.45
1:F:209:TYR:O	1:F:213:THR:HG23	2.16	0.45
1:F:237:GLU:HA	1:F:291:LEU:O	2.17	0.45
1:F:322:ILE:HD13	1:F:330:MET:CE	2.46	0.45
1:B:247:GLN:NE2	1:B:251:ARG:HH12	2.14	0.45
1:C:156:ILE:O	1:C:334:TYR:HE1	1.98	0.45
1:C:242:GLU:HA	1:F:117:ARG:HD3	1.99	0.45
1:C:257:GLY:C	1:C:259:ARG:H	2.19	0.45
1:C:371:LEU:HD22	1:C:437:MET:HB3	1.99	0.45
1:D:209:TYR:CD1	1:D:210:ILE:HD12	2.50	0.45
1:F:393:LYS:HG3	1:F:413:CYS:HB3	1.99	0.45
1:B:298:GLU:HA	1:B:298:GLU:OE2	2.17	0.45
1:C:428:LEU:HD22	1:C:430:ASN:N	2.32	0.45
1:D:216:LEU:HG	1:D:303:LEU:HD11	1.99	0.45
1:F:182:SER:O	1:F:184:GLU:N	2.50	0.45
1:F:218:THR:HA	1:F:219:PRO:HD3	1.72	0.45
1:A:154:ARG:NE	1:A:162:GLN:HE21	2.14	0.45
1:B:309:LYS:O	1:B:313:GLU:HB2	2.16	0.45
1:C:322:ILE:HA	1:C:322:ILE:HD12	1.73	0.45
1:D:391:LEU:HD23	1:D:391:LEU:HA	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:ASP:HB3	1:E:290:LYS:HE2	1.98	0.45
1:F:189:ALA:HB3	1:F:196:TYR:CE2	2.52	0.45
1:C:237:GLU:O	1:C:238:VAL:CG2	2.64	0.45
1:D:108:ASP:O	1:D:112:MET:HG3	2.16	0.45
1:D:199:GLY:CA	1:D:277:ALA:HB1	2.47	0.45
1:D:325:ARG:O	1:D:325:ARG:HG2	2.17	0.45
1:E:332:LEU:HD11	1:E:419:LEU:CD2	2.47	0.45
1:F:436:ILE:HG22	1:F:437:MET:HE3	1.99	0.45
1:A:146:PHE:CD2	1:A:205:SER:HA	2.52	0.45
1:A:309:LYS:HG3	1:A:361:PHE:CE1	2.52	0.45
1:B:119:ARG:NH1	1:B:154:ARG:O	2.50	0.45
1:C:278:LEU:O	1:C:281:TYR:HB3	2.17	0.45
1:D:218:THR:HA	1:D:219:PRO:HD3	1.83	0.45
1:D:324:GLU:OE2	1:D:411:HIS:HE1	1.99	0.45
1:E:247:GLN:HB3	1:E:251:ARG:NH1	2.32	0.45
1:F:206:PHE:CZ	1:F:210:ILE:HD11	2.52	0.45
1:A:401:ARG:CD	1:B:232:LEU:HD22	2.47	0.44
1:B:147:MET:HE2	1:B:151:ASP:HB3	1.99	0.44
1:B:316:ASP:N	1:B:317:PRO:HD3	2.33	0.44
1:D:326:GLN:HE21	1:D:326:GLN:HB2	1.66	0.44
1:F:419:LEU:HD12	1:F:419:LEU:H	1.82	0.44
1:B:313:GLU:O	1:B:315:HIS:N	2.49	0.44
1:F:373:ASN:O	1:F:374:ILE:C	2.56	0.44
1:B:293:ILE:CD1	1:B:293:ILE:H	2.30	0.44
1:B:453:PHE:CB	1:C:461:TRP:CE2	3.01	0.44
1:C:298:GLU:OE2	1:C:298:GLU:HA	2.17	0.44
1:C:457:MET:HE2	1:D:460:MET:HE1	1.99	0.44
1:D:198:LEU:HD23	1:D:278:LEU:HD23	1.98	0.44
1:D:349:LEU:HB3	1:D:355:GLU:OE2	2.17	0.44
1:A:134:LEU:N	1:A:171:TYR:HB3	2.33	0.44
1:A:228:LYS:HG2	1:A:235:ASP:O	2.16	0.44
1:A:322:ILE:HG13	1:A:326:GLN:NE2	2.32	0.44
1:A:334:TYR:CD1	1:A:443:ARG:HA	2.52	0.44
1:A:381:LEU:CD2	1:A:391:LEU:HD22	2.47	0.44
1:A:395:THR:O	1:A:398:GLN:N	2.50	0.44
1:B:115:GLU:OE1	1:B:161:LYS:HA	2.18	0.44
1:B:211:PHE:O	1:B:215:VAL:HG23	2.17	0.44
1:B:243:PHE:HZ	1:B:296:PHE:CE1	2.35	0.44
1:C:246:VAL:HG12	1:C:250:ILE:HD12	1.99	0.44
1:D:336:GLY:O	1:D:338:GLN:N	2.50	0.44
1:E:239:ASP:C	1:E:239:ASP:OD1	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ILE:CG2	1:A:302:LYS:HD3	2.47	0.44
1:B:166:LEU:CD2	1:B:172:ILE:HG13	2.42	0.44
1:B:286:ASP:O	1:B:287:LEU:HB2	2.18	0.44
1:B:375:ASN:O	1:B:379:THR:HG23	2.18	0.44
1:D:175:ARG:O	1:D:177:ASP:N	2.50	0.44
1:E:455:ARG:C	1:E:457:MET:H	2.20	0.44
1:F:350:LYS:HG2	1:F:355:GLU:OE2	2.18	0.44
1:C:187:LYS:HD3	1:C:201:CYS:HB3	1.99	0.44
1:C:246:VAL:O	1:C:247:GLN:C	2.56	0.44
1:C:347:ARG:O	1:C:350:LYS:HB3	2.16	0.44
1:D:138:SER:HB3	1:D:176:PHE:CB	2.48	0.44
1:E:218:THR:HG21	1:E:250:ILE:HG21	2.00	0.44
1:F:240:MET:HA	1:F:283:PHE:CE2	2.53	0.44
1:C:124:PRO:HG2	1:C:260:HIS:H	1.82	0.44
1:D:123:THR:O	1:D:124:PRO:C	2.55	0.44
1:A:168:LEU:O	1:A:170:GLN:HG3	2.18	0.44
1:A:410:ASP:O	1:A:413:CYS:HB2	2.18	0.44
1:C:115:GLU:OE1	1:C:161:LYS:HA	2.17	0.44
1:D:172:ILE:HG22	1:D:172:ILE:O	2.18	0.44
1:D:214:THR:HG21	1:D:251:ARG:CG	2.47	0.44
1:E:158:PRO:CD	1:E:334:TYR:CE1	3.01	0.44
1:F:190:ASP:O	1:F:196:TYR:CE2	2.70	0.44
1:F:408:LEU:HD23	1:F:408:LEU:HA	1.78	0.44
1:F:421:ASP:OD2	1:F:421:ASP:C	2.56	0.44
1:A:342:LEU:HD12	1:A:342:LEU:H	1.81	0.44
1:C:129:ARG:NH1	1:C:169:ASP:OD2	2.51	0.44
1:C:292:THR:CG2	1:C:293:ILE:HD12	2.48	0.44
1:C:393:LYS:HG3	1:C:413:CYS:HB3	2.00	0.44
1:D:216:LEU:HD23	1:D:216:LEU:HA	1.68	0.44
1:D:387:ALA:HB2	1:F:249:ILE:HD13	2.00	0.44
1:E:189:ALA:O	1:E:190:ASP:O	2.36	0.44
1:F:241:GLU:HG2	1:F:242:GLU:N	2.33	0.44
1:A:437:MET:HA	1:A:437:MET:CE	2.48	0.43
1:A:452:GLY:C	1:A:454:THR:H	2.18	0.43
1:D:154:ARG:NH2	1:D:162:GLN:NE2	2.63	0.43
1:D:417:PHE:O	1:D:418:ALA:C	2.55	0.43
1:F:221:ARG:HE	1:F:221:ARG:HA	1.82	0.43
1:B:334:TYR:CZ	1:B:443:ARG:HG2	2.54	0.43
1:C:137:ILE:HG22	1:C:143:ALA:HB2	1.98	0.43
1:E:119:ARG:HD3	1:E:155:SER:O	2.18	0.43
1:E:158:PRO:HD3	1:E:334:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LYS:NZ	1:B:186:GLU:OE2	2.52	0.43
1:B:245:GLN:HE22	1:E:117:ARG:HD3	1.83	0.43
1:E:154:ARG:HE	1:E:162:GLN:HE21	1.65	0.43
1:F:324:GLU:H	1:F:324:GLU:HG2	1.43	0.43
1:B:334:TYR:HD2	1:B:440:ARG:HD2	1.83	0.43
1:B:339:SER:HA	1:B:342:LEU:HB2	1.99	0.43
1:C:151:ASP:OD1	1:C:154:ARG:NH2	2.51	0.43
1:C:198:LEU:HD23	1:C:278:LEU:HD23	2.00	0.43
1:D:291:LEU:HD23	1:D:292:THR:H	1.84	0.43
1:E:375:ASN:O	1:E:379:THR:HG23	2.18	0.43
1:A:323:THR:HG22	1:A:324:GLU:N	2.34	0.43
1:A:395:THR:O	1:A:396:MET:C	2.57	0.43
1:C:390:SER:O	1:C:395:THR:HG21	2.18	0.43
1:C:396:MET:HE2	1:C:428:LEU:HD11	1.99	0.43
1:C:414:ASP:O	1:C:418:ALA:HB2	2.18	0.43
1:D:208:ASP:O	1:D:212:LEU:HG	2.19	0.43
1:F:133:THR:O	1:F:134:LEU:HD23	2.18	0.43
1:F:168:LEU:O	1:F:170:GLN:HG3	2.19	0.43
1:F:315:HIS:HB3	1:F:326:GLN:OE1	2.18	0.43
1:F:320:GLY:O	1:F:360:THR:HA	2.19	0.43
1:A:154:ARG:HH11	1:A:314:ARG:HH21	1.63	0.43
1:B:210:ILE:HG22	1:B:211:PHE:N	2.33	0.43
1:C:111:VAL:O	1:C:114:TYR:HB3	2.19	0.43
1:C:383:PHE:O	1:C:384:TYR:C	2.56	0.43
1:E:137:ILE:HG12	1:E:143:ALA:HB2	2.00	0.43
1:C:342:LEU:O	1:C:345:MET:HB3	2.18	0.43
1:C:417:PHE:O	1:C:421:ASP:HB3	2.19	0.43
1:C:454:THR:OG1	1:C:455:ARG:N	2.50	0.43
1:D:187:LYS:HG2	1:D:201:CYS:HB3	2.00	0.43
1:D:407:GLU:OE1	1:D:407:GLU:HA	2.18	0.43
1:F:278:LEU:O	1:F:281:TYR:HB3	2.19	0.43
1:A:194:ILE:O	1:A:194:ILE:HG13	2.17	0.43
1:A:209:TYR:O	1:A:213:THR:HG23	2.19	0.43
1:A:398:GLN:HE21	1:A:402:THR:HG23	1.84	0.43
1:B:146:PHE:HE1	1:B:200:GLU:OE2	2.01	0.43
1:B:233:ASN:N	1:B:233:ASN:ND2	2.67	0.43
1:C:218:THR:HG21	1:C:250:ILE:HG23	2.00	0.43
1:C:315:HIS:O	1:C:316:ASP:HB2	2.19	0.43
1:C:415:VAL:O	1:C:419:LEU:HD12	2.18	0.43
1:D:146:PHE:HE1	1:D:200:GLU:HG2	1.83	0.43
1:E:112:MET:HE3	1:E:112:MET:HB3	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:GLU:O	1:E:114:TYR:C	2.57	0.43
1:E:194:ILE:HG13	1:E:306:ASP:OD1	2.19	0.43
1:E:206:PHE:CE2	1:E:210:ILE:CD1	3.02	0.43
1:F:145:VAL:HG11	1:F:171:TYR:CE2	2.54	0.43
1:F:166:LEU:HD23	1:F:171:TYR:HA	2.01	0.43
1:B:293:ILE:HD12	1:B:293:ILE:H	1.82	0.43
1:D:305:HIS:HD2	1:D:365:GLU:OE2	2.02	0.43
1:E:137:ILE:HG22	1:E:138:SER:N	2.33	0.43
1:E:302:LYS:O	1:E:303:LEU:C	2.56	0.43
1:E:374:ILE:HD12	1:E:374:ILE:N	2.34	0.43
1:F:196:TYR:C	1:F:198:LEU:H	2.22	0.43
1:C:353:PHE:HD2	1:C:353:PHE:H	1.67	0.43
1:C:371:LEU:HB3	1:C:441:LEU:HD23	2.00	0.43
1:D:210:ILE:N	1:D:210:ILE:CD1	2.82	0.43
1:D:391:LEU:HD23	1:D:395:THR:HG21	2.00	0.43
1:F:346:GLN:O	1:F:350:LYS:CG	2.58	0.43
1:A:442:MET:HA	1:A:442:MET:HE2	2.01	0.42
1:B:464:ALA:HB2	1:E:457:MET:HG2	2.01	0.42
1:D:383:PHE:CE2	1:F:226:ALA:HB2	2.53	0.42
1:F:220:GLN:O	1:F:221:ARG:C	2.57	0.42
1:F:417:PHE:O	1:F:418:ALA:C	2.56	0.42
1:F:437:MET:HA	1:F:437:MET:HE3	2.00	0.42
1:A:148:THR:HB	1:A:149:PRO:HD3	2.01	0.42
1:A:314:ARG:HH11	1:A:314:ARG:HG2	1.84	0.42
1:B:316:ASP:H	1:B:317:PRO:HD3	1.83	0.42
1:B:342:LEU:O	1:B:345:MET:HB3	2.19	0.42
1:C:209:TYR:O	1:C:213:THR:HG23	2.19	0.42
1:C:239:ASP:OD1	1:C:242:GLU:HG3	2.18	0.42
1:C:377:VAL:O	1:C:381:LEU:HG	2.19	0.42
1:D:421:ASP:O	1:D:422:CYS:C	2.57	0.42
1:E:371:LEU:C	1:E:373:ASN:H	2.22	0.42
1:F:212:LEU:HD22	1:F:303:LEU:HD11	2.01	0.42
1:B:452:GLY:O	1:B:453:PHE:CB	2.66	0.42
1:C:244:GLU:HB3	1:F:121:TYR:CD1	2.55	0.42
1:D:112:MET:C	1:D:114:TYR:H	2.22	0.42
1:D:196:TYR:C	1:D:198:LEU:H	2.23	0.42
1:E:334:TYR:CE2	1:E:443:ARG:HA	2.55	0.42
1:E:460:MET:HB2	1:E:460:MET:HE3	1.91	0.42
1:E:462:LYS:O	1:E:465:GLN:CB	2.67	0.42
1:A:210:ILE:O	1:A:214:THR:HG23	2.19	0.42
1:A:298:GLU:OE2	1:A:298:GLU:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:SER:O	1:A:342:LEU:HD13	2.19	0.42
1:C:145:VAL:HG12	1:C:146:PHE:N	2.34	0.42
1:D:297:LEU:HA	1:D:297:LEU:HD23	1.63	0.42
1:D:324:GLU:OE2	1:D:411:HIS:CE1	2.72	0.42
1:A:459:ALA:O	1:D:456:LEU:HD21	2.20	0.42
1:C:335:SER:HA	1:C:439:GLN:CD	2.39	0.42
1:D:193:SER:C	1:D:195:PHE:N	2.70	0.42
1:D:214:THR:O	1:D:218:THR:HG23	2.19	0.42
1:D:323:THR:HB	1:D:326:GLN:H	1.85	0.42
1:E:322:ILE:HG23	1:E:323:THR:O	2.20	0.42
1:A:309:LYS:HG3	1:A:361:PHE:CZ	2.55	0.42
1:B:194:ILE:HD12	1:B:195:PHE:N	2.35	0.42
1:B:245:GLN:HE22	1:E:117:ARG:HH11	1.66	0.42
1:B:247:GLN:NE2	1:B:251:ARG:NH1	2.67	0.42
1:D:144:GLU:HB3	1:D:146:PHE:HE2	1.83	0.42
1:D:325:ARG:HA	1:D:345:MET:HE1	2.00	0.42
1:D:376:ASP:O	1:D:380:ALA:HB2	2.19	0.42
1:E:292:THR:HG22	1:E:294:LYS:N	2.35	0.42
1:A:206:PHE:CE2	1:A:210:ILE:HD11	2.54	0.42
1:A:395:THR:C	1:A:397:GLN:N	2.72	0.42
1:A:431:LYS:HG2	1:A:432:GLU:H	1.83	0.42
1:D:215:VAL:O	1:D:215:VAL:CG1	2.66	0.42
1:D:350:LYS:HB2	1:D:355:GLU:OE1	2.19	0.42
1:E:373:ASN:O	1:E:374:ILE:C	2.57	0.42
1:F:128:PHE:CE1	1:F:206:PHE:HA	2.54	0.42
1:A:347:ARG:HH12	1:F:425:ASN:HA	1.82	0.42
1:A:371:LEU:HD11	1:A:437:MET:SD	2.60	0.42
1:B:158:PRO:HD3	1:B:334:TYR:CE1	2.55	0.42
1:B:243:PHE:HA	1:B:246:VAL:CG1	2.48	0.42
1:B:433:PHE:CZ	1:B:437:MET:HG3	2.55	0.42
1:D:325:ARG:HA	1:D:345:MET:CE	2.50	0.42
1:E:323:THR:HG22	1:E:325:ARG:N	2.32	0.42
1:F:119:ARG:HD3	1:F:155:SER:O	2.20	0.42
1:F:323:THR:HB	1:F:326:GLN:H	1.84	0.42
1:A:331:LEU:O	1:A:333:ALA:N	2.53	0.42
1:B:137:ILE:HD12	1:B:137:ILE:N	2.34	0.42
1:C:149:PRO:HB3	1:C:310:LEU:HD21	2.02	0.42
1:D:421:ASP:O	1:D:421:ASP:OD2	2.38	0.42
1:F:374:ILE:O	1:F:378:ASP:HB2	2.20	0.42
1:A:123:THR:OG1	1:A:125:ASP:HB3	2.20	0.42
1:A:460:MET:HA	1:D:456:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ILE:HD12	1:B:322:ILE:HA	1.91	0.42
1:C:454:THR:HG22	1:E:460:MET:SD	2.60	0.42
1:D:307:VAL:HG12	1:D:308:LEU:N	2.33	0.42
1:D:352:HIS:O	1:D:353:PHE:HB2	2.20	0.42
1:E:327:PHE:CD2	1:E:359:LEU:HD13	2.55	0.42
1:F:352:HIS:O	1:F:353:PHE:HB2	2.20	0.42
1:A:119:ARG:NH2	1:A:159:ASN:H	2.18	0.41
1:A:198:LEU:CD1	1:A:204:ILE:HG12	2.47	0.41
1:A:342:LEU:O	1:A:345:MET:HB3	2.20	0.41
1:C:255:SER:O	1:C:259:ARG:NE	2.50	0.41
1:F:313:GLU:C	1:F:315:HIS:N	2.73	0.41
1:A:171:TYR:O	1:A:172:ILE:O	2.38	0.41
1:B:345:MET:HG3	1:B:418:ALA:HB1	2.02	0.41
1:B:359:LEU:HD23	1:B:363:GLU:OE2	2.19	0.41
1:B:398:GLN:O	1:B:402:THR:HG23	2.20	0.41
1:C:122:SER:HB3	1:C:126:LYS:HB3	2.01	0.41
1:C:283:PHE:O	1:C:284:GLY:O	2.36	0.41
1:D:160:GLU:HB3	1:D:314:ARG:NH1	2.24	0.41
1:E:348:GLN:CA	1:E:348:GLN:HE21	2.32	0.41
1:E:390:SER:N	1:F:337:VAL:HG21	2.35	0.41
1:F:210:ILE:O	1:F:211:PHE:C	2.58	0.41
1:A:133:THR:C	1:A:171:TYR:HB3	2.41	0.41
1:B:148:THR:O	1:B:151:ASP:N	2.53	0.41
1:B:305:HIS:HD2	1:B:365:GLU:OE2	2.02	0.41
1:B:393:LYS:HG3	1:B:413:CYS:HB3	2.01	0.41
1:B:396:MET:C	1:B:398:GLN:N	2.74	0.41
1:C:337:VAL:C	1:C:339:SER:N	2.72	0.41
1:D:146:PHE:N	1:D:146:PHE:CD2	2.88	0.41
1:D:196:TYR:O	1:D:198:LEU:N	2.54	0.41
1:D:231:ASP:HB3	1:D:236:GLY:HA2	2.01	0.41
1:D:367:PHE:O	1:D:370:PHE:HB3	2.20	0.41
1:F:308:LEU:HD13	1:F:361:PHE:CE1	2.55	0.41
1:F:350:LYS:HG2	1:F:355:GLU:CG	2.50	0.41
1:A:353:PHE:N	1:A:353:PHE:CD2	2.85	0.41
1:B:173:ILE:N	1:B:173:ILE:HD12	2.36	0.41
1:B:216:LEU:HA	1:B:216:LEU:HD23	1.81	0.41
1:D:420:PHE:CE1	1:D:436:ILE:HD12	2.55	0.41
1:E:295:ASN:O	1:E:298:GLU:N	2.54	0.41
1:E:298:GLU:OE2	1:E:298:GLU:HA	2.21	0.41
1:A:119:ARG:NH2	1:A:159:ASN:N	2.69	0.41
1:A:417:PHE:CE1	1:A:428:LEU:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:PRO:O	1:B:150:GLU:C	2.59	0.41
1:D:117:ARG:HG2	1:D:121:TYR:HD2	1.85	0.41
1:E:105:GLY:O	1:E:108:ASP:HB2	2.20	0.41
1:F:196:TYR:C	1:F:198:LEU:N	2.74	0.41
1:A:145:VAL:C	1:A:146:PHE:HD2	2.24	0.41
1:A:218:THR:HA	1:A:219:PRO:HD3	1.78	0.41
1:A:381:LEU:HD22	1:A:391:LEU:HD22	2.01	0.41
1:C:223:PHE:O	1:C:224:GLU:C	2.58	0.41
1:C:283:PHE:CE1	1:C:291:LEU:HB2	2.56	0.41
1:D:465:GLN:C	1:D:467:THR:H	2.24	0.41
1:E:315:HIS:HB2	1:E:322:ILE:HD11	2.02	0.41
1:E:352:HIS:O	1:E:354:LYS:N	2.53	0.41
1:A:119:ARG:HH21	1:A:159:ASN:H	1.67	0.41
1:A:147:MET:HE2	1:A:151:ASP:CB	2.50	0.41
1:A:292:THR:HG22	1:A:293:ILE:CD1	2.45	0.41
1:A:398:GLN:O	1:A:401:ARG:HB3	2.20	0.41
1:B:315:HIS:O	1:B:316:ASP:CB	2.62	0.41
1:C:162:GLN:O	1:C:163:PRO:C	2.59	0.41
1:C:216:LEU:HD23	1:C:216:LEU:HA	1.85	0.41
1:C:428:LEU:CD2	1:C:429:SER:N	2.84	0.41
1:A:198:LEU:O	1:A:277:ALA:HB1	2.19	0.41
1:B:187:LYS:HB3	1:B:196:TYR:OH	2.21	0.41
1:B:195:PHE:O	1:B:202:GLY:HA2	2.21	0.41
1:C:323:THR:CG2	1:C:324:GLU:N	2.83	0.41
1:C:351:LYS:HE2	1:C:352:HIS:HE1	1.85	0.41
1:D:387:ALA:HB2	1:F:249:ILE:HD11	2.02	0.41
1:F:350:LYS:HG2	1:F:355:GLU:HG3	2.03	0.41
1:A:222:ASN:ND2	1:B:383:PHE:HZ	2.11	0.41
1:A:231:ASP:OD2	1:A:234:GLY:HA3	2.21	0.41
1:A:323:THR:HB	1:A:326:GLN:CB	2.51	0.41
1:A:438:LYS:O	1:A:442:MET:CG	2.67	0.41
1:C:133:THR:HG22	1:C:166:LEU:HD13	2.02	0.41
1:C:238:VAL:HG12	1:C:243:PHE:HB2	2.03	0.41
1:D:160:GLU:CB	1:D:314:ARG:HH12	2.25	0.41
1:D:308:LEU:HD23	1:D:308:LEU:HA	1.83	0.41
1:D:332:LEU:HD11	1:D:419:LEU:CD2	2.50	0.41
1:D:350:LYS:N	1:D:355:GLU:OE2	2.54	0.41
1:E:286:ASP:OD2	1:E:288:LYS:HB2	2.21	0.41
1:E:378:ASP:CG	1:E:434:VAL:HG21	2.41	0.41
1:E:421:ASP:OD2	1:E:421:ASP:C	2.59	0.41
1:F:200:GLU:OE1	1:F:200:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:PHE:CZ	1:A:377:VAL:HG11	2.56	0.41
1:B:291:LEU:HD23	1:B:292:THR:N	2.36	0.41
1:B:371:LEU:C	1:B:373:ASN:N	2.73	0.41
1:C:115:GLU:OE1	1:C:160:GLU:O	2.39	0.41
1:C:136:VAL:CG2	1:C:174:LYS:HE2	2.51	0.41
1:C:397:GLN:NE2	1:C:413:CYS:SG	2.94	0.41
1:C:430:ASN:O	1:C:434:VAL:HG23	2.20	0.41
1:D:124:PRO:HG3	1:D:256:MET:HB3	2.02	0.41
1:D:221:ARG:HD3	1:F:376:ASP:OD1	2.21	0.41
1:D:436:ILE:HG22	1:D:437:MET:HE2	2.03	0.41
1:E:166:LEU:HD23	1:E:166:LEU:HA	1.66	0.41
1:E:199:GLY:HA3	1:E:277:ALA:CB	2.51	0.41
1:E:341:LYS:O	1:E:344:ALA:HB3	2.21	0.41
1:F:323:THR:CG2	1:F:324:GLU:N	2.82	0.41
1:A:145:VAL:O	1:A:146:PHE:HD2	2.04	0.40
1:A:239:ASP:OD1	1:A:242:GLU:HG3	2.21	0.40
1:C:205:SER:O	1:C:206:PHE:C	2.56	0.40
1:C:313:GLU:C	1:C:315:HIS:H	2.25	0.40
1:D:303:LEU:C	1:D:303:LEU:HD13	2.41	0.40
1:E:154:ARG:NH1	1:E:314:ARG:HH21	2.04	0.40
1:A:392:ASP:CG	1:A:394:VAL:HG23	2.42	0.40
1:B:453:PHE:CB	1:C:461:TRP:HE1	2.32	0.40
1:C:218:THR:HA	1:C:219:PRO:HD3	1.73	0.40
1:C:258:MET:C	1:C:259:ARG:HG3	2.41	0.40
1:E:108:ASP:O	1:E:112:MET:HG3	2.20	0.40
1:F:292:THR:HG22	1:F:293:ILE:HD12	2.04	0.40
1:F:404:ALA:O	1:F:405:LYS:C	2.57	0.40
1:A:106:PHE:CE2	1:D:241:GLU:HB2	2.57	0.40
1:A:206:PHE:CZ	1:A:210:ILE:HD11	2.56	0.40
1:A:297:LEU:HD23	1:A:297:LEU:HA	1.78	0.40
1:A:327:PHE:HD2	1:A:415:VAL:HG11	1.86	0.40
1:B:429:SER:O	1:B:431:LYS:N	2.54	0.40
1:C:322:ILE:HG13	1:C:326:GLN:HB2	2.02	0.40
1:C:368:PHE:HE2	1:C:440:ARG:HE	1.69	0.40
1:C:431:LYS:H	1:C:431:LYS:CD	2.33	0.40
1:D:154:ARG:CZ	1:D:162:GLN:HE21	2.33	0.40
1:E:193:SER:HG	1:E:195:PHE:HD2	1.69	0.40
1:E:308:LEU:HA	1:E:308:LEU:HD23	1.84	0.40
1:F:246:VAL:O	1:F:246:VAL:HG12	2.19	0.40
1:F:297:LEU:HA	1:F:297:LEU:HD23	1.85	0.40
1:B:411:HIS:O	1:B:415:VAL:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:ARG:HH11	1:C:117:ARG:HG3	1.85	0.40
1:C:163:PRO:O	1:C:165:HIS:N	2.55	0.40
1:A:327:PHE:CD2	1:A:415:VAL:HG11	2.56	0.40
1:B:108:ASP:O	1:B:111:VAL:N	2.54	0.40
1:B:258:MET:HE3	1:B:458:GLN:HG2	2.03	0.40
1:D:117:ARG:HG2	1:D:121:TYR:CD2	2.57	0.40
1:D:217:SER:HB2	1:D:445:LEU:CD2	2.43	0.40
1:E:119:ARG:NE	1:E:158:PRO:HA	2.36	0.40
1:E:154:ARG:HD3	1:E:314:ARG:NH2	2.36	0.40
1:E:247:GLN:NE2	1:E:251:ARG:HH12	2.10	0.40
1:E:335:SER:O	1:E:336:GLY:O	2.39	0.40
1:E:421:ASP:O	1:E:422:CYS:O	2.40	0.40
1:F:218:THR:HG21	1:F:250:ILE:CG2	2.51	0.40
1:F:337:VAL:HG12	1:F:340:LYS:HD3	2.03	0.40

All (1) 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 distance (Å)	Clash overlap (Å)
1:E:171:TYR:O	1:F:357:LYS:NZ[2_756]	2.10	0.10

## 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	Percentiles	
1	A	300/401 (75%)	227 (76%)	54 (18%)	19 (6%)	1	10
1	B	304/401 (76%)	235 (77%)	53 (17%)	16 (5%)	2	15
1	C	322/401 (80%)	248 (77%)	56 (17%)	18 (6%)	2	14
1	D	316/401 (79%)	262 (83%)	39 (12%)	15 (5%)	2	17
1	E	322/401 (80%)	261 (81%)	47 (15%)	14 (4%)	2	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	302/401 (75%)	237 (78%)	49 (16%)	16 (5%)	2	15
All	All	1866/2406 (78%)	1470 (79%)	298 (16%)	98 (5%)	2	15

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	LEU
1	A	172	ILE
1	A	354	LYS
1	A	453	PHE
1	B	374	ILE
1	B	453	PHE
1	C	200	GLU
1	C	338	GLN
1	C	422	CYS
1	C	450	ASP
1	D	176	PHE
1	D	190	ASP
1	D	314	ARG
1	E	190	ASP
1	E	194	ILE
1	E	336	GLY
1	E	353	PHE
1	E	422	CYS
1	E	430	ASN
1	F	164	GLU
1	F	200	GLU
1	F	253	GLN
1	F	422	CYS
1	A	200	GLU
1	A	221	ARG
1	A	332	LEU
1	B	166	LEU
1	B	190	ASP
1	B	200	GLU
1	B	430	ASN
1	C	164	GLU
1	C	168	LEU
1	C	254	THR
1	C	284	GLY
1	C	351	LYS
1	C	430	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	448	PRO
1	D	113	GLU
1	D	166	LEU
1	D	200	GLU
1	D	337	VAL
1	D	387	ALA
1	E	195	PHE
1	E	200	GLU
1	F	166	LEU
1	F	189	ALA
1	F	232	LEU
1	F	336	GLY
1	A	236	GLY
1	A	333	ALA
1	A	337	VAL
1	A	353	PHE
1	A	430	ASN
1	B	135	LYS
1	B	168	LEU
1	C	336	GLY
1	D	193	SER
1	D	389	ALA
1	D	422	CYS
1	E	338	GLN
1	F	159	ASN
1	F	231	ASP
1	F	314	ARG
1	A	228	LYS
1	A	232	LEU
1	B	195	PHE
1	B	236	GLY
1	B	314	ARG
1	B	372	LYS
1	C	163	PRO
1	C	372	LYS
1	C	447	LYS
1	C	462	LYS
1	D	208	ASP
1	D	425	ASN
1	E	389	ALA
1	F	183	GLN
1	F	277	ALA

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Mol	Chain	Res	Type
1	A	427	GLU
1	B	169	ASP
1	B	316	ASP
1	C	452	GLY
1	D	253	GLN
1	E	314	ARG
1	E	459	ALA
1	A	356	GLY
1	A	389	ALA
1	B	234	GLY
1	C	193	SER
1	F	190	ASP
1	A	374	ILE
1	B	163	PRO
1	D	173	ILE
1	E	374	ILE
1	F	337	VAL
1	A	127	ILE
1	F	374	ILE
1	E	140	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	A	259/354 (73%)	232 (90%)	27 (10%)	7	28
1	B	273/354 (77%)	243 (89%)	30 (11%)	6	26
1	C	274/354 (77%)	249 (91%)	25 (9%)	9	34
1	D	278/354 (78%)	256 (92%)	22 (8%)	12	43
1	E	269/354 (76%)	240 (89%)	29 (11%)	6	27
1	F	270/354 (76%)	241 (89%)	29 (11%)	6	27
All	All	1623/2124 (76%)	1461 (90%)	162 (10%)	7	30

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ARG
1	A	108	ASP
1	A	162	GLN
1	A	165	HIS
1	A	168	LEU
1	A	171	TYR
1	A	200	GLU
1	A	216	LEU
1	A	278	LEU
1	A	279	THR
1	A	291	LEU
1	A	292	THR
1	A	293	ILE
1	A	308	LEU
1	A	313	GLU
1	A	314	ARG
1	A	340	LYS
1	A	346	GLN
1	A	360	THR
1	A	365	GLU
1	A	371	LEU
1	A	374	ILE
1	A	396	MET
1	A	419	LEU
1	A	425	ASN
1	A	431	LYS
1	A	440	ARG
1	B	137	ILE
1	B	148	THR
1	B	149	PRO
1	B	162	GLN
1	B	190	ASP
1	B	194	ILE
1	B	200	GLU
1	B	205	SER
1	B	207	SER
1	B	221	ARG
1	B	235	ASP
1	B	241	GLU
1	B	246	VAL
1	B	247	GLN
1	B	275	CYS
1	B	279	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	291	LEU
1	B	293	ILE
1	B	303	LEU
1	B	308	LEU
1	B	346	GLN
1	B	360	THR
1	B	362	GLN
1	B	374	ILE
1	B	379	THR
1	B	398	GLN
1	B	419	LEU
1	B	430	ASN
1	B	431	LYS
1	B	463	CYS
1	C	168	LEU
1	C	171	TYR
1	C	194	ILE
1	C	200	GLU
1	C	221	ARG
1	C	241	GLU
1	C	258	MET
1	C	278	LEU
1	C	279	THR
1	C	293	ILE
1	C	301	ARG
1	C	308	LEU
1	C	313	GLU
1	C	346	GLN
1	C	348	GLN
1	C	353	PHE
1	C	379	THR
1	C	390	SER
1	C	396	MET
1	C	397	GLN
1	C	419	LEU
1	C	423	ASP
1	C	428	LEU
1	C	431	LYS
1	C	443	ARG
1	D	147	MET
1	D	162	GLN
1	D	168	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	190	ASP
1	D	200	GLU
1	D	214	THR
1	D	221	ARG
1	D	241	GLU
1	D	278	LEU
1	D	286	ASP
1	D	291	LEU
1	D	293	ILE
1	D	308	LEU
1	D	343	THR
1	D	349	LEU
1	D	407	GLU
1	D	412	VAL
1	D	419	LEU
1	D	428	LEU
1	D	431	LYS
1	D	440	ARG
1	D	445	LEU
1	E	108	ASP
1	E	112	MET
1	E	122	SER
1	E	150	GLU
1	E	162	GLN
1	E	164	GLU
1	E	216	LEU
1	E	248	SER
1	E	278	LEU
1	E	291	LEU
1	E	293	ILE
1	E	303	LEU
1	E	308	LEU
1	E	318	VAL
1	E	331	LEU
1	E	340	LYS
1	E	346	GLN
1	E	348	GLN
1	E	350	LYS
1	E	371	LEU
1	E	374	ILE
1	E	406	VAL
1	E	422	CYS

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Mol	Chain	Res	Type
1	E	423	ASP
1	E	425	ASN
1	E	428	LEU
1	E	430	ASN
1	E	431	LYS
1	E	434	VAL
1	F	137	ILE
1	F	150	GLU
1	F	162	GLN
1	F	166	LEU
1	F	171	TYR
1	F	194	ILE
1	F	200	GLU
1	F	214	THR
1	F	216	LEU
1	F	231	ASP
1	F	235	ASP
1	F	240	MET
1	F	241	GLU
1	F	278	LEU
1	F	280	THR
1	F	291	LEU
1	F	292	THR
1	F	293	ILE
1	F	294	LYS
1	F	303	LEU
1	F	322	ILE
1	F	324	GLU
1	F	374	ILE
1	F	379	THR
1	F	395	THR
1	F	419	LEU
1	F	423	ASP
1	F	431	LYS
1	F	437	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	GLN
1	A	222	ASN
1	A	233	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	245	GLN
1	A	247	GLN
1	A	295	ASN
1	A	304	GLN
1	A	326	GLN
1	A	346	GLN
1	A	373	ASN
1	A	375	ASN
1	A	397	GLN
1	A	398	GLN
1	A	439	GLN
1	B	162	GLN
1	B	233	ASN
1	B	245	GLN
1	B	247	GLN
1	B	315	HIS
1	B	326	GLN
1	B	346	GLN
1	B	352	HIS
1	B	366	ASN
1	B	430	ASN
1	C	162	GLN
1	C	170	GLN
1	C	220	GLN
1	C	233	ASN
1	C	245	GLN
1	C	300	GLN
1	C	326	GLN
1	C	346	GLN
1	C	397	GLN
1	C	411	HIS
1	C	425	ASN
1	C	439	GLN
1	D	162	GLN
1	D	170	GLN
1	D	245	GLN
1	D	247	GLN
1	D	253	GLN
1	D	295	ASN
1	D	300	GLN
1	D	305	HIS
1	D	315	HIS

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Mol	Chain	Res	Type
1	D	326	GLN
1	D	338	GLN
1	D	348	GLN
1	D	352	HIS
1	D	366	ASN
1	D	397	GLN
1	D	411	HIS
1	D	439	GLN
1	E	162	GLN
1	E	233	ASN
1	E	247	GLN
1	E	295	ASN
1	E	300	GLN
1	E	305	HIS
1	E	315	HIS
1	E	326	GLN
1	E	346	GLN
1	E	373	ASN
1	E	411	HIS
1	E	425	ASN
1	E	439	GLN
1	F	162	GLN
1	F	245	GLN
1	F	247	GLN
1	F	326	GLN
1	F	346	GLN
1	F	397	GLN
1	F	411	HIS
1	F	425	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	310/401 (77%)	0.09	7 (2%) 60 47	62, 86, 113, 127	0
1	B	316/401 (78%)	-0.11	2 (0%) 89 83	41, 73, 104, 122	0
1	C	330/401 (82%)	-0.15	6 (1%) 68 55	44, 70, 97, 114	0
1	D	326/401 (81%)	-0.17	3 (0%) 84 75	36, 60, 89, 111	0
1	E	330/401 (82%)	-0.30	2 (0%) 89 83	32, 59, 107, 122	0
1	F	310/401 (77%)	-0.33	0 100 100	36, 58, 95, 112	0
All	All	1922/2406 (79%)	-0.16	20 (1%) 82 72	32, 69, 104, 127	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	461	TRP	5.1
1	C	462	LYS	3.6
1	A	124	PRO	3.4
1	E	453	PHE	3.1
1	C	456	LEU	3.0
1	D	337	VAL	2.7
1	A	125	ASP	2.6
1	B	388	GLY	2.6
1	D	462	LYS	2.6
1	D	458	GLN	2.5
1	A	172	ILE	2.4
1	B	136	VAL	2.4
1	E	353	PHE	2.3
1	C	450	ASP	2.3
1	A	339	SER	2.2
1	C	164	GLU	2.2
1	C	451	MET	2.2
1	C	461	TRP	2.1
1	A	320	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	177	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.