



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:56 PM UTC

PDB ID : 4NSC / pdb_00004nsc
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

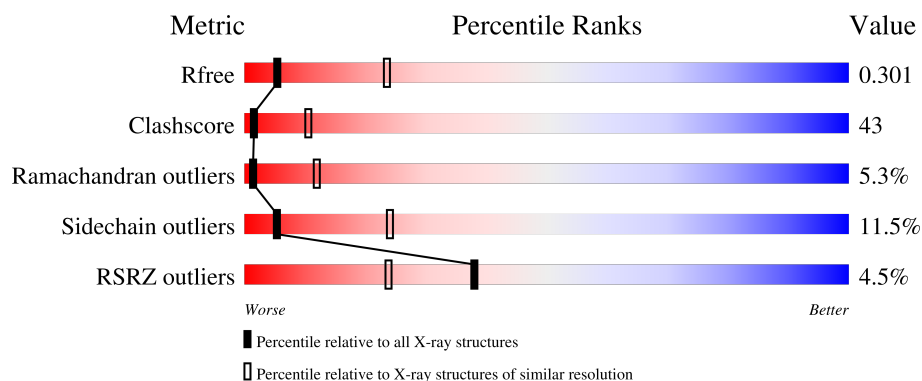
1 Overall quality at a glance

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 ≥ 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	5% 26% 38% 12% 23%
1	B	401	4% 28% 38% 10% 21%
1	C	401	5% 23% 49% 9% 18%
1	D	401	4% 31% 38% 11% 19%
1	E	401	2% 31% 38% 11% 18%

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Mol	Chain	Length	Quality of chain
1	F	401	2% 30% 36% 10% 23%

2 Entry composition

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

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

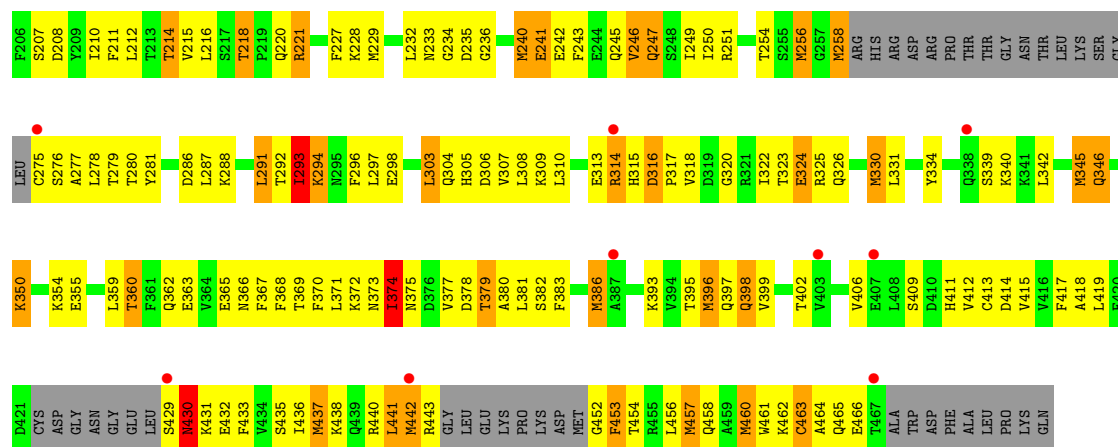
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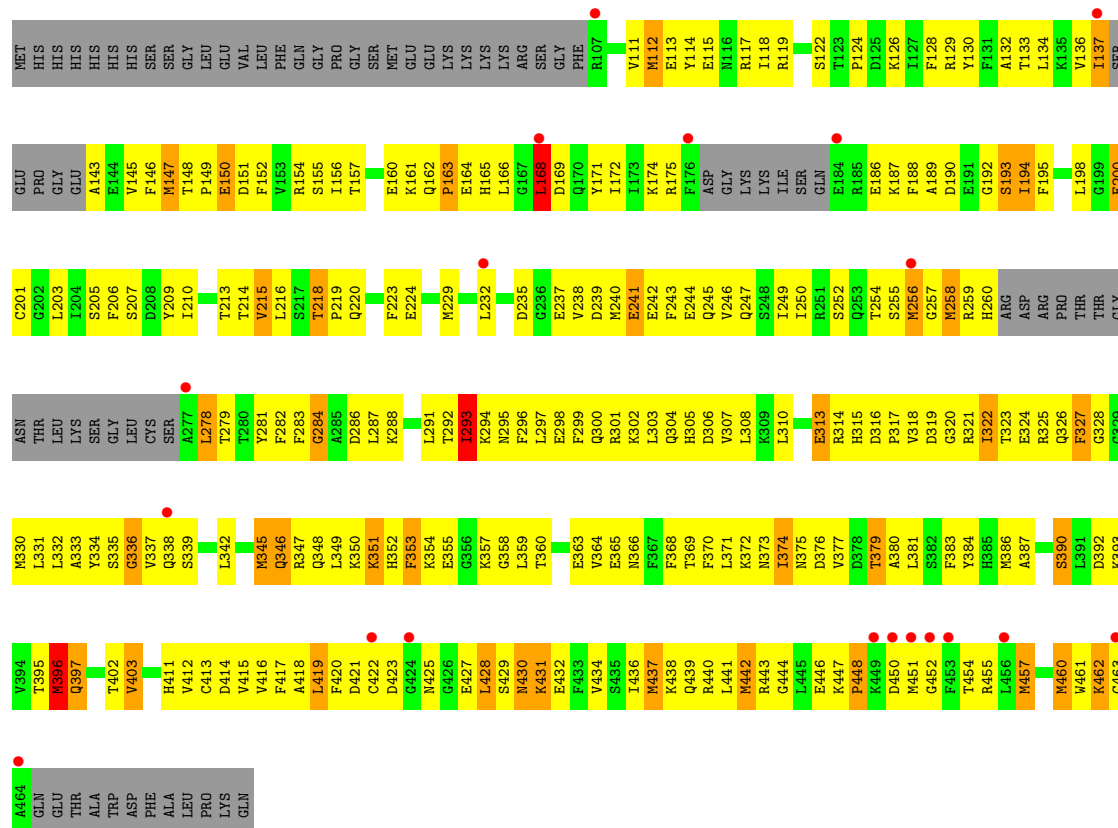
Chain	Residue	Modelled	Actual	Comment	Reference
E	93	PRO	-	expression tag	UNP Q9BPX6
E	94	GLY	-	expression tag	UNP Q9BPX6
E	95	SER	-	expression tag	UNP Q9BPX6
E	96	MET	-	expression tag	UNP Q9BPX6
F	76	MET	-	expression tag	UNP Q9BPX6
F	77	HIS	-	expression tag	UNP Q9BPX6
F	78	HIS	-	expression tag	UNP Q9BPX6
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

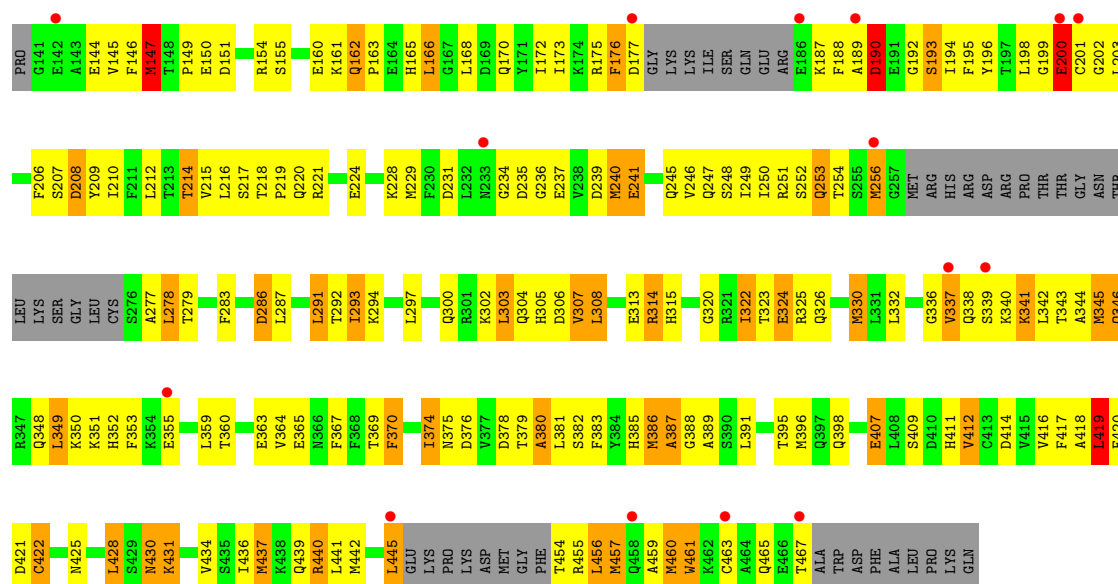


• Molecule 1: Calcium uptake protein 1, mitochondrial

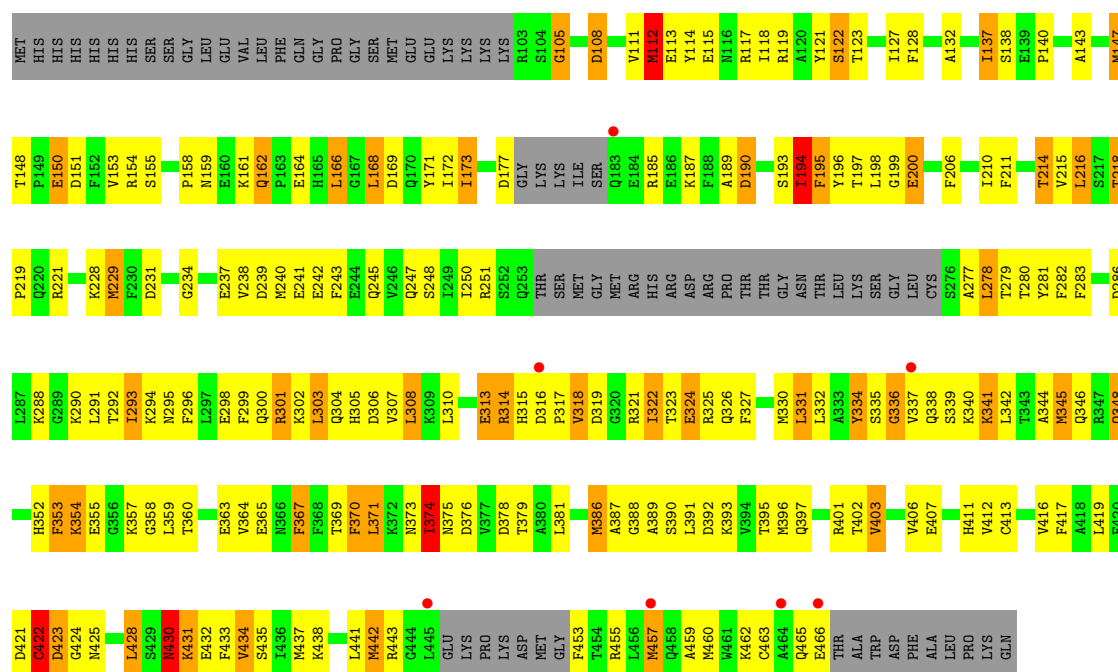


• Molecule 1: Calcium uptake protein 1, mitochondrial



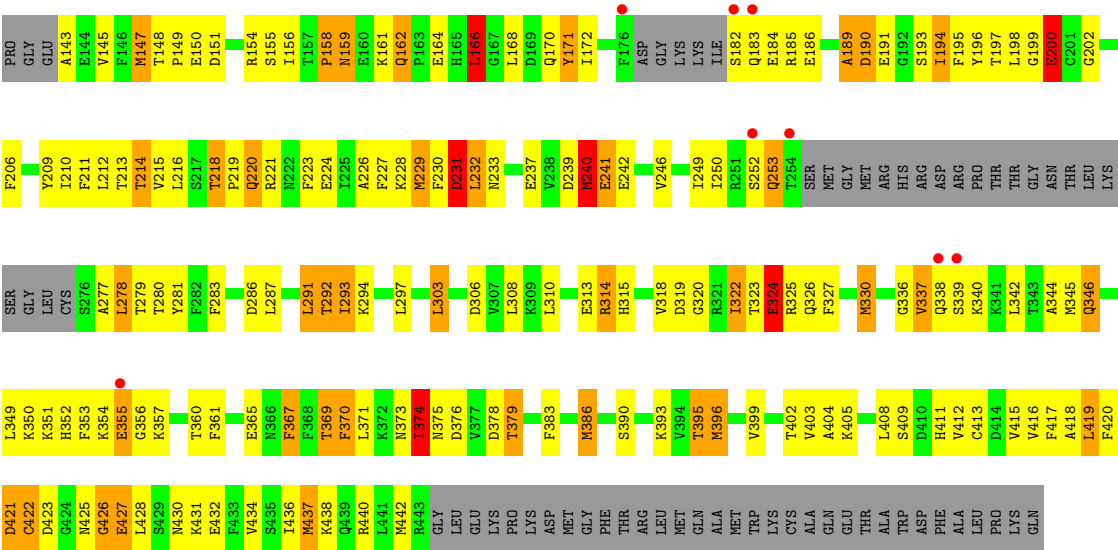


• Molecule 1: Calcium uptake protein 1, mitochondrial



• Molecule 1: Calcium uptake protein 1, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.88Å 146.82Å 115.87Å 90.00° 111.08° 90.00°	Depositor
Resolution (Å)	36.72 – 3.20 36.72 – 3.20	Depositor EDS
% Data completeness (in resolution range)	92.3 (36.72-3.20) 92.3 (36.72-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 3.18Å)	Xtriage
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 ²)	58.1	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15349	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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.

5 Model quality

5.1 Standard geometry

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	0.76	21/2517 (0.8%)	1.02	14/3379 (0.4%)
1	B	0.85	24/2581 (0.9%)	1.05	16/3456 (0.5%)
1	C	0.81	23/2665 (0.9%)	1.04	13/3577 (0.4%)
1	D	0.85	19/2649 (0.7%)	1.08	21/3551 (0.6%)
1	E	0.79	14/2644 (0.5%)	1.13	19/3550 (0.5%)
1	F	0.80	11/2549 (0.4%)	1.11	21/3418 (0.6%)
All	All	0.81	112/15605 (0.7%)	1.07	104/20931 (0.5%)

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 (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	147	MET	CG-SD	9.55	2.04	1.80
1	D	147	MET	CG-SD	8.58	2.02	1.80
1	D	229	MET	CG-SD	8.15	2.01	1.80
1	F	442	MET	CG-SD	8.13	2.01	1.80
1	D	256	MET	CG-SD	8.09	2.00	1.80
1	B	442	MET	CG-SD	8.00	2.00	1.80
1	F	147	MET	CG-SD	7.97	2.00	1.80
1	A	460	MET	CG-SD	7.84	2.00	1.80
1	A	147	MET	CG-SD	7.76	2.00	1.80
1	B	258	MET	CG-SD	7.48	1.99	1.80
1	E	147	MET	CG-SD	7.22	1.98	1.80
1	D	396	MET	CG-SD	7.17	1.98	1.80
1	E	229	MET	CG-SD	7.16	1.98	1.80
1	B	457	MET	CG-SD	7.14	1.98	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	457	MET	CG-SD	7.12	1.98	1.80
1	F	386	MET	SD-CE	7.04	1.97	1.79
1	F	442	MET	SD-CE	7.03	1.97	1.79
1	B	442	MET	SD-CE	6.93	1.96	1.79
1	A	442	MET	CG-SD	6.92	1.98	1.80
1	D	396	MET	SD-CE	6.86	1.96	1.79
1	C	330	MET	CG-SD	6.86	1.97	1.80
1	D	457	MET	SD-CE	6.82	1.96	1.79
1	D	442	MET	SD-CE	6.79	1.96	1.79
1	C	256	MET	SD-CE	6.73	1.96	1.79
1	B	147	MET	CG-SD	6.67	1.97	1.80
1	A	442	MET	SD-CE	6.65	1.96	1.79
1	E	442	MET	SD-CE	6.65	1.96	1.79
1	B	256	MET	SD-CE	6.62	1.96	1.79
1	E	240	MET	SD-CE	6.62	1.96	1.79
1	C	258	MET	SD-CE	6.62	1.96	1.79
1	D	256	MET	SD-CE	6.60	1.96	1.79
1	F	112	MET	SD-CE	6.56	1.96	1.79
1	B	240	MET	SD-CE	6.51	1.95	1.79
1	F	396	MET	CG-SD	6.47	1.97	1.80
1	D	437	MET	CG-SD	6.44	1.96	1.80
1	D	112	MET	SD-CE	6.40	1.95	1.79
1	F	386	MET	CG-SD	6.40	1.96	1.80
1	A	240	MET	SD-CE	6.39	1.95	1.79
1	A	457	MET	SD-CE	6.38	1.95	1.79
1	C	386	MET	SD-CE	6.36	1.95	1.79
1	D	386	MET	SD-CE	6.35	1.95	1.79
1	A	229	MET	SD-CE	6.35	1.95	1.79
1	F	229	MET	CG-SD	6.35	1.96	1.80
1	B	258	MET	SD-CE	6.31	1.95	1.79
1	C	229	MET	CG-SD	6.27	1.96	1.80
1	C	442	MET	CG-SD	6.26	1.96	1.80
1	C	442	MET	SD-CE	6.24	1.95	1.79
1	D	229	MET	SD-CE	6.23	1.95	1.79
1	B	457	MET	SD-CE	6.22	1.95	1.79
1	F	396	MET	SD-CE	6.21	1.95	1.79
1	E	396	MET	SD-CE	6.20	1.95	1.79
1	E	396	MET	CG-SD	6.17	1.96	1.80
1	C	457	MET	CG-SD	6.13	1.96	1.80
1	D	240	MET	SD-CE	6.13	1.94	1.79
1	C	112	MET	SD-CE	6.11	1.94	1.79
1	E	457	MET	SD-CE	6.11	1.94	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	112	MET	SD-CE	6.11	1.94	1.79
1	B	345	MET	CG-SD	6.08	1.96	1.80
1	B	256	MET	CG-SD	6.07	1.96	1.80
1	F	240	MET	SD-CE	6.04	1.94	1.79
1	C	396	MET	CG-SD	6.00	1.95	1.80
1	B	386	MET	SD-CE	5.99	1.94	1.79
1	A	345	MET	SD-CE	5.97	1.94	1.79
1	D	345	MET	CG-SD	5.97	1.95	1.80
1	D	330	MET	CG-SD	5.97	1.95	1.80
1	D	330	MET	SD-CE	5.94	1.94	1.79
1	F	330	MET	SD-CE	5.94	1.94	1.79
1	A	396	MET	SD-CE	5.91	1.94	1.79
1	B	345	MET	SD-CE	5.91	1.94	1.79
1	B	229	MET	CG-SD	5.90	1.95	1.80
1	E	112	MET	SD-CE	5.90	1.94	1.79
1	B	229	MET	SD-CE	5.89	1.94	1.79
1	A	147	MET	SD-CE	5.88	1.94	1.79
1	A	330	MET	CG-SD	5.88	1.95	1.80
1	C	240	MET	SD-CE	5.84	1.94	1.79
1	C	437	MET	SD-CE	5.83	1.94	1.79
1	A	345	MET	CG-SD	5.80	1.95	1.80
1	E	345	MET	SD-CE	5.79	1.94	1.79
1	A	330	MET	SD-CE	5.79	1.94	1.79
1	A	112	MET	CG-SD	5.78	1.95	1.80
1	B	112	MET	CG-SD	5.78	1.95	1.80
1	A	437	MET	SD-CE	5.76	1.94	1.79
1	A	229	MET	CG-SD	5.75	1.95	1.80
1	B	437	MET	SD-CE	5.74	1.93	1.79
1	C	258	MET	CG-SD	5.73	1.95	1.80
1	E	330	MET	SD-CE	5.69	1.93	1.79
1	A	437	MET	CG-SD	5.65	1.94	1.80
1	E	386	MET	SD-CE	5.64	1.93	1.79
1	A	386	MET	SD-CE	5.63	1.93	1.79
1	D	442	MET	CG-SD	5.59	1.94	1.80
1	B	147	MET	SD-CE	5.58	1.93	1.79
1	B	330	MET	SD-CE	5.58	1.93	1.79
1	B	396	MET	SD-CE	5.56	1.93	1.79
1	C	396	MET	SD-CE	5.55	1.93	1.79
1	D	460	MET	SD-CE	5.52	1.93	1.79
1	B	330	MET	CG-SD	5.49	1.94	1.80
1	B	437	MET	CG-SD	5.49	1.94	1.80
1	C	112	MET	CG-SD	5.48	1.94	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	460	MET	SD-CE	5.48	1.93	1.79
1	C	229	MET	SD-CE	5.48	1.93	1.79
1	A	386	MET	CG-SD	5.45	1.94	1.80
1	A	112	MET	SD-CE	5.44	1.93	1.79
1	C	345	MET	SD-CE	5.43	1.93	1.79
1	C	460	MET	CG-SD	5.40	1.94	1.80
1	E	442	MET	CG-SD	5.38	1.94	1.80
1	C	330	MET	SD-CE	5.36	1.93	1.79
1	D	345	MET	SD-CE	5.27	1.92	1.79
1	C	457	MET	SD-CE	5.23	1.92	1.79
1	C	460	MET	SD-CE	5.20	1.92	1.79
1	E	345	MET	CG-SD	5.19	1.93	1.80
1	E	330	MET	CG-SD	5.16	1.93	1.80
1	C	240	MET	CG-SD	5.08	1.93	1.80

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	454	THR	N-CA-C	-10.69	97.87	112.94
1	E	218	THR	CA-C-N	9.46	129.40	120.03
1	E	218	THR	C-N-CA	9.46	129.40	120.03
1	C	293	ILE	N-CA-C	-9.21	100.96	111.00
1	B	218	THR	CA-C-N	9.06	129.00	119.85
1	B	218	THR	C-N-CA	9.06	129.00	119.85
1	C	218	THR	CA-C-N	8.70	128.46	119.76
1	C	218	THR	C-N-CA	8.70	128.46	119.76
1	E	105	GLY	N-CA-C	-8.45	104.25	115.32
1	F	426	GLY	N-CA-C	-8.28	103.59	115.27
1	D	240	MET	N-CA-C	8.07	119.71	111.07
1	F	158	PRO	N-CA-C	7.81	123.50	112.26
1	B	280	THR	N-CA-C	-7.57	103.04	111.82
1	F	430	ASN	N-CA-C	7.53	120.15	111.11
1	F	131	PHE	N-CA-C	7.52	119.47	111.28
1	F	218	THR	CA-C-N	7.28	127.20	119.85
1	F	218	THR	C-N-CA	7.28	127.20	119.85
1	A	118	ILE	N-CA-C	-7.18	103.67	110.42
1	C	354	LYS	N-CA-C	-7.11	103.23	112.68
1	C	370	PHE	N-CA-C	-7.04	103.53	111.07
1	E	403	VAL	N-CA-C	6.92	116.93	110.42
1	C	448	PRO	N-CA-CB	6.92	110.52	103.25
1	F	338	GLN	N-CA-C	-6.81	103.97	113.37
1	D	324	GLU	N-CA-C	-6.74	104.31	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	380	ALA	N-CA-C	-6.73	105.07	113.55
1	D	131	PHE	N-CA-C	6.69	119.58	111.82
1	B	120	ALA	N-CA-C	6.59	119.47	111.82
1	F	369	THR	N-CA-C	-6.59	105.06	113.23
1	F	367	PHE	N-CA-C	-6.50	104.12	111.14
1	D	279	THR	N-CA-C	-6.41	104.51	112.90
1	B	294	LYS	N-CA-C	-6.39	103.22	111.02
1	E	457	MET	N-CA-C	-6.35	105.55	113.55
1	D	202	GLY	N-CA-C	-6.30	106.34	114.85
1	B	293	ILE	N-CA-C	-6.24	104.42	110.72
1	F	355	GLU	N-CA-C	6.22	119.97	112.38
1	A	111	VAL	N-CA-C	-6.21	104.58	110.42
1	F	356	GLY	N-CA-C	6.19	127.85	113.18
1	E	354	LYS	N-CA-C	-6.18	102.09	110.68
1	E	355	GLU	N-CA-C	6.10	119.92	112.23
1	E	370	PHE	N-CA-C	-6.07	104.74	111.36
1	D	460	MET	N-CA-C	-6.04	105.75	113.23
1	D	342	LEU	N-CA-C	-6.02	105.76	113.23
1	A	369	THR	N-CA-C	-6.00	104.80	111.71
1	D	455	ARG	N-CA-C	-6.00	105.04	113.20
1	D	351	LYS	N-CA-C	-5.99	104.88	111.82
1	D	419	LEU	N-CA-C	5.99	119.33	112.57
1	A	204	ILE	N-CA-C	5.96	116.19	107.37
1	F	106	PHE	N-CA-C	-5.96	105.78	113.16
1	F	324	GLU	N-CA-C	-5.94	105.29	112.54
1	F	220	GLN	N-CA-C	-5.90	104.85	111.28
1	C	218	THR	N-CA-C	5.80	117.19	109.83
1	D	344	ALA	N-CA-C	-5.74	106.24	113.18
1	D	120	ALA	N-CA-C	5.69	118.42	111.82
1	A	218	THR	CA-C-N	5.68	125.66	120.21
1	A	218	THR	C-N-CA	5.68	125.66	120.21
1	A	280	THR	N-CA-C	-5.66	105.64	112.54
1	D	456	LEU	N-CA-C	-5.62	104.63	112.45
1	E	367	PHE	N-CA-C	-5.62	105.15	111.28
1	B	324	GLU	N-CA-C	-5.62	105.16	111.28
1	D	341	LYS	N-CA-C	-5.60	106.21	113.16
1	E	240	MET	N-CA-C	5.59	117.18	111.14
1	E	402	THR	N-CA-C	5.59	117.06	111.07
1	E	172	ILE	N-CA-C	-5.58	100.36	108.17
1	B	350	LYS	N-CA-C	-5.57	106.16	113.12
1	E	324	GLU	N-CA-C	-5.57	104.84	111.69
1	F	370	PHE	N-CA-C	-5.56	104.85	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	369	THR	N-CA-C	-5.54	106.36	113.23
1	D	370	PHE	N-CA-C	-5.54	106.02	112.89
1	A	454	THR	N-CA-C	-5.51	106.69	113.41
1	C	327	PHE	N-CA-C	-5.48	105.38	111.36
1	B	277	ALA	N-CA-C	-5.46	106.29	113.17
1	A	293	ILE	N-CA-C	-5.43	104.26	111.05
1	C	369	THR	N-CA-C	-5.39	105.49	111.36
1	B	369	THR	N-CA-C	-5.38	105.31	111.07
1	F	421	ASP	N-CA-C	-5.38	103.51	110.19
1	D	430	ASN	N-CA-C	5.38	117.83	111.33
1	F	215	VAL	N-CA-C	-5.37	106.62	113.22
1	B	240	MET	N-CA-C	5.36	117.55	111.02
1	F	342	LEU	N-CA-C	-5.34	106.72	113.18
1	F	136	VAL	N-CA-C	5.33	115.57	108.11
1	A	240	MET	N-CA-C	5.32	116.89	111.14
1	E	166	LEU	N-CA-C	-5.32	99.48	110.80
1	D	340	LYS	N-CA-C	-5.31	107.17	113.97
1	A	164	GLU	N-CA-C	5.31	117.48	111.11
1	A	426	GLY	N-CA-C	-5.28	100.66	113.18
1	C	293	ILE	CB-CA-C	-5.28	105.17	112.24
1	C	215	VAL	N-CA-C	-5.25	107.29	111.81
1	E	341	LYS	N-CA-C	-5.25	105.61	112.23
1	A	222	ASN	N-CA-C	5.25	117.74	111.71
1	C	328	GLY	N-CA-C	-5.19	106.50	112.73
1	A	462	LYS	N-CA-C	-5.16	105.30	111.03
1	B	134	LEU	N-CA-C	5.12	118.50	109.80
1	E	369	THR	N-CA-C	-5.11	106.56	112.89
1	D	303	LEU	N-CA-C	-5.10	105.81	111.36
1	C	282	PHE	N-CA-C	5.09	117.61	111.40
1	B	397	GLN	N-CA-C	-5.09	106.17	112.38
1	F	240	MET	N-CA-C	5.07	117.46	111.33
1	F	344	ALA	N-CA-C	-5.04	106.39	112.54
1	E	334	TYR	N-CA-C	5.03	119.28	113.20
1	B	173	ILE	N-CA-C	5.02	116.51	108.87
1	E	280	THR	N-CA-C	-5.02	105.69	111.07
1	E	396	MET	N-CA-C	-5.01	105.73	111.14
1	B	196	TYR	N-CA-C	-5.01	106.86	113.12
1	D	461	TRP	N-CA-C	-5.01	105.73	111.14

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

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	245	0
1	B	2539	0	2496	229	0
1	C	2619	0	2542	262	0
1	D	2604	0	2547	228	0
1	E	2598	0	2494	204	1
1	F	2504	0	2458	204	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	1296	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 43.

All (1296) 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:A:460:MET:HG3	1:B:460:MET:HE1	1.31	1.06
1:D:323:THR:HG22	1:D:325:ARG:H	1.20	1.05
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:457:MET:HE3	1:D:460:MET:HE1	1.41	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: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:F:345:MET:HE2	1:F:419:LEU:HG	1.54	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:A:457:MET:HE2	1:B:463:CYS:HB3	1.56	0.87
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: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:D:325:ARG:HA	1:D:345:MET:HE1	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:D:315:HIS:CD2	1:D:330:MET:HE2	2.13	0.84
1:A:218:THR:HG21	1:A:250:ILE:CG2	2.08	0.83
1:F:437:MET:HA	1:F:437:MET:HE3	1.60	0.83
1:A:456:LEU:HD11	1:D:460:MET:HE3	1.61	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:E:325:ARG:HA	1:E:345:MET:HE1	1.63	0.80
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:E:331:LEU:HG	1:E:437:MET:HE1	1.64	0.79
1:F:252:SER:O	1:F:253:GLN:HG3	1.82	0.79
1:D:336:GLY:C	1:D:338:GLN:H	1.91	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:D:454:THR:C	1:D:456:LEU:H	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:460:MET:HE1	1:E:460:MET:SD	2.26	0.75
1:A:222:ASN:HD22	1:B:383:PHE:HZ	1.34	0.75
1:F:345:MET:CE	1:F:419:LEU:HG	2.16	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:C:315:HIS:HB3	1:C:322:ILE:HD11	1.70	0.74
1:C:239:ASP:CG	1:C:242:GLU:HG3	2.13	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:F:182:SER:C	1:F:184:GLU:H	1.95	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:D:386:MET:C	1:D:388:GLY:H	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:357:LYS:HB2	1:E:411:HIS:CE1	2.24	0.72
1:A:147:MET:HE2	1:A:151:ASP:C	2.14	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:C:457:MET:CE	1:D:460:MET:HE1	2.17	0.72
1:B:435:SER:O	1:B:438:LYS:HB2	1.90	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
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:D:313:GLU:C	1:D:315:HIS:H	1.99	0.70
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:B:190:ASP:CG	1:B:191:GLU:N	2.50	0.70
1:E:323:THR:CB	1:E:326:GLN:HG3	2.17	0.70
1:D:315:HIS:HD2	1:D:330:MET:HE2	1.57	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: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:373:ASN:C	1:A:377:VAL:HG23	2.17	0.69
1:A:459:ALA:CB	1:D:456:LEU:HD22	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:350:LYS:HG2	1:F:355:GLU:CD	2.18	0.69
1:A:237:GLU:HB3	1:A:290:LYS:HE3	1.75	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:227:PHE:C	1:A:229:MET:H	2.01	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
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:A:437:MET:HE2	1:A:437:MET:HA	1.75	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:194:ILE:HD12	1:D:194:ILE:C	2.20	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:240:MET:HE1	1:E:123:THR:HG23	1.77	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:F:148:THR:HG22	1:F:151:ASP:CG	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LEU:HD13	1:D:460:MET:HA	1.77	0.65
1:D:386:MET:C	1:D:388:GLY:N	2.53	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: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:C:442:MET:HE3	1:C:446:GLU:CB	2.27	0.65
1:D:445:LEU:HD13	1:D:445:LEU:O	1.96	0.65
1:A:457:MET:HE3	1:A:461:TRP:HE1	1.62	0.65
1:C:249:ILE:HG23	1:E:386:MET:HE2	1.77	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
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:C:337:VAL:C	1:C:339:SER:H	2.06	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:A:441:LEU:HD13	1:A:441:LEU:O	1.98	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:A:441:LEU:HD12	1:A:442:MET:HE3	1.79	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:C:345:MET:HE3	1:C:349:LEU:CD1	2.28	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:A:327:PHE:HA	1:A:330:MET:HE2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:437:MET:HE2	1:F:440:ARG:HG2	1.80	0.63
1:C:295:ASN:O	1:C:298:GLU:HB3	1.98	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
1:C:457:MET:HE3	1:D:460:MET:CE	2.24	0.62
1:D:190:ASP:O	1:D:196:TYR:HE2	1.82	0.62
1:E:460:MET:C	1:E:462:LYS:H	2.07	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: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:B:313:GLU:C	1:B:315:HIS:H	2.08	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:396:MET:HE1	1:C:416:VAL:HG11	1.81	0.60
1:C:462:LYS:O	1:C:462:LYS:HG2	2.00	0.60
1:F:375:ASN:O	1:F:379:THR:HG23	2.00	0.60
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:C:318:VAL:O	1:C:319:ASP:HB2	2.00	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:D:337:VAL:C	1:D:339:SER:H	2.09	0.59
1:D:436:ILE:HG22	1:D:437:MET:HE2	1.82	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:346:GLN:HA	1:B:346:GLN:NE2	2.17	0.59
1:C:332:LEU:HD12	1:C:332:LEU:N	2.17	0.59
1:C:457:MET:SD	1:E:460:MET:HE1	2.42	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:F:322:ILE:HD13	1:F:330:MET:HE2	1.84	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:F:313:GLU:C	1:F:315:HIS:H	2.10	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:F:240:MET:HE2	1:F:240:MET:O	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
1:B:371:LEU:C	1:B:373:ASN:H	2.11	0.58
1:C:128:PHE:CD1	1:C:147:MET:HE3	2.39	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:E:193:SER:O	1:E:194:ILE:C	2.45	0.58
1:C:303:LEU:HD23	1:C:303:LEU:C	2.29	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:C:345:MET:HE3	1:C:349:LEU:HD12	1.84	0.58
1:E:340:LYS:HD2	1:E:340:LYS:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:337:VAL:C	1:F:339:SER:H	2.11	0.58
1:F:395:THR:O	1:F:399:VAL:HG23	2.03	0.58
1:B:258:MET:HE3	1:B:458:GLN:HG2	1.85	0.57
1:A:243:PHE:O	1:A:247:GLN:HG3	2.04	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:D:454:THR:C	1:D:456:LEU:N	2.59	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:252:SER:HB2	1:E:386:MET:HE3	1.86	0.57
1:C:346:GLN:HE22	1:C:355:GLU:CG	2.06	0.57
1:C:425:ASN:C	1:C:427:GLU:H	2.13	0.57
1:C:461:TRP:C	1:C:463:CYS:H	2.12	0.57
1:D:313:GLU:C	1:D:315:HIS:N	2.63	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: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
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:D:350:LYS:HB2	1:D:355:GLU:CD	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:194:ILE:C	1:E:196:TYR:H	2.12	0.56
1:A:456:LEU:HD21	1:D:460:MET:HE2	1.87	0.56
1:D:323:THR:H	1:D:326:GLN:HE21	1.49	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: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:229:MET:HE2	1:F:230:PHE:CE2	2.41	0.56
1:F:425:ASN:HB3	1:F:427:GLU:HB2	1.88	0.56
1:A:147:MET:HE1	1:A:155:SER:HB3	1.88	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:C:371:LEU:C	1:C:373:ASN:H	2.14	0.55
1:D:122:SER:HB3	1:D:126:LYS:HB3	1.89	0.55
1:E:194:ILE:C	1:E:196:TYR:N	2.62	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
1:A:206:PHE:O	1:A:210:ILE:HD13	2.05	0.55
1:A:442:MET:HA	1:A:442:MET:HE2	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:325:ARG:HA	1:B:345:MET:HE1	1.87	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: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:B:240:MET:HE1	1:E:123:THR:CG2	2.38	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:E:460:MET:HA	1:E:463:CYS:CB	2.37	0.54
1:A:227:PHE:C	1:A:229:MET:N	2.65	0.54
1:C:314:ARG:HG2	1:C:314:ARG:HH11	1.72	0.54
1:C:235:ASP:HB2	1:C:293:ILE:HD11	1.89	0.54
1:C:331:LEU:HB3	1:C:437:MET:HE1	1.89	0.54
1:E:353:PHE:N	1:E:353:PHE:CD2	2.73	0.54
1:C:148:THR:O	1:C:149:PRO:C	2.50	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:337:VAL:C	1:D:339:SER:N	2.64	0.53
1:E:337:VAL:C	1:E:339:SER:H	2.16	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:C:293:ILE:H	1:C:293:ILE:CD1	2.03	0.53
1:C:296:PHE:O	1:C:299:PHE:N	2.42	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:B:148:THR:O	1:B:149:PRO:C	2.50	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:F:327:PHE:HA	1:F:330:MET:HE3	1.89	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:194:ILE:C	1:B:196:TYR:H	2.17	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:E:460:MET:C	1:E:462:LYS:N	2.66	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:336:GLY:C	1:A:338:GLN:H	2.15	0.53
1:A:422:CYS:HB2	1:A:425:ASN:OD1	2.09	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:283:PHE:CE1	1:F:291:LEU:HB2	2.44	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: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: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: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:B:462:LYS:O	1:B:463:CYS:C	2.53	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
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:D:437:MET:HE2	1:D:437:MET:HA	1.92	0.51
1:E:177:ASP:C	1:E:185:ARG:HD3	2.35	0.51
1:F:137:ILE:HD13	1:F:137:ILE:N	2.25	0.51
1:F:190:ASP:O	1:F:196:TYR:HE2	1.92	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:A:119:ARG:NH1	1:A:131:PHE:HE1	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:162:GLN:CD	1:B:163:PRO:HD2	2.35	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:D:239:ASP:OD1	1:D:239:ASP:C	2.54	0.51
1:E:119:ARG:NH1	1:E:154:ARG:O	2.43	0.51
1:F:182:SER:C	1:F:184:GLU:N	2.64	0.51
1:C:194:ILE:HG23	1:C:302:LYS:HG2	1.91	0.51
1:D:196:TYR:C	1:D:198:LEU:N	2.68	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:C:460:MET:HE1	1:D:461:TRP:CE3	2.46	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:D:194:ILE:C	1:D:194:ILE:CD1	2.83	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: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
1:D:364:VAL:O	1:D:365:GLU:C	2.53	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:PRO:O	1:A:159:ASN:HB2	2.11	0.50
1:A:345:MET:HE3	1:A:349:LEU:CD1	2.41	0.50
1:B:214:THR:HB	1:B:254:THR:HG21	1.93	0.50
1:C:239:ASP:C	1:C:239:ASP:OD1	2.53	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:B:373:ASN:O	1:B:374:ILE:C	2.55	0.50
1:C:147:MET:HB2	1:C:151:ASP:HB2	1.93	0.50
1:E:128:PHE:CD1	1:E:147:MET:HE3	2.46	0.50
1:E:433:PHE:C	1:E:435:SER:N	2.69	0.50
1:F:337:VAL:C	1:F:339:SER:N	2.69	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:112:MET:C	1:D:114:TYR:N	2.67	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:A:457:MET:CE	1:A:461:TRP:HE1	2.24	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:E:421:ASP:CG	1:E:424:GLY:HA2	2.36	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:398:GLN:NE2	1:B:232:LEU:HD21	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:MET:CE	1:B:463:CYS:HB3	2.36	0.49
1:B:115:GLU:HG2	1:B:130:TYR:OH	2.11	0.49
1:C:239:ASP:OD2	1:C:242:GLU:HG3	2.12	0.49
1:A:345:MET:HE3	1:A:349:LEU:HD12	1.93	0.49
1:B:258:MET:HE3	1:B:458:GLN:CG	2.41	0.49
1:C:238:VAL:HG12	1:C:239:ASP:O	2.11	0.49
1:C:257:GLY:C	1:C:259:ARG:H	2.19	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:A:396:MET:O	1:A:396:MET:HG3	2.06	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:A:456:LEU:HD11	1:D:460:MET:CE	2.36	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:B:315:HIS:CB	1:B:322:ILE:HD11	2.42	0.49
1:F:373:ASN:O	1:F:374:ILE:C	2.56	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:E:239:ASP:C	1:E:239:ASP:OD1	2.56	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: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:C:246:VAL:O	1:C:247:GLN:C	2.56	0.49
1:F:416:VAL:O	1:F:416:VAL:HG12	2.12	0.49
1:A:452:GLY:C	1:A:454:THR:H	2.18	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:455:ARG:C	1:E:457:MET:H	2.20	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:F:421:ASP:OD2	1:F:421:ASP:C	2.56	0.48
1:B:220:GLN:HG2	1:B:297:LEU:CD2	2.43	0.48
1:B:315:HIS:CD2	1:B:330:MET:HE2	2.48	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:A:442:MET:O	1:A:443:ARG:HB2	2.13	0.48
1:D:166:LEU:CD2	1:D:172:ILE:HG13	2.40	0.48
1:D:417:PHE:O	1:D:418:ALA:C	2.55	0.48
1:A:153:VAL:CG2	1:A:310:LEU:HD13	2.43	0.48
1:B:154:ARG:HD3	1:B:314:ARG:HH22	1.75	0.48
1:C:256:MET:HA	1:C:256:MET:HE2	1.94	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:395:THR:O	1:A:396:MET:C	2.57	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: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:C:383:PHE:O	1:C:384:TYR:C	2.56	0.48
1:D:123:THR:O	1:D:124:PRO:C	2.55	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:F:396:MET:HE3	1:F:428:LEU:HG	1.94	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:C:345:MET:HE3	1:C:349:LEU:HD11	1.95	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

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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	0.47
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:E:302:LYS:O	1:E:303:LEU:C	2.56	0.47
1:F:196:TYR:C	1:F:198:LEU:H	2.22	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:220:GLN:O	1:F:221:ARG:C	2.57	0.47
1:F:340:LYS:N	1:F:340:LYS:HD2	2.29	0.47
1:F:417:PHE:O	1:F:418:ALA:C	2.56	0.47
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:421:ASP:O	1:D:422:CYS:C	2.57	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:E:371:LEU:C	1:E:373:ASN:H	2.22	0.47
1:A:431:LYS:HD3	1:A:431:LYS:N	2.28	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:D:336:GLY:C	1:D:338:GLN:N	2.61	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:C:335:SER:HA	1:C:439:GLN:CD	2.39	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:H	2.23	0.47
1:D:457:MET:HE2	1:D:457:MET:N	2.29	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:D:112:MET:C	1:D:114:TYR:H	2.22	0.47
1:E:137:ILE:HG12	1:E:143:ALA:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:373:ASN:O	1:E:374:ILE:C	2.57	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:A:147:MET:HE2	1:A:152:PHE:N	2.28	0.46
1:B:371:LEU:O	1:B:373:ASN:N	2.46	0.46
1:C:387:ALA:HB2	1:E:229:MET:HE1	1.96	0.46
1:D:231:ASP:CB	1:D:237:GLU:H	2.21	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
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:210:ILE:O	1:F:211:PHE:C	2.58	0.46
1:C:232:LEU:N	1:C:232:LEU:CD1	2.79	0.46
1:D:465:GLN:C	1:D:467:THR:H	2.24	0.46
1:A:133:THR:C	1:A:171:TYR:HB3	2.41	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:C:396:MET:HE3	1:C:428:LEU:HD11	1.95	0.46
1:F:308:LEU:HD13	1:F:361:PHE:HE1	1.80	0.46
1:F:313:GLU:C	1:F:315:HIS:N	2.73	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:149:PRO:O	1:B:150:GLU:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:252:SER:HB2	1:F:386:MET:HG2	1.97	0.46
1:F:185:ARG:HG2	1:F:186:GLU:N	2.31	0.46
1:F:196:TYR:C	1:F:198:LEU:N	2.74	0.46
1:F:327:PHE:HD2	1:F:415:VAL:HG11	1.79	0.46
1:A:145:VAL:C	1:A:146:PHE:HD2	2.24	0.46
1:B:453:PHE:CB	1:C:461:TRP:CZ2	2.99	0.46
1:C:425:ASN:C	1:C:427:GLU:N	2.74	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:D:193:SER:C	1:D:195:PHE:N	2.70	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: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: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: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
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:E:378:ASP:CG	1:E:434:VAL:HG21	2.41	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:E:421:ASP:OD2	1:E:421:ASP:C	2.59	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:THR:HG21	1:B:250:ILE:HG23	1.98	0.45
1:B:371:LEU:C	1:B:373:ASN:N	2.73	0.45
1:C:205:SER:O	1:C:206:PHE:C	2.56	0.45
1:C:313:GLU:C	1:C:315:HIS:H	2.25	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:193:SER:C	1:D:195:PHE:H	2.25	0.45
1:D:303:LEU:C	1:D:303:LEU:HD13	2.41	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:A:392:ASP:CG	1:A:394:VAL:HG23	2.42	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:258:MET:C	1:C:259:ARG:HG3	2.41	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:350:LYS:HG2	1:B:355:GLU:CD	2.42	0.45
1:C:460:MET:HE3	1:C:460:MET:HB3	1.83	0.45
1:F:404:ALA:O	1:F:405:LYS:C	2.57	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
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:A:441:LEU:CD1	1:A:442:MET:HE3	2.46	0.45
1:C:237:GLU:O	1:C:238:VAL:CG2	2.64	0.45
1:C:387:ALA:CB	1:E:229:MET:HE1	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:395:THR:C	1:A:397:GLN:N	2.72	0.45
1:B:119:ARG:NH1	1:B:154:ARG:O	2.50	0.45
1:C:162:GLN:O	1:C:163:PRO:C	2.59	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:E:455:ARG:C	1:E:457:MET:N	2.74	0.45
1:F:206:PHE:CZ	1:F:210:ILE:HD11	2.52	0.45
1:A:194:ILE:C	1:A:196:TYR:H	2.25	0.44
1:A:401:ARG:CD	1:B:232:LEU:HD22	2.47	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:A:220:GLN:O	1:A:221:ARG:C	2.61	0.44
1:B:313:GLU:O	1:B:315:HIS:N	2.49	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:223:PHE:O	1:C:224:GLU:C	2.58	0.44
1:C:298:GLU:OE2	1:C:298:GLU:HA	2.17	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:A:194:ILE:CG2	1:A:302:LYS:HD3	2.47	0.44
1:A:339:SER:C	1:A:342:LEU:HD13	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:LEU:O	1:B:304:GLN:C	2.59	0.44
1:B:375:ASN:O	1:B:379:THR:HG23	2.18	0.44
1:C:206:PHE:O	1:C:207:SER:C	2.60	0.44
1:D:175:ARG:O	1:D:177:ASP:N	2.50	0.44
1:D:234:GLY:O	1:D:235:ASP:C	2.59	0.44
1:F:350:LYS:HG2	1:F:355:GLU:OE2	2.18	0.44
1:A:332:LEU:O	1:A:333:ALA:C	2.61	0.44
1:B:382:SER:HB2	1:B:386:MET:HE2	1.98	0.44
1:C:187:LYS:HD3	1:C:201:CYS:HB3	1.99	0.44
1:C:303:LEU:C	1:C:303:LEU:CD2	2.90	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:239:ASP:OD1	1:F:239:ASP:C	2.61	0.44
1:F:240:MET:HA	1:F:283:PHE:CE2	2.53	0.44
1:B:117:ARG:O	1:B:118:ILE:C	2.61	0.44
1:C:124:PRO:HG2	1:C:260:HIS:H	1.82	0.44
1:E:237:GLU:C	1:E:238:VAL:HG23	2.43	0.44
1:E:465:GLN:O	1:E:466:GLU:C	2.59	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:C:318:VAL:C	1:C:320:GLY:H	2.25	0.44
1:C:350:LYS:C	1:C:352:HIS:H	2.26	0.44
1:C:365:GLU:O	1:C:366:ASN:C	2.59	0.44
1:D:172:ILE:HG22	1:D:172:ILE:O	2.18	0.44
1:D:207:SER:O	1:D:208:ASP:C	2.59	0.44
1:D:214:THR:HG21	1:D:251:ARG:CG	2.47	0.44
1:D:247:GLN:O	1:D:248:SER:C	2.61	0.44
1:E:158:PRO:CD	1:E:334:TYR:CE1	3.01	0.44
1:E:278:LEU:O	1:E:279:THR:C	2.61	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:A:342:LEU:HD12	1:A:342:LEU:H	1.81	0.44
1:B:324:GLU:C	1:B:345:MET:HE1	2.42	0.44
1:B:417:PHE:O	1:B:418:ALA:C	2.61	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:C:436:ILE:HG22	1:C:437:MET:HE2	1.99	0.44
1:D:216:LEU:HD23	1:D:216:LEU:HA	1.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:373:ASN:C	1:B:375:ASN:N	2.76	0.43
1:D:154:ARG:NH2	1:D:162:GLN:NE2	2.63	0.43
1:E:441:LEU:HD13	1:E:441:LEU:C	2.43	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
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:A:196:TYR:HE1	1:A:201:CYS:C	2.26	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:D:305:HIS:ND1	1:D:305:HIS:C	2.76	0.43
1:E:375:ASN:O	1:E:379:THR:HG23	2.18	0.43
1:A:166:LEU:O	1:A:170:GLN:CD	2.61	0.43
1:A:323:THR:HG22	1:A:324:GLU:N	2.34	0.43
1:C:390:SER:O	1:C:395:THR:HG21	2.18	0.43
1:C:414:ASP:O	1:C:418:ALA:HB2	2.18	0.43
1:D:145:VAL:C	1:D:146:PHE:HD2	2.26	0.43
1:D:192:GLY:O	1:D:193:SER:C	2.61	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:194:ILE:C	1:B:196:TYR:N	2.76	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:D:385:HIS:ND1	1:D:385:HIS:C	2.77	0.43
1:E:137:ILE:HG12	1:E:143:ALA:HB2	2.00	0.43
1:E:293:ILE:O	1:E:294:LYS:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:LYS:HD3	1:B:414:ASP:CG	2.44	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:278:LEU:CD1	1:D:278:LEU:C	2.92	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: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:B:313:GLU:C	1:B:315:HIS:N	2.74	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:D:209:TYR:O	1:D:210:ILE:C	2.62	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:175:ARG:O	1:D:176:PHE:C	2.61	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:374:ILE:HD12	1:E:374:ILE:N	2.34	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: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:D:421:ASP:OD2	1:D:421:ASP:C	2.62	0.42
1:E:112:MET:HE3	1:E:112:MET:HB3	1.71	0.42
1:E:371:LEU:C	1:E:373:ASN:N	2.77	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:A:373:ASN:O	1:A:374:ILE:C	2.61	0.42
1:B:316:ASP:H	1:B:317:PRO:HD3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:212:LEU:HD22	1:F:303:LEU:HD11	2.01	0.42
1:A:386:MET:C	1:A:388:GLY:H	2.27	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:E:334:TYR:CE2	1:E:443:ARG:HA	2.55	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
1:A:298:GLU:CD	1:A:301:ARG:HH21	2.27	0.42
1:A:339:SER:O	1:A:342:LEU:HD13	2.19	0.42
1:B:378:ASP:C	1:B:380:ALA:N	2.77	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:E:315:HIS:O	1:E:316:ASP:C	2.62	0.42
1:A:164:GLU:O	1:A:165:HIS:C	2.60	0.42
1:A:427:GLU:O	1:A:428:LEU:C	2.61	0.42
1:A:459:ALA:O	1:D:456:LEU:HD21	2.20	0.42
1:B:123:THR:O	1:B:124:PRO:C	2.61	0.42
1:B:378:ASP:C	1:B:380:ALA:H	2.28	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:193:SER:C	1:E:195:PHE:N	2.77	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:167:GLY:O	1:B:168:LEU:C	2.62	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:B:318:VAL:C	1:B:320:GLY:N	2.77	0.42
1:C:252:SER:CB	1:E:386:MET:HE3	2.50	0.42
1:C:305:HIS:ND1	1:C:305:HIS:C	2.78	0.42
1:C:442:MET:C	1:C:444:GLY:N	2.75	0.42
1:D:144:GLU:HB3	1:D:146:PHE:HE2	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:293:ILE:O	1:B:294:LYS:C	2.63	0.42
1:B:429:SER:O	1:B:430:ASN:C	2.62	0.42
1:B:433:PHE:CZ	1:B:437:MET:HG3	2.55	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:B:196:TYR:C	1:B:198:LEU:H	2.27	0.42
1:B:256:MET:HE2	1:B:256:MET:HA	2.01	0.42
1:C:149:PRO:HB3	1:C:310:LEU:HD21	2.02	0.42
1:C:346:GLN:HE21	1:C:346:GLN:C	2.28	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
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:128:PHE:CD1	1:D:147:MET:HE3	2.55	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:196:TYR:CE1	1:A:201:CYS:C	2.98	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:B:168:LEU:C	1:B:170:GLN:N	2.78	0.41
1:C:255:SER:O	1:C:259:ARG:NE	2.50	0.41
1:E:433:PHE:C	1:E:435:SER:H	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:189:ALA:O	1:C:190:ASP:C	2.63	0.41
1:C:371:LEU:C	1:C:373:ASN:N	2.78	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:227:PHE:C	1:F:229:MET:N	2.77	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:B:241:GLU:CD	1:B:241:GLU:H	2.29	0.41
1:C:337:VAL:C	1:C:339:SER:N	2.72	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:337:VAL:C	1:A:339:SER:H	2.27	0.41
1:A:417:PHE:CE1	1:A:428:LEU:HB2	2.55	0.41
1:C:112:MET:O	1:C:113:GLU:C	2.64	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: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:B:190:ASP:CG	1:B:191:GLU:H	2.20	0.41
1:C:192:GLY:O	1:C:193:SER:C	2.63	0.41
1:C:283:PHE:CE1	1:C:291:LEU:HB2	2.56	0.41
1:D:436:ILE:O	1:D:437:MET:C	2.61	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:F:278:LEU:O	1:F:279:THR:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ARG:HH21	1:A:159:ASN:H	1.67	0.41
1:A:292:THR:HG22	1:A:293:ILE:CD1	2.45	0.41
1:A:292:THR:C	1:A:294:LYS:N	2.77	0.41
1:A:398:GLN:O	1:A:401:ARG:HB3	2.20	0.41
1:B:115:GLU:O	1:B:116:ASN:C	2.63	0.41
1:B:315:HIS:O	1:B:316:ASP:CB	2.62	0.41
1:C:216:LEU:HD23	1:C:216:LEU:HA	1.85	0.41
1:C:395:THR:C	1:C:397:GLN:N	2.79	0.41
1:C:428:LEU:CD2	1:C:429:SER:N	2.84	0.41
1:A:171:TYR:C	1:A:172:ILE:O	2.63	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:158:PRO:O	1:F:159:ASN:CG	2.63	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:B:305:HIS:ND1	1:B:305:HIS:C	2.77	0.41
1:B:318:VAL:C	1:B:320:GLY:H	2.27	0.41
1:B:436:ILE:C	1:B:438:LYS:N	2.79	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:F:200:GLU:OE1	1:F:200:GLU:N	2.54	0.41
1:F:223:PHE:O	1:F:224:GLU:C	2.63	0.41
1:A:209:TYR:C	1:A:211:PHE:N	2.79	0.41
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:457:MET:SD	1:E:460:MET:HE2	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:432:GLU:O	1:B:433:PHE:C	2.64	0.40
1:C:113:GLU:O	1:C:114:TYR:C	2.64	0.40
1:E:154:ARG:NH1	1:E:314:ARG:HH21	2.04	0.40
1:A:200:GLU:CD	1:A:200:GLU:H	2.30	0.40
1:A:457:MET:SD	1:B:460:MET:HE3	2.61	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:237:GLU:C	1:C:238:VAL:HG23	2.45	0.40
1:E:108:ASP:O	1:E:112:MET:HG3	2.20	0.40
1:F:126:LYS:O	1:F:127:ILE:C	2.63	0.40
1:F:292:THR:HG22	1:F:293:ILE:HD12	2.04	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:396:MET:C	1:B:398:GLN:N	2.74	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:D:251:ARG:C	1:D:253:GLN:H	2.29	0.40
1:E:308:LEU:HA	1:E:308:LEU:HD23	1.84	0.40
1:F:193:SER:C	1:F:195:PHE:H	2.28	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:A:194:ILE:O	1:A:194:ILE:HG13	2.17	0.40
1:B:331:LEU:HB3	1:B:437:MET:HE1	2.02	0.40
1:B:411:HIS:O	1:B:415:VAL:HG23	2.22	0.40
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:E:199:GLY:C	1:E:200:GLU:O	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:313:GLU:C	1:E:315:HIS:H	2.29	0.40
1:A:239:ASP:OD1	1:A:239:ASP:C	2.65	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: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	8
1	B	304/401 (76%)	235 (77%)	53 (17%)	16 (5%)	1	12
1	C	322/401 (80%)	248 (77%)	56 (17%)	18 (6%)	1	11
1	D	316/401 (79%)	262 (83%)	39 (12%)	15 (5%)	2	14
1	E	322/401 (80%)	261 (81%)	47 (15%)	14 (4%)	2	16
1	F	302/401 (75%)	237 (78%)	49 (16%)	16 (5%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1866/2406 (78%)	1470 (79%)	298 (16%)	98 (5%)	1	12

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
1	C	448	PRO

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Mol	Chain	Res	Type
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
1	A	427	GLU

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Mol	Chain	Res	Type
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 ⓘ

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%)	228 (88%)	31 (12%)	5	23
1	B	273/354 (77%)	242 (89%)	31 (11%)	5	24
1	C	274/354 (77%)	244 (89%)	30 (11%)	6	26
1	D	278/354 (78%)	250 (90%)	28 (10%)	7	30
1	E	269/354 (76%)	233 (87%)	36 (13%)	4	19
1	F	270/354 (76%)	239 (88%)	31 (12%)	5	24
All	All	1623/2124 (76%)	1436 (88%)	187 (12%)	5	24

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ARG
1	A	108	ASP
1	A	150	GLU
1	A	158	PRO
1	A	162	GLN
1	A	165	HIS
1	A	168	LEU
1	A	171	TYR
1	A	200	GLU
1	A	210	ILE
1	A	216	LEU
1	A	238	VAL
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	324	GLU
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	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	214	THR
1	B	221	ARG
1	B	235	ASP

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Mol	Chain	Res	Type
1	B	241	GLU
1	B	246	VAL
1	B	247	GLN
1	B	275	CYS
1	B	279	THR
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	441	LEU
1	B	463	CYS
1	C	118	ILE
1	C	137	ILE
1	C	150	GLU
1	C	168	LEU
1	C	171	TYR
1	C	194	ILE
1	C	200	GLU
1	C	241	GLU
1	C	245	GLN
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	322	ILE
1	C	346	GLN
1	C	348	GLN
1	C	353	PHE
1	C	374	ILE
1	C	379	THR
1	C	390	SER
1	C	396	MET

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Mol	Chain	Res	Type
1	C	397	GLN
1	C	403	VAL
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	150	GLU
1	D	162	GLN
1	D	168	LEU
1	D	190	ASP
1	D	200	GLU
1	D	214	THR
1	D	241	GLU
1	D	278	LEU
1	D	286	ASP
1	D	291	LEU
1	D	293	ILE
1	D	307	VAL
1	D	308	LEU
1	D	322	ILE
1	D	343	THR
1	D	346	GLN
1	D	348	GLN
1	D	349	LEU
1	D	374	ILE
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	441	LEU
1	D	445	LEU
1	E	108	ASP
1	E	112	MET
1	E	122	SER
1	E	137	ILE
1	E	150	GLU
1	E	162	GLN
1	E	164	GLU

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Mol	Chain	Res	Type
1	E	168	LEU
1	E	173	ILE
1	E	194	ILE
1	E	214	THR
1	E	216	LEU
1	E	241	GLU
1	E	248	SER
1	E	278	LEU
1	E	291	LEU
1	E	293	ILE
1	E	301	ARG
1	E	303	LEU
1	E	308	LEU
1	E	313	GLU
1	E	318	VAL
1	E	322	ILE
1	E	331	LEU
1	E	346	GLN
1	E	348	GLN
1	E	371	LEU
1	E	374	ILE
1	E	406	VAL
1	E	422	CYS
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	136	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	228	LYS
1	F	231	ASP
1	F	240	MET

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Mol	Chain	Res	Type
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	346	GLN
1	F	374	ILE
1	F	379	THR
1	F	395	THR
1	F	419	LEU
1	F	423	ASP
1	F	427	GLU
1	F	437	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	GLN
1	A	222	ASN
1	A	233	ASN
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	222	ASN
1	B	233	ASN
1	B	245	GLN
1	B	247	GLN
1	B	315	HIS

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Mol	Chain	Res	Type
1	B	326	GLN
1	B	346	GLN
1	B	352	HIS
1	B	366	ASN
1	B	397	GLN
1	B	398	GLN
1	B	430	ASN
1	B	439	GLN
1	C	162	GLN
1	C	220	GLN
1	C	233	ASN
1	C	300	GLN
1	C	315	HIS
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	326	GLN
1	D	338	GLN
1	D	352	HIS
1	D	366	ASN
1	D	375	ASN
1	D	397	GLN
1	D	411	HIS
1	D	439	GLN
1	E	162	GLN
1	E	220	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

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Mol	Chain	Res	Type
1	E	326	GLN
1	E	346	GLN
1	E	373	ASN
1	E	425	ASN
1	E	439	GLN
1	F	159	ASN
1	F	162	GLN
1	F	247	GLN
1	F	305	HIS
1	F	326	GLN
1	F	346	GLN
1	F	352	HIS
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 oligosaccharides 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, 95th 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 ²)	Q < 0.9
1	A	310/401 (77%)	0.79	21 (6%)	23 15	62, 86, 113, 127	0
1	B	316/401 (78%)	0.46	15 (4%)	36 23	41, 73, 104, 122	0
1	C	330/401 (82%)	0.49	19 (5%)	29 18	44, 70, 97, 114	0
1	D	326/401 (81%)	0.33	16 (4%)	35 22	36, 60, 89, 111	0
1	E	330/401 (82%)	0.18	7 (2%)	63 43	32, 59, 107, 122	0
1	F	310/401 (77%)	0.22	9 (2%)	53 35	36, 58, 95, 112	0
All	All	1922/2406 (79%)	0.41	87 (4%)	38 24	32, 69, 104, 127	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	ALA	4.9
1	C	450	ASP	4.9
1	A	124	PRO	4.5
1	A	339	SER	4.3
1	F	182	SER	3.7
1	F	339	SER	3.7
1	A	461	TRP	3.7
1	D	337	VAL	3.6
1	E	466	GLU	3.6
1	A	338	GLN	3.3
1	C	456	LEU	3.3
1	C	422	CYS	3.3
1	C	453	PHE	3.1
1	C	463	CYS	3.1
1	B	169	ASP	3.0
1	E	337	VAL	3.0
1	C	464	ALA	2.9
1	F	355	GLU	2.9
1	B	403	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	177	ASP	2.8
1	C	137	ILE	2.8
1	F	176	PHE	2.8
1	A	451	MET	2.8
1	C	184	GLU	2.8
1	B	467	THR	2.7
1	B	338	GLN	2.7
1	D	458	GLN	2.7
1	A	177	ASP	2.7
1	A	172	ILE	2.6
1	B	314	ARG	2.6
1	C	277	ALA	2.6
1	C	424	GLY	2.5
1	D	142	GLU	2.5
1	C	168	LEU	2.5
1	D	445	LEU	2.5
1	B	275	CYS	2.5
1	D	233	ASN	2.5
1	A	102	LYS	2.4
1	A	135	LYS	2.4
1	C	451	MET	2.4
1	A	203	LEU	2.4
1	B	442	MET	2.3
1	D	463	CYS	2.3
1	F	103	ARG	2.3
1	A	165	HIS	2.3
1	F	338	GLN	2.3
1	B	159	ASN	2.3
1	E	457	MET	2.3
1	A	168	LEU	2.3
1	A	453	PHE	2.3
1	E	183	GLN	2.3
1	F	254	THR	2.3
1	D	467	THR	2.2
1	F	252	SER	2.2
1	B	107	ARG	2.2
1	C	107	ARG	2.2
1	B	137	ILE	2.2
1	D	112	MET	2.2
1	B	429	SER	2.2
1	F	183	GLN	2.2
1	B	387	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	194	ILE	2.2
1	D	201	CYS	2.2
1	C	449	LYS	2.2
1	C	256	MET	2.2
1	D	186	GLU	2.2
1	D	200	GLU	2.2
1	B	121	TYR	2.1
1	A	232	LEU	2.1
1	C	338	GLN	2.1
1	D	256	MET	2.1
1	A	427	GLU	2.1
1	A	454	THR	2.1
1	C	452	GLY	2.1
1	C	176	PHE	2.1
1	A	201	CYS	2.1
1	C	232	LEU	2.1
1	E	316	ASP	2.1
1	E	445	LEU	2.1
1	D	189	ALA	2.1
1	A	237	GLU	2.1
1	D	339	SER	2.0
1	B	201	CYS	2.0
1	A	202	GLY	2.0
1	B	407	GLU	2.0
1	E	464	ALA	2.0
1	D	355	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.