Full wwPDB X-ray Structure Validation Report (i)

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

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

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

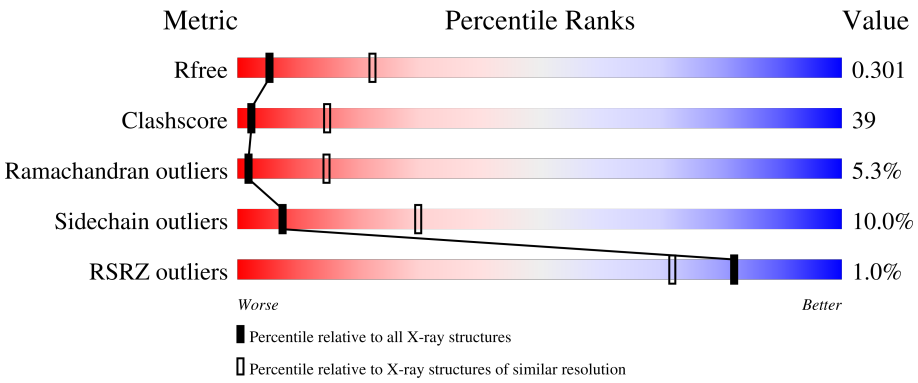
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	401	2%; 29%, 39%, 8%, 23%
1	B	401	35%, 36%, 7%, •, 21%
1	C	401	%; 28%, 47%, 6%, •, 18%
1	D	401	%; 37%, 36%, 7%, •, 19%
1	E	401	35%, 40%, 6%, •, 18%

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Mol	Chain	Length	Quality of chain
1	F	401	34% 35% 7% • 23%

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

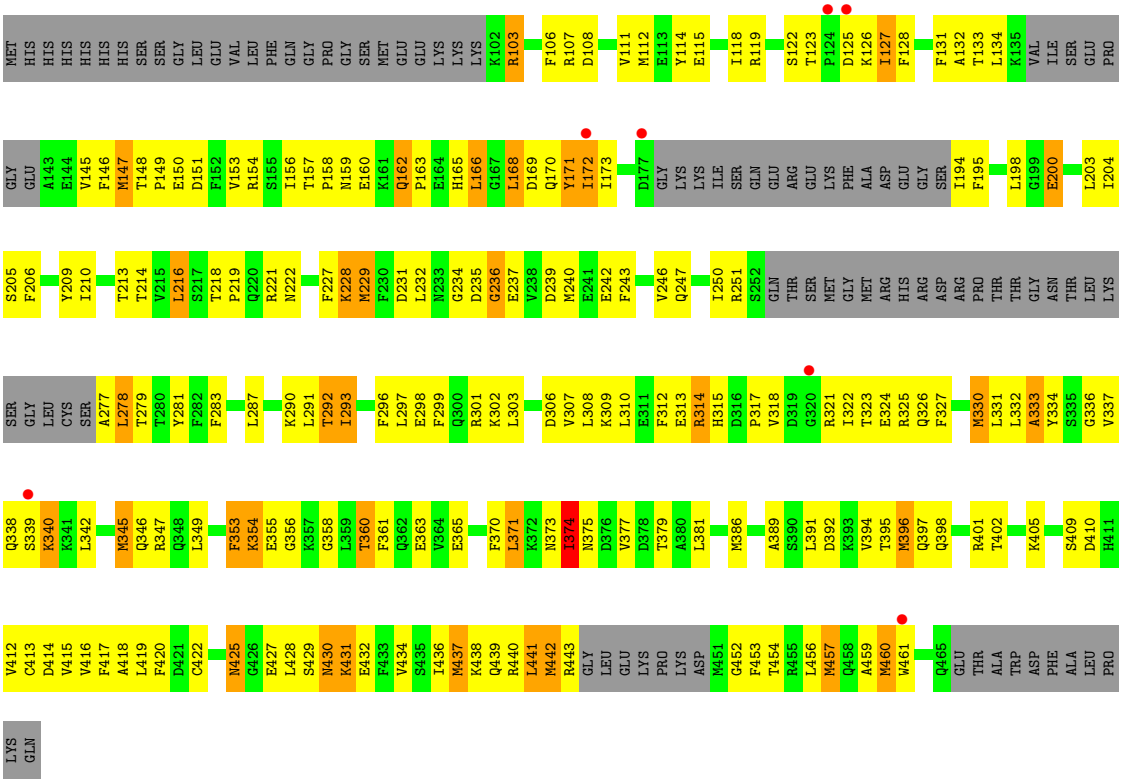
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	4	4	4	0	0
			Total	O		
2	B	3	3	3	0	0
			Total	O		
2	C	1	1	1	0	0
			Total	O		
2	D	1	1	1	0	0
			Total	O		
2	F	4	4	4	0	0

3 Residue-property plots (i)

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

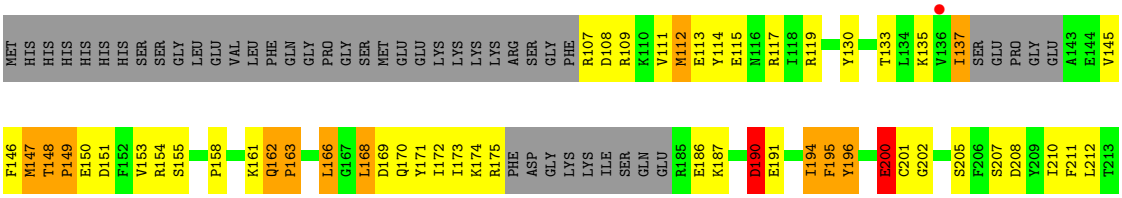
• Molecule 1: Calcium uptake protein 1, mitochondrial

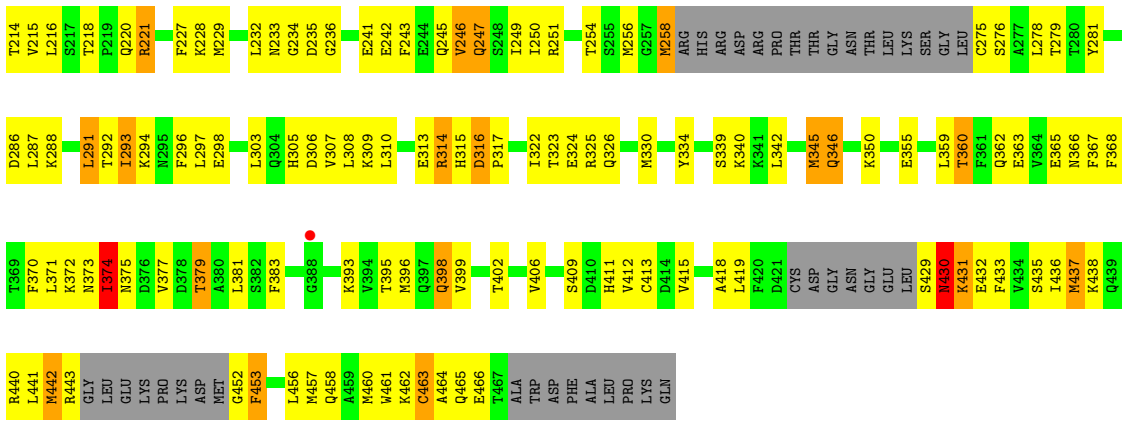
Chain A: 2% 29% 39% 8% 23%



• Molecule 1: Calcium uptake protein 1, mitochondrial

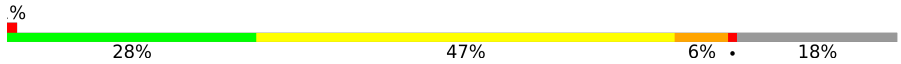
Chain B: 35% 36% 7% 21%

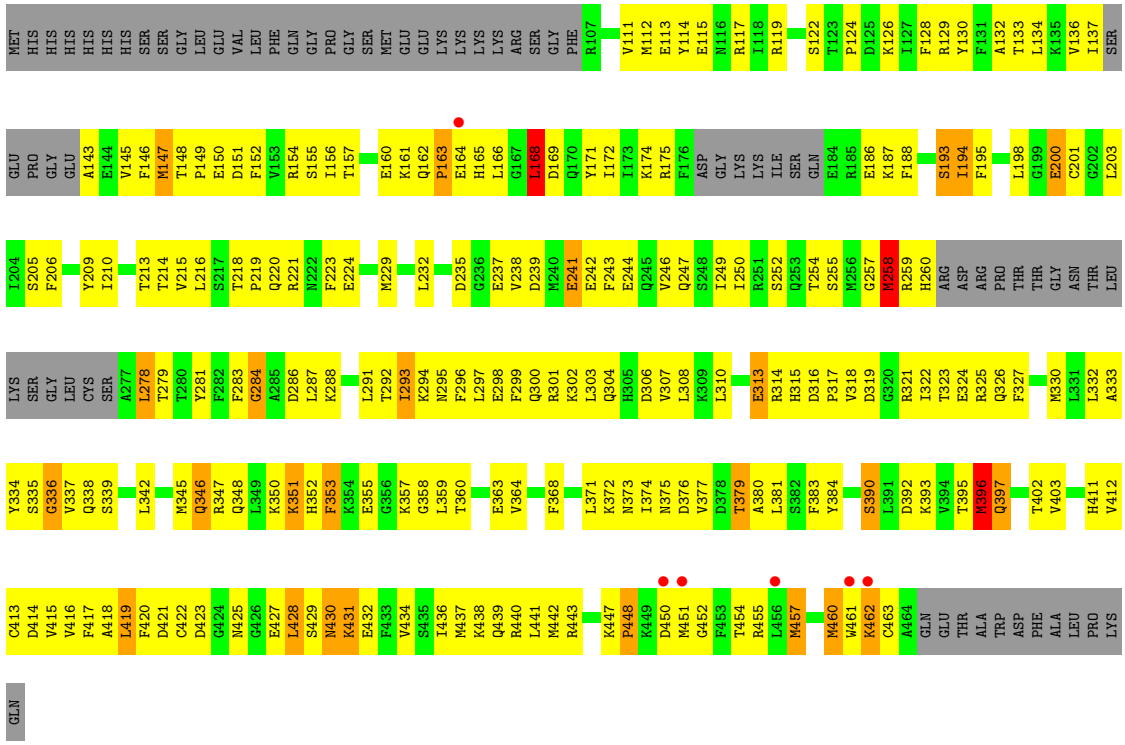




• Molecule 1: Calcium uptake protein 1, mitochondrial

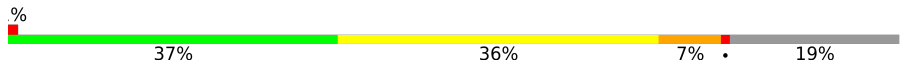
Chain C:

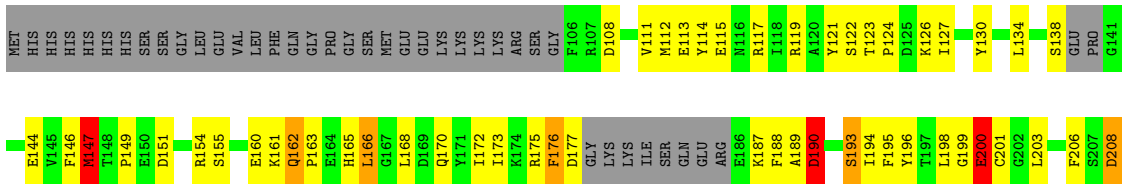


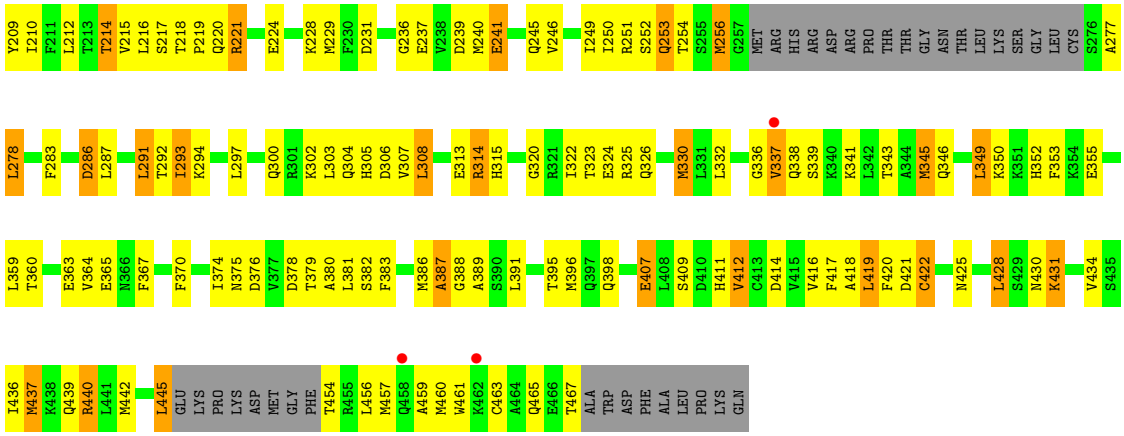


• Molecule 1: Calcium uptake protein 1, mitochondrial

Chain D:

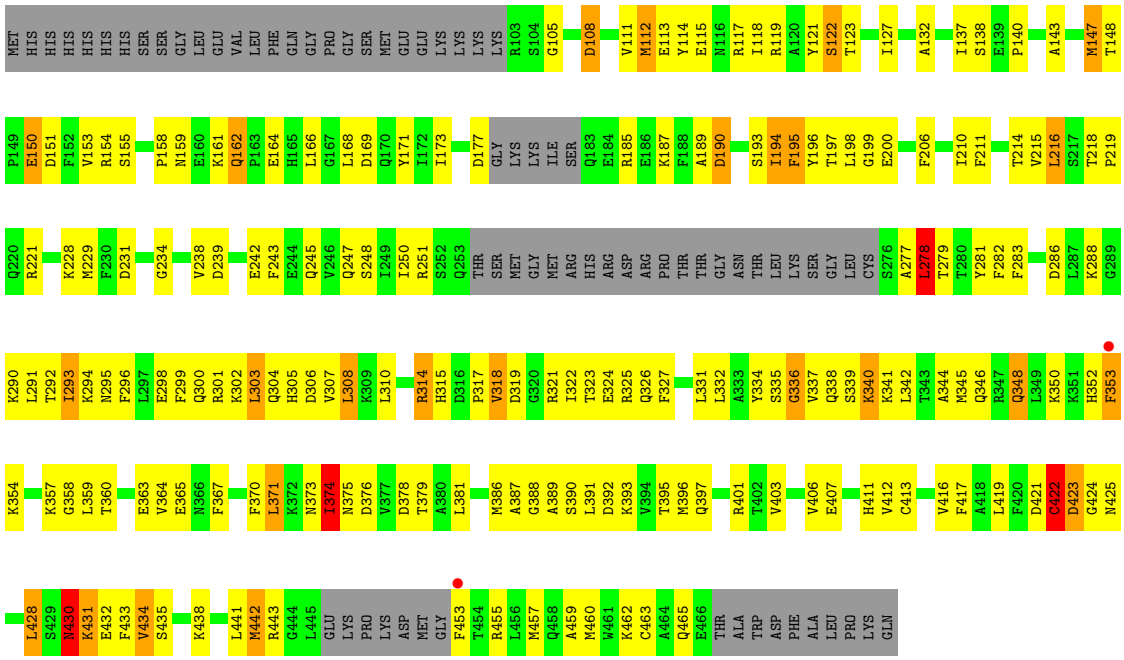






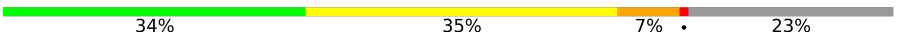
• Molecule 1: Calcium uptake protein 1, mitochondrial

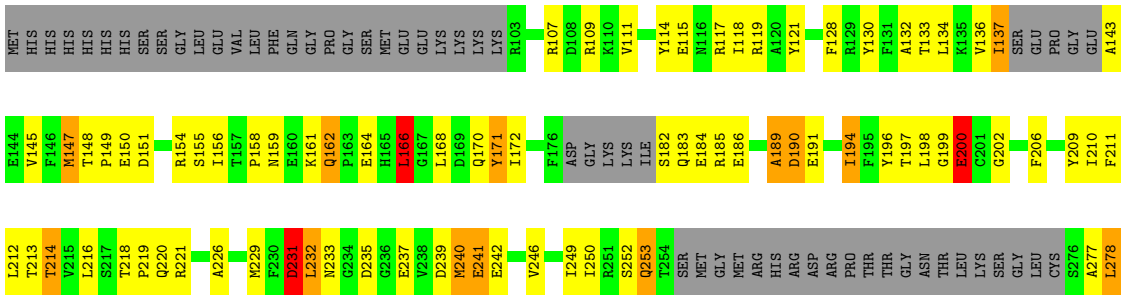
Chain E:

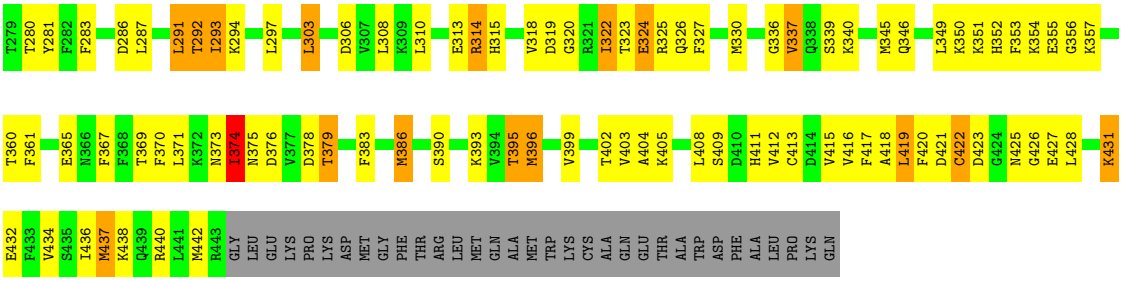


• Molecule 1: Calcium uptake protein 1, mitochondrial

Chain F:






T279 T280 Y281 F282 F283 D286 L287 L291 T292 I293 K294 L297 L303 D306 V307 L308 K309 L310 E313 R314 H315 V318 D319 G320 R321 I322 T323 E324 R325 Q326 F327 M330 G336 V337 Q338 S339 K340 M345 Q346 L349 K350 K351 H352 F353 K354 E355 G356 K357
T360 F361 E365 N366 F367 F368 T369 F370 L371 K372 N373 I374 N375 D376 V377 D378 T379 F383 M386 S390 K393 V394 T395 M396 V399 T402 V403 A404 K405 L408 S409 D410 H411 V412 C413 D414 V415 V416 F417 A418 L419 F420 D421 C422 D423 G424 N425 G426 E427 L428 K431
E432 F433 V434 S435 I436 M437 K438 Q439 R440 L441 M442 R443 GLY LEU GLU LYS PRO LYS ASP MET GLY PHE THR ARG LEU MET GLN ALA MET TRP LYS CYS ALA GLN GLU THR ALA TRP ASP PHE ALA LEU PRO LYS GLN

4 Data and refinement statistics (i)

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 36.71 – 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
$< I/\sigma(I) >$ [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)	0.29 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.88	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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(^{o})	Ideal(^{o})
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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Mol	Chain	Res	Type
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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Mol	Chain	Res	Type
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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Mol	Chain	Res	Type
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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Mol	Chain	Res	Type
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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.09	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.