



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:26 AM UTC

PDB ID : 1XO6 / pdb_00001xo6
Title : Acyl-CoA Carboxylase Beta Subunit from *S. coelicolor* (PccB), apo form #3
Authors : Diacovich, L.; Mitchell, D.L.; Pham, H.; Gago, G.; Melgar, M.M.; Khosla, C.; Gramajo, H.; Tsai, S.-C.
Deposited on : 2004-10-05
Resolution : 2.20 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

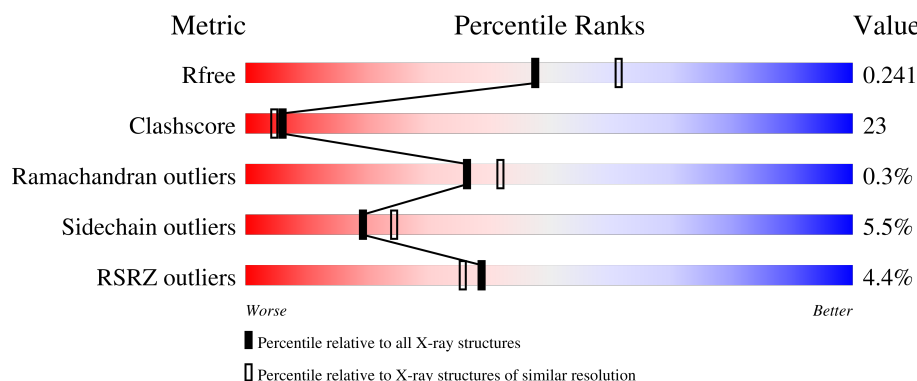
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	530	5% 62% 31% 5%
1	B	530	4% 67% 27%
1	C	530	4% 61% 34%
1	D	530	5% 64% 29% 5%
1	E	530	5% 63% 31%

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Mol	Chain	Length	Quality of chain
1	F	530	4% 67% 27% ...

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25641 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 propionyl-CoA carboxylase complex B subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	0	0
			3953	2481	698	761	13			
1	B	521	Total	C	N	O	S	0	0	0
			3953	2481	698	761	13			
1	C	521	Total	C	N	O	S	0	0	0
			3953	2481	698	761	13			
1	D	521	Total	C	N	O	S	0	0	0
			3953	2481	698	761	13			
1	E	521	Total	C	N	O	S	0	0	0
			3953	2481	698	761	13			
1	F	521	Total	C	N	O	S	0	0	0
			3953	2481	698	761	13			

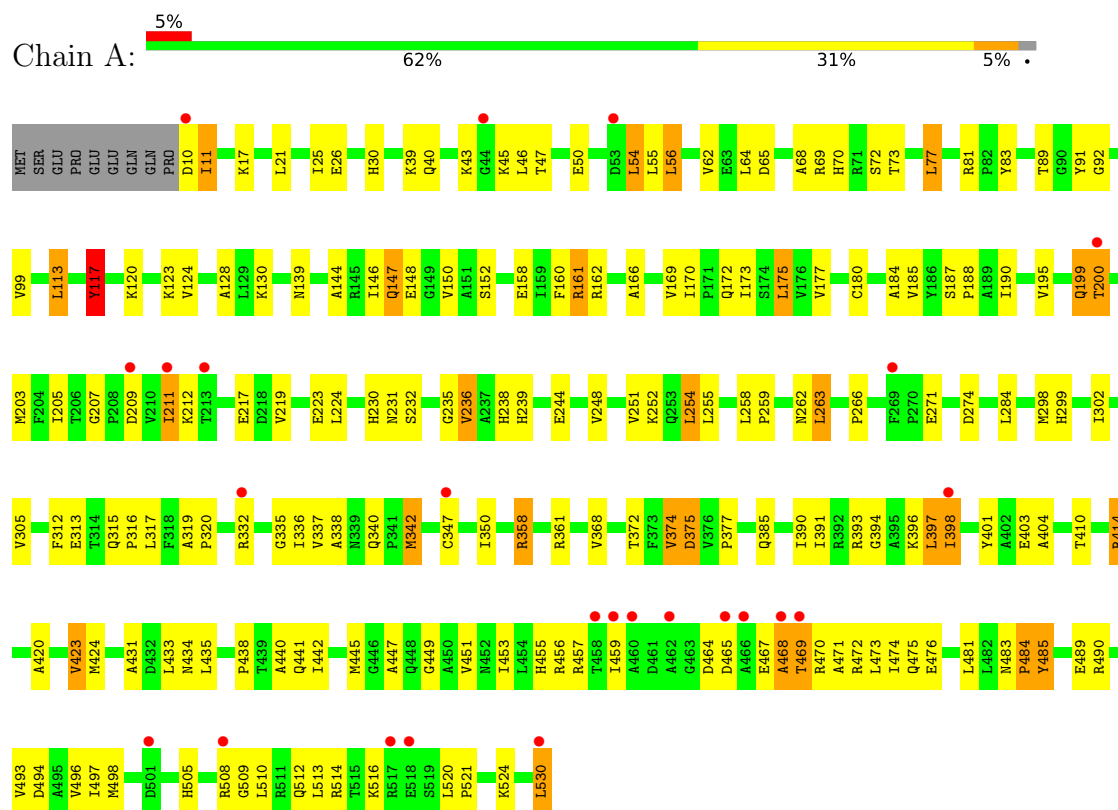
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	326	Total	O	0	0
			326	326		
2	B	320	Total	O	0	0
			320	320		
2	C	338	Total	O	0	0
			338	338		
2	D	332	Total	O	0	0
			332	332		
2	E	291	Total	O	0	0
			291	291		
2	F	316	Total	O	0	0
			316	316		

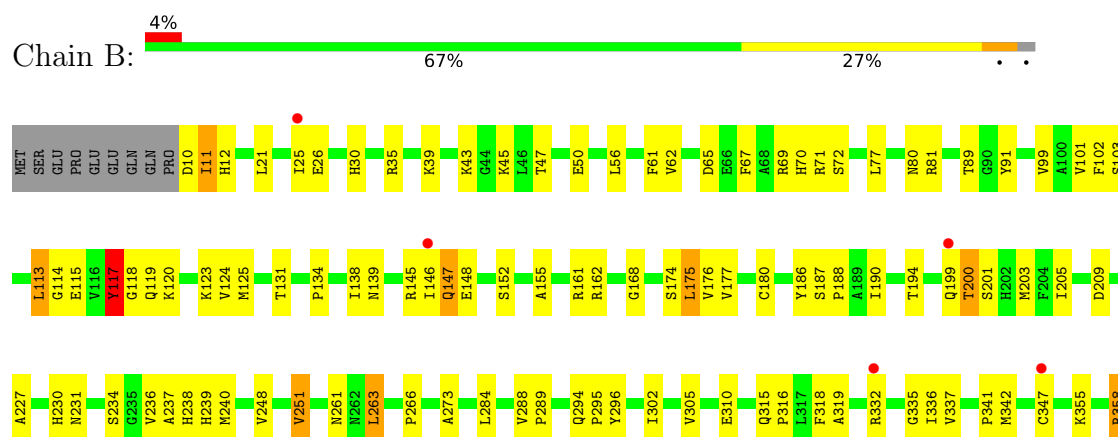
3 Residue-property plots

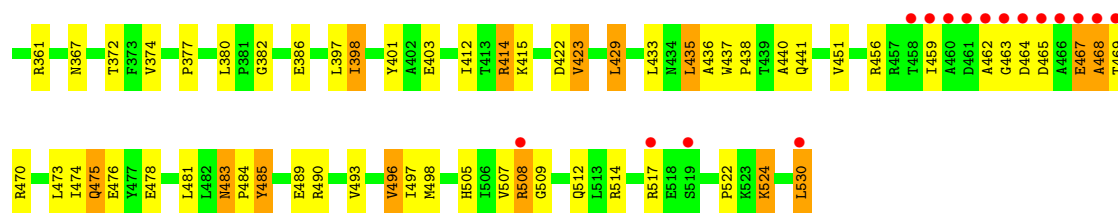
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: propionyl-CoA carboxylase complex B subunit

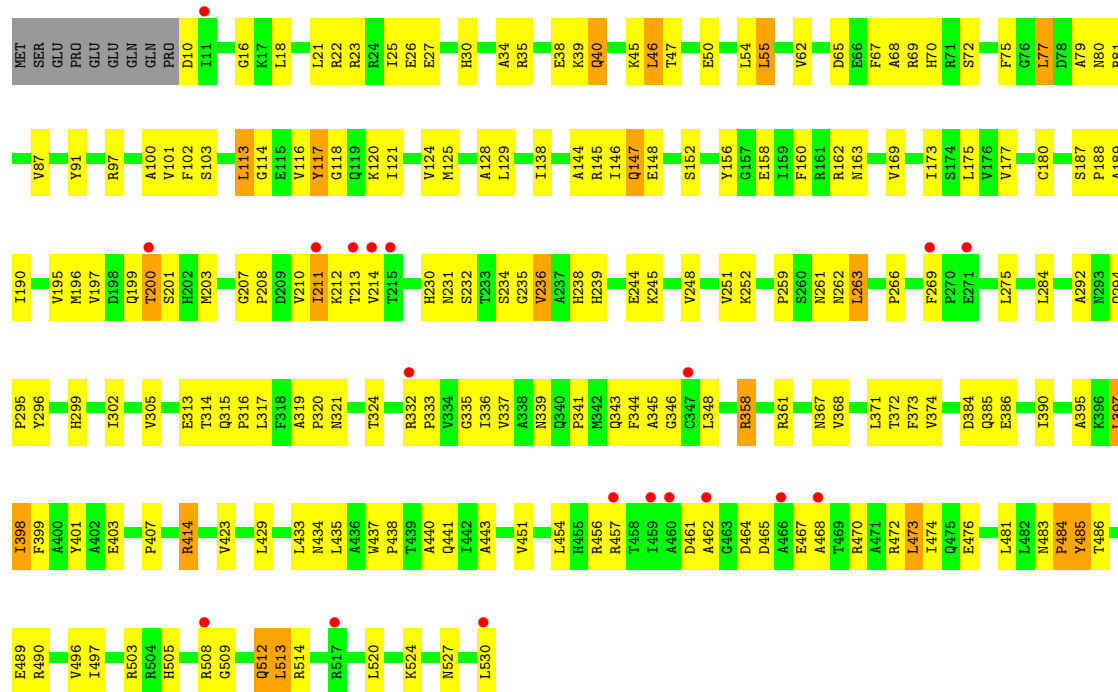


- Molecule 1: propionyl-CoA carboxylase complex B subunit

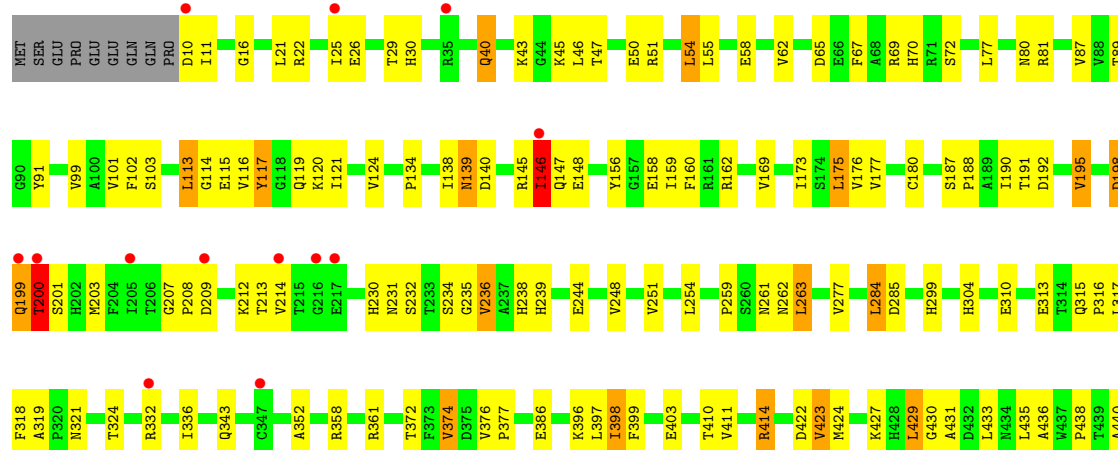




• Molecule 1: propionyl-CoA carboxylase complex B subunit

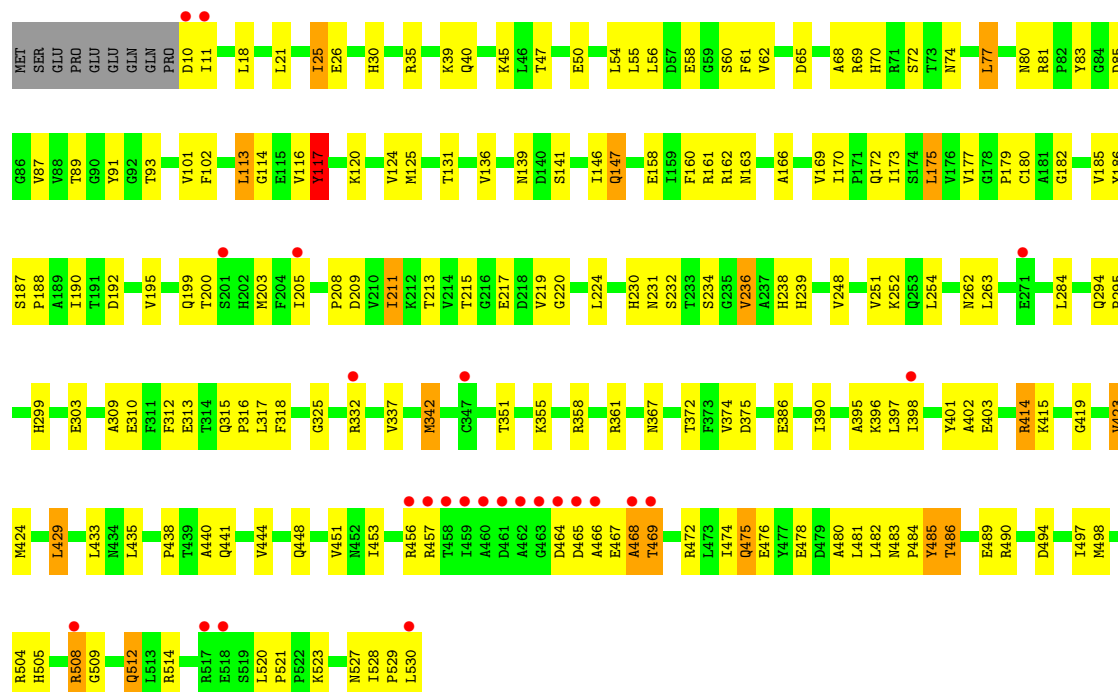


• Molecule 1: propionyl-CoA carboxylase complex B subunit

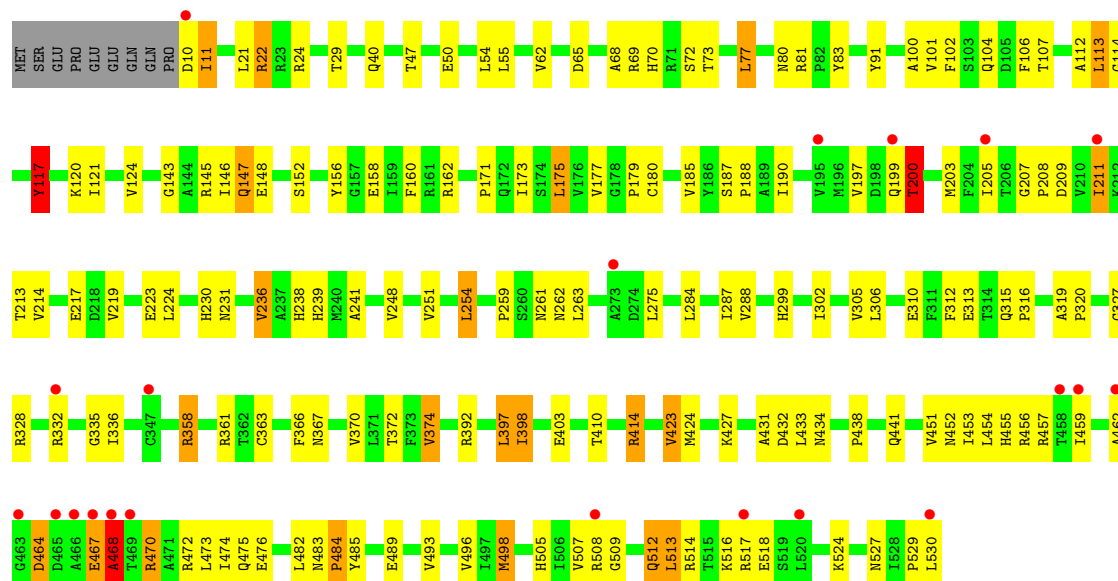




- Molecule 1: propionyl-CoA carboxylase complex B subunit



- Molecule 1: propionyl-CoA carboxylase complex B subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.77Å 178.95Å 296.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.41 – 2.20 49.41 – 2.20	Depositor EDS
% Data completeness (in resolution range)	86.0 (49.41-2.20) 86.0 (49.41-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.209 , 0.246 0.203 , 0.241	Depositor DCC
R_{free} test set	8903 reflections (3.10%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.947	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25641	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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	0.43	0/4033	1.05	18/5478 (0.3%)
1	B	0.42	0/4033	1.05	21/5478 (0.4%)
1	C	0.43	0/4033	1.07	22/5478 (0.4%)
1	D	0.43	0/4033	1.06	25/5478 (0.5%)
1	E	0.41	0/4033	0.95	14/5478 (0.3%)
1	F	0.41	0/4033	1.02	20/5478 (0.4%)
All	All	0.42	0/24198	1.03	120/32868 (0.4%)

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	A	0	1
1	B	0	1
1	D	0	1
1	E	0	1
All	All	0	4

There are no bond length outliers.

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	467	GLU	N-CA-C	26.92	145.22	112.38
1	C	467	GLU	N-CA-C	23.55	141.13	112.87
1	B	467	GLU	CB-CA-C	-21.00	75.70	111.41
1	D	467	GLU	N-CA-C	20.05	137.75	112.89
1	F	467	GLU	CB-CA-C	-19.40	79.09	111.68
1	D	468	ALA	N-CA-CB	-16.93	84.04	110.44
1	C	468	ALA	N-CA-CB	-15.96	86.86	110.49
1	A	468	ALA	N-CA-CB	-15.10	88.14	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	GLN	CB-CA-C	-14.98	89.92	111.80
1	B	468	ALA	CB-CA-C	-14.82	80.93	110.42
1	F	468	ALA	N-CA-C	-14.74	79.40	110.80
1	D	199	GLN	CB-CA-C	-13.83	91.60	111.80
1	F	199	GLN	CB-CA-C	-12.30	92.35	111.66
1	A	468	ALA	N-CA-C	-12.26	97.72	113.17
1	C	468	ALA	N-CA-C	-11.76	98.35	113.17
1	B	199	GLN	CB-CA-C	-11.64	94.81	111.80
1	F	467	GLU	N-CA-C	11.52	129.63	107.98
1	E	199	GLN	CB-CA-C	-11.30	93.92	111.66
1	B	469	THR	N-CA-C	-11.00	87.38	110.80
1	B	468	ALA	N-CA-C	-10.69	88.03	110.80
1	B	469	THR	N-CA-CB	10.14	127.63	110.49
1	E	468	ALA	CB-CA-C	-8.93	97.64	111.66
1	A	467	GLU	CB-CA-C	-8.77	91.81	110.32
1	B	467	GLU	CA-CB-CG	-8.74	96.61	114.10
1	C	200	THR	N-CA-C	-8.74	104.66	114.62
1	D	467	GLU	CB-CA-C	-8.72	91.76	109.99
1	A	199	GLN	CB-CA-C	-8.53	93.44	110.42
1	D	374	VAL	N-CA-C	8.44	119.99	108.17
1	D	485	TYR	N-CA-C	8.38	121.54	111.82
1	B	374	VAL	N-CA-C	8.34	120.28	108.36
1	F	374	VAL	N-CA-C	8.32	119.82	108.17
1	B	467	GLU	N-CA-C	8.26	124.09	107.41
1	C	467	GLU	CB-CA-C	-8.18	92.30	110.21
1	F	464	ASP	N-CA-C	-8.11	97.87	109.96
1	F	200	THR	N-CA-C	-7.97	104.71	114.75
1	B	200	THR	N-CA-CB	7.91	123.85	110.49
1	D	200	THR	N-CA-CB	7.83	123.73	110.49
1	E	374	VAL	N-CA-C	7.79	119.08	108.17
1	E	200	THR	N-CA-CB	7.78	125.51	110.88
1	C	414	ARG	N-CA-C	7.66	127.11	110.80
1	B	467	GLU	CB-CG-CD	7.61	125.53	112.60
1	A	200	THR	N-CA-C	-7.60	104.91	114.56
1	F	200	THR	N-CA-CB	7.47	122.06	111.15
1	E	469	THR	N-CA-C	-7.42	94.99	110.80
1	A	374	VAL	N-CA-C	7.39	118.52	108.17
1	F	288	VAL	N-CA-C	7.22	114.13	107.56
1	C	55	LEU	N-CA-C	7.18	118.90	111.14
1	E	200	THR	N-CA-C	-7.16	103.56	114.16
1	D	414	ARG	N-CA-C	7.08	125.88	110.80
1	C	200	THR	N-CA-CB	7.06	122.34	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	485	TYR	N-CA-C	7.05	119.81	111.71
1	C	374	VAL	N-CA-C	6.93	118.27	108.36
1	D	198	ASP	CB-CA-C	6.74	120.91	109.72
1	D	200	THR	N-CA-C	-6.71	96.51	110.80
1	D	468	ALA	N-CA-C	-6.65	104.98	113.23
1	C	496	VAL	N-CA-C	-6.58	98.38	107.99
1	D	199	GLN	N-CA-C	6.57	120.47	111.54
1	B	468	ALA	N-CA-CB	-6.44	99.61	110.49
1	F	468	ALA	CB-CA-C	6.25	122.85	110.42
1	E	485	TYR	N-CA-C	6.21	120.12	112.54
1	A	200	THR	N-CA-CB	6.19	119.24	111.00
1	F	498	MET	N-CA-C	-6.01	102.48	109.93
1	D	464	ASP	N-CA-C	-6.00	100.77	109.59
1	F	524	LYS	N-CA-C	-5.92	104.91	111.36
1	A	414	ARG	N-CA-C	5.90	123.37	110.80
1	C	485	TYR	N-CA-C	5.87	118.63	111.82
1	D	55	LEU	N-CA-C	5.86	118.55	111.40
1	B	414	ARG	N-CA-C	5.86	123.28	110.80
1	B	463	GLY	N-CA-C	-5.84	105.50	113.27
1	F	214	VAL	N-CA-C	5.76	117.28	111.00
1	E	423	VAL	N-CA-C	5.75	115.94	110.42
1	F	414	ARG	N-CA-C	5.70	122.93	110.80
1	D	496	VAL	N-CA-C	-5.69	99.69	107.99
1	B	524	LYS	N-CA-C	-5.68	105.17	111.36
1	A	496	VAL	N-CA-C	-5.65	99.75	107.99
1	A	423	VAL	N-CA-C	5.64	116.37	110.62
1	C	169	VAL	N-CA-C	-5.62	107.18	111.62
1	A	485	TYR	N-CA-C	5.58	118.29	111.82
1	E	414	ARG	N-CA-C	5.58	122.69	110.80
1	D	207	GLY	CA-C-N	5.57	125.03	119.24
1	D	207	GLY	C-N-CA	5.57	125.03	119.24
1	D	192	ASP	N-CA-C	5.54	117.40	111.36
1	C	367	ASN	N-CA-C	5.50	119.29	112.24
1	A	493	VAL	N-CA-C	-5.50	100.56	108.48
1	E	486	THR	N-CA-C	-5.50	105.30	112.23
1	F	55	LEU	N-CA-C	5.49	117.07	111.14
1	B	496	VAL	N-CA-C	-5.47	99.86	107.80
1	B	497	ILE	N-CA-C	5.47	117.52	108.99
1	E	199	GLN	N-CA-C	5.43	119.07	111.90
1	D	146	ILE	N-CA-C	5.41	120.59	109.34
1	E	192	ASP	N-CA-C	5.40	118.09	111.82
1	D	463	GLY	N-CA-C	-5.40	106.09	113.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	486	THR	N-CA-C	-5.40	105.48	111.36
1	A	469	THR	N-CA-C	-5.39	105.06	111.69
1	F	493	VAL	N-CA-C	-5.38	100.72	108.53
1	D	139	ASN	N-CA-C	5.38	118.01	109.24
1	E	469	THR	N-CA-CB	5.34	119.52	110.49
1	D	497	ILE	N-CA-C	5.33	116.53	108.96
1	A	524	LYS	N-CA-C	-5.30	105.58	111.36
1	C	524	LYS	N-CA-C	-5.29	105.68	111.82
1	A	56	LEU	N-CA-C	5.28	117.68	110.55
1	C	199	GLN	N-CA-C	5.27	118.71	111.54
1	F	496	VAL	N-CA-C	-5.25	100.33	107.99
1	C	207	GLY	CA-C-N	5.24	125.29	119.32
1	C	207	GLY	C-N-CA	5.24	125.29	119.32
1	C	486	THR	N-CA-C	-5.23	105.66	111.36
1	C	269	PHE	CA-C-N	5.16	125.45	119.93
1	C	269	PHE	C-N-CA	5.16	125.45	119.93
1	F	423	VAL	N-CA-C	5.16	115.38	110.42
1	E	424	MET	N-CA-C	5.16	117.59	109.39
1	D	199	GLN	N-CA-CB	-5.14	104.18	111.84
1	F	117	TYR	N-CA-C	-5.14	105.68	111.28
1	C	296	TYR	N-CA-C	-5.13	101.27	109.07
1	D	423	VAL	N-CA-C	5.12	115.84	110.62
1	B	493	VAL	N-CA-C	-5.12	101.11	108.48
1	B	423	VAL	N-CA-C	5.09	115.81	110.62
1	A	375	ASP	N-CA-C	-5.03	100.08	110.80
1	A	404	ALA	N-CA-C	5.02	117.32	110.24
1	B	367	ASN	N-CA-C	5.01	118.66	112.24
1	F	470	ARG	N-CA-C	-5.01	105.29	111.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	TYR	Sidechain
1	B	117	TYR	Sidechain
1	D	117	TYR	Sidechain
1	E	117	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	3953	0	3880	202	0
1	B	3953	0	3880	183	0
1	C	3953	0	3880	201	0
1	D	3953	0	3880	205	0
1	E	3953	0	3880	193	0
1	F	3953	0	3880	181	0
2	A	326	0	0	52	0
2	B	320	0	0	43	0
2	C	338	0	0	71	0
2	D	332	0	0	79	0
2	E	291	0	0	50	0
2	F	316	0	0	46	0
All	All	25641	0	23280	1061	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (1061) 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:E:295:PRO:HB2	1:E:342:MET:HE3	1.29	1.08
1:B:295:PRO:HB2	1:B:342:MET:HE2	1.38	1.05
1:D:99:VAL:HA	2:D:778:HOH:O	1.54	1.04
1:B:99:VAL:HA	2:B:833:HOH:O	1.55	1.03
1:D:62:VAL:HG21	1:E:508:ARG:HG3	1.42	1.02
1:D:414:ARG:O	2:D:851:HOH:O	1.79	1.01
1:D:89:THR:HG23	2:D:723:HOH:O	1.65	0.96
1:A:147:GLN:H	1:A:147:GLN:HE21	1.13	0.95
1:B:147:GLN:H	1:B:147:GLN:HE21	0.97	0.95
1:C:160:PHE:HB3	1:F:398:ILE:HD13	1.47	0.93
1:A:358:ARG:HG2	2:D:725:HOH:O	1.68	0.92
1:B:147:GLN:H	1:B:147:GLN:NE2	1.65	0.92
1:D:262:ASN:HB3	2:D:832:HOH:O	1.69	0.92
1:D:483:ASN:HD22	1:D:485:TYR:H	1.18	0.91
1:C:70:HIS:HD2	1:C:72:SER:H	1.18	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:VAL:HG23	2:D:838:HOH:O	1.70	0.90
1:E:187:SER:HB3	1:E:188:PRO:HD3	1.53	0.90
1:B:194:THR:HB	2:B:746:HOH:O	1.74	0.88
1:D:498:MET:HE2	1:F:21:LEU:HD23	1.56	0.87
1:F:372:THR:HG23	1:F:410:THR:HG23	1.56	0.87
1:E:62:VAL:HG21	1:F:508:ARG:HG3	1.53	0.87
1:E:483:ASN:HD22	1:E:485:TYR:H	1.18	0.85
1:A:393:ARG:HB2	2:A:625:HOH:O	1.76	0.85
1:E:435:LEU:HD13	2:E:773:HOH:O	1.75	0.85
1:F:147:GLN:H	1:F:147:GLN:HE21	1.22	0.85
1:E:55:LEU:HA	2:E:600:HOH:O	1.76	0.85
1:D:70:HIS:HD2	1:D:72:SER:H	1.23	0.84
1:C:483:ASN:HD22	1:C:485:TYR:H	1.26	0.84
1:B:71:ARG:HH22	1:B:119:GLN:HE22	1.24	0.84
1:E:147:GLN:H	1:E:147:GLN:NE2	1.75	0.83
1:A:483:ASN:HD22	1:A:485:TYR:H	1.24	0.83
1:B:508:ARG:NE	1:C:91:TYR:OH	2.13	0.82
1:F:77:LEU:HB3	2:F:809:HOH:O	1.78	0.82
1:D:508:ARG:HG3	1:F:62:VAL:HG21	1.61	0.82
1:B:147:GLN:HE21	1:B:147:GLN:N	1.78	0.81
1:F:70:HIS:HD2	1:F:72:SER:H	1.27	0.81
2:C:754:HOH:O	1:F:529:PRO:HG2	1.79	0.81
1:B:65:ASP:HB2	1:B:120:LYS:HE3	1.63	0.81
1:C:187:SER:HB3	1:C:188:PRO:HD3	1.61	0.81
1:B:295:PRO:HB2	1:B:342:MET:CE	2.11	0.80
1:D:140:ASP:HB2	2:D:838:HOH:O	1.81	0.80
1:E:295:PRO:HB2	1:E:342:MET:CE	2.11	0.80
1:E:147:GLN:H	1:E:147:GLN:HE21	1.27	0.80
1:A:62:VAL:HG21	1:C:508:ARG:HG3	1.61	0.80
1:A:508:ARG:HG3	1:B:62:VAL:HG21	1.61	0.80
1:A:398:ILE:HD13	1:D:160:PHE:HB3	1.63	0.80
1:B:508:ARG:HG3	1:C:62:VAL:HG21	1.63	0.80
1:A:484:PRO:HD3	2:A:856:HOH:O	1.83	0.79
1:C:147:GLN:H	1:C:147:GLN:HE21	1.29	0.79
1:F:261:ASN:HA	2:F:819:HOH:O	1.83	0.79
1:F:508:ARG:HD3	1:F:509:GLY:N	1.97	0.79
1:C:138:ILE:HD12	1:C:175:LEU:HD23	1.65	0.79
1:F:187:SER:HB3	1:F:188:PRO:HD3	1.62	0.78
1:A:128:ALA:HA	2:A:794:HOH:O	1.83	0.78
1:B:187:SER:HB3	1:B:188:PRO:HD3	1.64	0.78
1:C:197:VAL:HB	2:C:786:HOH:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ARG:CZ	1:A:514:ARG:HH21	1.97	0.78
1:E:505:HIS:HA	1:E:508:ARG:HD2	1.65	0.78
1:A:70:HIS:HD2	1:A:72:SER:H	1.32	0.78
1:E:367:ASN:HA	2:E:768:HOH:O	1.83	0.77
1:D:187:SER:HB3	1:D:188:PRO:HD3	1.65	0.77
1:D:121:ILE:HA	2:D:801:HOH:O	1.85	0.77
1:F:451:VAL:HG21	1:F:474:ILE:HG12	1.66	0.77
1:A:266:PRO:HG3	2:A:731:HOH:O	1.85	0.77
1:A:187:SER:HB3	1:A:188:PRO:HD3	1.68	0.76
1:C:368:VAL:HG13	2:C:839:HOH:O	1.85	0.76
1:D:508:ARG:NE	1:F:91:TYR:OH	2.18	0.76
1:B:99:VAL:HB	2:B:846:HOH:O	1.84	0.76
1:C:147:GLN:H	1:C:147:GLN:NE2	1.82	0.76
1:A:248:VAL:O	1:A:251:VAL:HG22	1.84	0.76
1:F:171:PRO:HD3	2:F:819:HOH:O	1.85	0.76
1:C:177:VAL:HA	2:C:786:HOH:O	1.86	0.75
1:D:159:ILE:HG12	2:D:788:HOH:O	1.86	0.75
1:F:50:GLU:O	1:F:54:LEU:HD13	1.85	0.75
1:A:258:LEU:HD12	2:A:669:HOH:O	1.87	0.75
1:E:175:LEU:HD22	1:E:177:VAL:HG13	1.67	0.75
1:C:252:LYS:HD2	2:C:775:HOH:O	1.86	0.75
1:A:508:ARG:HE	1:B:62:VAL:HG11	1.52	0.74
1:A:332:ARG:NE	1:A:514:ARG:HH21	1.86	0.74
1:A:147:GLN:H	1:A:147:GLN:NE2	1.84	0.74
1:C:398:ILE:HG13	2:F:721:HOH:O	1.85	0.74
1:C:128:ALA:HA	2:C:832:HOH:O	1.85	0.74
1:D:361:ARG:HD2	1:D:403:GLU:OE2	1.88	0.74
1:F:483:ASN:HD22	1:F:485:TYR:H	1.34	0.74
1:C:314:THR:HG23	2:C:678:HOH:O	1.87	0.74
1:E:248:VAL:O	1:E:251:VAL:HG22	1.87	0.73
1:F:457:ARG:N	1:F:457:ARG:HD2	2.02	0.73
1:F:254:LEU:HD13	1:F:312:PHE:HE2	1.53	0.73
1:D:457:ARG:H	1:D:457:ARG:HD2	1.52	0.73
1:D:462:ALA:HB3	2:D:685:HOH:O	1.87	0.73
1:F:147:GLN:H	1:F:147:GLN:NE2	1.86	0.73
1:D:508:ARG:HE	1:F:62:VAL:HG11	1.52	0.73
1:C:34:ALA:O	1:C:38:GLU:HG3	1.87	0.73
1:C:336:ILE:HG23	2:C:856:HOH:O	1.89	0.73
1:A:91:TYR:OH	1:C:508:ARG:NE	2.22	0.73
1:D:62:VAL:HG11	1:E:508:ARG:HE	1.53	0.72
1:A:433:LEU:HD21	1:A:508:ARG:NH1	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ALA:HA	2:B:746:HOH:O	1.88	0.72
1:C:485:TYR:O	1:C:489:GLU:HG3	1.89	0.72
1:E:45:LYS:HG2	2:E:801:HOH:O	1.89	0.72
1:C:275:LEU:HD23	2:C:771:HOH:O	1.89	0.72
1:C:23:ARG:HB3	1:C:23:ARG:HH11	1.53	0.71
1:C:230:HIS:HB3	1:C:236:VAL:HG22	1.71	0.71
1:C:292:ALA:HB1	2:C:599:HOH:O	1.90	0.71
1:C:508:ARG:HD3	1:C:509:GLY:N	2.05	0.71
1:B:398:ILE:HD13	1:E:160:PHE:HB3	1.73	0.71
1:C:113:LEU:HD22	2:C:843:HOH:O	1.91	0.71
1:D:473:LEU:HD13	2:D:655:HOH:O	1.90	0.71
1:E:504:ARG:HD3	2:E:570:HOH:O	1.90	0.71
1:A:65:ASP:HB2	1:A:120:LYS:HE3	1.73	0.71
1:D:457:ARG:HD2	1:D:457:ARG:N	2.05	0.71
1:E:508:ARG:HD3	1:E:509:GLY:N	2.06	0.71
1:B:438:PRO:HG3	1:C:21:LEU:HD22	1.72	0.70
1:D:45:LYS:HE2	2:D:824:HOH:O	1.89	0.70
1:D:482:LEU:HD21	2:D:690:HOH:O	1.91	0.70
1:D:65:ASP:HB2	1:D:120:LYS:HE3	1.72	0.70
1:D:508:ARG:HD3	1:D:509:GLY:N	2.06	0.70
1:A:451:VAL:HG21	1:A:474:ILE:HG12	1.73	0.70
1:D:456:ARG:HH11	1:D:457:ARG:NH1	1.90	0.70
1:A:62:VAL:HG11	1:C:508:ARG:HE	1.56	0.70
1:A:438:PRO:HG3	1:B:21:LEU:HD22	1.72	0.70
1:A:508:ARG:HD3	1:A:509:GLY:N	2.06	0.70
1:B:288:VAL:HG13	2:B:743:HOH:O	1.91	0.69
1:C:372:THR:HG23	2:C:606:HOH:O	1.92	0.69
1:D:508:ARG:HH21	1:F:62:VAL:HG11	1.56	0.69
1:B:113:LEU:HD22	1:B:117:TYR:CD1	2.28	0.69
1:C:152:SER:HB2	2:C:854:HOH:O	1.93	0.69
1:E:117:TYR:HA	2:E:785:HOH:O	1.93	0.69
1:A:62:VAL:HG11	1:C:508:ARG:HH21	1.57	0.69
1:E:89:THR:HB	1:E:124:VAL:HG21	1.75	0.69
1:F:121:ILE:O	1:F:124:VAL:HG12	1.92	0.69
1:A:175:LEU:HD22	1:A:177:VAL:HG13	1.72	0.69
1:D:40:GLN:HA	2:D:824:HOH:O	1.93	0.69
1:F:457:ARG:HD2	1:F:457:ARG:H	1.57	0.69
1:D:433:LEU:HD21	1:D:508:ARG:NH1	2.09	0.68
1:D:446:GLY:HA2	2:D:690:HOH:O	1.94	0.68
1:E:62:VAL:HG11	1:F:508:ARG:HE	1.57	0.68
1:A:505:HIS:HA	1:A:508:ARG:HD2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ILE:HA	2:A:625:HOH:O	1.94	0.68
1:B:341:PRO:HD2	2:B:745:HOH:O	1.92	0.68
1:D:91:TYR:OH	1:E:508:ARG:NE	2.27	0.68
1:C:208:PRO:HA	1:C:211:ILE:HD12	1.74	0.68
1:E:91:TYR:OH	1:F:508:ARG:NE	2.27	0.68
1:A:431:ALA:HB1	2:A:623:HOH:O	1.94	0.67
1:C:341:PRO:HD2	2:C:851:HOH:O	1.94	0.67
1:A:459:ILE:HG21	1:A:470:ARG:HH21	1.58	0.67
1:F:372:THR:HG22	2:F:532:HOH:O	1.94	0.67
1:D:87:VAL:HG13	2:D:723:HOH:O	1.95	0.67
1:B:161:ARG:CZ	2:E:758:HOH:O	2.41	0.67
1:F:431:ALA:HB1	2:F:823:HOH:O	1.93	0.67
1:D:148:GLU:HG3	2:D:786:HOH:O	1.95	0.67
1:A:451:VAL:HG21	1:A:474:ILE:CG1	2.25	0.66
1:E:185:VAL:HG21	1:E:205:ILE:HG12	1.78	0.66
1:B:152:SER:HB3	2:B:669:HOH:O	1.96	0.66
1:D:469:THR:O	1:D:473:LEU:HD22	1.96	0.66
1:F:361:ARG:HD2	1:F:403:GLU:OE2	1.95	0.66
1:B:398:ILE:HG22	1:B:423:VAL:HG22	1.77	0.66
1:C:505:HIS:HA	1:C:508:ARG:HD2	1.77	0.66
1:F:113:LEU:HD22	1:F:117:TYR:CD1	2.29	0.66
1:D:501:ASP:HB2	2:D:779:HOH:O	1.95	0.66
1:E:433:LEU:HD21	1:E:508:ARG:NH1	2.11	0.66
1:A:508:ARG:HH21	1:B:62:VAL:HG11	1.59	0.66
1:A:170:ILE:HG13	2:A:760:HOH:O	1.95	0.66
1:C:23:ARG:HB3	1:C:23:ARG:NH1	2.11	0.66
1:D:113:LEU:HD22	1:D:117:TYR:CD1	2.31	0.65
1:E:47:THR:OG1	1:E:50:GLU:HG3	1.96	0.65
1:A:508:ARG:NE	1:B:91:TYR:OH	2.29	0.65
1:D:410:THR:HG22	2:D:814:HOH:O	1.94	0.65
1:D:230:HIS:HB3	1:D:236:VAL:HG22	1.79	0.65
1:A:394:GLY:N	2:A:843:HOH:O	2.28	0.65
1:D:43:LYS:HD2	2:D:824:HOH:O	1.95	0.65
1:A:259:PRO:HG2	2:A:807:HOH:O	1.95	0.65
1:D:497:ILE:HD12	2:D:779:HOH:O	1.97	0.65
1:D:508:ARG:NE	1:F:62:VAL:HG11	2.12	0.65
1:C:433:LEU:HD21	1:C:508:ARG:NH1	2.11	0.65
1:D:497:ILE:HB	2:D:779:HOH:O	1.96	0.65
1:E:65:ASP:HB2	1:E:120:LYS:HE3	1.77	0.65
1:E:70:HIS:HD2	1:E:72:SER:H	1.44	0.65
1:F:315:GLN:N	1:F:316:PRO:HD3	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ALA:HB3	2:A:842:HOH:O	1.97	0.64
1:F:65:ASP:HB2	1:F:120:LYS:HE3	1.79	0.64
1:C:65:ASP:HB2	1:C:120:LYS:HE3	1.79	0.64
1:E:395:ALA:O	1:E:398:ILE:HG12	1.97	0.64
1:A:494:ASP:HA	2:A:782:HOH:O	1.97	0.64
1:B:315:GLN:N	1:B:316:PRO:HD3	2.13	0.64
1:B:508:ARG:HD3	1:B:509:GLY:N	2.13	0.64
1:D:231:ASN:HD21	1:D:239:HIS:N	1.96	0.64
1:B:433:LEU:HD21	1:B:508:ARG:NH1	2.13	0.64
1:A:469:THR:O	1:A:473:LEU:HD13	1.98	0.64
1:C:248:VAL:O	1:C:251:VAL:HG22	1.98	0.64
1:C:395:ALA:O	1:C:398:ILE:HG23	1.98	0.64
2:C:801:HOH:O	1:F:146:ILE:HG22	1.97	0.64
1:D:70:HIS:CD2	1:D:72:SER:H	2.12	0.64
1:D:508:ARG:NH2	1:F:62:VAL:HG11	2.13	0.64
1:B:70:HIS:HD2	1:B:72:SER:H	1.44	0.63
1:C:372:THR:HG21	1:C:401:TYR:OH	1.97	0.63
1:C:196:MET:HE1	2:C:722:HOH:O	1.97	0.63
1:D:438:PRO:HG3	1:F:21:LEU:HD22	1.80	0.63
1:F:512:GLN:HB3	2:F:707:HOH:O	1.98	0.63
1:B:498:MET:HE1	1:C:18:LEU:HD13	1.80	0.63
1:F:197:VAL:HG13	2:F:829:HOH:O	1.96	0.63
1:B:175:LEU:HD22	1:B:177:VAL:HG13	1.80	0.63
1:E:325:GLY:HA2	2:E:700:HOH:O	1.98	0.63
1:E:429:LEU:C	2:E:758:HOH:O	2.42	0.63
1:C:266:PRO:HG3	2:C:839:HOH:O	1.98	0.63
1:C:457:ARG:HD2	1:C:457:ARG:N	2.12	0.63
1:D:505:HIS:HA	1:D:508:ARG:HD2	1.81	0.63
1:F:179:PRO:HD2	2:F:818:HOH:O	1.98	0.63
1:D:120:LYS:HE2	2:D:723:HOH:O	1.99	0.63
1:D:212:LYS:HG3	2:D:598:HOH:O	1.98	0.62
1:D:21:LEU:HD22	1:E:438:PRO:HG3	1.80	0.62
1:D:436:ALA:HB3	2:D:834:HOH:O	1.98	0.62
1:E:81:ARG:HB3	2:E:777:HOH:O	1.99	0.62
1:B:512:GLN:HG3	1:C:91:TYR:CE1	2.34	0.62
1:B:437:TRP:HB3	2:B:834:HOH:O	1.98	0.62
1:A:158:GLU:O	1:A:162:ARG:HG2	2.00	0.62
1:A:160:PHE:HB3	1:D:398:ILE:HD13	1.80	0.62
1:D:198:ASP:O	1:D:199:GLN:HB2	1.99	0.62
1:E:332:ARG:HD3	1:E:514:ARG:NH2	2.15	0.62
1:F:284:LEU:O	1:F:287:ILE:HG22	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:GLY:C	1:A:336:ILE:HD12	2.24	0.62
1:B:456:ARG:O	1:B:459:ILE:HG22	2.00	0.62
1:C:259:PRO:HD3	2:C:571:HOH:O	2.00	0.62
1:D:10:ASP:CG	1:D:11:ILE:H	2.07	0.62
1:E:170:ILE:HG13	2:E:691:HOH:O	1.99	0.62
1:A:147:GLN:HE21	1:A:147:GLN:N	1.94	0.62
1:C:160:PHE:HB3	1:F:398:ILE:CD1	2.24	0.62
1:E:113:LEU:HD22	1:E:117:TYR:CD1	2.35	0.62
1:F:505:HIS:C	1:F:508:ARG:HH11	2.07	0.62
1:F:453:ILE:HB	2:F:775:HOH:O	2.00	0.61
1:B:415:LYS:HE2	2:B:666:HOH:O	1.99	0.61
1:F:433:LEU:HD21	1:F:508:ARG:CZ	2.30	0.61
1:A:368:VAL:HG13	2:A:731:HOH:O	2.00	0.61
1:B:524:LYS:NZ	2:E:768:HOH:O	2.32	0.61
1:A:298:MET:HE3	2:A:749:HOH:O	2.01	0.61
1:D:485:TYR:O	1:D:489:GLU:HG3	2.01	0.61
1:F:10:ASP:CG	1:F:11:ILE:H	2.08	0.61
1:F:328:ARG:NH2	2:F:846:HOH:O	2.33	0.61
1:A:54:LEU:HD13	2:A:604:HOH:O	2.01	0.61
1:A:271:GLU:HB3	2:A:736:HOH:O	2.00	0.61
1:A:361:ARG:HD2	1:A:403:GLU:OE2	2.00	0.61
1:A:440:ALA:N	2:A:856:HOH:O	2.33	0.61
1:E:172:GLN:C	1:E:173:ILE:HD12	2.26	0.61
1:E:456:ARG:HD2	1:E:457:ARG:NH1	2.15	0.61
1:A:47:THR:OG1	1:A:50:GLU:HG3	2.01	0.61
1:C:465:ASP:HB3	2:C:688:HOH:O	2.01	0.61
1:D:459:ILE:HD11	1:D:466:ALA:O	2.01	0.61
1:E:361:ARG:HD3	2:E:739:HOH:O	2.01	0.61
1:C:232:SER:HB3	1:C:317:LEU:HB3	1.83	0.60
1:A:485:TYR:O	1:A:489:GLU:HG3	2.01	0.60
1:B:39:LYS:NZ	1:B:39:LYS:HB3	2.16	0.60
1:F:366:PHE:HB2	2:F:753:HOH:O	2.01	0.60
1:A:530:LEU:HG	1:D:396:LYS:HD3	1.83	0.60
1:B:296:TYR:C	1:B:342:MET:HE3	2.25	0.60
1:C:113:LEU:HD13	2:C:843:HOH:O	2.01	0.60
1:C:262:ASN:HA	2:C:850:HOH:O	2.01	0.60
1:D:259:PRO:HG2	2:D:854:HOH:O	2.00	0.60
1:B:238:HIS:ND1	2:B:746:HOH:O	2.32	0.60
1:C:25:ILE:HD13	1:C:67:PHE:HZ	1.67	0.60
1:A:254:LEU:HD13	1:A:312:PHE:HE2	1.66	0.60
1:C:10:ASP:O	1:C:16:GLY:HA3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:PRO:HB3	2:C:571:HOH:O	2.02	0.60
1:C:399:PHE:HA	2:F:721:HOH:O	2.00	0.60
1:D:483:ASN:HB2	1:D:484:PRO:HD2	1.82	0.60
1:B:21:LEU:O	1:B:25:ILE:HG23	2.02	0.60
1:D:147:GLN:HB2	2:D:786:HOH:O	2.00	0.60
1:A:113:LEU:HD22	1:A:117:TYR:CD1	2.37	0.59
1:B:490:ARG:HG3	2:B:698:HOH:O	2.00	0.59
1:E:21:LEU:HD22	1:F:438:PRO:HG3	1.83	0.59
1:E:523:LYS:HB2	2:E:797:HOH:O	2.01	0.59
1:D:332:ARG:HD2	2:D:536:HOH:O	2.02	0.59
1:D:530:LEU:HD22	2:D:725:HOH:O	2.01	0.59
1:F:231:ASN:HD21	1:F:239:HIS:N	2.00	0.59
1:A:70:HIS:CD2	1:A:72:SER:H	2.16	0.59
1:A:508:ARG:NE	1:B:62:VAL:HG11	2.17	0.59
1:A:508:ARG:CG	1:B:62:VAL:HG21	2.33	0.59
1:D:248:VAL:O	1:D:251:VAL:HG22	2.02	0.59
1:A:490:ARG:HH22	1:D:115:GLU:CD	2.10	0.59
1:D:62:VAL:HG11	1:E:508:ARG:NE	2.16	0.59
1:E:68:ALA:HB3	2:E:735:HOH:O	2.03	0.59
1:E:215:THR:HB	2:E:659:HOH:O	2.03	0.59
1:E:451:VAL:HG21	1:E:474:ILE:CG1	2.32	0.59
1:E:483:ASN:HD22	1:E:485:TYR:N	1.95	0.59
1:B:47:THR:OG1	1:B:50:GLU:HG3	2.03	0.59
1:F:77:LEU:N	2:F:724:HOH:O	2.34	0.59
1:A:266:PRO:HB3	2:A:815:HOH:O	2.02	0.59
1:A:332:ARG:HE	1:A:514:ARG:HE	1.49	0.59
1:D:62:VAL:HG21	1:E:508:ARG:CG	2.26	0.59
1:F:433:LEU:HD21	1:F:508:ARG:NH2	2.17	0.59
1:C:40:GLN:HE21	1:C:40:GLN:HA	1.65	0.59
1:A:315:GLN:N	1:A:316:PRO:HD3	2.18	0.58
1:D:399:PHE:HB2	2:D:857:HOH:O	2.02	0.58
1:E:361:ARG:HD2	1:E:403:GLU:OE2	2.03	0.58
1:A:148:GLU:HG3	2:A:712:HOH:O	2.03	0.58
1:A:459:ILE:HD11	1:A:473:LEU:HD22	1.86	0.58
1:A:483:ASN:HB2	1:A:484:PRO:HD2	1.85	0.58
1:D:433:LEU:HD21	1:D:508:ARG:HH12	1.68	0.58
1:E:21:LEU:O	1:E:25:ILE:HG22	2.03	0.58
1:E:372:THR:HG21	1:E:401:TYR:OH	2.03	0.58
1:A:505:HIS:O	1:A:508:ARG:HD3	2.03	0.58
1:B:56:LEU:HD22	2:B:846:HOH:O	2.02	0.58
1:C:472:ARG:O	1:C:476:GLU:HG3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:GLN:N	1:D:316:PRO:HD3	2.19	0.58
1:C:316:PRO:HD2	2:C:639:HOH:O	2.03	0.58
1:D:433:LEU:HD13	2:D:858:HOH:O	2.03	0.58
1:C:138:ILE:HG13	2:C:865:HOH:O	2.03	0.58
1:C:505:HIS:O	1:C:508:ARG:HD3	2.02	0.58
1:B:248:VAL:O	1:B:251:VAL:HG13	2.04	0.58
1:D:209:ASP:HB2	2:D:840:HOH:O	2.03	0.58
1:B:186:TYR:O	1:B:190:ILE:HG12	2.04	0.58
1:C:147:GLN:HE21	1:C:147:GLN:N	2.01	0.58
1:F:72:SER:HB3	2:F:809:HOH:O	2.04	0.58
1:C:371:LEU:HB2	2:C:856:HOH:O	2.03	0.57
1:C:520:LEU:HD13	2:C:692:HOH:O	2.03	0.57
1:E:215:THR:HG21	2:E:770:HOH:O	2.02	0.57
1:E:456:ARG:HH11	1:E:457:ARG:NH1	2.02	0.57
1:A:139:ASN:HB3	2:A:685:HOH:O	2.03	0.57
1:A:70:HIS:CE1	1:A:81:ARG:HG2	2.39	0.57
1:B:335:GLY:C	1:B:336:ILE:HD12	2.30	0.57
1:C:145:ARG:HD2	1:C:148:GLU:OE2	2.05	0.57
1:E:456:ARG:HD2	1:E:457:ARG:CZ	2.34	0.57
1:F:262:ASN:OD1	1:F:263:LEU:HD22	2.03	0.57
1:F:483:ASN:HB2	1:F:484:PRO:HD2	1.85	0.57
1:A:433:LEU:HD21	1:A:508:ARG:HH12	1.67	0.57
1:B:125:MET:HG3	2:B:711:HOH:O	2.05	0.57
1:B:230:HIS:HB3	1:B:236:VAL:HG22	1.85	0.57
1:B:436:ALA:HB3	2:B:839:HOH:O	2.04	0.57
1:B:505:HIS:O	1:B:508:ARG:HD3	2.04	0.57
1:C:230:HIS:HD2	2:C:722:HOH:O	1.86	0.57
1:D:254:LEU:HG	2:D:856:HOH:O	2.04	0.57
1:D:121:ILE:HG22	2:D:788:HOH:O	2.04	0.57
1:D:134:PRO:HD2	2:D:778:HOH:O	2.04	0.57
1:E:230:HIS:HB3	1:E:236:VAL:HG22	1.84	0.57
1:E:451:VAL:HG21	1:E:474:ILE:HG13	1.86	0.57
1:A:508:ARG:NH2	1:B:62:VAL:HG11	2.20	0.57
1:B:273:ALA:HB3	2:B:841:HOH:O	2.05	0.57
1:B:438:PRO:HD2	2:B:834:HOH:O	2.03	0.57
1:C:201:SER:HB3	2:C:786:HOH:O	2.05	0.57
1:B:174:SER:HB3	2:B:811:HOH:O	2.04	0.57
1:C:47:THR:OG1	1:C:50:GLU:HG3	2.04	0.57
1:E:89:THR:HB	1:E:124:VAL:CG2	2.34	0.57
1:A:64:LEU:HB3	2:C:829:HOH:O	2.04	0.57
1:D:498:MET:HE3	1:F:22:ARG:HD3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:LEU:HD12	2:E:600:HOH:O	2.04	0.57
1:E:474:ILE:O	1:E:478:GLU:HG2	2.04	0.57
1:A:10:ASP:OD1	1:A:11:ILE:N	2.37	0.57
1:B:147:GLN:NE2	1:B:147:GLN:N	2.45	0.57
1:C:113:LEU:HD22	1:C:117:TYR:CD1	2.40	0.57
1:E:231:ASN:HD21	1:E:239:HIS:C	2.13	0.57
1:B:113:LEU:HD13	1:B:114:GLY:N	2.20	0.57
1:E:472:ARG:O	1:E:476:GLU:HG3	2.05	0.57
1:F:175:LEU:HD22	1:F:177:VAL:HG13	1.86	0.57
1:A:62:VAL:HG11	1:C:508:ARG:NH2	2.20	0.56
1:A:173:ILE:HD11	2:A:669:HOH:O	2.03	0.56
1:E:62:VAL:HG21	1:F:508:ARG:CG	2.29	0.56
1:F:175:LEU:CD2	1:F:177:VAL:HG13	2.35	0.56
1:F:262:ASN:HA	2:F:828:HOH:O	2.04	0.56
1:C:35:ARG:O	1:C:39:LYS:HG3	2.05	0.56
1:D:173:ILE:HA	2:D:835:HOH:O	2.05	0.56
2:D:803:HOH:O	1:F:21:LEU:HA	2.04	0.56
1:E:523:LYS:HD3	2:E:797:HOH:O	2.05	0.56
1:F:173:ILE:HG21	1:F:251:VAL:HG23	1.87	0.56
1:A:161:ARG:NH2	1:D:430:GLY:HA2	2.21	0.56
1:A:424:MET:HE3	2:A:691:HOH:O	2.04	0.56
1:B:467:GLU:HB3	2:B:656:HOH:O	2.05	0.56
1:C:505:HIS:C	1:C:508:ARG:HH11	2.14	0.56
1:D:456:ARG:O	1:D:459:ILE:HG22	2.04	0.56
1:E:85:ASP:HB3	2:E:785:HOH:O	2.04	0.56
1:F:230:HIS:HB3	1:F:236:VAL:HG22	1.87	0.56
1:F:374:VAL:HG22	1:F:424:MET:HB3	1.86	0.56
1:F:397:LEU:HD13	1:F:423:VAL:CG1	2.34	0.56
1:C:55:LEU:HA	2:C:775:HOH:O	2.06	0.56
1:E:217:GLU:HB3	2:E:659:HOH:O	2.04	0.56
1:E:482:LEU:HD11	2:E:804:HOH:O	2.04	0.56
1:A:190:ILE:HG12	2:D:857:HOH:O	2.05	0.56
1:C:190:ILE:CD1	1:F:398:ILE:HD11	2.35	0.56
1:E:315:GLN:N	1:E:316:PRO:HD3	2.20	0.56
1:A:219:VAL:HG23	1:A:223:GLU:OE1	2.05	0.56
1:A:350:ILE:HG12	2:A:625:HOH:O	2.05	0.56
1:C:23:ARG:O	1:C:27:GLU:HG3	2.04	0.56
1:E:315:GLN:HB2	1:E:355:LYS:HE3	1.87	0.56
1:F:433:LEU:HD21	1:F:508:ARG:NH1	2.20	0.56
1:C:438:PRO:HG3	2:C:811:HOH:O	2.05	0.56
1:A:45:LYS:HG2	1:A:200:THR:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:LEU:HD13	1:A:423:VAL:HG12	1.87	0.56
1:B:10:ASP:OD1	1:B:11:ILE:N	2.39	0.56
1:B:361:ARG:HD2	1:B:403:GLU:OE2	2.06	0.56
1:D:508:ARG:CG	1:F:62:VAL:HG21	2.35	0.56
1:E:62:VAL:HG11	1:F:508:ARG:HH21	1.71	0.56
1:E:414:ARG:O	1:E:441:GLN:N	2.38	0.55
1:A:505:HIS:C	1:A:508:ARG:HH11	2.14	0.55
1:E:208:PRO:HA	1:E:211:ILE:HD11	1.88	0.55
1:D:62:VAL:CG2	1:E:508:ARG:HG3	2.29	0.55
1:E:485:TYR:O	1:E:489:GLU:HG3	2.07	0.55
1:A:17:LYS:HE2	2:C:730:HOH:O	2.06	0.55
1:B:56:LEU:HD12	1:B:61:PHE:HB2	1.88	0.55
1:E:131:THR:HG21	2:F:707:HOH:O	2.05	0.55
1:F:398:ILE:HG22	1:F:423:VAL:HG22	1.88	0.55
1:A:211:ILE:HG13	1:A:212:LYS:N	2.20	0.55
1:D:102:PHE:HB3	2:D:801:HOH:O	2.05	0.55
1:E:113:LEU:HD13	1:E:113:LEU:C	2.32	0.55
1:B:489:GLU:HG2	1:C:69:ARG:HG3	1.88	0.55
1:C:211:ILE:HD13	1:C:212:LYS:N	2.22	0.55
1:F:248:VAL:O	1:F:251:VAL:HG12	2.06	0.55
2:A:782:HOH:O	1:B:123:LYS:NZ	2.38	0.55
1:B:332:ARG:HD3	1:B:514:ARG:NH2	2.22	0.55
1:D:483:ASN:HD22	1:D:485:TYR:N	1.97	0.55
1:A:332:ARG:HH22	1:A:510:LEU:HB3	1.72	0.55
1:B:70:HIS:HE1	1:B:80:ASN:O	1.90	0.55
1:B:148:GLU:HB2	2:B:669:HOH:O	2.06	0.55
1:C:117:TYR:HB3	2:C:843:HOH:O	2.05	0.55
1:E:69:ARG:HD3	1:E:83:TYR:CD2	2.42	0.55
1:D:208:PRO:HD2	2:D:836:HOH:O	2.07	0.55
1:C:333:PRO:HB2	2:C:839:HOH:O	2.07	0.55
1:A:232:SER:HB3	1:A:317:LEU:HB3	1.89	0.54
1:B:231:ASN:HD21	1:B:239:HIS:N	2.04	0.54
1:B:412:ILE:HG23	2:B:732:HOH:O	2.07	0.54
1:B:433:LEU:HD21	1:B:508:ARG:HH12	1.71	0.54
1:B:530:LEU:HG	1:E:396:LYS:HD3	1.89	0.54
1:B:505:HIS:C	1:B:508:ARG:HH11	2.15	0.54
1:D:101:VAL:HG13	2:D:837:HOH:O	2.07	0.54
1:E:262:ASN:OD1	1:E:263:LEU:HD22	2.07	0.54
1:A:512:GLN:HG3	1:B:91:TYR:CE1	2.42	0.54
1:B:414:ARG:O	1:B:441:GLN:N	2.39	0.54
1:C:483:ASN:ND2	1:C:485:TYR:H	2.01	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:HIS:HA	1:E:116:VAL:HG21	1.90	0.54
1:B:81:ARG:HD3	2:B:632:HOH:O	2.06	0.54
1:B:451:VAL:HG21	1:B:474:ILE:CG1	2.38	0.54
1:E:231:ASN:HD21	1:E:239:HIS:N	2.06	0.54
1:A:459:ILE:HD12	1:A:470:ARG:HB3	1.88	0.54
1:D:441:GLN:HG3	2:D:851:HOH:O	2.07	0.54
1:F:24:ARG:HG2	2:F:835:HOH:O	2.05	0.54
1:C:69:ARG:HD3	1:C:81:ARG:O	2.07	0.54
1:A:340:GLN:CD	1:A:342:MET:HB2	2.33	0.54
1:C:121:ILE:O	1:C:124:VAL:HG12	2.08	0.54
1:E:173:ILE:HD12	1:E:173:ILE:N	2.23	0.54
1:A:332:ARG:NE	1:A:514:ARG:HE	2.06	0.54
1:C:361:ARG:HD2	1:C:403:GLU:OE2	2.08	0.54
1:C:398:ILE:HD12	1:C:398:ILE:O	2.07	0.54
1:C:483:ASN:HB2	1:C:484:PRO:HD2	1.88	0.54
1:F:254:LEU:CD1	1:F:312:PHE:HE2	2.20	0.54
1:B:89:THR:HB	1:B:124:VAL:HG21	1.89	0.54
1:B:451:VAL:HG21	1:B:474:ILE:HG12	1.89	0.54
1:B:508:ARG:NE	1:C:62:VAL:HG11	2.24	0.53
1:D:277:VAL:HG22	2:D:780:HOH:O	2.08	0.53
1:B:39:LYS:O	1:B:43:LYS:HG3	2.08	0.53
1:B:261:ASN:OD1	1:B:263:LEU:HB2	2.08	0.53
1:B:475:GLN:HE22	1:B:476:GLU:HG3	1.74	0.53
1:D:45:LYS:CD	1:D:200:THR:HG23	2.37	0.53
1:F:472:ARG:O	1:F:476:GLU:HG3	2.08	0.53
1:A:259:PRO:HD3	2:A:815:HOH:O	2.07	0.53
1:D:25:ILE:O	1:D:29:THR:HG23	2.08	0.53
1:D:46:LEU:HD13	1:D:244:GLU:OE2	2.07	0.53
1:E:254:LEU:HD13	1:E:312:PHE:HE2	1.74	0.53
1:E:505:HIS:O	1:E:508:ARG:HD3	2.08	0.53
1:F:147:GLN:HE21	1:F:147:GLN:N	2.00	0.53
1:A:21:LEU:HD22	1:C:438:PRO:HG3	1.90	0.53
1:B:25:ILE:HG22	1:B:67:PHE:HZ	1.73	0.53
1:B:89:THR:HB	1:B:124:VAL:CG2	2.39	0.53
1:E:120:LYS:HD2	2:E:735:HOH:O	2.07	0.53
1:F:70:HIS:HE1	1:F:80:ASN:O	1.91	0.53
1:A:21:LEU:HB2	2:C:811:HOH:O	2.08	0.53
1:C:97:ARG:HB2	2:C:721:HOH:O	2.09	0.53
1:C:315:GLN:N	1:C:316:PRO:HD3	2.23	0.53
1:E:316:PRO:HD2	2:E:699:HOH:O	2.09	0.53
1:D:414:ARG:O	1:D:441:GLN:N	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:VAL:HG12	2:E:785:HOH:O	2.07	0.53
1:B:134:PRO:HD2	2:B:833:HOH:O	2.08	0.53
1:D:398:ILE:C	1:D:398:ILE:HD12	2.34	0.53
1:D:70:HIS:HA	1:D:116:VAL:HG21	1.91	0.53
1:D:398:ILE:HG22	1:D:423:VAL:HG22	1.91	0.53
1:D:427:LYS:HA	1:D:431:ALA:HB3	1.90	0.53
1:E:433:LEU:HD21	1:E:508:ARG:CZ	2.39	0.53
1:E:505:HIS:C	1:E:508:ARG:HH11	2.16	0.53
1:A:372:THR:OG1	1:A:410:THR:HG23	2.09	0.52
1:A:414:ARG:O	1:A:441:GLN:N	2.42	0.52
1:C:373:PHE:HE1	2:C:856:HOH:O	1.92	0.52
1:D:212:LYS:HD2	2:D:795:HOH:O	2.09	0.52
1:E:62:VAL:HG11	1:F:508:ARG:NE	2.23	0.52
1:E:372:THR:HG23	2:E:545:HOH:O	2.08	0.52
1:A:62:VAL:HG11	1:C:508:ARG:NE	2.22	0.52
1:A:113:LEU:C	1:A:113:LEU:HD13	2.34	0.52
1:B:114:GLY:HA2	2:B:669:HOH:O	2.09	0.52
1:B:161:ARG:HG3	2:E:758:HOH:O	2.07	0.52
1:B:508:ARG:CG	1:C:62:VAL:HG21	2.34	0.52
1:C:324:THR:HA	1:C:336:ILE:O	2.10	0.52
1:D:377:PRO:HD3	2:D:806:HOH:O	2.09	0.52
2:D:641:HOH:O	1:F:65:ASP:HA	2.10	0.52
1:E:70:HIS:N	2:E:777:HOH:O	2.41	0.52
1:E:139:ASN:HB3	2:E:702:HOH:O	2.09	0.52
1:C:414:ARG:O	1:C:441:GLN:N	2.41	0.52
1:D:456:ARG:HH11	1:D:457:ARG:HH12	1.57	0.52
1:E:166:ALA:HB1	2:E:691:HOH:O	2.09	0.52
1:A:207:GLY:O	1:A:211:ILE:HG23	2.10	0.52
1:B:113:LEU:HD13	1:B:113:LEU:C	2.34	0.52
1:B:464:ASP:O	1:B:465:ASP:HB2	2.08	0.52
1:F:485:TYR:O	1:F:489:GLU:HG3	2.10	0.52
1:B:134:PRO:N	2:B:833:HOH:O	2.42	0.52
1:E:263:LEU:HD22	1:E:263:LEU:N	2.24	0.52
1:E:299:HIS:HE1	1:E:313:GLU:OE2	1.93	0.52
1:C:433:LEU:HD21	1:C:508:ARG:CZ	2.39	0.52
1:F:414:ARG:O	1:F:441:GLN:N	2.40	0.52
1:C:230:HIS:HA	1:C:234:SER:OG	2.10	0.52
1:A:438:PRO:HD3	1:A:497:ILE:O	2.08	0.52
1:E:457:ARG:HD2	1:E:457:ARG:N	2.24	0.52
1:F:197:VAL:HG22	2:F:829:HOH:O	2.09	0.52
1:F:470:ARG:O	1:F:474:ILE:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:363:CYS:HA	2:F:753:HOH:O	2.09	0.52
1:A:62:VAL:HG21	1:C:508:ARG:CG	2.37	0.52
1:B:505:HIS:HA	1:B:508:ARG:HD2	1.91	0.52
2:B:792:HOH:O	1:E:444:VAL:HG21	2.09	0.52
1:D:505:HIS:C	1:D:508:ARG:HH11	2.16	0.52
1:D:508:ARG:CZ	1:F:62:VAL:HG11	2.40	0.52
1:A:455:HIS:O	1:A:459:ILE:HG12	2.10	0.51
1:D:124:VAL:HB	2:D:801:HOH:O	2.09	0.51
1:F:498:MET:HE2	2:F:729:HOH:O	2.09	0.51
1:B:168:GLY:HA3	2:E:797:HOH:O	2.09	0.51
1:C:343:GLN:N	2:C:810:HOH:O	2.43	0.51
1:A:391:ILE:C	2:A:843:HOH:O	2.53	0.51
1:C:336:ILE:HD12	2:C:856:HOH:O	2.10	0.51
1:A:211:ILE:CD1	1:A:217:GLU:HB2	2.40	0.51
1:B:39:LYS:HB3	1:B:39:LYS:HZ3	1.74	0.51
1:B:139:ASN:HB3	2:B:554:HOH:O	2.10	0.51
1:C:158:GLU:O	1:C:162:ARG:HG2	2.09	0.51
1:E:498:MET:HE2	2:E:708:HOH:O	2.09	0.51
1:E:505:HIS:ND1	1:E:508:ARG:CZ	2.74	0.51
1:A:262:ASN:OD1	1:A:263:LEU:HD13	2.11	0.51
1:A:472:ARG:O	1:A:476:GLU:HG3	2.10	0.51
1:C:25:ILE:HD13	1:C:67:PHE:CZ	2.46	0.51
1:E:62:VAL:CG2	1:F:508:ARG:HG3	2.33	0.51
1:A:457:ARG:HB2	2:A:675:HOH:O	2.09	0.51
1:C:261:ASN:OD1	1:C:263:LEU:HB2	2.10	0.51
1:E:70:HIS:HE1	1:E:80:ASN:O	1.94	0.51
1:E:175:LEU:HD23	1:E:195:VAL:HG13	1.92	0.51
1:F:259:PRO:HG3	2:F:828:HOH:O	2.11	0.51
1:D:235:GLY:HA2	2:D:783:HOH:O	2.11	0.51
1:F:238:HIS:HA	1:F:315:GLN:HG2	1.93	0.51
1:B:398:ILE:C	1:B:398:ILE:HD12	2.36	0.51
1:C:129:LEU:HD23	2:C:862:HOH:O	2.10	0.51
1:A:447:ALA:O	1:A:451:VAL:HG22	2.11	0.51
1:E:68:ALA:HA	1:F:489:GLU:HA	1.93	0.51
1:E:147:GLN:HE21	1:E:147:GLN:N	2.03	0.51
1:B:336:ILE:HD12	1:B:336:ILE:N	2.25	0.50
1:C:238:HIS:HA	1:C:315:GLN:HG2	1.92	0.50
1:A:230:HIS:HB3	1:A:236:VAL:HG22	1.91	0.50
1:B:26:GLU:O	1:B:30:HIS:HD2	1.94	0.50
1:E:475:GLN:HA	1:E:478:GLU:OE1	2.10	0.50
1:A:271:GLU:O	1:A:271:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:337:VAL:O	1:E:372:THR:HA	2.11	0.50
1:F:332:ARG:HD3	1:F:514:ARG:NH2	2.26	0.50
1:B:35:ARG:O	1:B:39:LYS:HG3	2.11	0.50
2:C:714:HOH:O	1:F:392:ARG:HG2	2.11	0.50
1:C:203:MET:N	2:C:722:HOH:O	2.45	0.50
1:C:470:ARG:O	1:C:474:ILE:HG13	2.11	0.50
1:E:505:HIS:HB3	1:E:508:ARG:NH1	2.27	0.50
1:C:101:VAL:HG22	1:C:102:PHE:N	2.27	0.50
1:D:176:VAL:HG22	2:D:855:HOH:O	2.11	0.50
1:E:231:ASN:HD21	1:E:239:HIS:CA	2.24	0.50
1:F:505:HIS:O	1:F:508:ARG:HD3	2.12	0.50
1:E:481:LEU:N	1:E:481:LEU:HD22	2.27	0.50
1:A:160:PHE:HB3	1:D:398:ILE:CD1	2.40	0.50
1:B:414:ARG:HG2	2:B:823:HOH:O	2.12	0.50
1:C:100:ALA:HB1	1:C:124:VAL:HG22	1.94	0.50
1:C:438:PRO:HD3	1:C:497:ILE:O	2.12	0.50
1:F:211:ILE:HD11	2:F:531:HOH:O	2.12	0.50
1:F:451:VAL:HG21	1:F:474:ILE:CG1	2.39	0.50
1:A:255:LEU:HA	2:A:669:HOH:O	2.12	0.49
1:A:398:ILE:C	1:A:398:ILE:HD12	2.37	0.49
1:F:106:PHE:HB3	2:F:815:HOH:O	2.12	0.49
1:F:336:ILE:HD12	1:F:336:ILE:N	2.27	0.49
1:A:180:CYS:HB3	1:A:203:MET:HG2	1.94	0.49
1:A:224:LEU:HD11	1:D:386:GLU:HG3	1.93	0.49
1:C:70:HIS:HA	1:C:116:VAL:HG21	1.93	0.49
1:C:113:LEU:HG	1:C:156:TYR:CE1	2.47	0.49
1:C:345:ALA:N	2:C:810:HOH:O	2.45	0.49
1:D:119:GLN:HG3	2:D:729:HOH:O	2.10	0.49
1:D:191:THR:HB	2:D:835:HOH:O	2.11	0.49
1:E:169:VAL:HA	1:E:262:ASN:ND2	2.26	0.49
1:B:481:LEU:HD22	1:B:481:LEU:N	2.27	0.49
1:C:266:PRO:HG2	2:C:543:HOH:O	2.12	0.49
1:D:180:CYS:HB3	1:D:203:MET:HG2	1.93	0.49
1:E:93:THR:HG23	2:E:771:HOH:O	2.11	0.49
1:F:241:ALA:HB3	2:F:829:HOH:O	2.12	0.49
1:F:397:LEU:HD13	1:F:423:VAL:HG12	1.94	0.49
1:A:62:VAL:CG1	1:C:508:ARG:HH21	2.24	0.49
1:B:231:ASN:HD21	1:B:239:HIS:C	2.20	0.49
1:B:289:PRO:HD2	2:B:743:HOH:O	2.11	0.49
1:D:505:HIS:O	1:D:508:ARG:HD3	2.12	0.49
1:B:113:LEU:HD22	1:B:117:TYR:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:VAL:HA	1:D:262:ASN:ND2	2.28	0.49
1:F:24:ARG:HA	2:F:835:HOH:O	2.11	0.49
1:F:302:ILE:O	1:F:305:VAL:HG22	2.12	0.49
1:A:99:VAL:HB	2:A:830:HOH:O	2.12	0.49
1:A:147:GLN:HB2	2:A:712:HOH:O	2.11	0.49
1:B:11:ILE:HG23	1:B:12:HIS:ND1	2.28	0.49
1:D:318:PHE:O	1:D:319:ALA:C	2.56	0.49
1:F:100:ALA:HB1	1:F:124:VAL:HG22	1.94	0.49
1:A:398:ILE:HG22	1:A:423:VAL:HG22	1.94	0.49
1:C:332:ARG:HD3	1:C:514:ARG:HH21	1.78	0.49
1:F:335:GLY:C	1:F:336:ILE:HD12	2.37	0.49
1:A:231:ASN:HD21	1:A:239:HIS:CA	2.25	0.49
1:F:505:HIS:HA	1:F:508:ARG:HD2	1.95	0.49
1:A:238:HIS:HA	1:A:315:GLN:HG2	1.95	0.49
1:A:481:LEU:N	1:A:481:LEU:HD22	2.28	0.49
1:D:145:ARG:HG2	2:D:786:HOH:O	2.13	0.49
1:E:113:LEU:C	1:E:113:LEU:CD1	2.86	0.49
1:F:69:ARG:HD2	1:F:81:ARG:O	2.12	0.49
1:C:236:VAL:HG12	2:C:714:HOH:O	2.12	0.49
1:D:212:LYS:C	1:D:214:VAL:H	2.21	0.49
1:D:456:ARG:NH1	1:D:457:ARG:HH12	2.11	0.49
1:E:101:VAL:HG23	1:E:136:VAL:O	2.13	0.49
1:E:186:TYR:O	1:E:190:ILE:HG12	2.13	0.49
1:A:231:ASN:HD21	1:A:239:HIS:N	2.11	0.48
1:A:498:MET:HE2	2:B:810:HOH:O	2.13	0.48
1:B:231:ASN:HD21	1:B:239:HIS:CA	2.26	0.48
1:D:464:ASP:O	1:D:465:ASP:HB2	2.12	0.48
1:E:451:VAL:HB	2:E:703:HOH:O	2.12	0.48
1:E:483:ASN:HB2	1:E:484:PRO:HD2	1.94	0.48
1:A:169:VAL:CG2	1:D:523:LYS:HE2	2.43	0.48
1:A:299:HIS:HE1	1:A:313:GLU:OE2	1.95	0.48
1:B:101:VAL:HG22	1:B:102:PHE:N	2.28	0.48
1:B:162:ARG:HG2	1:B:162:ARG:HH11	1.78	0.48
1:C:490:ARG:HG3	2:C:824:HOH:O	2.12	0.48
1:D:508:ARG:HH21	1:F:62:VAL:CG1	2.24	0.48
1:A:219:VAL:HG12	2:A:576:HOH:O	2.12	0.48
1:B:113:LEU:C	1:B:113:LEU:CD1	2.86	0.48
1:F:107:THR:HG23	2:F:815:HOH:O	2.12	0.48
1:F:306:LEU:HD13	1:F:327:GLY:HA3	1.95	0.48
1:A:211:ILE:HD12	1:A:217:GLU:HB2	1.94	0.48
1:B:433:LEU:HD21	1:B:508:ARG:CZ	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:434:ASN:HB3	2:C:825:HOH:O	2.13	0.48
1:C:527:ASN:HD21	1:F:358:ARG:HD3	1.78	0.48
1:E:70:HIS:CE1	1:E:77:LEU:HD22	2.47	0.48
1:A:483:ASN:HB2	1:A:484:PRO:CD	2.43	0.48
1:B:190:ILE:HD11	1:E:398:ILE:HD11	1.94	0.48
1:D:158:GLU:O	1:D:162:ARG:HG2	2.13	0.48
1:D:501:ASP:CB	2:D:779:HOH:O	2.59	0.48
1:C:180:CYS:HB3	1:C:203:MET:HG2	1.96	0.48
1:F:114:GLY:HA2	2:F:685:HOH:O	2.13	0.48
1:F:454:LEU:HG	2:F:775:HOH:O	2.13	0.48
1:A:73:THR:C	2:A:723:HOH:O	2.57	0.48
1:A:336:ILE:HD12	1:A:336:ILE:N	2.29	0.48
1:A:340:GLN:OE1	1:A:342:MET:HB2	2.14	0.48
1:A:396:LYS:HD3	1:D:530:LEU:HG	1.96	0.48
1:B:176:VAL:HG12	1:B:201:SER:HB2	1.95	0.48
1:C:259:PRO:HG3	2:C:850:HOH:O	2.13	0.48
1:C:503:ARG:NH1	2:C:771:HOH:O	2.47	0.48
1:D:54:LEU:HD13	2:D:608:HOH:O	2.13	0.48
1:E:317:LEU:HD13	2:E:748:HOH:O	2.13	0.48
1:A:372:THR:HG21	1:A:401:TYR:OH	2.14	0.48
1:B:508:ARG:CZ	1:C:62:VAL:HG11	2.43	0.48
1:D:414:ARG:C	2:D:851:HOH:O	2.44	0.48
1:D:496:VAL:HG22	2:D:834:HOH:O	2.14	0.48
1:B:146:ILE:HA	2:B:792:HOH:O	2.14	0.48
1:C:299:HIS:HE1	1:C:313:GLU:OE2	1.97	0.48
1:C:337:VAL:O	1:C:372:THR:HA	2.13	0.48
1:C:397:LEU:HD13	1:C:423:VAL:HG12	1.96	0.48
1:D:47:THR:OG1	1:D:50:GLU:HG3	2.13	0.48
1:D:411:VAL:C	2:D:814:HOH:O	2.57	0.48
1:E:438:PRO:HD3	1:E:497:ILE:O	2.14	0.48
1:B:508:ARG:NH2	1:C:62:VAL:HG11	2.29	0.47
1:C:70:HIS:CD2	1:C:72:SER:H	2.11	0.47
1:D:483:ASN:HB2	1:D:484:PRO:CD	2.44	0.47
1:E:230:HIS:HA	1:E:234:SER:OG	2.14	0.47
1:B:459:ILE:HD11	1:B:470:ARG:HB2	1.96	0.47
1:B:496:VAL:HG22	2:B:839:HOH:O	2.14	0.47
1:E:209:ASP:O	1:E:213:THR:HG23	2.14	0.47
1:A:56:LEU:HD13	1:A:92:GLY:HA3	1.96	0.47
1:A:89:THR:HB	1:A:124:VAL:HG21	1.95	0.47
1:D:321:ASN:ND2	1:D:352:ALA:HB2	2.29	0.47
1:F:319:ALA:N	1:F:320:PRO:HD3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:ASP:O	1:C:465:ASP:HB3	2.14	0.47
1:D:40:GLN:CD	1:D:45:LYS:HE3	2.39	0.47
1:E:125:MET:HE1	1:E:163:ASN:ND2	2.28	0.47
1:D:58:GLU:HG3	2:D:745:HOH:O	2.14	0.47
1:D:398:ILE:HG13	1:D:399:PHE:N	2.28	0.47
1:E:238:HIS:HA	1:E:315:GLN:HG2	1.95	0.47
1:B:45:LYS:HG2	1:B:200:THR:CG2	2.45	0.47
1:B:230:HIS:HA	1:B:234:SER:OG	2.15	0.47
1:C:70:HIS:HE1	1:C:80:ASN:O	1.96	0.47
1:D:70:HIS:HE1	1:D:80:ASN:O	1.96	0.47
1:A:338:ALA:HB1	2:A:749:HOH:O	2.14	0.47
1:C:512:GLN:HE21	1:C:512:GLN:HB3	1.54	0.47
1:D:101:VAL:HG22	1:D:102:PHE:N	2.29	0.47
1:E:50:GLU:O	1:E:54:LEU:HD13	2.15	0.47
1:E:113:LEU:HD13	1:E:114:GLY:N	2.29	0.47
1:F:73:THR:C	2:F:724:HOH:O	2.58	0.47
1:F:209:ASP:O	1:F:213:THR:HG23	2.14	0.47
1:F:456:ARG:HB3	1:F:457:ARG:NH1	2.30	0.47
1:F:512:GLN:HB3	1:F:512:GLN:HE21	1.57	0.47
1:B:134:PRO:CD	2:B:833:HOH:O	2.63	0.47
1:B:302:ILE:O	1:B:305:VAL:HG22	2.15	0.47
1:C:346:GLY:N	2:C:810:HOH:O	2.46	0.47
1:F:516:LYS:HE2	1:F:518:GLU:HG3	1.97	0.47
1:B:372:THR:HG21	1:B:401:TYR:OH	2.15	0.47
1:C:341:PRO:C	2:C:810:HOH:O	2.57	0.47
1:F:70:HIS:CE1	1:F:81:ARG:HG2	2.50	0.47
1:B:296:TYR:CA	1:B:342:MET:HE3	2.45	0.47
1:B:522:PRO:HG2	2:B:793:HOH:O	2.15	0.47
1:A:391:ILE:O	2:A:843:HOH:O	2.19	0.46
1:A:393:ARG:HD3	2:A:625:HOH:O	2.14	0.46
1:B:505:HIS:CA	1:B:508:ARG:HH11	2.27	0.46
1:C:118:GLY:N	2:C:843:HOH:O	2.47	0.46
1:C:386:GLU:HG3	1:F:224:LEU:HD11	1.96	0.46
1:C:433:LEU:HD21	1:C:508:ARG:HH12	1.80	0.46
1:C:451:VAL:HG21	1:C:474:ILE:CG1	2.45	0.46
1:D:238:HIS:HA	1:D:315:GLN:HG2	1.97	0.46
1:D:422:ASP:O	1:D:429:LEU:HD22	2.15	0.46
1:E:187:SER:HB3	1:E:188:PRO:CD	2.34	0.46
1:A:89:THR:HB	1:A:124:VAL:CG2	2.46	0.46
1:A:77:LEU:HB3	2:A:723:HOH:O	2.14	0.46
1:A:146:ILE:HD12	1:D:453:ILE:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:GLU:HG3	1:E:224:LEU:HD11	1.97	0.46
1:E:69:ARG:HG3	1:F:489:GLU:HG2	1.96	0.46
1:A:508:ARG:HH21	1:B:62:VAL:CG1	2.27	0.46
1:B:358:ARG:HD3	1:E:527:ASN:HD21	1.80	0.46
1:B:435:LEU:N	1:B:435:LEU:HD22	2.31	0.46
1:C:208:PRO:O	1:C:211:ILE:HD13	2.15	0.46
1:D:139:ASN:HB3	2:D:720:HOH:O	2.15	0.46
1:D:191:THR:CB	2:D:835:HOH:O	2.63	0.46
1:D:299:HIS:HE1	1:D:313:GLU:OE2	1.97	0.46
1:E:35:ARG:NH1	1:E:39:LYS:NZ	2.64	0.46
1:F:101:VAL:HG22	1:F:102:PHE:N	2.30	0.46
1:F:508:ARG:HD3	1:F:509:GLY:H	1.75	0.46
1:E:68:ALA:C	1:E:69:ARG:HG2	2.41	0.46
1:A:10:ASP:N	2:A:823:HOH:O	2.47	0.46
1:B:507:VAL:HG11	2:B:841:HOH:O	2.16	0.46
1:C:302:ILE:O	1:C:305:VAL:HG22	2.15	0.46
1:D:261:ASN:OD1	1:D:263:LEU:HB2	2.16	0.46
1:E:62:VAL:HG11	1:F:508:ARG:NH2	2.31	0.46
1:E:69:ARG:HD2	1:E:81:ARG:O	2.15	0.46
1:E:101:VAL:HG22	1:E:102:PHE:N	2.31	0.46
1:E:466:ALA:O	1:E:469:THR:HB	2.16	0.46
1:F:219:VAL:CG2	1:F:223:GLU:HB3	2.45	0.46
1:A:166:ALA:HB1	2:A:760:HOH:O	2.16	0.46
1:D:62:VAL:HG11	1:E:508:ARG:HH21	1.81	0.46
1:D:134:PRO:CD	2:D:778:HOH:O	2.63	0.46
1:F:158:GLU:O	1:F:162:ARG:HG2	2.16	0.46
1:F:190:ILE:HD13	2:F:721:HOH:O	2.16	0.46
1:F:231:ASN:HD21	1:F:239:HIS:CA	2.29	0.46
1:A:358:ARG:HD3	1:D:527:ASN:HD21	1.81	0.46
1:C:457:ARG:HD2	1:C:457:ARG:H	1.80	0.46
1:F:10:ASP:HB2	2:F:834:HOH:O	2.16	0.46
1:F:483:ASN:HB2	1:F:484:PRO:CD	2.45	0.46
1:E:172:GLN:HG3	2:E:691:HOH:O	2.14	0.45
1:E:482:LEU:HD21	2:E:804:HOH:O	2.15	0.45
1:B:294:GLN:HA	1:B:295:PRO:HD3	1.83	0.45
1:C:173:ILE:HD12	1:C:173:ILE:N	2.31	0.45
1:D:438:PRO:HD3	1:D:497:ILE:O	2.17	0.45
2:A:845:HOH:O	1:B:131:THR:HG22	2.15	0.45
1:D:65:ASP:HA	2:E:604:HOH:O	2.16	0.45
1:E:375:ASP:CG	1:E:414:ARG:HB3	2.40	0.45
1:E:419:GLY:O	1:E:423:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:520:LEU:HB3	1:E:521:PRO:CD	2.46	0.45
1:F:275:LEU:HD21	1:F:507:VAL:HG11	1.98	0.45
1:A:453:ILE:HG23	1:A:456:ARG:HH22	1.80	0.45
1:A:468:ALA:HA	1:A:471:ALA:HB3	1.99	0.45
1:B:315:GLN:HB2	1:B:355:LYS:HE3	1.99	0.45
1:B:337:VAL:O	1:B:372:THR:HA	2.17	0.45
1:D:175:LEU:HD22	1:D:177:VAL:HG13	1.98	0.45
1:F:47:THR:OG1	1:F:50:GLU:HG3	2.16	0.45
1:F:468:ALA:O	1:F:472:ARG:N	2.48	0.45
1:A:68:ALA:HA	1:C:489:GLU:HA	1.98	0.45
1:C:398:ILE:HD11	1:F:160:PHE:HB3	1.98	0.45
1:D:530:LEU:HB2	2:D:725:HOH:O	2.16	0.45
1:F:113:LEU:C	1:F:113:LEU:HD13	2.41	0.45
1:F:148:GLU:HB2	2:F:685:HOH:O	2.17	0.45
1:B:489:GLU:HG3	2:C:728:HOH:O	2.17	0.45
1:C:144:ALA:HA	2:C:854:HOH:O	2.17	0.45
1:D:25:ILE:HG22	1:D:67:PHE:HZ	1.81	0.45
1:E:180:CYS:HB3	1:E:203:MET:HG2	1.98	0.45
1:C:343:GLN:C	2:C:810:HOH:O	2.60	0.45
1:E:303:GLU:O	1:E:309:ALA:HA	2.17	0.45
1:F:432:ASP:HB2	1:F:513:LEU:HD21	1.99	0.45
1:F:455:HIS:O	1:F:459:ILE:HG22	2.17	0.45
1:D:176:VAL:HG12	1:D:201:SER:HB2	1.97	0.45
1:E:483:ASN:ND2	2:E:654:HOH:O	2.44	0.45
1:C:245:LYS:HB2	1:C:245:LYS:NZ	2.31	0.45
1:C:358:ARG:HD3	1:F:527:ASN:HD21	1.82	0.45
1:D:483:ASN:ND2	1:D:485:TYR:H	2.00	0.45
1:A:21:LEU:O	1:A:25:ILE:HG13	2.16	0.44
1:A:398:ILE:HD11	1:D:190:ILE:CD1	2.47	0.44
1:B:398:ILE:CD1	1:E:160:PHE:HB3	2.42	0.44
1:C:146:ILE:HG21	2:F:775:HOH:O	2.17	0.44
1:C:440:ALA:HB3	1:C:484:PRO:HB3	1.98	0.44
1:D:134:PRO:N	2:D:778:HOH:O	2.50	0.44
1:D:321:ASN:HD21	1:D:352:ALA:HB2	1.81	0.44
1:E:415:LYS:HD2	2:E:620:HOH:O	2.17	0.44
1:A:508:ARG:HG3	1:B:62:VAL:CG2	2.38	0.44
1:A:254:LEU:CD1	1:A:312:PHE:HE2	2.31	0.44
1:C:339:ASN:ND2	2:C:724:HOH:O	2.50	0.44
1:E:10:ASP:N	2:E:634:HOH:O	2.49	0.44
1:E:18:LEU:HD13	1:F:498:MET:HE1	1.98	0.44
1:E:26:GLU:O	1:E:30:HIS:HD2	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:402:ALA:HA	1:E:429:LEU:O	2.17	0.44
1:E:464:ASP:O	1:E:465:ASP:HB3	2.16	0.44
1:F:162:ARG:HG2	1:F:162:ARG:HH11	1.83	0.44
1:F:475:GLN:NE2	2:F:652:HOH:O	2.50	0.44
1:B:318:PHE:O	1:B:319:ALA:C	2.60	0.44
1:B:433:LEU:HD21	1:B:508:ARG:NH2	2.32	0.44
1:B:483:ASN:HD22	1:B:485:TYR:H	1.65	0.44
1:D:11:ILE:N	2:D:581:HOH:O	2.50	0.44
1:D:43:LYS:HB2	2:D:824:HOH:O	2.18	0.44
1:D:46:LEU:N	1:D:46:LEU:HD12	2.32	0.44
1:E:494:ASP:HB2	2:E:773:HOH:O	2.17	0.44
1:F:434:ASN:HB3	2:F:747:HOH:O	2.17	0.44
1:A:505:HIS:O	1:A:508:ARG:CD	2.66	0.44
1:A:516:LYS:N	2:A:845:HOH:O	2.49	0.44
1:B:161:ARG:NE	2:E:758:HOH:O	2.50	0.44
1:C:336:ILE:CD1	2:C:856:HOH:O	2.66	0.44
1:D:70:HIS:CE1	1:D:81:ARG:HG2	2.53	0.44
1:E:483:ASN:ND2	1:E:485:TYR:H	1.99	0.44
1:C:483:ASN:ND2	2:C:831:HOH:O	2.49	0.44
1:D:21:LEU:O	1:D:25:ILE:HG23	2.17	0.44
1:A:464:ASP:O	1:A:465:ASP:HB3	2.17	0.44
1:A:512:GLN:NE2	2:A:715:HOH:O	2.50	0.44
1:B:474:ILE:O	1:B:478:GLU:HG2	2.17	0.44
2:B:549:HOH:O	1:E:386:GLU:HG2	2.18	0.44
1:C:77:LEU:C	1:C:79:ALA:H	2.26	0.44
1:D:489:GLU:HA	1:F:68:ALA:HA	2.00	0.44
1:E:70:HIS:HD2	1:E:72:SER:N	2.12	0.44
1:E:480:ALA:HB3	1:E:481:LEU:HD22	1.98	0.44
1:F:211:ILE:C	1:F:211:ILE:HD12	2.43	0.44
1:A:235:GLY:HA2	2:A:642:HOH:O	2.17	0.44
1:B:145:ARG:HD2	1:B:148:GLU:OE2	2.18	0.44
1:C:212:LYS:C	1:C:214:VAL:H	2.26	0.44
1:B:422:ASP:O	1:B:429:LEU:HD22	2.17	0.44
1:C:210:VAL:HA	1:C:213:THR:HG22	1.99	0.44
1:D:230:HIS:HA	1:D:234:SER:OG	2.18	0.44
1:D:232:SER:HB3	1:D:317:LEU:HB3	1.99	0.44
1:E:56:LEU:HD12	1:E:61:PHE:HB2	2.00	0.44
1:E:332:ARG:HD3	1:E:514:ARG:CZ	2.48	0.44
1:F:208:PRO:O	1:F:211:ILE:HG13	2.17	0.44
1:B:227:ALA:HB1	1:B:240:MET:HG3	2.00	0.43
1:F:29:THR:HG21	2:F:795:HOH:O	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:VAL:HG22	2:B:741:HOH:O	2.16	0.43
1:C:87:VAL:O	1:C:120:LYS:NZ	2.50	0.43
1:D:507:VAL:O	1:D:511:ARG:HG3	2.18	0.43
1:F:248:VAL:O	1:F:251:VAL:CG1	2.66	0.43
1:F:427:LYS:HA	1:F:431:ALA:HB3	2.00	0.43
1:C:438:PRO:HD3	2:C:806:HOH:O	2.19	0.43
1:E:35:ARG:NH1	1:E:39:LYS:HZ1	2.16	0.43
1:E:60:SER:HB2	2:E:771:HOH:O	2.18	0.43
1:E:467:GLU:O	1:E:468:ALA:HB3	2.18	0.43
1:A:319:ALA:N	1:A:320:PRO:HD3	2.32	0.43
1:E:332:ARG:HD2	2:E:629:HOH:O	2.19	0.43
1:F:452:ASN:ND2	1:F:470:ARG:HH11	2.16	0.43
1:B:200:THR:HG22	1:B:200:THR:O	2.17	0.43
1:C:103:SER:HA	1:C:138:ILE:HB	2.00	0.43
1:C:231:ASN:HD21	1:C:239:HIS:CA	2.32	0.43
1:C:483:ASN:HD22	1:C:485:TYR:N	2.04	0.43
1:C:483:ASN:HB2	1:C:484:PRO:CD	2.49	0.43
1:E:486:THR:O	1:E:490:ARG:HG2	2.18	0.43
1:A:302:ILE:O	1:A:305:VAL:HG22	2.19	0.43
1:A:350:ILE:HG13	1:A:385:GLN:OE1	2.19	0.43
1:A:375:ASP:CG	1:A:414:ARG:HB3	2.44	0.43
1:C:45:LYS:HG2	1:C:200:THR:HG23	1.99	0.43
1:D:495:ALA:HB2	2:D:554:HOH:O	2.19	0.43
1:E:113:LEU:HD22	1:E:117:TYR:CE1	2.53	0.43
1:F:29:THR:O	1:F:29:THR:HG22	2.17	0.43
1:A:144:ALA:HB1	1:A:152:SER:OG	2.19	0.43
1:A:442:ILE:HD12	1:A:484:PRO:HA	2.00	0.43
1:C:454:LEU:HD11	2:C:801:HOH:O	2.18	0.43
1:F:254:LEU:HD13	1:F:312:PHE:CE2	2.41	0.43
1:A:69:ARG:HD3	1:A:83:TYR:CD2	2.53	0.43
1:A:146:ILE:H	1:A:146:ILE:HG13	1.62	0.43
1:C:75:PHE:CZ	1:F:454:LEU:HD13	2.54	0.43
1:D:456:ARG:NH1	1:D:457:ARG:NH1	2.64	0.43
1:D:473:LEU:HA	2:D:655:HOH:O	2.18	0.43
1:F:70:HIS:CD2	1:F:72:SER:H	2.19	0.43
1:F:112:ALA:HA	1:F:143:GLY:O	2.19	0.43
1:A:398:ILE:CG1	1:D:190:ILE:HD11	2.48	0.43
1:B:361:ARG:NH2	1:E:528:ILE:HG22	2.33	0.43
1:C:294:GLN:HA	1:C:295:PRO:HD3	1.82	0.43
1:D:374:VAL:HG23	2:D:814:HOH:O	2.19	0.43
1:D:472:ARG:NH1	2:D:655:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:414:ARG:O	1:E:440:ALA:HA	2.19	0.43
1:E:512:GLN:HE21	1:E:512:GLN:HB3	1.56	0.43
1:F:299:HIS:HE1	1:F:313:GLU:OE2	2.01	0.43
1:A:172:GLN:HG3	2:A:760:HOH:O	2.18	0.42
1:A:266:PRO:HG2	2:A:593:HOH:O	2.19	0.42
1:B:209:ASP:HB2	2:B:803:HOH:O	2.19	0.42
1:D:101:VAL:CG2	1:D:102:PHE:N	2.81	0.42
1:E:147:GLN:NE2	1:E:147:GLN:N	2.57	0.42
1:E:453:ILE:HG23	1:E:456:ARG:HH22	1.84	0.42
1:A:508:ARG:CZ	1:B:62:VAL:HG11	2.49	0.42
1:B:512:GLN:HE21	1:B:512:GLN:HB3	1.66	0.42
1:C:21:LEU:O	1:C:25:ILE:HG12	2.18	0.42
1:C:231:ASN:HD21	1:C:239:HIS:N	2.17	0.42
1:C:407:PRO:HB3	1:C:513:LEU:HB3	2.01	0.42
1:C:508:ARG:HD3	1:C:509:GLY:H	1.80	0.42
1:D:16:GLY:HA3	2:D:581:HOH:O	2.18	0.42
1:D:212:LYS:NZ	2:D:598:HOH:O	2.52	0.42
1:D:483:ASN:ND2	1:D:485:TYR:HB2	2.34	0.42
1:E:141:SER:O	1:E:179:PRO:HB2	2.19	0.42
1:A:372:THR:HB	2:A:763:HOH:O	2.19	0.42
1:F:370:VAL:HG22	2:F:675:HOH:O	2.18	0.42
1:A:347:CYS:SG	1:A:377:PRO:HG2	2.59	0.42
1:B:508:ARG:HG3	1:C:62:VAL:CG2	2.41	0.42
1:C:429:LEU:HG	2:F:730:HOH:O	2.18	0.42
1:D:69:ARG:HH21	1:D:81:ARG:HB2	1.85	0.42
1:D:514:ARG:HD2	2:D:808:HOH:O	2.18	0.42
1:F:180:CYS:HB3	1:F:203:MET:HG2	2.01	0.42
1:A:46:LEU:HD13	1:A:244:GLU:OE2	2.18	0.42
1:A:420:ALA:HB3	2:A:707:HOH:O	2.20	0.42
1:B:382:GLY:N	1:E:211:ILE:HG22	2.35	0.42
1:B:414:ARG:O	1:B:440:ALA:HA	2.20	0.42
1:B:505:HIS:O	1:B:508:ARG:NH1	2.48	0.42
1:C:45:LYS:HG2	1:C:200:THR:CG2	2.49	0.42
1:C:114:GLY:H	1:C:117:TYR:HB3	1.85	0.42
1:D:113:LEU:HD22	1:D:117:TYR:CE1	2.54	0.42
1:A:55:LEU:O	1:A:252:LYS:HE2	2.20	0.42
1:A:332:ARG:CZ	1:A:514:ARG:NH2	2.75	0.42
1:B:103:SER:HA	1:B:138:ILE:HB	2.01	0.42
1:C:235:GLY:HA2	2:C:638:HOH:O	2.20	0.42
1:D:87:VAL:C	2:D:723:HOH:O	2.62	0.42
1:D:114:GLY:H	1:D:117:TYR:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:324:THR:HA	1:D:336:ILE:O	2.19	0.42
1:D:374:VAL:HG22	1:D:424:MET:HB3	2.01	0.42
1:E:527:ASN:HB2	2:E:745:HOH:O	2.19	0.42
1:F:152:SER:HB2	2:F:685:HOH:O	2.19	0.42
1:F:207:GLY:O	1:F:211:ILE:HG23	2.19	0.42
1:A:374:VAL:HG22	1:A:424:MET:HB3	2.02	0.42
1:A:505:HIS:HB3	1:A:508:ARG:NH1	2.34	0.42
1:C:26:GLU:O	1:C:30:HIS:HD2	2.02	0.42
1:C:46:LEU:HB2	1:C:244:GLU:OE2	2.19	0.42
1:C:190:ILE:HD11	1:F:398:ILE:HD11	2.00	0.42
1:C:319:ALA:N	1:C:320:PRO:HD3	2.33	0.42
1:D:361:ARG:NH2	2:D:533:HOH:O	2.40	0.42
1:E:70:HIS:HA	1:E:116:VAL:CG2	2.49	0.42
1:F:177:VAL:HG12	1:F:197:VAL:CG2	2.49	0.42
1:A:26:GLU:O	1:A:30:HIS:HD2	2.03	0.42
1:A:520:LEU:HB3	1:A:521:PRO:CD	2.49	0.42
1:F:77:LEU:HD12	2:F:809:HOH:O	2.20	0.42
1:F:185:VAL:O	1:F:188:PRO:HD2	2.19	0.42
1:A:130:LYS:HE2	2:C:807:HOH:O	2.19	0.42
1:B:483:ASN:HB2	1:B:484:PRO:HD2	2.01	0.42
1:B:489:GLU:HA	1:C:68:ALA:HA	2.00	0.42
1:C:315:GLN:NE2	2:C:559:HOH:O	2.42	0.42
1:E:182:GLY:O	1:E:185:VAL:HG22	2.19	0.42
1:E:231:ASN:ND2	1:E:239:HIS:C	2.78	0.42
1:A:231:ASN:HD21	1:A:239:HIS:C	2.28	0.42
1:B:115:GLU:HG3	2:B:760:HOH:O	2.19	0.42
1:C:125:MET:HE1	1:C:163:ASN:ND2	2.34	0.42
1:C:437:TRP:CG	2:C:806:HOH:O	2.72	0.42
1:D:89:THR:HB	1:D:124:VAL:CG2	2.50	0.42
1:E:195:VAL:HG13	1:E:195:VAL:O	2.20	0.42
1:E:448:GLN:O	1:E:451:VAL:HG22	2.20	0.42
1:F:230:HIS:HB2	2:F:831:HOH:O	2.19	0.42
1:A:490:ARG:HD3	2:A:659:HOH:O	2.20	0.41
1:B:361:ARG:HH21	1:E:528:ILE:HG22	1.85	0.41
1:C:390:ILE:HG13	1:F:205:ILE:CD1	2.50	0.41
1:F:104:GLN:HB3	2:F:630:HOH:O	2.20	0.41
1:A:445:MET:HE2	1:A:449:GLY:HA3	2.01	0.41
1:A:530:LEU:HD12	1:A:530:LEU:HA	1.85	0.41
1:B:188:PRO:HG2	2:B:741:HOH:O	2.19	0.41
1:F:69:ARG:HD3	1:F:83:TYR:CD2	2.55	0.41
1:F:441:GLN:HG2	1:F:482:LEU:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:THR:HG21	2:A:620:HOH:O	2.20	0.41
1:B:118:GLY:HA3	1:B:155:ALA:HB1	2.02	0.41
1:B:347:CYS:SG	1:B:377:PRO:HG2	2.61	0.41
1:B:508:ARG:HE	1:C:62:VAL:HG11	1.86	0.41
1:C:456:ARG:HD2	1:C:457:ARG:NH2	2.36	0.41
1:D:46:LEU:HD13	1:D:244:GLU:CD	2.45	0.41
1:D:285:ASP:OD1	1:D:499:PRO:HD2	2.19	0.41
1:A:219:VAL:HG23	1:A:223:GLU:CD	2.45	0.41
1:B:10:ASP:CG	1:B:11:ILE:H	2.26	0.41
1:B:26:GLU:O	1:B:30:HIS:CD2	2.72	0.41
1:B:238:HIS:HA	1:B:315:GLN:HG2	2.03	0.41
1:B:462:ALA:C	1:B:464:ASP:N	2.75	0.41
1:C:443:ALA:HB1	2:C:834:HOH:O	2.20	0.41
1:D:376:VAL:HG13	1:D:376:VAL:O	2.20	0.41
1:A:332:ARG:CD	1:A:514:ARG:HH21	2.34	0.41
1:A:337:VAL:O	1:A:372:THR:HA	2.20	0.41
1:B:266:PRO:HG2	2:B:583:HOH:O	2.19	0.41
1:B:414:ARG:HA	1:B:440:ALA:HA	2.03	0.41
1:C:473:LEU:HD12	1:C:473:LEU:HA	1.92	0.41
1:D:146:ILE:H	1:D:146:ILE:HG13	1.69	0.41
1:A:77:LEU:N	2:A:723:HOH:O	2.54	0.41
1:A:185:VAL:HG13	2:A:842:HOH:O	2.20	0.41
1:B:71:ARG:NH2	1:B:119:GLN:HE22	2.05	0.41
1:C:348:LEU:HG	2:C:724:HOH:O	2.19	0.41
1:D:62:VAL:HG11	1:E:508:ARG:NH2	2.35	0.41
1:D:508:ARG:HB3	2:D:797:HOH:O	2.20	0.41
1:A:434:ASN:HB3	2:A:670:HOH:O	2.20	0.41
1:B:70:HIS:O	1:B:81:ARG:HD2	2.21	0.41
1:C:398:ILE:HD12	1:C:398:ILE:C	2.45	0.41
1:E:528:ILE:HD12	2:E:739:HOH:O	2.20	0.41
1:A:62:VAL:CG2	1:C:508:ARG:HG3	2.43	0.41
1:B:517:ARG:NH2	2:B:629:HOH:O	2.46	0.41
1:D:509:GLY:O	1:D:513:LEU:HB2	2.21	0.41
1:F:145:ARG:HD2	1:F:148:GLU:OE2	2.20	0.41
1:A:10:ASP:CG	1:A:11:ILE:H	2.26	0.41
1:A:150:VAL:HG23	2:D:706:HOH:O	2.20	0.41
1:A:508:ARG:HD3	1:A:509:GLY:H	1.85	0.41
1:B:180:CYS:HB3	1:B:203:MET:HG2	2.01	0.41
1:B:296:TYR:N	1:B:342:MET:HE3	2.36	0.41
1:B:315:GLN:N	1:B:316:PRO:CD	2.82	0.41
1:C:114:GLY:O	2:C:843:HOH:O	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:ALA:C	2:C:754:HOH:O	2.63	0.41
1:D:81:ARG:HD3	2:D:656:HOH:O	2.21	0.41
1:D:284:LEU:HD13	1:D:304:HIS:CD2	2.55	0.41
1:D:321:ASN:HA	1:D:343:GLN:HB2	2.01	0.41
1:D:508:ARG:HG3	1:F:62:VAL:CG2	2.41	0.41
1:E:74:ASN:O	1:E:77:LEU:HB2	2.21	0.41
1:E:219:VAL:HG22	1:E:220:GLY:N	2.36	0.41
1:C:321:ASN:HA	1:C:343:GLN:HB2	2.03	0.41
1:C:344:PHE:O	1:C:345:ALA:HB3	2.21	0.41
1:D:195:VAL:HG11	1:D:251:VAL:HG12	2.03	0.41
1:D:231:ASN:HD21	1:D:239:HIS:CA	2.34	0.41
1:D:505:HIS:HB3	1:D:508:ARG:NH1	2.36	0.41
1:E:69:ARG:HB3	2:E:777:HOH:O	2.21	0.41
1:E:318:PHE:CZ	1:E:351:THR:HB	2.56	0.41
1:F:68:ALA:C	1:F:69:ARG:HG2	2.45	0.41
1:F:177:VAL:HG12	1:F:197:VAL:HG21	2.03	0.41
1:A:39:LYS:O	1:A:43:LYS:HG3	2.21	0.40
1:B:517:ARG:HG3	1:B:517:ARG:HH11	1.86	0.40
1:C:473:LEU:HD12	1:C:476:GLU:OE1	2.21	0.40
1:D:51:ARG:NH1	2:D:838:HOH:O	2.52	0.40
1:D:440:ALA:HB3	1:D:484:PRO:HB3	2.02	0.40
1:D:462:ALA:C	1:D:464:ASP:N	2.78	0.40
1:D:490:ARG:HG3	2:D:706:HOH:O	2.21	0.40
1:E:158:GLU:O	1:E:162:ARG:HG2	2.21	0.40
1:E:252:LYS:HE2	2:E:600:HOH:O	2.20	0.40
1:E:483:ASN:HB2	1:E:484:PRO:CD	2.51	0.40
1:F:24:ARG:HD3	1:F:83:TYR:OH	2.21	0.40
1:F:104:GLN:HB3	1:F:117:TYR:OH	2.21	0.40
1:A:172:GLN:CG	2:A:760:HOH:O	2.69	0.40
1:B:230:HIS:HB3	1:B:236:VAL:CG2	2.51	0.40
1:F:113:LEU:HG	1:F:156:TYR:CE1	2.56	0.40
1:F:200:THR:O	1:F:200:THR:CG2	2.69	0.40
1:F:248:VAL:HA	1:F:251:VAL:HG12	2.03	0.40
1:F:367:ASN:ND2	2:F:828:HOH:O	2.54	0.40
1:F:370:VAL:HG13	2:F:675:HOH:O	2.19	0.40
1:A:123:LYS:HD2	2:C:569:HOH:O	2.21	0.40
1:A:433:LEU:HD21	1:A:508:ARG:CZ	2.50	0.40
1:A:455:HIS:CB	1:A:473:LEU:HD23	2.51	0.40
1:C:332:ARG:HD3	1:C:514:ARG:NH2	2.36	0.40
1:D:26:GLU:O	1:D:30:HIS:HD2	2.03	0.40
1:E:232:SER:HB3	1:E:317:LEU:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:520:LEU:HD12	1:E:520:LEU:N	2.36	0.40
1:F:315:GLN:N	1:F:316:PRO:CD	2.82	0.40
1:F:462:ALA:O	1:F:464:ASP:O	2.40	0.40
1:B:398:ILE:HD12	1:B:398:ILE:O	2.21	0.40
1:C:437:TRP:CD1	2:C:806:HOH:O	2.74	0.40
1:D:103:SER:HA	1:D:138:ILE:HB	2.04	0.40
1:D:113:LEU:HG	1:D:156:TYR:CE1	2.57	0.40
1:E:294:GLN:HA	1:E:295:PRO:HD3	1.87	0.40
1:E:386:GLU:HA	1:E:390:ILE:HG22	2.03	0.40
1:F:211:ILE:CD1	1:F:217:GLU:HB2	2.51	0.40
1:A:146:ILE:CD1	1:D:453:ILE:HG21	2.52	0.40
1:A:332:ARG:NE	1:A:514:ARG:NH2	2.62	0.40
1:B:43:LYS:HE2	2:B:686:HOH:O	2.22	0.40
1:B:316:PRO:HG2	2:B:683:HOH:O	2.21	0.40
1:C:335:GLY:HA3	2:C:777:HOH:O	2.22	0.40
1:C:384:ASP:CG	1:C:385:GLN:N	2.80	0.40
1:C:461:ASP:O	1:C:462:ALA:HB3	2.22	0.40
1:D:10:ASP:CG	1:D:11:ILE:N	2.76	0.40
1:D:40:GLN:OE1	1:D:45:LYS:HE3	2.20	0.40
1:E:529:PRO:HD3	2:E:766:HOH:O	2.22	0.40
1:F:517:ARG:NH2	2:F:718:HOH:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	519/530 (98%)	499 (96%)	18 (4%)	2 (0%)	30	34
1	B	519/530 (98%)	496 (96%)	21 (4%)	2 (0%)	30	34
1	C	519/530 (98%)	501 (96%)	18 (4%)	0	100	100
1	D	519/530 (98%)	499 (96%)	18 (4%)	2 (0%)	30	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	519/530 (98%)	500 (96%)	17 (3%)	2 (0%)	30	34
1	F	519/530 (98%)	497 (96%)	20 (4%)	2 (0%)	30	34
All	All	3114/3180 (98%)	2992 (96%)	112 (4%)	10 (0%)	36	42

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	E	11	ILE
1	A	199	GLN
1	B	11	ILE
1	B	468	ALA
1	F	468	ALA
1	D	146	ILE
1	D	213	THR
1	E	146	ILE
1	F	11	ILE

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	412/421 (98%)	386 (94%)	26 (6%)	16	19
1	B	412/421 (98%)	390 (95%)	22 (5%)	20	26
1	C	412/421 (98%)	389 (94%)	23 (6%)	19	24
1	D	412/421 (98%)	388 (94%)	24 (6%)	18	22
1	E	412/421 (98%)	391 (95%)	21 (5%)	21	27
1	F	412/421 (98%)	391 (95%)	21 (5%)	21	27
All	All	2472/2526 (98%)	2335 (94%)	137 (6%)	19	24

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	54	LEU
1	A	77	LEU
1	A	113	LEU
1	A	117	TYR
1	A	147	GLN
1	A	161	ARG
1	A	175	LEU
1	A	195	VAL
1	A	205	ILE
1	A	209	ASP
1	A	211	ILE
1	A	236	VAL
1	A	254	LEU
1	A	263	LEU
1	A	274	ASP
1	A	284	LEU
1	A	342	MET
1	A	358	ARG
1	A	397	LEU
1	A	398	ILE
1	A	435	LEU
1	A	475	GLN
1	A	484	PRO
1	A	513	LEU
1	A	530	LEU
1	B	69	ARG
1	B	77	LEU
1	B	113	LEU
1	B	117	TYR
1	B	147	GLN
1	B	175	LEU
1	B	205	ILE
1	B	251	VAL
1	B	263	LEU
1	B	284	LEU
1	B	310	GLU
1	B	358	ARG
1	B	380	LEU
1	B	397	LEU
1	B	398	ILE
1	B	429	LEU
1	B	435	LEU

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Mol	Chain	Res	Type
1	B	473	LEU
1	B	475	GLN
1	B	483	ASN
1	B	508	ARG
1	B	530	LEU
1	C	22	ARG
1	C	40	GLN
1	C	46	LEU
1	C	54	LEU
1	C	77	LEU
1	C	113	LEU
1	C	117	TYR
1	C	147	GLN
1	C	195	VAL
1	C	211	ILE
1	C	236	VAL
1	C	263	LEU
1	C	284	LEU
1	C	358	ARG
1	C	397	LEU
1	C	398	ILE
1	C	435	LEU
1	C	473	LEU
1	C	481	LEU
1	C	484	PRO
1	C	512	GLN
1	C	513	LEU
1	C	530	LEU
1	D	22	ARG
1	D	40	GLN
1	D	54	LEU
1	D	77	LEU
1	D	113	LEU
1	D	175	LEU
1	D	195	VAL
1	D	200	THR
1	D	236	VAL
1	D	263	LEU
1	D	284	LEU
1	D	310	GLU
1	D	358	ARG
1	D	372	THR

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Mol	Chain	Res	Type
1	D	397	LEU
1	D	398	ILE
1	D	429	LEU
1	D	435	LEU
1	D	473	LEU
1	D	484	PRO
1	D	508	ARG
1	D	512	GLN
1	D	513	LEU
1	D	530	LEU
1	E	25	ILE
1	E	40	GLN
1	E	58	GLU
1	E	77	LEU
1	E	113	LEU
1	E	117	TYR
1	E	147	GLN
1	E	161	ARG
1	E	175	LEU
1	E	211	ILE
1	E	236	VAL
1	E	284	LEU
1	E	310	GLU
1	E	342	MET
1	E	358	ARG
1	E	397	LEU
1	E	429	LEU
1	E	475	GLN
1	E	508	ARG
1	E	512	GLN
1	E	530	LEU
1	F	22	ARG
1	F	40	GLN
1	F	77	LEU
1	F	113	LEU
1	F	117	TYR
1	F	147	GLN
1	F	175	LEU
1	F	200	THR
1	F	211	ILE
1	F	236	VAL
1	F	254	LEU

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Mol	Chain	Res	Type
1	F	310	GLU
1	F	358	ARG
1	F	397	LEU
1	F	398	ILE
1	F	467	GLU
1	F	473	LEU
1	F	484	PRO
1	F	512	GLN
1	F	513	LEU
1	F	530	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	70	HIS
1	A	74	ASN
1	A	147	GLN
1	A	163	ASN
1	A	199	GLN
1	A	231	ASN
1	A	294	GLN
1	A	299	HIS
1	A	315	GLN
1	A	387	HIS
1	A	441	GLN
1	A	475	GLN
1	A	483	ASN
1	A	512	GLN
1	A	527	ASN
1	B	30	HIS
1	B	40	GLN
1	B	70	HIS
1	B	119	GLN
1	B	147	GLN
1	B	163	ASN
1	B	231	ASN
1	B	239	HIS
1	B	299	HIS
1	B	315	GLN
1	B	475	GLN
1	B	483	ASN

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Mol	Chain	Res	Type
1	B	512	GLN
1	B	527	ASN
1	C	30	HIS
1	C	40	GLN
1	C	70	HIS
1	C	74	ASN
1	C	119	GLN
1	C	147	GLN
1	C	163	ASN
1	C	199	GLN
1	C	231	ASN
1	C	299	HIS
1	C	448	GLN
1	C	455	HIS
1	C	483	ASN
1	C	512	GLN
1	C	527	ASN
1	D	30	HIS
1	D	40	GLN
1	D	70	HIS
1	D	74	ASN
1	D	163	ASN
1	D	199	GLN
1	D	231	ASN
1	D	299	HIS
1	D	448	GLN
1	D	455	HIS
1	D	475	GLN
1	D	483	ASN
1	D	512	GLN
1	D	527	ASN
1	E	30	HIS
1	E	40	GLN
1	E	70	HIS
1	E	74	ASN
1	E	147	GLN
1	E	163	ASN
1	E	199	GLN
1	E	231	ASN
1	E	299	HIS
1	E	441	GLN
1	E	455	HIS

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Mol	Chain	Res	Type
1	E	483	ASN
1	E	512	GLN
1	E	527	ASN
1	F	12	HIS
1	F	40	GLN
1	F	70	HIS
1	F	74	ASN
1	F	139	ASN
1	F	147	GLN
1	F	163	ASN
1	F	199	GLN
1	F	231	ASN
1	F	299	HIS
1	F	448	GLN
1	F	452	ASN
1	F	455	HIS
1	F	483	ASN
1	F	512	GLN
1	F	527	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	521/530 (98%)	0.23	24 (4%)	37	34	20, 32, 51, 98	0
1	B	521/530 (98%)	0.29	21 (4%)	42	39	23, 34, 54, 100	0
1	C	521/530 (98%)	0.20	19 (3%)	46	43	21, 32, 51, 84	0
1	D	521/530 (98%)	0.21	26 (4%)	34	31	19, 31, 50, 86	0
1	E	521/530 (98%)	0.36	25 (4%)	35	32	22, 35, 53, 99	0
1	F	521/530 (98%)	0.30	21 (4%)	42	39	18, 34, 55, 100	0
All	All	3126/3180 (98%)	0.26	136 (4%)	39	36	18, 33, 53, 100	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	508	ARG	7.5
1	E	508	ARG	7.0
1	B	508	ARG	5.8
1	C	508	ARG	5.4
1	A	508	ARG	5.3
1	B	462	ALA	4.7
1	D	508	ARG	4.4
1	C	466	ALA	4.3
1	D	462	ALA	4.1
1	F	466	ALA	4.1
1	E	466	ALA	4.1
1	A	466	ALA	4.0
1	B	466	ALA	3.9
1	E	462	ALA	3.9
1	F	347	CYS	3.8
1	C	11	ILE	3.8
1	E	468	ALA	3.7
1	C	462	ALA	3.7
1	D	466	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	468	ALA	3.5
1	D	459	ILE	3.5
1	F	459	ILE	3.4
1	B	469	THR	3.4
1	A	462	ALA	3.4
1	D	217	GLU	3.4
1	D	347	CYS	3.4
1	C	211	ILE	3.4
1	F	517	ARG	3.3
1	F	462	ALA	3.3
1	C	347	CYS	3.2
1	D	464	ASP	3.2
1	E	460	ALA	3.1
1	A	332	ARG	3.1
1	E	398	ILE	3.1
1	F	468	ALA	3.1
1	C	269	PHE	3.0
1	C	530	LEU	3.0
1	E	459	ILE	3.0
1	E	332	ARG	2.9
1	D	199	GLN	2.9
1	E	347	CYS	2.9
1	A	458	THR	2.8
1	F	469	THR	2.8
1	F	199	GLN	2.8
1	B	463	GLY	2.8
1	D	200	THR	2.8
1	C	271	GLU	2.8
1	E	458	THR	2.7
1	A	517	ARG	2.7
1	A	459	ILE	2.7
1	D	216	GLY	2.7
1	D	517	ARG	2.7
1	F	463	GLY	2.7
1	E	461	ASP	2.6
1	B	25	ILE	2.6
1	C	459	ILE	2.6
1	E	465	ASP	2.6
1	D	214	VAL	2.6
1	C	332	ARG	2.6
1	D	35	ARG	2.6
1	A	213	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	459	ILE	2.6
1	B	465	ASP	2.5
1	B	146	ILE	2.5
1	F	332	ARG	2.5
1	D	209	ASP	2.5
1	B	458	THR	2.5
1	C	517	ARG	2.5
1	E	456	ARG	2.5
1	C	460	ALA	2.5
1	C	200	THR	2.5
1	B	332	ARG	2.5
1	E	463	GLY	2.5
1	A	469	THR	2.4
1	E	457	ARG	2.4
1	C	214	VAL	2.4
1	F	530	LEU	2.4
1	B	467	GLU	2.4
1	D	458	THR	2.4
1	C	457	ARG	2.4
1	C	468	ALA	2.4
1	E	11	ILE	2.4
1	D	332	ARG	2.4
1	E	517	ARG	2.4
1	B	461	ASP	2.4
1	A	460	ALA	2.3
1	A	269	PHE	2.3
1	B	347	CYS	2.3
1	A	501	ASP	2.3
1	F	465	ASP	2.3
1	E	469	THR	2.3
1	A	211	ILE	2.3
1	F	467	GLU	2.3
1	A	53	ASP	2.3
1	E	464	ASP	2.3
1	D	463	GLY	2.3
1	A	347	CYS	2.3
1	D	468	ALA	2.3
1	D	25	ILE	2.3
1	B	530	LEU	2.2
1	A	10	ASP	2.2
1	D	10	ASP	2.2
1	D	146	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	205	ILE	2.2
1	B	464	ASP	2.2
1	A	44	GLY	2.2
1	B	199	GLN	2.2
1	A	200	THR	2.2
1	F	458	THR	2.2
1	D	465	ASP	2.2
1	E	271	GLU	2.2
1	A	468	ALA	2.2
1	E	205	ILE	2.1
1	C	213	THR	2.1
1	E	201	SER	2.1
1	F	273	ALA	2.1
1	A	209	ASP	2.1
1	D	452	ASN	2.1
1	F	195	VAL	2.1
1	A	518	GLU	2.1
1	A	398	ILE	2.1
1	D	457	ARG	2.1
1	B	519	SER	2.1
1	B	460	ALA	2.1
1	E	530	LEU	2.1
1	D	205	ILE	2.1
1	E	10	ASP	2.1
1	F	10	ASP	2.1
1	B	517	ARG	2.1
1	C	215	THR	2.0
1	A	530	LEU	2.0
1	F	211	ILE	2.0
1	D	469	THR	2.0
1	E	518	GLU	2.0
1	A	465	ASP	2.0
1	F	520	LEU	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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.