



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:26 AM UTC

PDB ID : 5A9V / pdb_00005a9v
Title : Structure of apo BipA
Authors : Kumar, V.; Chen, Y.; Ero, R.; Li, Z.; Gao, Y.
Deposited on : 2015-07-23
Resolution : 3.31 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

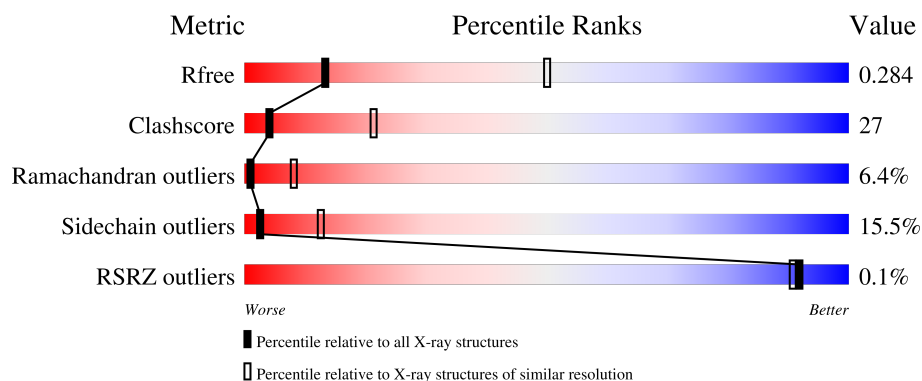
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

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	607	
1	B	607	
1	C	607	
1	D	607	
1	E	607	

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Mol	Chain	Length	Quality of chain
1	F	607	58% 24% 8% • 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25398 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.

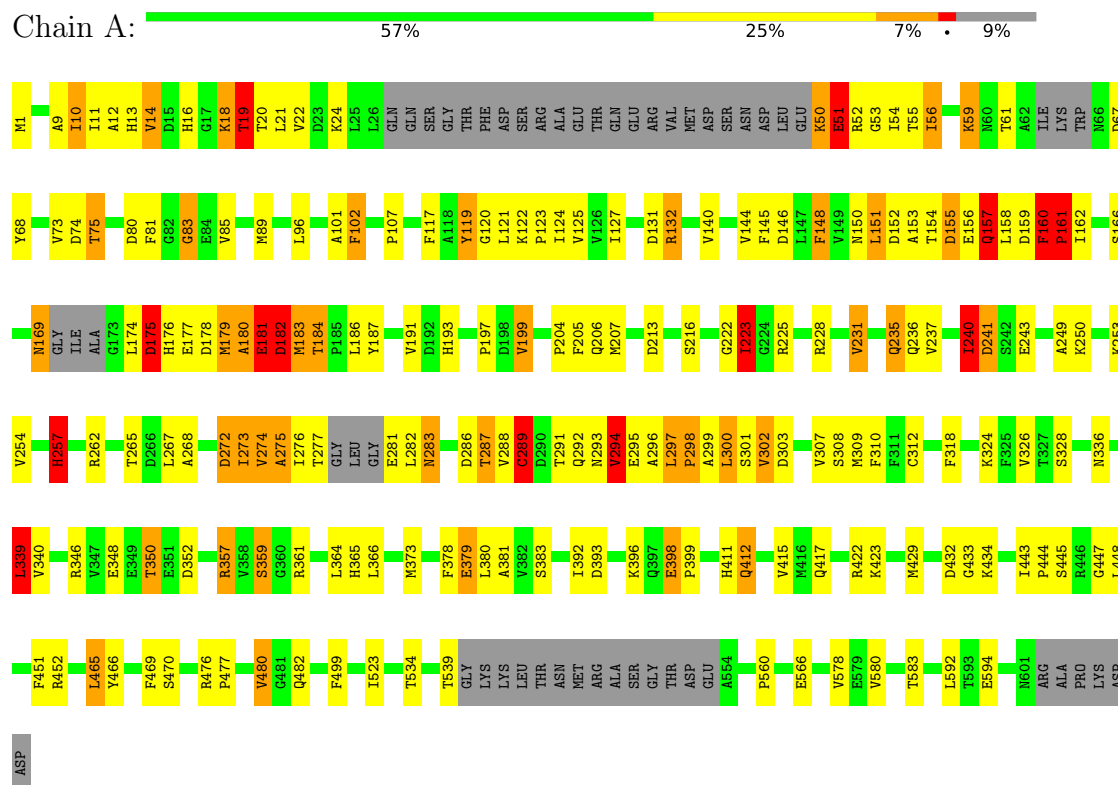
- Molecule 1 is a protein called GTP-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4233	2675	736	806	16			
1	B	555	Total	C	N	O	S	0	0	0
			4233	2675	736	806	16			
1	C	555	Total	C	N	O	S	0	0	0
			4233	2675	736	806	16			
1	D	555	Total	C	N	O	S	0	0	0
			4233	2675	736	806	16			
1	E	555	Total	C	N	O	S	0	0	0
			4233	2675	736	806	16			
1	F	555	Total	C	N	O	S	0	0	0
			4233	2675	736	806	16			

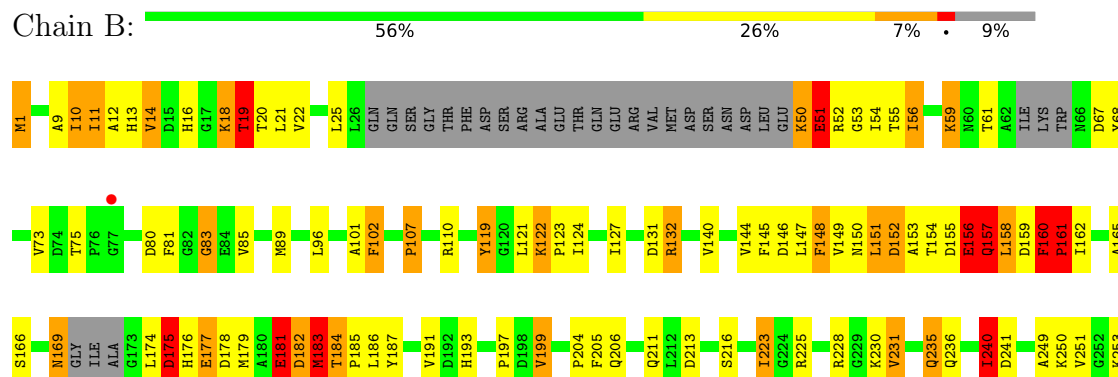
3 Residue-property plots

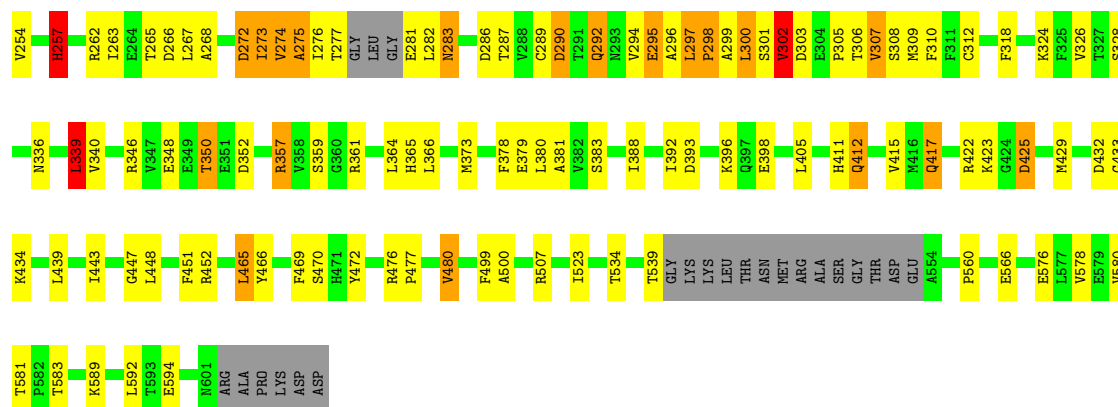
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: GTP-BINDING PROTEIN



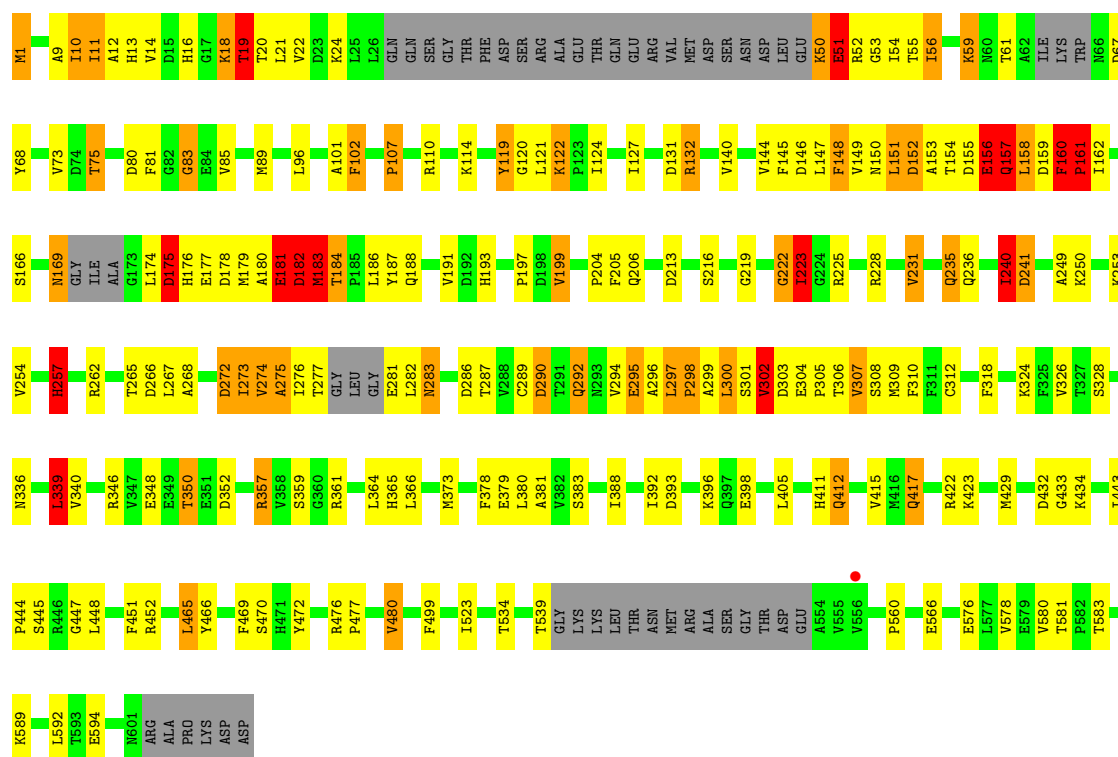
• Molecule 1: GTP-BINDING PROTEIN





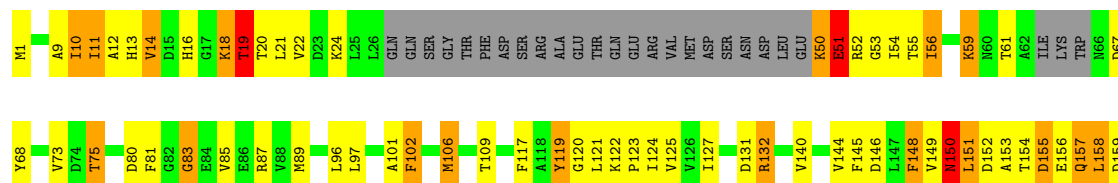
• Molecule 1: GTP-BINDING PROTEIN

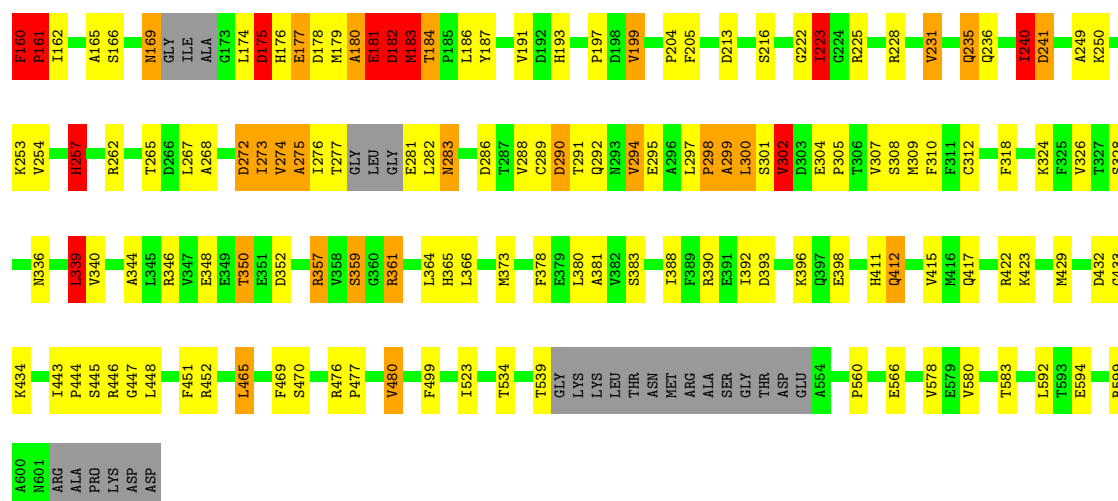
Chain C: 57% 25% 7% 9%



• Molecule 1: GTP-BINDING PROTEIN

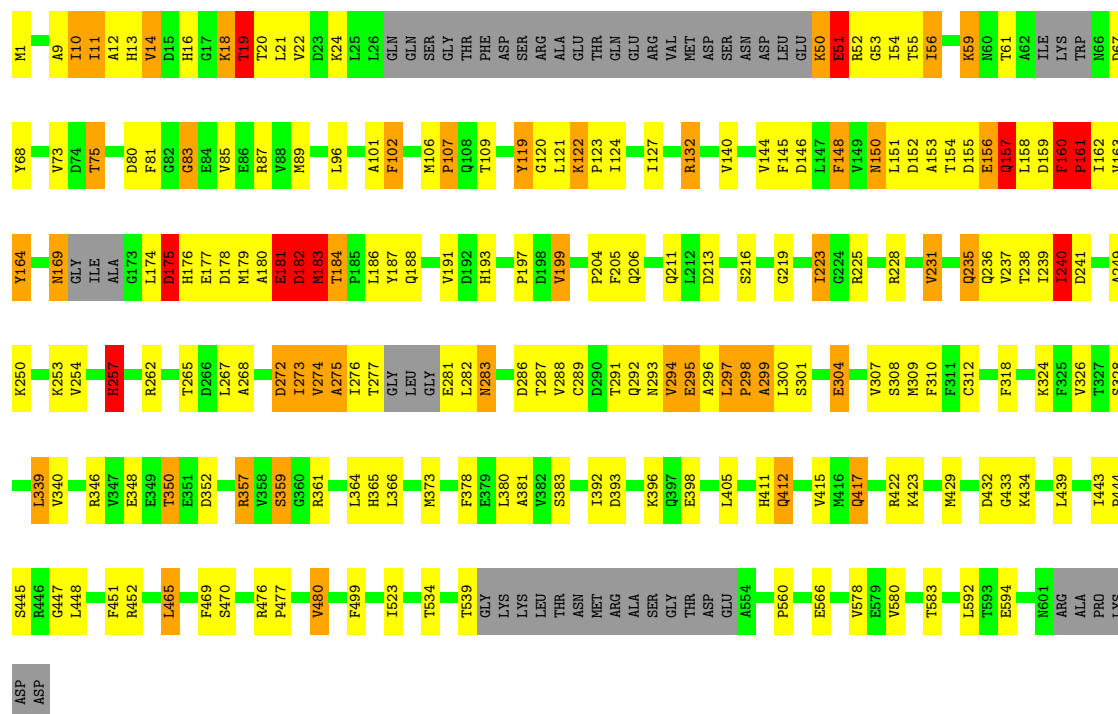
Chain D: 57% 25% 7% 9%





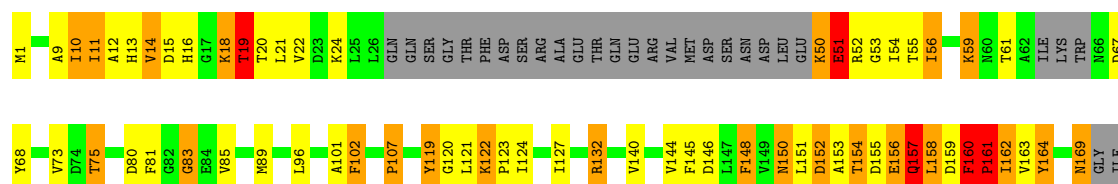
• Molecule 1: GTP-BINDING PROTEIN

Chain E: 58% 25% 7% 9%



• Molecule 1: GTP-BINDING PROTEIN

Chain F: 58% 24% 8% 9%



ALA	G173	L174	D175	H176	E177	D178	M179	A180	E181	D182	M183	T184	F185	L186	Y187	V191	D192	H193	P197	D198	V199	P204	F205	Q206	Q211	I212	D213	S216	G219	I223	G224	R225	R228	V231	Q235	Q236	V237	T238	I239	I240	D241	A249	K250	K253	V254	H257		
R346	V347	E348	E349	T350	E351	D352	R357	V358	S359	G360	R361	L364	H365	L366	M373	F378	E379	L380	A381	V382	S383	I392	D393	K396	G397	E398	L405	H411	Q412	V415	M416	Q417	R422	K423	M429	D432	G433	K434	L439	I443	P444	S445	R446	G447	L448			
F451	R452	L465	F469	S470	R476	P477	V480	F499	I523	T534	T539	GLY	LYS	LYS	LEU	THR	ASN	MET	ARG	ALA	SER	GLY	THR	ASP	GLU	A554	P560	M563	E566	V578	E579	V580	T583	L592	T593	E594	N601	ARG	ALA	PRO	LYS	ASP	ASP					
R262	T265	D266	A268	D272	I273	V274	A275	I276	T277	GLY	LEU	GLY	E281	L282	N283	D286	T287	V288	G289	D290	T291	Q292	N293	V294	E295	A296	L297	P298	A299	L300	S301	V302	D303	V307	S308	M309	F310	F311	C312	F318	K324	F325	V326	T327	S328	N336	L339	V340

4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	241.95Å 241.95Å 241.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 3.31 49.39 – 3.31	Depositor EDS
% Data completeness (in resolution range)	91.8 (49.39-3.31) 91.8 (49.39-3.31)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.263 , 0.288 0.277 , 0.284	Depositor DCC
R_{free} test set	9472 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	114.3	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 267.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.429 for l,-k,h 0.429 for -l,-k,-h 0.429 for -h,-l,-k 0.429 for -h,l,k 0.439 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25398	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% 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	0.85	3/4292 (0.1%)	1.14	23/5786 (0.4%)
1	B	0.86	3/4292 (0.1%)	1.15	23/5786 (0.4%)
1	C	0.86	2/4292 (0.0%)	1.14	24/5786 (0.4%)
1	D	0.85	3/4292 (0.1%)	1.14	20/5786 (0.3%)
1	E	0.85	3/4292 (0.1%)	1.13	24/5786 (0.4%)
1	F	0.85	3/4292 (0.1%)	1.13	22/5786 (0.4%)
All	All	0.85	17/25752 (0.1%)	1.14	136/34716 (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	4
1	B	0	4
1	C	0	4
1	D	0	5
1	E	0	4
1	F	0	4
All	All	0	25

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	ILE	CA-C	6.29	1.60	1.52
1	D	240	ILE	CA-C	6.15	1.60	1.52
1	F	240	ILE	CA-C	6.15	1.60	1.52
1	E	240	ILE	CA-C	5.89	1.60	1.52
1	C	240	ILE	CA-C	5.89	1.60	1.52
1	B	240	ILE	CA-C	5.68	1.59	1.52
1	F	257	HIS	CA-C	5.40	1.60	1.52
1	A	257	HIS	CA-C	5.37	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	257	HIS	CA-C	5.37	1.59	1.52
1	D	257	HIS	CA-C	5.33	1.59	1.52
1	C	257	HIS	CA-C	5.29	1.59	1.52
1	B	14	VAL	N-CA	5.24	1.52	1.46
1	E	257	HIS	CA-C	5.19	1.59	1.52
1	F	14	VAL	N-CA	5.08	1.52	1.46
1	E	14	VAL	N-CA	5.07	1.52	1.46
1	D	14	VAL	N-CA	5.04	1.52	1.46
1	A	14	VAL	N-CA	5.03	1.52	1.46

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	476	ARG	CA-C-N	-11.37	105.62	119.84
1	A	476	ARG	C-N-CA	-11.37	105.62	119.84
1	C	476	ARG	CA-C-N	-11.28	105.75	119.84
1	C	476	ARG	C-N-CA	-11.28	105.75	119.84
1	B	476	ARG	CA-C-N	-11.25	105.78	119.84
1	B	476	ARG	C-N-CA	-11.25	105.78	119.84
1	D	476	ARG	CA-C-N	-11.19	105.85	119.84
1	D	476	ARG	C-N-CA	-11.19	105.85	119.84
1	F	476	ARG	CA-C-N	-11.05	106.03	119.84
1	F	476	ARG	C-N-CA	-11.05	106.03	119.84
1	E	476	ARG	CA-C-N	-10.80	106.34	119.84
1	E	476	ARG	C-N-CA	-10.80	106.34	119.84
1	C	222	GLY	N-CA-C	8.74	124.70	113.24
1	F	223	ILE	N-CA-C	-7.39	97.82	108.17
1	E	223	ILE	N-CA-C	-7.32	97.92	108.53
1	F	563	MET	CA-CB-CG	-7.22	99.66	114.10
1	F	119	TYR	N-CA-C	-7.20	98.23	109.25
1	A	119	TYR	N-CA-C	-7.20	98.24	109.25
1	B	223	ILE	N-CA-C	-7.19	98.08	108.36
1	B	161	PRO	N-CA-CB	7.16	110.48	102.60
1	F	161	PRO	N-CA-CB	7.16	110.47	102.60
1	A	161	PRO	N-CA-CB	7.15	110.46	102.60
1	C	161	PRO	N-CA-CB	7.12	110.43	102.60
1	E	161	PRO	N-CA-CB	7.11	110.42	102.60
1	D	161	PRO	N-CA-CB	7.10	110.41	102.60
1	D	119	TYR	N-CA-C	-6.99	98.56	109.25
1	B	119	TYR	N-CA-C	-6.95	98.62	109.25
1	D	106	MET	CA-C-N	-6.94	111.16	119.84
1	D	106	MET	C-N-CA	-6.94	111.16	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	119	TYR	N-CA-C	-6.87	98.73	109.25
1	C	119	TYR	N-CA-C	-6.83	98.80	109.25
1	B	240	ILE	N-CA-C	6.54	122.95	109.34
1	F	240	ILE	N-CA-C	6.48	122.82	109.34
1	E	240	ILE	N-CA-C	6.48	122.82	109.34
1	D	59	LYS	N-CA-C	6.48	118.88	107.61
1	C	59	LYS	N-CA-C	6.39	118.73	107.61
1	C	240	ILE	N-CA-C	6.38	122.61	109.34
1	A	59	LYS	N-CA-C	6.36	118.67	107.61
1	F	59	LYS	N-CA-C	6.36	118.67	107.61
1	E	59	LYS	N-CA-C	6.32	118.60	107.61
1	B	59	LYS	N-CA-C	6.30	118.58	107.61
1	D	240	ILE	N-CA-C	6.30	122.45	109.34
1	A	240	ILE	N-CA-C	6.22	122.29	109.34
1	C	318	PHE	N-CA-C	-6.22	102.92	110.88
1	B	500	ALA	CB-CA-C	-6.19	100.83	110.37
1	A	350	THR	N-CA-C	6.03	118.38	109.69
1	A	318	PHE	N-CA-C	-6.01	103.19	110.88
1	C	19	THR	CB-CA-C	-5.98	103.28	110.94
1	F	318	PHE	N-CA-C	-5.97	103.23	110.88
1	B	523	ILE	N-CA-C	-5.96	101.85	109.30
1	E	318	PHE	N-CA-C	-5.93	103.29	110.88
1	B	318	PHE	N-CA-C	-5.92	103.30	110.88
1	B	350	THR	N-CA-C	5.92	118.21	109.69
1	B	19	THR	CA-C-N	5.89	132.30	121.70
1	B	19	THR	C-N-CA	5.89	132.30	121.70
1	C	19	THR	CA-C-N	5.86	132.25	121.70
1	C	19	THR	C-N-CA	5.86	132.25	121.70
1	A	19	THR	CA-C-N	5.86	132.24	121.70
1	A	19	THR	C-N-CA	5.86	132.24	121.70
1	C	350	THR	N-CA-C	5.85	118.12	109.69
1	F	19	THR	CB-CA-C	-5.85	103.45	110.94
1	D	19	THR	CA-C-N	5.83	132.19	121.70
1	D	19	THR	C-N-CA	5.83	132.19	121.70
1	D	318	PHE	N-CA-C	-5.83	103.42	110.88
1	D	350	THR	N-CA-C	5.82	118.07	109.69
1	F	592	LEU	N-CA-C	5.81	120.41	112.68
1	F	350	THR	N-CA-C	5.81	118.06	109.69
1	A	324	LYS	N-CA-C	5.81	120.41	112.04
1	A	19	THR	CB-CA-C	-5.81	103.51	110.94
1	E	19	THR	CA-C-N	5.79	132.13	121.70
1	E	19	THR	C-N-CA	5.79	132.13	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	19	THR	CA-C-N	5.78	132.10	121.70
1	F	19	THR	C-N-CA	5.78	132.10	121.70
1	F	523	ILE	N-CA-C	-5.78	102.08	109.30
1	D	19	THR	CB-CA-C	-5.75	103.58	110.94
1	D	592	LEU	N-CA-C	5.74	120.31	112.68
1	A	592	LEU	N-CA-C	5.72	120.29	112.68
1	B	592	LEU	N-CA-C	5.71	120.27	112.68
1	E	324	LYS	N-CA-C	5.71	120.26	112.04
1	B	19	THR	CB-CA-C	-5.70	103.65	110.94
1	E	19	THR	CB-CA-C	-5.69	103.66	110.94
1	C	592	LEU	N-CA-C	5.68	120.23	112.68
1	E	350	THR	N-CA-C	5.66	117.84	109.69
1	A	523	ILE	N-CA-C	-5.59	102.32	109.30
1	E	304	GLU	N-CA-C	5.58	116.02	109.60
1	B	415	VAL	CB-CA-C	-5.57	104.62	111.92
1	E	415	VAL	CB-CA-C	-5.56	104.64	111.92
1	E	592	LEU	N-CA-C	5.56	120.08	112.68
1	D	523	ILE	N-CA-C	-5.50	102.42	109.30
1	C	324	LYS	N-CA-C	5.50	119.95	112.04
1	B	324	LYS	N-CA-C	5.49	119.94	112.04
1	E	286	ASP	CB-CA-C	-5.49	100.94	109.61
1	C	132	ARG	CA-C-N	5.47	126.68	119.84
1	C	132	ARG	C-N-CA	5.47	126.68	119.84
1	D	415	VAL	CB-CA-C	-5.46	104.76	111.92
1	C	286	ASP	CB-CA-C	-5.46	100.98	109.61
1	E	523	ILE	N-CA-C	-5.46	102.48	109.30
1	F	415	VAL	CB-CA-C	-5.45	104.78	111.92
1	B	132	ARG	CA-C-N	5.44	126.64	119.84
1	B	132	ARG	C-N-CA	5.44	126.64	119.84
1	C	415	VAL	CB-CA-C	-5.43	104.80	111.92
1	F	15	ASP	CB-CG-OD2	5.43	130.90	118.40
1	D	324	LYS	N-CA-C	5.42	119.85	112.04
1	D	132	ARG	CA-C-N	5.41	126.60	119.84
1	D	132	ARG	C-N-CA	5.41	126.60	119.84
1	A	243	GLU	N-CA-CB	-5.39	103.45	111.43
1	C	523	ILE	N-CA-C	-5.38	102.57	109.30
1	D	283	ASN	N-CA-C	5.38	117.59	109.41
1	B	107	PRO	N-CA-C	5.36	123.51	112.47
1	C	219	GLY	N-CA-C	-5.33	106.17	111.56
1	E	132	ARG	CA-C-N	5.33	126.50	119.84
1	E	132	ARG	C-N-CA	5.33	126.50	119.84
1	A	132	ARG	CA-C-N	5.32	126.49	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	ARG	C-N-CA	5.32	126.49	119.84
1	A	415	VAL	CB-CA-C	-5.32	104.96	111.92
1	C	283	ASN	N-CA-C	5.30	117.47	109.41
1	F	132	ARG	CA-C-N	5.29	126.45	119.84
1	F	132	ARG	C-N-CA	5.29	126.45	119.84
1	E	107	PRO	N-CA-C	5.28	123.34	112.47
1	A	107	PRO	N-CA-C	5.27	123.32	112.47
1	F	107	PRO	N-CA-C	5.25	123.29	112.47
1	A	379	GLU	CB-CA-C	5.25	118.53	110.14
1	A	283	ASN	N-CA-C	5.23	117.36	109.41
1	F	324	LYS	N-CA-C	5.23	119.57	112.04
1	C	188	GLN	N-CA-C	-5.23	105.27	110.97
1	A	466	TYR	CA-CB-CG	5.19	123.25	113.90
1	B	283	ASN	N-CA-C	5.19	117.30	109.41
1	B	466	TYR	CA-CB-CG	5.19	123.24	113.90
1	E	283	ASN	N-CA-C	5.17	117.27	109.41
1	C	107	PRO	N-CA-C	5.16	123.09	112.47
1	C	466	TYR	CA-CB-CG	5.15	123.17	113.90
1	F	219	GLY	N-CA-C	-5.14	106.37	111.56
1	E	219	GLY	N-CA-C	-5.10	106.41	111.56
1	A	287	THR	N-CA-C	5.05	117.67	109.24
1	E	188	GLN	N-CA-C	-5.02	105.50	110.97
1	B	263	ILE	N-CA-C	-5.02	105.81	110.53

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	ARG	Peptide
1	A	19	THR	Peptide
1	A	240	ILE	Peptide
1	A	465	LEU	Peptide
1	B	132	ARG	Peptide
1	B	19	THR	Peptide
1	B	240	ILE	Peptide
1	B	465	LEU	Peptide
1	C	132	ARG	Peptide
1	C	19	THR	Peptide
1	C	240	ILE	Peptide
1	C	465	LEU	Peptide
1	D	132	ARG	Peptide
1	D	19	THR	Peptide

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Mol	Chain	Res	Type	Group
1	D	240	ILE	Peptide
1	D	291	THR	Peptide
1	D	465	LEU	Peptide
1	E	132	ARG	Peptide
1	E	19	THR	Peptide
1	E	240	ILE	Peptide
1	E	465	LEU	Peptide
1	F	132	ARG	Peptide
1	F	19	THR	Peptide
1	F	240	ILE	Peptide
1	F	465	LEU	Peptide

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	4233	0	4156	224	0
1	B	4233	0	4156	247	0
1	C	4233	0	4156	250	0
1	D	4233	0	4155	223	0
1	E	4233	0	4156	228	0
1	F	4233	0	4156	229	0
All	All	25398	0	24935	1383	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 27.

All (1383) 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:A:287:THR:HB	1:A:297:LEU:CD1	1.13	1.55
1:B:169:ASN:HD21	1:B:182:ASP:N	1.09	1.48
1:A:287:THR:CB	1:A:297:LEU:CD1	1.94	1.45
1:B:169:ASN:CG	1:B:182:ASP:HB2	1.02	1.41
1:C:287:THR:CB	1:C:297:LEU:HD11	1.53	1.39
1:D:169:ASN:OD1	1:D:182:ASP:CB	1.70	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ASN:CG	1:B:182:ASP:CB	1.98	1.37
1:B:287:THR:CB	1:B:297:LEU:HD11	1.56	1.33
1:C:287:THR:HB	1:C:297:LEU:CD1	1.57	1.32
1:A:287:THR:OG1	1:A:297:LEU:HG	1.22	1.30
1:B:287:THR:HB	1:B:297:LEU:CD1	1.59	1.30
1:E:123:PRO:HG2	1:E:156:GLU:OE2	1.14	1.29
1:B:289:CYS:CB	1:B:294:VAL:HG11	1.66	1.25
1:A:287:THR:CB	1:A:297:LEU:CG	2.15	1.25
1:C:289:CYS:CB	1:C:294:VAL:HG11	1.66	1.24
1:A:287:THR:CB	1:A:297:LEU:HG	1.65	1.24
1:B:169:ASN:OD1	1:B:182:ASP:HB2	1.28	1.24
1:F:123:PRO:CG	1:F:156:GLU:OE2	1.85	1.24
1:A:287:THR:CG2	1:A:297:LEU:HD12	1.69	1.22
1:C:287:THR:CB	1:C:297:LEU:CD1	2.15	1.21
1:B:169:ASN:ND2	1:B:182:ASP:N	1.90	1.19
1:D:289:CYS:SG	1:D:294:VAL:HG11	1.83	1.18
1:A:178:ASP:HB2	1:A:179:MET:HB2	1.19	1.17
1:B:183:MET:O	1:B:187:TYR:CD2	1.98	1.17
1:A:398:GLU:OE1	1:A:399:PRO:HD2	1.45	1.16
1:B:169:ASN:ND2	1:B:182:ASP:HB2	1.60	1.16
1:F:156:GLU:HG2	1:F:159:ASP:HB2	1.23	1.15
1:F:239:ILE:CD1	1:F:288:VAL:HG13	1.75	1.15
1:B:287:THR:CB	1:B:297:LEU:CD1	2.18	1.14
1:E:289:CYS:HB2	1:E:294:VAL:HG11	1.30	1.13
1:A:287:THR:HB	1:A:297:LEU:HD12	1.27	1.13
1:B:289:CYS:HB2	1:B:294:VAL:HG11	1.13	1.13
1:C:289:CYS:SG	1:C:294:VAL:HG11	1.89	1.12
1:C:178:ASP:HB2	1:C:179:MET:HB2	1.25	1.12
1:C:287:THR:CG2	1:C:297:LEU:HD12	1.79	1.12
1:D:169:ASN:OD1	1:D:182:ASP:HB2	0.96	1.11
1:F:123:PRO:HG2	1:F:156:GLU:OE2	0.94	1.11
1:A:156:GLU:HG3	1:A:159:ASP:HB2	1.22	1.10
1:B:289:CYS:SG	1:B:294:VAL:HG11	1.91	1.10
1:C:289:CYS:HB2	1:C:294:VAL:HG11	1.16	1.10
1:F:239:ILE:HD13	1:F:288:VAL:HG13	1.26	1.09
1:C:287:THR:HG21	1:C:297:LEU:HD12	1.33	1.09
1:E:178:ASP:HB2	1:E:179:MET:HB2	1.26	1.09
1:B:287:THR:CG2	1:B:297:LEU:HD12	1.82	1.09
1:D:178:ASP:HB2	1:D:179:MET:HB2	1.34	1.09
1:E:123:PRO:CG	1:E:156:GLU:OE2	1.99	1.09
1:A:287:THR:HB	1:A:297:LEU:CG	1.81	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:THR:HG21	1:A:297:LEU:HB2	1.23	1.08
1:D:97:LEU:CD2	1:D:148:PHE:HZ	1.65	1.08
1:B:178:ASP:HB2	1:B:179:MET:HB2	1.27	1.08
1:F:178:ASP:HB2	1:F:179:MET:HB2	1.25	1.08
1:A:289:CYS:HB2	1:A:294:VAL:HG11	1.20	1.08
1:B:169:ASN:OD1	1:B:182:ASP:CB	1.93	1.08
1:A:123:PRO:HG2	1:A:156:GLU:OE1	1.54	1.07
1:F:289:CYS:HB2	1:F:294:VAL:HG11	1.35	1.07
1:E:156:GLU:HG2	1:E:159:ASP:HB2	1.07	1.07
1:C:287:THR:CG2	1:C:297:LEU:CD1	2.32	1.07
1:B:287:THR:CG2	1:B:297:LEU:CD1	2.34	1.05
1:B:169:ASN:HD21	1:B:182:ASP:CA	1.68	1.05
1:C:305:PRO:HG3	1:C:346:ARG:HG3	1.33	1.05
1:B:305:PRO:HG3	1:B:346:ARG:HG3	1.30	1.05
1:D:160:PHE:CE2	1:D:162:ILE:HD12	1.91	1.04
1:D:123:PRO:HG2	1:D:156:GLU:OE1	1.56	1.04
1:A:287:THR:CB	1:A:297:LEU:HD12	1.71	1.04
1:C:156:GLU:HG2	1:C:159:ASP:HB2	1.38	1.04
1:B:287:THR:HG21	1:B:297:LEU:HD12	1.35	1.03
1:C:157:GLN:HG2	1:D:599:ARG:HD3	1.41	1.03
1:B:156:GLU:HG2	1:B:159:ASP:HB2	1.37	1.02
1:F:287:THR:HG21	1:F:297:LEU:HG	1.41	1.01
1:B:289:CYS:SG	1:B:294:VAL:CG1	2.49	1.00
1:B:156:GLU:HA	1:B:158:LEU:N	1.77	1.00
1:C:156:GLU:HA	1:C:158:LEU:N	1.77	1.00
1:F:160:PHE:CE2	1:F:162:ILE:HD12	1.96	1.00
1:A:124:ILE:HA	1:A:161:PRO:CB	1.90	1.00
1:A:287:THR:HG21	1:A:297:LEU:CB	1.89	1.00
1:C:289:CYS:SG	1:C:294:VAL:CG1	2.48	1.00
1:E:156:GLU:HA	1:E:158:LEU:N	1.77	1.00
1:D:169:ASN:CG	1:D:182:ASP:CB	2.34	1.00
1:F:156:GLU:HA	1:F:158:LEU:N	1.77	1.00
1:A:156:GLU:HG3	1:A:159:ASP:CB	1.92	1.00
1:A:178:ASP:CB	1:A:179:MET:HB2	1.91	1.00
1:B:156:GLU:CG	1:B:159:ASP:HB2	1.92	0.99
1:C:156:GLU:CG	1:C:159:ASP:HB2	1.92	0.99
1:D:156:GLU:HA	1:D:158:LEU:N	1.78	0.99
1:B:169:ASN:ND2	1:B:182:ASP:CB	2.18	0.99
1:A:156:GLU:HA	1:A:158:LEU:N	1.77	0.99
1:B:160:PHE:CD2	1:B:162:ILE:HD12	1.98	0.99
1:A:160:PHE:CE2	1:A:162:ILE:HD12	1.97	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ILE:HD12	1:A:296:ALA:HB1	1.43	0.98
1:D:124:ILE:HA	1:D:161:PRO:CB	1.93	0.98
1:C:289:CYS:HB2	1:C:294:VAL:CG1	1.94	0.98
1:B:289:CYS:HB2	1:B:294:VAL:CG1	1.92	0.98
1:E:160:PHE:CE2	1:E:162:ILE:HD12	1.99	0.98
1:F:289:CYS:CB	1:F:294:VAL:HG11	1.92	0.98
1:C:169:ASN:ND2	1:C:182:ASP:O	1.97	0.97
1:B:294:VAL:HG12	1:B:295:GLU:H	1.26	0.97
1:B:169:ASN:ND2	1:B:182:ASP:CA	2.25	0.97
1:B:306:THR:CA	1:B:388:ILE:HD12	1.94	0.97
1:C:294:VAL:HG12	1:C:295:GLU:H	1.24	0.97
1:C:160:PHE:CD2	1:C:162:ILE:HD12	1.99	0.97
1:D:124:ILE:HG23	1:D:161:PRO:HA	1.46	0.97
1:E:294:VAL:HG12	1:E:295:GLU:H	1.27	0.97
1:E:289:CYS:CB	1:E:294:VAL:HG11	1.94	0.96
1:D:156:GLU:HG3	1:D:159:ASP:HB2	1.47	0.96
1:D:156:GLU:CG	1:D:159:ASP:HB2	1.95	0.96
1:E:169:ASN:ND2	1:E:182:ASP:O	1.97	0.96
1:F:169:ASN:ND2	1:F:182:ASP:O	1.97	0.96
1:A:124:ILE:HG23	1:A:161:PRO:HA	1.48	0.96
1:A:287:THR:HB	1:A:297:LEU:HD11	0.97	0.95
1:A:176:HIS:CG	1:A:177:GLU:HA	2.02	0.95
1:B:166:SER:N	1:B:182:ASP:OD2	2.00	0.95
1:D:97:LEU:CD2	1:D:148:PHE:CZ	2.49	0.95
1:C:160:PHE:CD1	1:C:162:ILE:HB	2.03	0.94
1:F:160:PHE:CD2	1:F:162:ILE:HD12	2.03	0.94
1:B:160:PHE:CD1	1:B:162:ILE:HB	2.02	0.94
1:C:287:THR:HG21	1:C:297:LEU:CD1	1.95	0.94
1:D:160:PHE:CD1	1:D:162:ILE:HB	2.02	0.93
1:B:287:THR:HG21	1:B:297:LEU:CD1	1.97	0.93
1:C:306:THR:CA	1:C:388:ILE:HD12	1.98	0.93
1:A:160:PHE:CD1	1:A:162:ILE:HB	2.04	0.93
1:B:122:LYS:NZ	1:B:158:LEU:O	2.00	0.93
1:E:156:GLU:CG	1:E:159:ASP:HB2	1.99	0.93
1:A:50:LYS:HE3	1:A:51:GLU:HG3	1.50	0.93
1:C:122:LYS:NZ	1:C:158:LEU:O	2.01	0.92
1:D:97:LEU:HD23	1:D:148:PHE:HZ	1.30	0.92
1:F:156:GLU:CG	1:F:159:ASP:HB2	1.97	0.92
1:D:305:PRO:HD2	1:D:390:ARG:CZ	1.99	0.92
1:A:169:ASN:HD21	1:A:182:ASP:C	1.78	0.92
1:E:160:PHE:CD2	1:E:162:ILE:HD12	2.05	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:ASN:CG	1:D:182:ASP:HB2	1.94	0.91
1:D:160:PHE:CD2	1:D:162:ILE:HD12	2.05	0.91
1:A:287:THR:HG1	1:A:297:LEU:HG	1.22	0.91
1:E:156:GLU:HA	1:E:158:LEU:H	1.35	0.91
1:C:160:PHE:CE2	1:C:162:ILE:HD12	2.06	0.90
1:E:156:GLU:HG2	1:E:159:ASP:CB	2.01	0.90
1:C:178:ASP:CB	1:C:179:MET:HB2	2.02	0.90
1:A:287:THR:CG2	1:A:297:LEU:CD1	2.39	0.90
1:A:289:CYS:CB	1:A:294:VAL:HG11	2.02	0.90
1:F:178:ASP:CB	1:F:179:MET:HB2	2.02	0.90
1:B:183:MET:O	1:B:187:TYR:HD2	1.42	0.89
1:D:160:PHE:CE1	1:D:162:ILE:HB	2.07	0.89
1:F:123:PRO:HG2	1:F:156:GLU:CD	1.96	0.89
1:F:52:ARG:HB3	1:F:53:GLY:HA3	1.55	0.89
1:E:52:ARG:HB3	1:E:53:GLY:HA3	1.55	0.89
1:E:178:ASP:CB	1:E:179:MET:HB2	2.02	0.89
1:B:160:PHE:CE2	1:B:162:ILE:HD12	2.07	0.89
1:B:169:ASN:HD21	1:B:182:ASP:H	1.17	0.89
1:B:178:ASP:CB	1:B:179:MET:HB2	2.03	0.88
1:F:294:VAL:HG12	1:F:295:GLU:H	1.37	0.88
1:F:239:ILE:HD12	1:F:288:VAL:HG22	1.54	0.88
1:F:287:THR:HB	1:F:297:LEU:HD11	1.52	0.88
1:E:160:PHE:CD1	1:E:162:ILE:HB	2.08	0.88
1:D:156:GLU:HA	1:D:158:LEU:H	1.38	0.88
1:C:147:LEU:HA	1:C:150:ASN:OD1	1.74	0.88
1:B:52:ARG:HB3	1:B:53:GLY:HA3	1.55	0.88
1:E:296:ALA:C	1:E:297:LEU:HD23	1.98	0.88
1:F:160:PHE:CD1	1:F:162:ILE:HB	2.09	0.88
1:A:153:ALA:HB3	1:A:154:THR:C	1.99	0.88
1:A:160:PHE:CD2	1:A:162:ILE:HD12	2.09	0.88
1:C:50:LYS:HE3	1:C:51:GLU:HG3	1.56	0.88
1:D:169:ASN:ND2	1:D:182:ASP:O	2.07	0.87
1:A:156:GLU:HA	1:A:158:LEU:H	1.39	0.87
1:D:153:ALA:HB3	1:D:154:THR:C	2.00	0.87
1:C:289:CYS:CB	1:C:294:VAL:CG1	2.51	0.86
1:E:169:ASN:HD21	1:E:182:ASP:C	1.83	0.86
1:F:169:ASN:HD21	1:F:182:ASP:C	1.83	0.86
1:A:54:ILE:CG2	1:A:55:THR:HG22	2.05	0.86
1:B:147:LEU:HA	1:B:150:ASN:OD1	1.75	0.86
1:C:54:ILE:CG2	1:C:55:THR:HG22	2.06	0.86
1:D:54:ILE:CG2	1:D:55:THR:HG22	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:153:ALA:HB3	1:F:154:THR:C	2.00	0.86
1:F:239:ILE:CD1	1:F:288:VAL:CG1	2.53	0.86
1:A:287:THR:HG22	1:A:297:LEU:HD12	1.58	0.86
1:A:160:PHE:CE1	1:A:162:ILE:HB	2.11	0.86
1:A:169:ASN:ND2	1:A:182:ASP:O	2.09	0.86
1:C:156:GLU:HA	1:C:158:LEU:H	1.40	0.86
1:E:153:ALA:HB3	1:E:154:THR:C	2.00	0.86
1:B:169:ASN:ND2	1:B:182:ASP:H	1.69	0.85
1:B:169:ASN:OD1	1:B:182:ASP:CG	2.19	0.85
1:B:289:CYS:CB	1:B:294:VAL:CG1	2.50	0.85
1:A:287:THR:CG2	1:A:297:LEU:CG	2.53	0.85
1:B:156:GLU:HA	1:B:158:LEU:H	1.40	0.85
1:B:160:PHE:CE1	1:B:162:ILE:HB	2.12	0.85
1:C:169:ASN:HD21	1:C:182:ASP:C	1.83	0.85
1:D:97:LEU:HD23	1:D:148:PHE:CZ	2.11	0.85
1:D:178:ASP:HB2	1:D:179:MET:CB	2.06	0.85
1:D:294:VAL:HG12	1:D:295:GLU:H	1.39	0.85
1:B:153:ALA:HB3	1:B:154:THR:C	2.02	0.84
1:B:61:THR:OG1	1:B:67:ASP:HA	1.78	0.84
1:C:174:LEU:HG	1:C:175:ASP:OD2	1.77	0.84
1:D:156:GLU:N	1:D:157:GLN:HB2	1.92	0.84
1:D:289:CYS:CB	1:D:294:VAL:HG11	2.07	0.84
1:B:1:MET:HE1	1:B:266:ASP:OD2	1.78	0.84
1:C:153:ALA:HB3	1:C:154:THR:C	2.02	0.84
1:A:61:THR:OG1	1:A:67:ASP:HA	1.78	0.84
1:D:169:ASN:CG	1:D:182:ASP:HB3	2.02	0.84
1:F:156:GLU:HA	1:F:158:LEU:H	1.40	0.84
1:C:22:VAL:CG1	1:C:56:ILE:HG21	2.08	0.84
1:D:61:THR:OG1	1:D:67:ASP:HA	1.78	0.84
1:E:123:PRO:HG2	1:E:156:GLU:CD	2.01	0.84
1:A:181:GLU:O	1:A:183:MET:N	2.11	0.83
1:C:160:PHE:CE1	1:C:162:ILE:HB	2.12	0.83
1:F:174:LEU:HG	1:F:175:ASP:OD2	1.77	0.83
1:A:294:VAL:HG12	1:A:295:GLU:H	1.42	0.83
1:F:61:THR:OG1	1:F:67:ASP:HA	1.77	0.83
1:C:61:THR:OG1	1:C:67:ASP:HA	1.78	0.83
1:A:287:THR:HG21	1:A:297:LEU:CG	2.08	0.83
1:A:176:HIS:NE2	1:A:177:GLU:OE1	2.12	0.83
1:B:25:LEU:HD23	1:B:183:MET:SD	2.18	0.83
1:D:289:CYS:SG	1:D:294:VAL:CG1	2.67	0.83
1:D:22:VAL:CG1	1:D:56:ILE:HG21	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:PHE:CE1	1:E:162:ILE:HB	2.14	0.82
1:E:61:THR:OG1	1:E:67:ASP:HA	1.78	0.82
1:F:160:PHE:CE1	1:F:162:ILE:HB	2.14	0.82
1:D:169:ASN:HD21	1:D:182:ASP:CA	1.92	0.82
1:F:178:ASP:HB2	1:F:179:MET:CB	2.09	0.82
1:E:178:ASP:HB2	1:E:179:MET:CB	2.09	0.82
1:D:157:GLN:HB3	1:D:158:LEU:HD12	1.61	0.82
1:D:169:ASN:HD21	1:D:182:ASP:C	1.88	0.82
1:E:300:LEU:HB2	1:E:301:SER:HA	1.61	0.82
1:A:169:ASN:HD21	1:A:182:ASP:CA	1.88	0.82
1:A:289:CYS:HB2	1:A:294:VAL:CG1	2.08	0.81
1:D:176:HIS:HA	1:D:177:GLU:C	2.05	0.81
1:A:287:THR:OG1	1:A:297:LEU:CG	2.15	0.81
1:D:157:GLN:O	1:D:159:ASP:HB3	1.80	0.81
1:D:169:ASN:OD1	1:D:182:ASP:HB3	1.78	0.81
1:F:160:PHE:CZ	1:F:162:ILE:HD12	2.14	0.81
1:E:174:LEU:HG	1:E:175:ASP:OD2	1.79	0.81
1:C:176:HIS:HA	1:C:177:GLU:C	2.05	0.81
1:F:176:HIS:HA	1:F:177:GLU:C	2.05	0.81
1:C:169:ASN:HD21	1:C:182:ASP:CA	1.93	0.81
1:D:178:ASP:CB	1:D:179:MET:HB2	2.11	0.81
1:D:50:LYS:HE3	1:D:51:GLU:HG3	1.63	0.81
1:A:177:GLU:N	1:A:178:ASP:HA	1.96	0.80
1:B:176:HIS:CG	1:B:177:GLU:HA	2.17	0.80
1:E:157:GLN:O	1:E:159:ASP:HB3	1.80	0.80
1:E:156:GLU:N	1:E:157:GLN:HB2	1.96	0.80
1:F:239:ILE:HD11	1:F:288:VAL:HG13	1.63	0.80
1:A:240:ILE:CD1	1:A:296:ALA:HB1	2.11	0.79
1:B:178:ASP:HB2	1:B:179:MET:CB	2.11	0.79
1:E:169:ASN:HD21	1:E:182:ASP:CA	1.93	0.79
1:F:156:GLU:N	1:F:157:GLN:HB2	1.97	0.79
1:B:176:HIS:HA	1:B:177:GLU:C	2.06	0.79
1:E:160:PHE:CZ	1:E:162:ILE:HD12	2.17	0.79
1:F:157:GLN:O	1:F:159:ASP:HB3	1.81	0.79
1:B:160:PHE:HA	1:B:161:PRO:C	2.08	0.79
1:F:169:ASN:HD21	1:F:182:ASP:CA	1.93	0.79
1:E:287:THR:HG21	1:E:297:LEU:HG	1.64	0.78
1:F:160:PHE:HA	1:F:161:PRO:C	2.08	0.78
1:B:287:THR:OG1	1:B:297:LEU:HG	1.83	0.78
1:E:176:HIS:HA	1:E:177:GLU:C	2.08	0.78
1:B:177:GLU:H	1:B:179:MET:HG3	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:ILE:CG2	1:D:161:PRO:HA	2.14	0.78
1:E:160:PHE:HA	1:E:161:PRO:C	2.08	0.78
1:B:306:THR:HA	1:B:388:ILE:HD12	1.67	0.77
1:F:287:THR:CG2	1:F:297:LEU:HG	2.14	0.77
1:A:160:PHE:HA	1:A:161:PRO:C	2.10	0.77
1:C:178:ASP:HB2	1:C:179:MET:CB	2.09	0.77
1:B:306:THR:N	1:B:388:ILE:HD12	1.99	0.77
1:C:158:LEU:HA	1:C:159:ASP:HB3	1.67	0.77
1:C:287:THR:OG1	1:C:297:LEU:HG	1.84	0.77
1:D:174:LEU:HG	1:D:175:ASP:OD2	1.85	0.77
1:A:117:PHE:CD2	1:A:152:ASP:O	2.37	0.77
1:A:156:GLU:CG	1:A:159:ASP:HB2	2.09	0.77
1:D:156:GLU:H	1:D:157:GLN:HB2	1.49	0.77
1:B:158:LEU:HA	1:B:159:ASP:HB3	1.66	0.76
1:E:239:ILE:CD1	1:E:288:VAL:HG13	2.15	0.76
1:E:300:LEU:HB2	1:E:301:SER:CA	2.16	0.76
1:A:50:LYS:CE	1:A:51:GLU:HG3	2.15	0.76
1:A:124:ILE:CG2	1:A:161:PRO:HA	2.15	0.76
1:C:160:PHE:HA	1:C:161:PRO:C	2.08	0.76
1:A:157:GLN:O	1:A:159:ASP:HB3	1.86	0.75
1:D:180:ALA:O	1:D:182:ASP:N	2.19	0.75
1:C:306:THR:N	1:C:388:ILE:HD12	2.01	0.75
1:E:294:VAL:C	1:E:295:GLU:HG2	2.10	0.75
1:E:300:LEU:HB3	1:E:304:GLU:HG3	1.67	0.75
1:D:158:LEU:HA	1:D:159:ASP:HB3	1.69	0.74
1:A:169:ASN:ND2	1:A:182:ASP:C	2.45	0.74
1:A:182:ASP:O	1:A:183:MET:HE2	1.88	0.74
1:B:181:GLU:O	1:B:183:MET:N	2.20	0.74
1:D:156:GLU:CA	1:D:157:GLN:HB2	2.17	0.74
1:A:174:LEU:HG	1:A:175:ASP:OD2	1.86	0.74
1:C:289:CYS:SG	1:C:294:VAL:HG12	2.27	0.74
1:A:22:VAL:CG1	1:A:56:ILE:HG21	2.18	0.73
1:E:287:THR:HB	1:E:297:LEU:CD1	2.19	0.73
1:F:163:VAL:HG13	1:F:176:HIS:CD2	2.24	0.73
1:F:297:LEU:HD23	1:F:297:LEU:N	2.03	0.73
1:A:54:ILE:HG22	1:A:55:THR:HG22	1.69	0.73
1:C:294:VAL:HG12	1:C:295:GLU:N	2.03	0.73
1:D:117:PHE:HZ	1:D:148:PHE:CD1	2.07	0.73
1:B:160:PHE:O	1:B:193:HIS:NE2	2.22	0.73
1:B:289:CYS:SG	1:B:294:VAL:HG12	2.28	0.73
1:B:294:VAL:C	1:B:295:GLU:HG2	2.13	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:297:LEU:HD23	1:E:297:LEU:N	2.03	0.73
1:C:54:ILE:HG22	1:C:55:THR:HG22	1.70	0.72
1:C:294:VAL:C	1:C:295:GLU:HG2	2.14	0.72
1:D:106:MET:O	1:D:109:THR:OG1	2.06	0.72
1:E:153:ALA:HB3	1:E:154:THR:CA	2.20	0.72
1:F:287:THR:HB	1:F:297:LEU:CD1	2.19	0.72
1:D:54:ILE:HG22	1:D:55:THR:HG22	1.70	0.72
1:D:289:CYS:HB2	1:D:294:VAL:HG11	1.69	0.72
1:C:306:THR:HA	1:C:388:ILE:HB	1.72	0.72
1:E:287:THR:HG21	1:E:297:LEU:CG	2.19	0.72
1:A:240:ILE:CD1	1:A:296:ALA:CB	2.67	0.72
1:C:156:GLU:N	1:C:157:GLN:HB2	2.05	0.71
1:F:240:ILE:HD12	1:F:287:THR:OG1	1.89	0.71
1:A:297:LEU:HD23	1:A:297:LEU:N	2.04	0.71
1:B:177:GLU:N	1:B:178:ASP:HA	2.04	0.71
1:B:183:MET:O	1:B:187:TYR:CE2	2.43	0.71
1:F:158:LEU:HA	1:F:159:ASP:HB3	1.71	0.71
1:D:156:GLU:HG2	1:D:159:ASP:HB2	1.70	0.71
1:E:87:ARG:NH2	1:E:300:LEU:O	2.23	0.71
1:F:153:ALA:HB3	1:F:154:THR:CA	2.21	0.71
1:D:22:VAL:CG1	1:D:56:ILE:HD13	2.21	0.71
1:C:22:VAL:CG1	1:C:56:ILE:HD13	2.21	0.71
1:C:160:PHE:O	1:C:193:HIS:NE2	2.22	0.71
1:A:176:HIS:HA	1:A:177:GLU:C	2.15	0.71
1:B:300:LEU:CB	1:B:301:SER:HA	2.19	0.71
1:D:160:PHE:HA	1:D:161:PRO:C	2.15	0.71
1:A:22:VAL:CG1	1:A:56:ILE:HD13	2.21	0.70
1:A:237:VAL:HA	1:A:291:THR:HG23	1.72	0.70
1:C:287:THR:CB	1:C:297:LEU:CG	2.69	0.70
1:F:277:THR:HB	1:F:281:GLU:N	2.06	0.70
1:A:178:ASP:CA	1:A:179:MET:HB2	2.20	0.70
1:C:222:GLY:O	1:C:223:ILE:O	2.09	0.70
1:C:300:LEU:CB	1:C:301:SER:HA	2.19	0.70
1:B:150:ASN:ND2	1:B:151:LEU:HD22	2.06	0.70
1:C:306:THR:HA	1:C:388:ILE:HD12	1.71	0.70
1:C:150:ASN:ND2	1:C:151:LEU:HD22	2.06	0.70
1:C:157:GLN:O	1:C:159:ASP:HB3	1.92	0.70
1:B:52:ARG:CB	1:B:53:GLY:HA3	2.21	0.70
1:B:306:THR:HB	1:B:472:TYR:OH	1.91	0.70
1:C:301:SER:O	1:C:302:VAL:HG13	1.92	0.70
1:D:153:ALA:HB3	1:D:154:THR:CA	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ALA:HB3	1:C:154:THR:CA	2.21	0.70
1:B:156:GLU:N	1:B:157:GLN:HB2	2.06	0.70
1:B:306:THR:HA	1:B:388:ILE:HB	1.72	0.70
1:F:52:ARG:CB	1:F:53:GLY:HA3	2.21	0.70
1:B:153:ALA:HB3	1:B:154:THR:CA	2.21	0.70
1:C:277:THR:HB	1:C:281:GLU:N	2.07	0.70
1:D:182:ASP:O	1:D:183:MET:HE2	1.92	0.70
1:E:158:LEU:HA	1:E:159:ASP:HB3	1.74	0.70
1:F:13:HIS:O	1:F:16:HIS:CE1	2.45	0.70
1:B:294:VAL:HG12	1:B:295:GLU:N	2.05	0.70
1:C:13:HIS:O	1:C:16:HIS:CE1	2.45	0.70
1:E:52:ARG:CB	1:E:53:GLY:HA3	2.21	0.70
1:D:169:ASN:HD21	1:D:182:ASP:N	1.89	0.69
1:F:239:ILE:CD1	1:F:288:VAL:HG22	2.21	0.69
1:E:182:ASP:O	1:E:183:MET:HE2	1.91	0.69
1:F:294:VAL:C	1:F:295:GLU:HG2	2.16	0.69
1:B:287:THR:CB	1:B:297:LEU:CG	2.70	0.69
1:F:287:THR:HG21	1:F:297:LEU:CG	2.20	0.69
1:B:13:HIS:O	1:B:16:HIS:CE1	2.46	0.69
1:C:54:ILE:HG23	1:C:55:THR:HG22	1.75	0.69
1:C:182:ASP:O	1:C:183:MET:HE2	1.91	0.69
1:E:13:HIS:O	1:E:16:HIS:CE1	2.45	0.69
1:C:50:LYS:CE	1:C:51:GLU:HG3	2.23	0.69
1:D:13:HIS:O	1:D:16:HIS:CE1	2.45	0.69
1:A:54:ILE:HG22	1:A:55:THR:CG2	2.23	0.69
1:B:301:SER:O	1:B:302:VAL:HG13	1.93	0.69
1:D:22:VAL:HG12	1:D:56:ILE:HG21	1.75	0.69
1:E:239:ILE:HD13	1:E:288:VAL:HG13	1.73	0.69
1:F:182:ASP:O	1:F:183:MET:HE2	1.91	0.69
1:B:157:GLN:O	1:B:159:ASP:HB3	1.93	0.69
1:D:54:ILE:HG22	1:D:55:THR:CG2	2.23	0.69
1:F:296:ALA:C	1:F:297:LEU:HD23	2.18	0.68
1:E:50:LYS:HE3	1:E:51:GLU:HG3	1.75	0.68
1:D:22:VAL:HG11	1:D:56:ILE:HD13	1.76	0.68
1:F:300:LEU:CB	1:F:301:SER:HA	2.23	0.68
1:C:292:GLN:O	1:C:294:VAL:HG23	1.94	0.68
1:D:277:THR:HB	1:D:281:GLU:N	2.07	0.68
1:C:54:ILE:HG22	1:C:55:THR:CG2	2.23	0.68
1:D:169:ASN:ND2	1:D:182:ASP:C	2.50	0.68
1:A:160:PHE:CZ	1:A:162:ILE:HD12	2.28	0.68
1:C:22:VAL:HG11	1:C:56:ILE:HD13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:287:THR:CB	1:E:297:LEU:HG	2.23	0.68
1:E:294:VAL:HG12	1:E:295:GLU:N	2.07	0.68
1:F:160:PHE:CG	1:F:162:ILE:HD12	2.29	0.68
1:F:169:ASN:ND2	1:F:182:ASP:C	2.47	0.68
1:A:13:HIS:O	1:A:16:HIS:CE1	2.46	0.68
1:E:150:ASN:ND2	1:E:151:LEU:HD22	2.07	0.68
1:E:277:THR:HB	1:E:281:GLU:N	2.09	0.68
1:F:239:ILE:HD13	1:F:288:VAL:CG1	2.13	0.67
1:E:160:PHE:CG	1:E:162:ILE:HD12	2.30	0.67
1:E:169:ASN:ND2	1:E:182:ASP:C	2.47	0.67
1:A:398:GLU:OE1	1:A:399:PRO:CD	2.34	0.67
1:A:145:PHE:O	1:A:148:PHE:HB3	1.94	0.67
1:B:179:MET:HE2	1:B:182:ASP:OD1	1.94	0.67
1:C:169:ASN:ND2	1:C:182:ASP:C	2.48	0.67
1:B:150:ASN:O	1:C:423:LYS:NZ	2.27	0.67
1:D:290:ASP:O	1:D:294:VAL:HG21	1.94	0.67
1:D:301:SER:O	1:D:302:VAL:HG13	1.94	0.67
1:A:153:ALA:HB3	1:A:154:THR:CA	2.24	0.67
1:B:160:PHE:O	1:B:193:HIS:CE1	2.48	0.67
1:A:156:GLU:N	1:A:157:GLN:HB2	2.10	0.67
1:B:145:PHE:O	1:B:148:PHE:HB3	1.95	0.67
1:B:277:THR:HB	1:B:281:GLU:N	2.09	0.67
1:B:297:LEU:N	1:B:297:LEU:HD23	2.10	0.67
1:E:287:THR:HB	1:E:297:LEU:HD11	1.76	0.67
1:A:54:ILE:HG23	1:A:55:THR:HG22	1.75	0.66
1:C:160:PHE:CG	1:C:162:ILE:HD12	2.30	0.66
1:D:54:ILE:HG23	1:D:55:THR:HG22	1.75	0.66
1:D:300:LEU:CB	1:D:301:SER:HA	2.22	0.66
1:F:50:LYS:HE3	1:F:51:GLU:HG3	1.77	0.66
1:C:22:VAL:HG12	1:C:56:ILE:HG21	1.75	0.66
1:B:50:LYS:HE3	1:B:51:GLU:HG3	1.75	0.66
1:F:240:ILE:CD1	1:F:287:THR:OG1	2.43	0.66
1:A:240:ILE:HD13	1:A:296:ALA:HB2	1.78	0.66
1:B:292:GLN:O	1:B:294:VAL:HG23	1.96	0.66
1:A:22:VAL:HG11	1:A:56:ILE:HD13	1.78	0.66
1:A:296:ALA:C	1:A:297:LEU:HD23	2.20	0.66
1:E:300:LEU:N	1:E:300:LEU:HD12	2.11	0.66
1:B:300:LEU:HB2	1:B:301:SER:HA	1.77	0.66
1:C:306:THR:HB	1:C:472:TYR:OH	1.95	0.66
1:A:294:VAL:C	1:A:295:GLU:HG2	2.20	0.65
1:B:160:PHE:CG	1:B:162:ILE:HD12	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:PHE:HZ	1:D:148:PHE:CE1	2.13	0.65
1:C:160:PHE:O	1:C:193:HIS:CE1	2.48	0.65
1:A:277:THR:HB	1:A:281:GLU:N	2.10	0.65
1:C:145:PHE:O	1:C:148:PHE:HB3	1.94	0.65
1:F:181:GLU:O	1:F:183:MET:N	2.30	0.65
1:F:373:MET:O	1:F:378:PHE:HB2	1.96	0.65
1:E:163:VAL:HG13	1:E:176:HIS:CD2	2.32	0.65
1:E:287:THR:CG2	1:E:297:LEU:HG	2.25	0.65
1:A:174:LEU:HD23	1:A:174:LEU:H	1.62	0.65
1:C:300:LEU:HB2	1:C:301:SER:HA	1.77	0.65
1:E:181:GLU:O	1:E:183:MET:N	2.30	0.65
1:B:165:ALA:HA	1:B:182:ASP:OD2	1.97	0.65
1:C:373:MET:O	1:C:378:PHE:HB2	1.97	0.65
1:E:373:MET:O	1:E:378:PHE:HB2	1.97	0.65
1:B:287:THR:HG21	1:B:297:LEU:CG	2.27	0.64
1:F:239:ILE:HD11	1:F:288:VAL:CG1	2.24	0.64
1:A:123:PRO:CG	1:A:156:GLU:OE1	2.40	0.64
1:B:158:LEU:CA	1:B:159:ASP:HB3	2.27	0.64
1:A:300:LEU:CB	1:A:301:SER:HA	2.25	0.64
1:A:249:ALA:HB3	1:A:275:ALA:HB2	1.80	0.64
1:C:177:GLU:N	1:C:178:ASP:HA	2.13	0.64
1:C:297:LEU:N	1:C:297:LEU:HD23	2.12	0.64
1:D:373:MET:O	1:D:378:PHE:HB2	1.97	0.64
1:F:150:ASN:ND2	1:F:151:LEU:HD22	2.12	0.64
1:A:176:HIS:ND1	1:A:177:GLU:HA	2.12	0.64
1:B:176:HIS:NE2	1:B:177:GLU:OE1	2.31	0.64
1:D:177:GLU:CB	1:D:178:ASP:HA	2.25	0.64
1:D:249:ALA:HB3	1:D:275:ALA:HB2	1.80	0.64
1:C:287:THR:HG21	1:C:297:LEU:CG	2.27	0.64
1:E:177:GLU:N	1:E:178:ASP:HA	2.12	0.64
1:B:249:ALA:HB3	1:B:275:ALA:HB2	1.80	0.64
1:D:169:ASN:ND2	1:D:182:ASP:CB	2.61	0.64
1:F:249:ALA:HB3	1:F:275:ALA:HB2	1.80	0.64
1:A:151:LEU:O	1:A:152:ASP:HB2	1.97	0.63
1:C:157:GLN:C	1:C:159:ASP:HB3	2.23	0.63
1:C:181:GLU:O	1:C:183:MET:N	2.30	0.63
1:B:373:MET:O	1:B:378:PHE:HB2	1.97	0.63
1:A:22:VAL:HG12	1:A:56:ILE:HG21	1.80	0.63
1:A:373:MET:O	1:A:378:PHE:HB2	1.98	0.63
1:E:249:ALA:HB3	1:E:275:ALA:HB2	1.80	0.63
1:D:155:ASP:O	1:D:156:GLU:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:GLU:H	1:E:179:MET:HG3	1.64	0.63
1:A:22:VAL:HG11	1:A:56:ILE:CD1	2.29	0.63
1:B:423:LYS:NZ	1:C:150:ASN:O	2.32	0.63
1:C:158:LEU:CA	1:C:159:ASP:HB3	2.28	0.63
1:F:177:GLU:N	1:F:178:ASP:HA	2.13	0.63
1:C:249:ALA:HB3	1:C:275:ALA:HB2	1.80	0.63
1:E:123:PRO:HG3	1:E:148:PHE:HZ	1.63	0.63
1:B:157:GLN:C	1:B:159:ASP:HB3	2.24	0.62
1:D:181:GLU:O	1:D:183:MET:N	2.31	0.62
1:F:160:PHE:HA	1:F:162:ILE:HG13	1.81	0.62
1:F:180:ALA:O	1:F:182:ASP:N	2.32	0.62
1:B:169:ASN:CG	1:B:182:ASP:H	2.07	0.62
1:B:432:ASP:O	1:B:434:LYS:N	2.33	0.62
1:C:180:ALA:O	1:C:182:ASP:N	2.32	0.62
1:C:287:THR:OG1	1:C:297:LEU:CG	2.47	0.62
1:E:180:ALA:O	1:E:182:ASP:N	2.32	0.62
1:F:432:ASP:O	1:F:434:LYS:N	2.32	0.62
1:B:287:THR:OG1	1:B:297:LEU:CG	2.47	0.62
1:E:432:ASP:O	1:E:434:LYS:N	2.32	0.62
1:A:287:THR:CG2	1:A:297:LEU:HG	2.23	0.62
1:A:300:LEU:HB2	1:A:301:SER:HA	1.80	0.62
1:A:50:LYS:HD3	1:A:51:GLU:HB2	1.81	0.61
1:A:117:PHE:HD2	1:A:152:ASP:O	1.83	0.61
1:C:50:LYS:HD3	1:C:51:GLU:HB2	1.81	0.61
1:D:300:LEU:HB2	1:D:301:SER:HA	1.81	0.61
1:E:123:PRO:CB	1:E:156:GLU:OE2	2.47	0.61
1:F:157:GLN:HB3	1:F:158:LEU:HD12	1.83	0.61
1:D:22:VAL:HG11	1:D:56:ILE:CD1	2.31	0.61
1:A:176:HIS:CD2	1:A:177:GLU:HA	2.35	0.61
1:A:287:THR:CB	1:A:297:LEU:HD11	1.93	0.61
1:E:160:PHE:HA	1:E:162:ILE:HG13	1.82	0.61
1:A:432:ASP:O	1:A:434:LYS:N	2.32	0.61
1:D:432:ASP:O	1:D:434:LYS:N	2.33	0.61
1:F:123:PRO:HG3	1:F:148:PHE:HZ	1.65	0.61
1:A:123:PRO:HG2	1:A:156:GLU:CD	2.24	0.61
1:E:157:GLN:C	1:E:159:ASP:HB3	2.24	0.61
1:D:169:ASN:ND2	1:D:182:ASP:CA	2.63	0.61
1:F:289:CYS:SG	1:F:294:VAL:HG11	2.41	0.61
1:C:160:PHE:HD1	1:C:161:PRO:O	1.85	0.60
1:C:22:VAL:HG11	1:C:56:ILE:CD1	2.30	0.60
1:C:432:ASP:O	1:C:434:LYS:N	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:MET:HE2	1:D:182:ASP:OD1	2.00	0.60
1:E:162:ILE:HG22	1:E:162:ILE:O	2.02	0.60
1:C:160:PHE:HA	1:C:162:ILE:HG13	1.82	0.60
1:F:162:ILE:HG22	1:F:162:ILE:O	2.02	0.60
1:B:160:PHE:HA	1:B:162:ILE:HG13	1.84	0.60
1:E:240:ILE:HD12	1:E:287:THR:OG1	2.01	0.60
1:B:107:PRO:HB2	1:C:417:GLN:HG3	1.83	0.60
1:A:155:ASP:O	1:A:156:GLU:HB3	2.00	0.60
1:C:174:LEU:HD23	1:C:174:LEU:H	1.66	0.60
1:F:174:LEU:HD23	1:F:174:LEU:H	1.66	0.60
1:A:153:ALA:N	1:A:154:THR:HA	2.16	0.60
1:D:176:HIS:HA	1:D:177:GLU:O	2.02	0.60
1:E:22:VAL:CG1	1:E:56:ILE:HG21	2.32	0.60
1:E:160:PHE:HD1	1:E:161:PRO:O	1.85	0.60
1:B:156:GLU:HG3	1:B:159:ASP:HB2	1.79	0.59
1:B:287:THR:HB	1:B:297:LEU:HD11	0.71	0.59
1:D:153:ALA:H	1:D:154:THR:HA	1.67	0.59
1:D:156:GLU:HG3	1:D:159:ASP:CB	2.25	0.59
1:D:158:LEU:HA	1:D:159:ASP:C	2.26	0.59
1:A:160:PHE:CE1	1:A:162:ILE:CB	2.86	0.59
1:C:156:GLU:HG3	1:C:159:ASP:HB2	1.80	0.59
1:F:160:PHE:CE1	1:F:162:ILE:CB	2.86	0.59
1:F:22:VAL:CG1	1:F:56:ILE:HG21	2.32	0.59
1:B:160:PHE:HD1	1:B:161:PRO:O	1.85	0.59
1:C:177:GLU:H	1:C:179:MET:HG3	1.67	0.59
1:D:157:GLN:C	1:D:159:ASP:HB3	2.27	0.59
1:E:160:PHE:CE1	1:E:162:ILE:CB	2.86	0.59
1:A:177:GLU:H	1:A:179:MET:HG3	1.66	0.59
1:D:153:ALA:N	1:D:154:THR:HA	2.18	0.59
1:F:153:ALA:H	1:F:154:THR:HA	1.68	0.59
1:F:160:PHE:HD1	1:F:161:PRO:O	1.86	0.59
1:B:22:VAL:CG1	1:B:56:ILE:HG21	2.33	0.59
1:D:10:ILE:O	1:D:75:THR:OG1	2.20	0.59
1:D:50:LYS:CE	1:D:51:GLU:HG3	2.32	0.59
1:F:160:PHE:CE1	1:F:162:ILE:HD12	2.38	0.59
1:A:197:PRO:O	1:A:199:VAL:HG22	2.03	0.59
1:B:417:GLN:HG3	1:C:107:PRO:HB2	1.85	0.59
1:C:158:LEU:HA	1:C:159:ASP:C	2.28	0.59
1:C:162:ILE:HG22	1:C:162:ILE:O	2.02	0.59
1:A:158:LEU:HA	1:A:159:ASP:HB3	1.85	0.58
1:D:197:PRO:O	1:D:199:VAL:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:179:MET:HE2	1:F:182:ASP:CG	2.27	0.58
1:B:162:ILE:O	1:B:162:ILE:HG22	2.02	0.58
1:D:160:PHE:CE1	1:D:162:ILE:CB	2.86	0.58
1:E:156:GLU:HG3	1:E:159:ASP:N	2.18	0.58
1:A:158:LEU:HA	1:A:159:ASP:C	2.27	0.58
1:F:177:GLU:H	1:F:179:MET:HG3	1.68	0.58
1:F:153:ALA:N	1:F:154:THR:HA	2.19	0.58
1:F:174:LEU:HD23	1:F:174:LEU:N	2.18	0.58
1:B:307:VAL:N	1:B:388:ILE:HD12	2.18	0.58
1:D:290:ASP:O	1:D:294:VAL:CG2	2.51	0.58
1:E:153:ALA:H	1:E:154:THR:HA	1.68	0.58
1:E:158:LEU:HA	1:E:159:ASP:C	2.28	0.58
1:E:197:PRO:O	1:E:199:VAL:HG22	2.03	0.58
1:F:300:LEU:HB2	1:F:301:SER:HA	1.85	0.58
1:A:158:LEU:HA	1:A:159:ASP:CB	2.33	0.58
1:C:179:MET:HE2	1:C:182:ASP:CG	2.28	0.58
1:C:197:PRO:O	1:C:199:VAL:HG22	2.03	0.58
1:F:123:PRO:CB	1:F:156:GLU:OE2	2.49	0.58
1:F:197:PRO:O	1:F:199:VAL:HG22	2.03	0.58
1:A:287:THR:HG21	1:A:297:LEU:CD1	2.31	0.58
1:B:153:ALA:N	1:B:154:THR:HA	2.18	0.58
1:C:145:PHE:O	1:C:146:ASP:C	2.47	0.58
1:E:160:PHE:CE1	1:E:162:ILE:HD12	2.39	0.58
1:C:1:MET:HE1	1:C:266:ASP:OD2	2.04	0.58
1:D:179:MET:HE2	1:D:182:ASP:CG	2.29	0.58
1:F:157:GLN:C	1:F:159:ASP:HB3	2.28	0.58
1:F:169:ASN:HD21	1:F:182:ASP:N	2.02	0.58
1:B:158:LEU:HA	1:B:159:ASP:C	2.28	0.58
1:B:197:PRO:O	1:B:199:VAL:HG22	2.03	0.58
1:E:169:ASN:HD21	1:E:182:ASP:N	2.02	0.58
1:A:240:ILE:HD13	1:A:296:ALA:CB	2.32	0.57
1:B:306:THR:C	1:B:388:ILE:HD12	2.29	0.57
1:C:307:VAL:N	1:C:388:ILE:HD12	2.19	0.57
1:F:85:VAL:HG12	1:F:89:MET:HE2	1.87	0.57
1:A:156:GLU:HA	1:A:157:GLN:C	2.26	0.57
1:B:131:ASP:OD2	1:B:166:SER:OG	2.20	0.57
1:E:85:VAL:HG12	1:E:89:MET:HE2	1.87	0.57
1:C:153:ALA:N	1:C:154:THR:HA	2.18	0.57
1:C:169:ASN:HD21	1:C:182:ASP:N	2.02	0.57
1:F:239:ILE:HD12	1:F:288:VAL:CG2	2.30	0.57
1:A:145:PHE:O	1:A:146:ASP:C	2.47	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:LEU:HA	1:F:159:ASP:C	2.28	0.57
1:F:179:MET:HE2	1:F:182:ASP:OD1	2.04	0.57
1:D:178:ASP:HB2	1:D:179:MET:CG	2.34	0.57
1:E:157:GLN:HB3	1:E:158:LEU:HD12	1.86	0.57
1:C:174:LEU:HD23	1:C:174:LEU:N	2.19	0.57
1:A:178:ASP:HB2	1:A:179:MET:CB	2.13	0.57
1:C:160:PHE:CD1	1:C:162:ILE:CB	2.86	0.57
1:E:153:ALA:N	1:E:154:THR:HA	2.20	0.57
1:D:97:LEU:HD21	1:D:148:PHE:CZ	2.39	0.56
1:E:145:PHE:O	1:E:146:ASP:C	2.47	0.56
1:E:176:HIS:CG	1:E:177:GLU:HA	2.40	0.56
1:E:300:LEU:HB2	1:E:301:SER:C	2.30	0.56
1:F:52:ARG:HB3	1:F:53:GLY:CA	2.33	0.56
1:F:176:HIS:CG	1:F:177:GLU:HA	2.40	0.56
1:F:298:PRO:O	1:F:299:ALA:HB3	2.05	0.56
1:F:156:GLU:HG2	1:F:159:ASP:CB	2.16	0.56
1:A:176:HIS:CG	1:A:177:GLU:CA	2.86	0.56
1:A:180:ALA:O	1:A:182:ASP:N	2.38	0.56
1:C:176:HIS:CG	1:C:177:GLU:HA	2.41	0.56
1:D:162:ILE:O	1:D:162:ILE:HG22	2.05	0.56
1:D:298:PRO:O	1:D:299:ALA:HB3	2.05	0.56
1:F:145:PHE:O	1:F:146:ASP:C	2.48	0.56
1:F:158:LEU:HA	1:F:159:ASP:CB	2.31	0.56
1:D:158:LEU:CA	1:D:159:ASP:HB3	2.35	0.56
1:E:52:ARG:HB3	1:E:53:GLY:CA	2.33	0.56
1:E:175:ASP:O	1:E:178:ASP:HB3	2.05	0.56
1:E:174:LEU:H	1:E:174:LEU:HD23	1.70	0.56
1:F:289:CYS:SG	1:F:294:VAL:CG1	2.94	0.56
1:D:304:GLU:CD	1:D:390:ARG:CZ	2.79	0.56
1:C:85:VAL:HG12	1:C:89:MET:HE2	1.87	0.56
1:E:237:VAL:HA	1:E:291:THR:HG23	1.86	0.56
1:C:160:PHE:CZ	1:C:162:ILE:HD12	2.41	0.56
1:E:153:ALA:HB3	1:E:154:THR:HA	1.87	0.56
1:F:350:THR:OG1	1:F:352:ASP:O	2.23	0.56
1:B:85:VAL:HG12	1:B:89:MET:HE2	1.86	0.56
1:B:177:GLU:N	1:B:179:MET:HG3	2.18	0.56
1:C:296:ALA:C	1:C:297:LEU:HD23	2.31	0.56
1:D:12:ALA:HB3	1:D:18:LYS:HG3	1.88	0.56
1:D:131:ASP:OD2	1:D:166:SER:OG	2.21	0.56
1:E:107:PRO:HB2	1:F:417:GLN:HG3	1.87	0.56
1:E:287:THR:CG2	1:E:297:LEU:HD12	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:350:THR:OG1	1:E:352:ASP:O	2.23	0.56
1:C:157:GLN:CG	1:D:599:ARG:HD3	2.27	0.56
1:E:160:PHE:CD1	1:E:162:ILE:CB	2.87	0.56
1:F:213:ASP:HA	1:F:340:VAL:HG22	1.88	0.56
1:D:150:ASN:ND2	1:D:151:LEU:HD22	2.19	0.55
1:F:240:ILE:HD12	1:F:296:ALA:HB1	1.88	0.55
1:C:179:MET:HE2	1:C:182:ASP:OD1	2.06	0.55
1:E:179:MET:HE2	1:E:182:ASP:CG	2.31	0.55
1:A:176:HIS:O	1:A:179:MET:HE3	2.06	0.55
1:D:85:VAL:HG12	1:D:89:MET:HE2	1.86	0.55
1:A:85:VAL:HG12	1:A:89:MET:HE2	1.86	0.55
1:C:287:THR:HB	1:C:297:LEU:HD11	0.68	0.55
1:B:145:PHE:O	1:B:146:ASP:C	2.47	0.55
1:C:175:ASP:O	1:C:178:ASP:HB3	2.07	0.55
1:D:145:PHE:O	1:D:146:ASP:C	2.47	0.55
1:F:238:THR:OG1	1:F:291:THR:HG22	2.07	0.55
1:E:300:LEU:HB2	1:E:301:SER:O	2.06	0.55
1:B:124:ILE:HG23	1:B:161:PRO:CB	2.36	0.55
1:D:179:MET:O	1:D:180:ALA:HB2	2.05	0.55
1:E:206:GLN:CD	1:E:297:LEU:HD22	2.31	0.55
1:B:176:HIS:ND1	1:B:177:GLU:HA	2.22	0.55
1:C:298:PRO:O	1:C:299:ALA:HB3	2.07	0.55
1:C:350:THR:OG1	1:C:352:ASP:O	2.23	0.55
1:D:13:HIS:C	1:D:16:HIS:CE1	2.85	0.55
1:E:213:ASP:HA	1:E:340:VAL:HG22	1.89	0.55
1:F:206:GLN:CG	1:F:297:LEU:HD22	2.37	0.55
1:B:165:ALA:C	1:B:182:ASP:OD2	2.50	0.55
1:B:306:THR:HA	1:B:388:ILE:CD1	2.34	0.55
1:C:13:HIS:C	1:C:16:HIS:CE1	2.85	0.55
1:C:158:LEU:HA	1:C:159:ASP:CB	2.31	0.55
1:E:417:GLN:HG3	1:F:107:PRO:HB2	1.88	0.55
1:F:175:ASP:O	1:F:178:ASP:HB3	2.06	0.55
1:A:175:ASP:O	1:A:178:ASP:HB3	2.07	0.55
1:A:213:ASP:HA	1:A:340:VAL:HG22	1.89	0.55
1:B:153:ALA:HB3	1:B:154:THR:HA	1.88	0.55
1:D:50:LYS:HD3	1:D:51:GLU:HB2	1.88	0.55
1:A:53:GLY:O	1:A:74:ASP:HB2	2.08	0.54
1:B:153:ALA:H	1:B:154:THR:HA	1.72	0.54
1:B:294:VAL:CG1	1:B:295:GLU:H	2.10	0.54
1:E:156:GLU:CA	1:E:157:GLN:CB	2.85	0.54
1:F:12:ALA:HB3	1:F:18:LYS:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:LEU:CA	1:F:159:ASP:HB3	2.37	0.54
1:B:277:THR:OG1	1:B:282:LEU:N	2.40	0.54
1:C:124:ILE:HG23	1:C:161:PRO:CB	2.37	0.54
1:C:153:ALA:H	1:C:154:THR:HA	1.71	0.54
1:D:213:ASP:HA	1:D:340:VAL:HG22	1.89	0.54
1:F:13:HIS:C	1:F:16:HIS:CE1	2.85	0.54
1:B:174:LEU:HG	1:B:175:ASP:N	2.22	0.54
1:F:156:GLU:CA	1:F:157:GLN:CB	2.86	0.54
1:F:240:ILE:HD12	1:F:287:THR:HG1	1.72	0.54
1:A:158:LEU:CA	1:A:159:ASP:CB	2.86	0.54
1:A:350:THR:OG1	1:A:352:ASP:O	2.23	0.54
1:B:213:ASP:HA	1:B:340:VAL:HG22	1.89	0.54
1:D:176:HIS:CE1	1:D:177:GLU:CD	2.86	0.54
1:F:277:THR:OG1	1:F:282:LEU:N	2.40	0.54
1:B:298:PRO:O	1:B:299:ALA:HB3	2.08	0.54
1:C:12:ALA:HB3	1:C:18:LYS:HG3	1.88	0.54
1:E:87:ARG:CZ	1:E:300:LEU:O	2.55	0.54
1:F:160:PHE:CD1	1:F:162:ILE:CB	2.88	0.54
1:F:300:LEU:CB	1:F:301:SER:CA	2.86	0.54
1:B:158:LEU:CA	1:B:159:ASP:CB	2.86	0.54
1:B:296:ALA:C	1:B:297:LEU:HD23	2.32	0.54
1:C:156:GLU:CA	1:C:157:GLN:CB	2.86	0.54
1:C:158:LEU:CA	1:C:159:ASP:CB	2.86	0.54
1:C:277:THR:OG1	1:C:282:LEU:N	2.40	0.54
1:F:240:ILE:HD13	1:F:296:ALA:HB2	1.88	0.54
1:A:176:HIS:CE1	1:A:177:GLU:CD	2.86	0.54
1:B:287:THR:CB	1:B:297:LEU:HG	2.36	0.54
1:C:156:GLU:HA	1:C:157:GLN:C	2.27	0.54
1:D:350:THR:OG1	1:D:352:ASP:O	2.23	0.54
1:E:277:THR:OG1	1:E:282:LEU:N	2.40	0.54
1:F:206:GLN:CD	1:F:297:LEU:HD22	2.33	0.54
1:A:277:THR:OG1	1:A:282:LEU:N	2.40	0.54
1:C:9:ALA:HA	1:C:73:VAL:O	2.08	0.54
1:C:306:THR:C	1:C:388:ILE:HD12	2.32	0.54
1:D:176:HIS:ND1	1:D:177:GLU:HA	2.22	0.54
1:E:176:HIS:CE1	1:E:177:GLU:CD	2.86	0.54
1:F:176:HIS:CE1	1:F:177:GLU:CD	2.86	0.54
1:F:239:ILE:CD1	1:F:288:VAL:CG2	2.86	0.54
1:B:306:THR:CA	1:B:388:ILE:HB	2.38	0.54
1:D:277:THR:OG1	1:D:282:LEU:N	2.40	0.54
1:E:158:LEU:CA	1:E:159:ASP:HB3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:LEU:CA	1:E:159:ASP:CB	2.86	0.54
1:F:153:ALA:HB3	1:F:154:THR:HA	1.89	0.54
1:A:9:ALA:HA	1:A:73:VAL:O	2.07	0.54
1:A:131:ASP:OD2	1:A:166:SER:OG	2.21	0.54
1:A:178:ASP:CA	1:A:179:MET:CB	2.86	0.54
1:A:300:LEU:CB	1:A:301:SER:CA	2.86	0.54
1:B:156:GLU:CA	1:B:157:GLN:CB	2.86	0.54
1:B:307:VAL:N	1:B:388:ILE:CD1	2.70	0.54
1:C:213:ASP:HA	1:C:340:VAL:HG22	1.89	0.54
1:E:238:THR:OG1	1:E:291:THR:HG22	2.08	0.54
1:F:158:LEU:CA	1:F:159:ASP:CB	2.86	0.54
1:E:13:HIS:C	1:E:16:HIS:CE1	2.86	0.53
1:A:156:GLU:CA	1:A:157:GLN:CB	2.86	0.53
1:B:300:LEU:CB	1:B:301:SER:CA	2.86	0.53
1:C:158:LEU:HD21	1:D:599:ARG:HH12	1.73	0.53
1:A:153:ALA:H	1:A:154:THR:HA	1.73	0.53
1:B:9:ALA:HA	1:B:73:VAL:O	2.08	0.53
1:B:13:HIS:C	1:B:16:HIS:CE1	2.87	0.53
1:B:176:HIS:CE1	1:B:177:GLU:CD	2.86	0.53
1:E:179:MET:HE2	1:E:182:ASP:OD1	2.08	0.53
1:D:156:GLU:HG3	1:D:159:ASP:N	2.24	0.53
1:A:13:HIS:C	1:A:16:HIS:CE1	2.87	0.53
1:E:140:VAL:O	1:E:144:VAL:HG23	2.08	0.53
1:F:140:VAL:O	1:F:144:VAL:HG23	2.08	0.53
1:F:164:TYR:CD1	1:F:164:TYR:N	2.77	0.53
1:B:174:LEU:HG	1:B:175:ASP:OD2	2.09	0.53
1:C:176:HIS:CE1	1:C:177:GLU:CD	2.86	0.53
1:D:178:ASP:HB2	1:D:179:MET:SD	2.49	0.53
1:F:160:PHE:O	1:F:193:HIS:CE1	2.61	0.53
1:A:156:GLU:H	1:A:157:GLN:HB2	1.73	0.53
1:E:174:LEU:HD23	1:E:174:LEU:N	2.23	0.53
1:F:163:VAL:HG13	1:F:176:HIS:HD2	1.71	0.53
1:F:199:VAL:HB	1:F:267:LEU:HD11	1.91	0.53
1:D:140:VAL:O	1:D:144:VAL:HG23	2.08	0.53
1:A:140:VAL:O	1:A:144:VAL:HG23	2.08	0.53
1:A:169:ASN:HD21	1:A:182:ASP:N	2.05	0.53
1:C:307:VAL:N	1:C:388:ILE:CD1	2.72	0.53
1:E:9:ALA:HA	1:E:73:VAL:O	2.08	0.53
1:E:199:VAL:HB	1:E:267:LEU:HD11	1.91	0.53
1:C:140:VAL:O	1:C:144:VAL:HG23	2.08	0.52
1:E:300:LEU:H	1:E:301:SER:HA	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:VAL:HG12	1:A:289:CYS:H	1.74	0.52
1:D:153:ALA:HB3	1:D:154:THR:HA	1.91	0.52
1:D:174:LEU:HD23	1:D:174:LEU:H	1.74	0.52
1:F:160:PHE:CD1	1:F:162:ILE:HD12	2.44	0.52
1:F:287:THR:CB	1:F:297:LEU:HG	2.40	0.52
1:A:160:PHE:HD1	1:A:161:PRO:O	1.92	0.52
1:D:9:ALA:HA	1:D:73:VAL:O	2.08	0.52
1:E:156:GLU:CA	1:E:157:GLN:HB2	2.40	0.52
1:C:153:ALA:HB3	1:C:154:THR:HA	1.89	0.52
1:D:160:PHE:CZ	1:D:162:ILE:HD12	2.43	0.52
1:D:300:LEU:CB	1:D:301:SER:CA	2.86	0.52
1:F:9:ALA:HA	1:F:73:VAL:O	2.09	0.52
1:A:145:PHE:O	1:A:148:PHE:CB	2.58	0.52
1:B:350:THR:OG1	1:B:352:ASP:O	2.23	0.52
1:D:310:PHE:HB2	1:D:357:ARG:NH2	2.24	0.52
1:A:205:PHE:O	1:A:289:CYS:HA	2.10	0.52
1:C:276:ILE:HG22	1:C:277:THR:HG23	1.92	0.52
1:C:300:LEU:CB	1:C:301:SER:CA	2.86	0.52
1:E:276:ILE:HG22	1:E:277:THR:HG23	1.92	0.52
1:B:160:PHE:N	1:B:161:PRO:CB	2.73	0.52
1:B:306:THR:HA	1:B:388:ILE:CB	2.40	0.52
1:C:150:ASN:ND2	1:C:151:LEU:CD2	2.73	0.52
1:C:158:LEU:HD21	1:D:599:ARG:NH1	2.24	0.52
1:E:160:PHE:CD1	1:E:162:ILE:HD12	2.44	0.52
1:E:160:PHE:N	1:E:161:PRO:CB	2.73	0.52
1:B:150:ASN:ND2	1:B:151:LEU:CD2	2.73	0.52
1:B:160:PHE:CD1	1:B:162:ILE:CB	2.86	0.52
1:D:117:PHE:CZ	1:D:148:PHE:CD1	2.94	0.52
1:E:310:PHE:HB2	1:E:357:ARG:NH2	2.25	0.52
1:F:310:PHE:HB2	1:F:357:ARG:NH2	2.25	0.52
1:B:160:PHE:CE1	1:B:162:ILE:CB	2.91	0.52
1:C:199:VAL:HB	1:C:267:LEU:HD11	1.91	0.52
1:D:305:PRO:HG2	1:D:388:ILE:CD1	2.39	0.52
1:F:160:PHE:N	1:F:161:PRO:CB	2.73	0.52
1:F:177:GLU:CB	1:F:178:ASP:HA	2.39	0.52
1:F:276:ILE:HG22	1:F:277:THR:HG23	1.92	0.52
1:A:222:GLY:O	1:A:223:ILE:C	2.51	0.51
1:C:160:PHE:N	1:C:161:PRO:CB	2.73	0.51
1:C:287:THR:CB	1:C:297:LEU:HG	2.37	0.51
1:C:310:PHE:HB2	1:C:357:ARG:NH2	2.25	0.51
1:D:199:VAL:HB	1:D:267:LEU:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:VAL:HB	1:A:267:LEU:HD11	1.91	0.51
1:A:294:VAL:HG12	1:A:295:GLU:N	2.20	0.51
1:C:177:GLU:CB	1:C:178:ASP:HA	2.39	0.51
1:F:156:GLU:CA	1:F:157:GLN:HB2	2.40	0.51
1:A:117:PHE:HD2	1:A:153:ALA:HA	1.74	0.51
1:A:207:MET:O	1:A:297:LEU:HD11	2.10	0.51
1:A:287:THR:HG21	1:A:297:LEU:HD12	1.81	0.51
1:B:140:VAL:O	1:B:144:VAL:HG23	2.09	0.51
1:B:54:ILE:HG23	1:B:73:VAL:HG13	1.91	0.51
1:B:199:VAL:HB	1:B:267:LEU:HD11	1.91	0.51
1:C:294:VAL:CG1	1:C:295:GLU:H	2.08	0.51
1:D:150:ASN:ND2	1:D:151:LEU:CD2	2.73	0.51
1:D:160:PHE:N	1:D:161:PRO:CB	2.73	0.51
1:E:164:TYR:N	1:E:164:TYR:CD1	2.79	0.51
1:E:239:ILE:HD11	1:E:288:VAL:HG13	1.91	0.51
1:A:276:ILE:HG22	1:A:277:THR:HG23	1.92	0.51
1:B:276:ILE:HG22	1:B:277:THR:HG23	1.92	0.51
1:D:300:LEU:H	1:D:301:SER:HA	1.76	0.51
1:D:304:GLU:HB3	1:D:390:ARG:CZ	2.40	0.51
1:E:159:ASP:O	1:E:162:ILE:HD11	2.11	0.51
1:F:156:GLU:N	1:F:157:GLN:CB	2.73	0.51
1:C:131:ASP:OD2	1:C:166:SER:OG	2.21	0.51
1:D:276:ILE:HG22	1:D:277:THR:HG23	1.92	0.51
1:E:184:THR:HA	1:E:187:TYR:HD2	1.76	0.51
1:E:300:LEU:N	1:E:300:LEU:CD1	2.74	0.51
1:F:184:THR:HA	1:F:187:TYR:HD2	1.76	0.51
1:B:174:LEU:H	1:B:174:LEU:HD23	1.75	0.51
1:B:310:PHE:HB2	1:B:357:ARG:NH2	2.25	0.51
1:C:184:THR:HA	1:C:187:TYR:HD2	1.76	0.51
1:D:158:LEU:HA	1:D:159:ASP:CB	2.31	0.51
1:E:50:LYS:HD3	1:E:51:GLU:HB2	1.93	0.51
1:E:160:PHE:HA	1:E:161:PRO:O	2.10	0.51
1:A:160:PHE:N	1:A:161:PRO:CB	2.73	0.51
1:C:306:THR:CA	1:C:388:ILE:HB	2.39	0.51
1:D:158:LEU:CA	1:D:159:ASP:CB	2.88	0.51
1:D:301:SER:OG	1:D:302:VAL:HG22	2.11	0.51
1:F:160:PHE:HA	1:F:161:PRO:O	2.09	0.51
1:B:156:GLU:HA	1:B:157:GLN:C	2.27	0.51
1:C:145:PHE:O	1:C:148:PHE:CB	2.57	0.51
1:F:176:HIS:HA	1:F:177:GLU:O	2.11	0.51
1:B:160:PHE:CZ	1:B:162:ILE:HD12	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:50:LYS:HD3	1:F:51:GLU:HB2	1.93	0.50
1:C:156:GLU:N	1:C:157:GLN:CB	2.73	0.50
1:C:176:HIS:HA	1:C:177:GLU:O	2.10	0.50
1:D:222:GLY:O	1:D:223:ILE:C	2.52	0.50
1:E:289:CYS:SG	1:E:294:VAL:HG11	2.51	0.50
1:B:50:LYS:HD3	1:B:51:GLU:HB2	1.93	0.50
1:E:160:PHE:O	1:E:193:HIS:CE1	2.64	0.50
1:D:184:THR:HA	1:D:187:TYR:HD2	1.75	0.50
1:F:156:GLU:HG3	1:F:159:ASP:N	2.26	0.50
1:F:159:ASP:O	1:F:162:ILE:HD11	2.12	0.50
1:B:145:PHE:O	1:B:148:PHE:CB	2.58	0.50
1:B:157:GLN:HB3	1:B:158:LEU:HD12	1.94	0.50
1:D:24:LYS:HG2	1:D:183:MET:HE3	1.93	0.50
1:B:309:MET:HG2	1:B:366:LEU:HD13	1.94	0.50
1:B:25:LEU:CD2	1:B:183:MET:SD	2.96	0.50
1:B:425:ASP:CG	1:C:114:LYS:HE2	2.36	0.50
1:C:157:GLN:HB3	1:C:158:LEU:HD12	1.93	0.50
1:C:306:THR:HA	1:C:388:ILE:CD1	2.38	0.50
1:E:177:GLU:CB	1:E:178:ASP:HA	2.41	0.50
1:E:309:MET:HG2	1:E:366:LEU:HD13	1.94	0.50
1:F:176:HIS:NE2	1:F:177:GLU:OE1	2.45	0.50
1:A:160:PHE:O	1:A:193:HIS:CE1	2.65	0.49
1:F:153:ALA:CB	1:F:154:THR:CA	2.88	0.49
1:F:160:PHE:CD2	1:F:162:ILE:CD1	2.86	0.49
1:F:287:THR:CG2	1:F:297:LEU:CD1	2.90	0.49
1:A:162:ILE:HG22	1:A:162:ILE:O	2.12	0.49
1:A:310:PHE:HB2	1:A:357:ARG:NH2	2.26	0.49
1:C:222:GLY:O	1:C:223:ILE:C	2.50	0.49
1:C:240:ILE:HD12	1:C:296:ALA:HB1	1.94	0.49
1:C:253:LYS:HG2	1:C:254:VAL:N	2.28	0.49
1:F:160:PHE:O	1:F:193:HIS:NE2	2.45	0.49
1:F:309:MET:HG2	1:F:366:LEU:HD13	1.94	0.49
1:A:309:MET:HG2	1:A:366:LEU:HD13	1.94	0.49
1:C:22:VAL:HG12	1:C:56:ILE:HD13	1.94	0.49
1:E:123:PRO:HB2	1:E:156:GLU:OE2	2.12	0.49
1:C:52:ARG:CB	1:C:53:GLY:HA3	2.42	0.49
1:C:158:LEU:HG	1:D:599:ARG:NH1	2.27	0.49
1:D:174:LEU:HD23	1:D:174:LEU:N	2.27	0.49
1:F:50:LYS:HA	1:F:51:GLU:CB	2.41	0.49
1:A:12:ALA:HB3	1:A:18:LYS:HG3	1.95	0.49
1:A:125:VAL:H	1:A:161:PRO:CB	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:PRO:C	1:C:306:THR:CG2	2.86	0.49
1:E:54:ILE:HG23	1:E:73:VAL:HG13	1.93	0.49
1:B:149:VAL:C	1:B:151:LEU:H	2.21	0.49
1:B:156:GLU:N	1:B:157:GLN:CB	2.73	0.49
1:C:309:MET:HG2	1:C:366:LEU:HD13	1.95	0.49
1:D:177:GLU:N	1:D:178:ASP:HA	2.27	0.49
1:E:150:ASN:ND2	1:E:151:LEU:CD2	2.76	0.49
1:E:293:ASN:C	1:E:294:VAL:CG2	2.86	0.49
1:B:287:THR:HG21	1:B:297:LEU:HG	1.95	0.49
1:D:309:MET:HG2	1:D:366:LEU:HD13	1.95	0.49
1:E:160:PHE:CD2	1:E:162:ILE:CD1	2.88	0.49
1:E:176:HIS:NE2	1:E:177:GLU:OE1	2.46	0.49
1:E:300:LEU:N	1:E:301:SER:HA	2.26	0.49
1:B:305:PRO:C	1:B:306:THR:CG2	2.86	0.49
1:C:178:ASP:CA	1:C:179:MET:HB2	2.43	0.49
1:D:305:PRO:HG2	1:D:388:ILE:HD13	1.94	0.49
1:E:253:LYS:HG2	1:E:254:VAL:N	2.27	0.49
1:E:287:THR:CG2	1:E:297:LEU:CD1	2.91	0.49
1:E:287:THR:CG2	1:E:297:LEU:CG	2.88	0.49
1:A:293:ASN:C	1:A:294:VAL:CG2	2.86	0.49
1:B:50:LYS:HA	1:B:51:GLU:CB	2.42	0.49
1:D:156:GLU:HA	1:D:157:GLN:CB	2.42	0.49
1:E:122:LYS:NZ	1:E:158:LEU:O	2.38	0.49
1:E:153:ALA:CB	1:E:154:THR:CA	2.87	0.49
1:E:205:PHE:CE1	1:E:231:VAL:HG22	2.48	0.49
1:F:122:LYS:NZ	1:F:158:LEU:O	2.39	0.49
1:A:22:VAL:HG12	1:A:56:ILE:HD13	1.93	0.48
1:B:178:ASP:CA	1:B:179:MET:HB2	2.42	0.48
1:B:240:ILE:HD12	1:B:296:ALA:HB1	1.95	0.48
1:C:176:HIS:NE2	1:C:177:GLU:OE1	2.46	0.48
1:D:124:ILE:HG23	1:D:161:PRO:CA	2.30	0.48
1:D:160:PHE:O	1:D:193:HIS:CE1	2.66	0.48
1:E:50:LYS:HA	1:E:51:GLU:CB	2.42	0.48
1:E:287:THR:CB	1:E:297:LEU:CD1	2.91	0.48
1:B:205:PHE:CE1	1:B:231:VAL:HG22	2.48	0.48
1:C:411:HIS:O	1:C:412:GLN:C	2.56	0.48
1:A:124:ILE:HG23	1:A:161:PRO:CA	2.31	0.48
1:B:12:ALA:HB3	1:B:18:LYS:HG3	1.94	0.48
1:D:160:PHE:CZ	1:D:162:ILE:HG21	2.48	0.48
1:F:240:ILE:HD13	1:F:296:ALA:CB	2.42	0.48
1:A:205:PHE:CE1	1:A:231:VAL:HG22	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:156:GLU:HA	1:F:157:GLN:C	2.27	0.48
1:F:205:PHE:CE1	1:F:231:VAL:HG22	2.49	0.48
1:F:253:LYS:HG2	1:F:254:VAL:N	2.28	0.48
1:F:293:ASN:C	1:F:294:VAL:CG2	2.86	0.48
1:A:300:LEU:N	1:A:301:SER:HA	2.28	0.48
1:C:159:ASP:O	1:C:162:ILE:HD11	2.14	0.48
1:F:54:ILE:HG23	1:F:73:VAL:HG13	1.94	0.48
1:B:159:ASP:O	1:B:162:ILE:HG13	2.13	0.48
1:D:294:VAL:HG12	1:D:295:GLU:N	2.18	0.48
1:B:54:ILE:HG21	1:B:211:GLN:OE1	2.13	0.48
1:C:205:PHE:CE1	1:C:231:VAL:HG22	2.48	0.48
1:C:306:THR:HA	1:C:388:ILE:CB	2.41	0.48
1:D:87:ARG:NH2	1:D:301:SER:HB3	2.29	0.48
1:A:10:ILE:O	1:A:75:THR:OG1	2.19	0.48
1:A:50:LYS:CE	1:A:51:GLU:CG	2.90	0.48
1:D:22:VAL:HG12	1:D:56:ILE:HD13	1.94	0.48
1:E:12:ALA:HB3	1:E:18:LYS:HG3	1.95	0.48
1:E:52:ARG:CB	1:E:53:GLY:CA	2.91	0.48
1:F:249:ALA:HB3	1:F:275:ALA:CB	2.44	0.48
1:F:52:ARG:CB	1:F:53:GLY:CA	2.91	0.48
1:A:153:ALA:HB3	1:A:154:THR:HA	1.95	0.48
1:B:165:ALA:CA	1:B:182:ASP:OD2	2.61	0.48
1:C:160:PHE:CD2	1:C:162:ILE:CD1	2.86	0.48
1:D:253:LYS:HG2	1:D:254:VAL:N	2.28	0.48
1:E:249:ALA:HB3	1:E:275:ALA:CB	2.44	0.48
1:F:300:LEU:N	1:F:301:SER:HA	2.29	0.48
1:A:55:THR:HB	1:A:73:VAL:HA	1.94	0.47
1:A:157:GLN:C	1:A:159:ASP:HB3	2.39	0.47
1:B:411:HIS:O	1:B:412:GLN:C	2.57	0.47
1:E:293:ASN:O	1:E:294:VAL:HG22	2.14	0.47
1:E:411:HIS:O	1:E:412:GLN:C	2.57	0.47
1:F:411:HIS:O	1:F:412:GLN:C	2.57	0.47
1:B:178:ASP:CA	1:B:179:MET:CB	2.92	0.47
1:C:149:VAL:C	1:C:151:LEU:H	2.22	0.47
1:D:290:ASP:HB3	1:D:292:GLN:HB3	1.95	0.47
1:E:310:PHE:CG	1:E:383:SER:HB3	2.49	0.47
1:F:10:ILE:O	1:F:75:THR:OG1	2.20	0.47
1:F:240:ILE:CD1	1:F:296:ALA:HB1	2.43	0.47
1:A:50:LYS:CD	1:A:51:GLU:HB2	2.44	0.47
1:A:253:LYS:HG2	1:A:254:VAL:N	2.29	0.47
1:F:178:ASP:CA	1:F:179:MET:HB2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:287:THR:CB	1:F:297:LEU:CD1	2.92	0.47
1:A:176:HIS:CE1	1:A:177:GLU:HA	2.50	0.47
1:A:411:HIS:O	1:A:412:GLN:C	2.57	0.47
1:B:177:GLU:N	1:B:178:ASP:CA	2.76	0.47
1:C:305:PRO:O	1:C:306:THR:HG22	2.15	0.47
1:B:159:ASP:O	1:B:162:ILE:HD11	2.15	0.47
1:B:305:PRO:O	1:B:306:THR:HG22	2.15	0.47
1:D:205:PHE:CE1	1:D:231:VAL:HG22	2.49	0.47
1:D:423:LYS:HG3	1:D:480:VAL:HG11	1.96	0.47
1:E:10:ILE:O	1:E:75:THR:OG1	2.20	0.47
1:B:253:LYS:HG2	1:B:254:VAL:N	2.29	0.47
1:B:423:LYS:HG3	1:B:480:VAL:HG11	1.97	0.47
1:D:176:HIS:CG	1:D:177:GLU:HA	2.49	0.47
1:E:54:ILE:HG21	1:E:211:GLN:OE1	2.14	0.47
1:E:163:VAL:HG13	1:E:176:HIS:HD2	1.77	0.47
1:E:178:ASP:CA	1:E:179:MET:HB2	2.44	0.47
1:E:240:ILE:HD12	1:E:296:ALA:HB1	1.96	0.47
1:F:54:ILE:HG21	1:F:211:GLN:OE1	2.14	0.47
1:F:293:ASN:O	1:F:294:VAL:HG22	2.15	0.47
1:B:301:SER:OG	1:B:302:VAL:HG22	2.15	0.47
1:C:423:LYS:HG3	1:C:480:VAL:HG11	1.97	0.47
1:D:156:GLU:CA	1:D:157:GLN:CB	2.86	0.47
1:F:150:ASN:ND2	1:F:151:LEU:CD2	2.78	0.47
1:F:423:LYS:HG3	1:F:480:VAL:HG11	1.97	0.47
1:B:52:ARG:CB	1:B:53:GLY:CA	2.91	0.47
1:E:423:LYS:HG3	1:E:480:VAL:HG11	1.97	0.47
1:A:293:ASN:O	1:A:294:VAL:HG22	2.15	0.47
1:D:411:HIS:O	1:D:412:GLN:C	2.57	0.47
1:E:160:PHE:O	1:E:193:HIS:NE2	2.48	0.47
1:E:289:CYS:SG	1:E:294:VAL:CG1	3.03	0.47
1:F:164:TYR:H	1:F:164:TYR:HD1	1.63	0.47
1:A:423:LYS:HG3	1:A:480:VAL:HG11	1.97	0.46
1:B:249:ALA:HB3	1:B:275:ALA:CB	2.44	0.46
1:B:306:THR:C	1:B:307:VAL:HG23	2.41	0.46
1:C:206:GLN:CG	1:C:297:LEU:HD22	2.46	0.46
1:C:301:SER:OG	1:C:302:VAL:HG22	2.15	0.46
1:E:10:ILE:HG22	1:E:11:ILE:N	2.30	0.46
1:E:176:HIS:ND1	1:E:177:GLU:HA	2.30	0.46
1:A:249:ALA:HB3	1:A:275:ALA:CB	2.44	0.46
1:A:469:PHE:CD1	1:A:469:PHE:C	2.93	0.46
1:C:249:ALA:HB3	1:C:275:ALA:CB	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:PHE:CZ	1:D:148:PHE:CE1	2.99	0.46
1:D:294:VAL:O	1:D:295:GLU:HB2	2.14	0.46
1:E:22:VAL:HG12	1:E:56:ILE:HG21	1.96	0.46
1:E:176:HIS:HA	1:E:177:GLU:O	2.14	0.46
1:B:160:PHE:CD2	1:B:162:ILE:CD1	2.86	0.46
1:C:55:THR:O	1:C:56:ILE:HB	2.16	0.46
1:C:146:ASP:O	1:C:150:ASN:OD1	2.33	0.46
1:C:306:THR:C	1:C:307:VAL:HG23	2.41	0.46
1:D:52:ARG:CB	1:D:53:GLY:HA3	2.44	0.46
1:A:144:VAL:O	1:A:148:PHE:CD2	2.69	0.46
1:C:176:HIS:ND1	1:C:177:GLU:HA	2.31	0.46
1:C:240:ILE:HD13	1:C:296:ALA:HB2	1.98	0.46
1:D:148:PHE:N	1:D:150:ASN:OD1	2.48	0.46
1:D:249:ALA:HB3	1:D:275:ALA:CB	2.44	0.46
1:D:469:PHE:CD1	1:D:469:PHE:C	2.93	0.46
1:E:156:GLU:HA	1:E:157:GLN:C	2.30	0.46
1:E:283:ASN:OD1	1:E:346:ARG:HA	2.16	0.46
1:A:156:GLU:N	1:A:157:GLN:CB	2.78	0.46
1:A:283:ASN:OD1	1:A:346:ARG:HA	2.16	0.46
1:C:160:PHE:CE1	1:C:162:ILE:CB	2.90	0.46
1:D:151:LEU:O	1:D:152:ASP:HB2	2.16	0.46
1:E:239:ILE:HD12	1:E:288:VAL:HG22	1.97	0.46
1:A:101:ALA:HB2	1:A:127:ILE:HG22	1.98	0.46
1:A:237:VAL:C	1:A:291:THR:HG22	2.41	0.46
1:A:422:ARG:NH1	1:A:447:GLY:O	2.48	0.46
1:B:274:VAL:O	1:B:275:ALA:HB3	2.16	0.46
1:C:159:ASP:O	1:C:162:ILE:HG13	2.15	0.46
1:C:469:PHE:CD1	1:C:469:PHE:C	2.93	0.46
1:B:22:VAL:HG12	1:B:56:ILE:HG21	1.98	0.46
1:B:469:PHE:CD1	1:B:469:PHE:C	2.93	0.46
1:C:101:ALA:HB2	1:C:127:ILE:HG22	1.98	0.46
1:C:144:VAL:O	1:C:148:PHE:CD2	2.69	0.46
1:D:156:GLU:HA	1:D:157:GLN:HB2	1.97	0.46
1:E:287:THR:HG21	1:E:297:LEU:HB2	1.98	0.46
1:F:283:ASN:OD1	1:F:346:ARG:HA	2.16	0.46
1:A:310:PHE:CG	1:A:383:SER:HB3	2.51	0.46
1:B:273:ILE:HD11	1:B:276:ILE:HD11	1.98	0.46
1:D:55:THR:O	1:D:56:ILE:HB	2.16	0.46
1:D:283:ASN:OD1	1:D:346:ARG:HA	2.16	0.46
1:A:237:VAL:HA	1:A:291:THR:CG2	2.44	0.46
1:C:287:THR:HG21	1:C:297:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:22:VAL:HG12	1:F:56:ILE:HG21	1.97	0.46
1:F:176:HIS:ND1	1:F:177:GLU:HA	2.31	0.46
1:F:287:THR:CG2	1:F:297:LEU:CG	2.88	0.46
1:B:146:ASP:O	1:B:150:ASN:OD1	2.34	0.46
1:C:283:ASN:OD1	1:C:346:ARG:HA	2.16	0.46
1:E:156:GLU:H	1:E:157:GLN:HB2	1.76	0.46
1:D:101:ALA:HB2	1:D:127:ILE:HG22	1.98	0.45
1:D:422:ARG:NH1	1:D:447:GLY:O	2.48	0.45
1:E:273:ILE:HD11	1:E:276:ILE:HD11	1.98	0.45
1:E:274:VAL:O	1:E:275:ALA:HB3	2.16	0.45
1:E:469:PHE:CD1	1:E:469:PHE:C	2.93	0.45
1:F:156:GLU:H	1:F:157:GLN:HB2	1.76	0.45
1:A:124:ILE:CA	1:A:161:PRO:CB	2.80	0.45
1:A:206:GLN:HG2	1:A:297:LEU:HD22	1.99	0.45
1:A:288:VAL:C	1:A:289:CYS:SG	3.00	0.45
1:B:144:VAL:O	1:B:148:PHE:CD2	2.69	0.45
1:C:160:PHE:CA	1:C:162:ILE:HG13	2.47	0.45
1:C:273:ILE:HD11	1:C:276:ILE:HD11	1.98	0.45
1:D:101:ALA:HA	1:D:140:VAL:HG21	1.98	0.45
1:F:273:ILE:HD11	1:F:276:ILE:HD11	1.98	0.45
1:F:274:VAL:O	1:F:275:ALA:HB3	2.16	0.45
1:B:175:ASP:O	1:B:178:ASP:HB3	2.16	0.45
1:C:274:VAL:O	1:C:275:ALA:HB3	2.16	0.45
1:E:96:LEU:HD23	1:E:96:LEU:HA	1.74	0.45
1:C:61:THR:HG1	1:C:67:ASP:HA	1.76	0.45
1:C:422:ARG:NH1	1:C:447:GLY:O	2.49	0.45
1:A:101:ALA:HA	1:A:140:VAL:HG21	1.99	0.45
1:B:290:ASP:O	1:B:294:VAL:HG21	2.16	0.45
1:B:300:LEU:N	1:B:301:SER:HA	2.32	0.45
1:C:12:ALA:HB3	1:C:18:LYS:CG	2.46	0.45
1:E:177:GLU:N	1:E:178:ASP:CA	2.79	0.45
1:E:240:ILE:HD13	1:E:296:ALA:HB2	1.98	0.45
1:A:288:VAL:HG12	1:A:289:CYS:N	2.32	0.45
1:B:176:HIS:CG	1:B:177:GLU:CA	2.95	0.45
1:B:294:VAL:O	1:B:295:GLU:HG2	2.16	0.45
1:B:310:PHE:CG	1:B:383:SER:HB3	2.51	0.45
1:F:237:VAL:HA	1:F:291:THR:HG23	1.98	0.45
1:F:239:ILE:HA	1:F:287:THR:O	2.16	0.45
1:F:301:SER:OG	1:F:302:VAL:HG22	2.16	0.45
1:C:160:PHE:CA	1:C:161:PRO:C	2.86	0.45
1:C:534:THR:HG21	1:C:594:GLU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:ILE:HA	1:E:55:THR:HA	1.47	0.45
1:F:24:LYS:HG2	1:F:183:MET:HE3	1.99	0.45
1:A:61:THR:HG1	1:A:67:ASP:HA	1.79	0.45
1:B:283:ASN:OD1	1:B:346:ARG:HA	2.17	0.45
1:D:149:VAL:C	1:D:151:LEU:N	2.74	0.45
1:E:534:THR:HG21	1:E:594:GLU:HB2	1.99	0.45
1:F:54:ILE:HA	1:F:55:THR:HA	1.47	0.45
1:A:178:ASP:HA	1:A:179:MET:CB	2.45	0.45
1:A:273:ILE:HD11	1:A:276:ILE:HD11	1.98	0.45
1:D:61:THR:HG1	1:D:67:ASP:HA	1.79	0.45
1:F:534:THR:HG21	1:F:594:GLU:HB2	1.99	0.45
1:A:160:PHE:CG	1:A:162:ILE:HD12	2.51	0.45
1:A:274:VAL:O	1:A:275:ALA:HB3	2.17	0.45
1:B:101:ALA:HB2	1:B:127:ILE:HG22	1.98	0.45
1:B:119:TYR:O	1:B:121:LEU:N	2.50	0.45
1:B:534:THR:HG21	1:B:594:GLU:HB2	1.99	0.45
1:C:10:ILE:O	1:C:75:THR:OG1	2.20	0.45
1:C:50:LYS:HA	1:C:51:GLU:CB	2.46	0.45
1:C:178:ASP:CA	1:C:179:MET:CB	2.95	0.45
1:D:50:LYS:HA	1:D:51:GLU:CB	2.47	0.45
1:D:146:ASP:O	1:D:150:ASN:OD1	2.34	0.45
1:D:156:GLU:HA	1:D:157:GLN:C	2.27	0.45
1:E:300:LEU:CB	1:E:304:GLU:HG3	2.43	0.45
1:F:124:ILE:HA	1:F:161:PRO:CB	2.47	0.45
1:F:164:TYR:CE1	1:F:175:ASP:HB2	2.51	0.45
1:A:12:ALA:HB3	1:A:18:LYS:CG	2.48	0.44
1:B:206:GLN:CG	1:B:297:LEU:HD22	2.46	0.44
1:E:237:VAL:CA	1:E:291:THR:HG23	2.46	0.44
1:F:119:TYR:O	1:F:121:LEU:N	2.50	0.44
1:B:101:ALA:HA	1:B:140:VAL:HG21	1.98	0.44
1:C:153:ALA:CB	1:C:154:THR:CA	2.88	0.44
1:C:158:LEU:CD2	1:D:599:ARG:HH12	2.30	0.44
1:C:300:LEU:N	1:C:301:SER:HA	2.32	0.44
1:B:12:ALA:HB3	1:B:18:LYS:CG	2.46	0.44
1:B:204:PRO:O	1:B:228:ARG:HB3	2.17	0.44
1:D:274:VAL:O	1:D:275:ALA:HB3	2.16	0.44
1:E:287:THR:HG21	1:E:297:LEU:CB	2.46	0.44
1:C:290:ASP:O	1:C:294:VAL:HG21	2.17	0.44
1:D:12:ALA:HB3	1:D:18:LYS:CG	2.47	0.44
1:E:101:ALA:HB2	1:E:127:ILE:HG22	1.98	0.44
1:E:119:TYR:O	1:E:121:LEU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:ASP:N	1:E:272:ASP:OD1	2.50	0.44
1:F:101:ALA:HA	1:F:140:VAL:HG21	1.99	0.44
1:F:174:LEU:C	1:F:175:ASP:CG	2.86	0.44
1:F:12:ALA:HB3	1:F:18:LYS:CG	2.47	0.44
1:F:272:ASP:OD1	1:F:272:ASP:N	2.50	0.44
1:A:267:LEU:HG	1:A:268:ALA:N	2.33	0.44
1:B:240:ILE:HD13	1:B:296:ALA:HB2	1.99	0.44
1:C:287:THR:CG2	1:C:297:LEU:CG	2.89	0.44
1:D:160:PHE:CA	1:D:161:PRO:CB	2.95	0.44
1:D:160:PHE:HD1	1:D:161:PRO:O	2.01	0.44
1:D:165:ALA:HA	1:D:182:ASP:OD2	2.17	0.44
1:F:301:SER:O	1:F:302:VAL:HG13	2.17	0.44
1:A:54:ILE:HA	1:A:55:THR:HA	1.71	0.44
1:A:156:GLU:H	1:A:157:GLN:CB	2.31	0.44
1:A:174:LEU:HD23	1:A:174:LEU:N	2.32	0.44
1:B:273:ILE:HD11	1:B:276:ILE:CD1	2.48	0.44
1:B:305:PRO:C	1:B:306:THR:HG23	2.42	0.44
1:C:305:PRO:C	1:C:306:THR:HG23	2.42	0.44
1:D:534:THR:HG21	1:D:594:GLU:HB2	1.99	0.44
1:E:150:ASN:HB2	1:F:423:LYS:NZ	2.33	0.44
1:E:273:ILE:HD11	1:E:276:ILE:CD1	2.48	0.44
1:C:267:LEU:HG	1:C:268:ALA:N	2.33	0.44
1:D:273:ILE:HD11	1:D:276:ILE:HD11	1.98	0.44
1:D:289:CYS:HB2	1:D:294:VAL:CG1	2.43	0.44
1:E:24:LYS:HG2	1:E:183:MET:HE3	2.00	0.44
1:E:101:ALA:HA	1:E:140:VAL:HG21	1.99	0.44
1:E:293:ASN:C	1:E:294:VAL:HG23	2.42	0.44
1:F:101:ALA:HB2	1:F:127:ILE:HG22	1.98	0.44
1:F:469:PHE:CD1	1:F:469:PHE:C	2.95	0.44
1:A:272:ASP:OD1	1:A:272:ASP:N	2.51	0.44
1:B:425:ASP:OD1	1:C:114:LYS:HD3	2.17	0.44
1:C:174:LEU:C	1:C:175:ASP:CG	2.86	0.44
1:C:174:LEU:O	1:C:178:ASP:HB3	2.18	0.44
1:C:204:PRO:O	1:C:228:ARG:HB3	2.18	0.44
1:D:124:ILE:CA	1:D:161:PRO:CB	2.83	0.44
1:D:272:ASP:OD1	1:D:272:ASP:N	2.51	0.44
1:D:310:PHE:CG	1:D:383:SER:HB3	2.53	0.44
1:E:160:PHE:CD1	1:E:162:ILE:CG1	3.01	0.44
1:E:267:LEU:HG	1:E:268:ALA:N	2.33	0.44
1:F:160:PHE:CD1	1:F:162:ILE:CG1	3.01	0.44
1:F:178:ASP:CA	1:F:179:MET:CB	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:273:ILE:HD11	1:F:276:ILE:CD1	2.48	0.44
1:B:159:ASP:O	1:B:160:PHE:HB2	2.18	0.43
1:B:272:ASP:OD1	1:B:272:ASP:N	2.51	0.43
1:D:149:VAL:O	1:D:151:LEU:N	2.51	0.43
1:E:178:ASP:CA	1:E:179:MET:CB	2.95	0.43
1:F:177:GLU:N	1:F:178:ASP:CA	2.80	0.43
1:F:240:ILE:CD1	1:F:296:ALA:CB	2.95	0.43
1:F:310:PHE:CG	1:F:383:SER:HB3	2.53	0.43
1:A:273:ILE:HD11	1:A:276:ILE:CD1	2.48	0.43
1:B:287:THR:CG2	1:B:297:LEU:HG	2.48	0.43
1:C:101:ALA:HA	1:C:140:VAL:HG21	1.99	0.43
1:C:110:ARG:NH2	1:C:151:LEU:HD11	2.33	0.43
1:C:160:PHE:CG	1:C:162:ILE:CD1	3.01	0.43
1:C:240:ILE:HD13	1:C:296:ALA:CB	2.49	0.43
1:E:12:ALA:HB3	1:E:18:LYS:CG	2.47	0.43
1:F:422:ARG:NH1	1:F:447:GLY:O	2.48	0.43
1:A:156:GLU:O	1:A:156:GLU:HG2	2.18	0.43
1:A:204:PRO:O	1:A:228:ARG:HB3	2.17	0.43
1:B:177:GLU:CB	1:B:178:ASP:HA	2.48	0.43
1:D:117:PHE:HZ	1:D:148:PHE:HD1	1.62	0.43
1:D:344:ALA:HB1	1:D:361:ARG:HB2	2.00	0.43
1:A:160:PHE:CD1	1:A:162:ILE:CB	2.91	0.43
1:A:534:THR:HG21	1:A:594:GLU:HB2	1.99	0.43
1:B:54:ILE:HA	1:B:55:THR:HA	1.46	0.43
1:C:119:TYR:O	1:C:121:LEU:N	2.50	0.43
1:F:204:PRO:O	1:F:228:ARG:HB3	2.18	0.43
1:B:176:HIS:HA	1:B:177:GLU:O	2.18	0.43
1:B:348:GLU:HB2	1:B:357:ARG:HB3	2.00	0.43
1:C:158:LEU:CD2	1:D:599:ARG:NH1	2.81	0.43
1:C:348:GLU:HB2	1:C:357:ARG:HB3	2.01	0.43
1:D:204:PRO:O	1:D:228:ARG:HB3	2.17	0.43
1:E:380:LEU:O	1:E:580:VAL:HG22	2.18	0.43
1:F:152:ASP:N	1:F:152:ASP:OD1	2.52	0.43
1:B:50:LYS:CE	1:B:51:GLU:HG3	2.46	0.43
1:B:174:LEU:C	1:B:175:ASP:CG	2.85	0.43
1:B:184:THR:HB	1:B:185:PRO:HD3	2.01	0.43
1:B:267:LEU:HG	1:B:268:ALA:N	2.33	0.43
1:D:300:LEU:N	1:D:301:SER:HA	2.29	0.43
1:E:204:PRO:O	1:E:228:ARG:HB3	2.18	0.43
1:F:160:PHE:CG	1:F:162:ILE:CD1	3.00	0.43
1:A:174:LEU:C	1:A:175:ASP:CG	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ASN:HD21	1:B:181:GLU:C	2.04	0.43
1:C:144:VAL:O	1:C:144:VAL:HG12	2.19	0.43
1:C:287:THR:HG1	1:C:297:LEU:HG	1.80	0.43
1:E:156:GLU:N	1:E:157:GLN:CB	2.73	0.43
1:E:422:ARG:NH1	1:E:447:GLY:O	2.48	0.43
1:E:451:PHE:O	1:E:452:ARG:C	2.62	0.43
1:F:144:VAL:HG12	1:F:144:VAL:O	2.19	0.43
1:A:177:GLU:N	1:A:178:ASP:CA	2.73	0.43
1:C:273:ILE:HD11	1:C:276:ILE:CD1	2.48	0.43
1:D:174:LEU:C	1:D:175:ASP:CG	2.86	0.43
1:D:273:ILE:HD11	1:D:276:ILE:CD1	2.49	0.43
1:E:144:VAL:HG12	1:E:144:VAL:O	2.19	0.43
1:E:174:LEU:C	1:E:175:ASP:CG	2.87	0.43
1:E:287:THR:CB	1:E:297:LEU:CG	2.95	0.43
1:F:19:THR:HG22	1:F:22:VAL:HB	2.01	0.43
1:F:294:VAL:HG12	1:F:295:GLU:N	2.16	0.43
1:F:348:GLU:HB2	1:F:357:ARG:HB3	2.01	0.43
1:C:19:THR:HG22	1:C:22:VAL:HB	2.01	0.43
1:C:294:VAL:O	1:C:295:GLU:HG2	2.18	0.43
1:E:160:PHE:CG	1:E:162:ILE:CD1	3.01	0.43
1:C:24:LYS:HG2	1:C:183:MET:HE3	2.00	0.43
1:C:240:ILE:CD1	1:C:296:ALA:HB1	2.49	0.43
1:E:106:MET:O	1:E:109:THR:OG1	2.33	0.43
1:A:169:ASN:ND2	1:A:182:ASP:CA	2.62	0.42
1:B:144:VAL:O	1:B:144:VAL:HG12	2.19	0.42
1:B:169:ASN:ND2	1:B:182:ASP:C	2.77	0.42
1:C:177:GLU:N	1:C:178:ASP:CA	2.81	0.42
1:D:158:LEU:N	1:D:158:LEU:HD12	2.33	0.42
1:D:267:LEU:HG	1:D:268:ALA:N	2.34	0.42
1:E:297:LEU:N	1:E:297:LEU:CD2	2.73	0.42
1:F:451:PHE:O	1:F:452:ARG:C	2.62	0.42
1:A:292:GLN:O	1:A:294:VAL:HG23	2.18	0.42
1:B:240:ILE:HD13	1:B:296:ALA:CB	2.50	0.42
1:C:54:ILE:HA	1:C:55:THR:HA	1.71	0.42
1:C:300:LEU:HG	1:C:304:GLU:OE1	2.19	0.42
1:E:298:PRO:O	1:E:299:ALA:HB3	2.18	0.42
1:F:174:LEU:O	1:F:178:ASP:HB3	2.19	0.42
1:F:267:LEU:HG	1:F:268:ALA:N	2.34	0.42
1:F:380:LEU:O	1:F:580:VAL:HG22	2.19	0.42
1:B:169:ASN:CB	1:B:182:ASP:HB2	2.19	0.42
1:D:125:VAL:H	1:D:161:PRO:CB	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:ILE:HA	1:E:161:PRO:CB	2.49	0.42
1:E:348:GLU:HB2	1:E:357:ARG:HB3	2.01	0.42
1:A:119:TYR:O	1:A:121:LEU:N	2.50	0.42
1:C:451:PHE:O	1:C:452:ARG:C	2.62	0.42
1:D:348:GLU:HB2	1:D:357:ARG:HB3	2.01	0.42
1:E:87:ARG:NH1	1:E:300:LEU:O	2.52	0.42
1:E:423:LYS:NZ	1:F:150:ASN:HB2	2.35	0.42
1:F:61:THR:HG1	1:F:67:ASP:HA	1.80	0.42
1:B:10:ILE:HG22	1:B:11:ILE:N	2.35	0.42
1:D:307:VAL:O	1:D:359:SER:HA	2.20	0.42
1:E:19:THR:HG22	1:E:22:VAL:HB	2.01	0.42
1:E:237:VAL:C	1:E:291:THR:CG2	2.92	0.42
1:A:156:GLU:HA	1:A:157:GLN:CB	2.49	0.42
1:A:298:PRO:O	1:A:299:ALA:HB3	2.19	0.42
1:A:380:LEU:O	1:A:580:VAL:HG22	2.19	0.42
1:B:160:PHE:CA	1:B:162:ILE:HG13	2.47	0.42
1:C:159:ASP:O	1:C:160:PHE:HB2	2.19	0.42
1:D:119:TYR:O	1:D:121:LEU:N	2.50	0.42
1:D:444:PRO:O	1:D:447:GLY:N	2.53	0.42
1:E:61:THR:HG1	1:E:67:ASP:HA	1.80	0.42
1:E:164:TYR:O	1:E:179:MET:CE	2.67	0.42
1:E:444:PRO:O	1:E:445:SER:C	2.62	0.42
1:F:307:VAL:O	1:F:359:SER:HA	2.20	0.42
1:A:307:VAL:O	1:A:359:SER:HA	2.20	0.42
1:C:68:TYR:CZ	1:C:191:VAL:HG11	2.55	0.42
1:D:54:ILE:HA	1:D:55:THR:HA	1.71	0.42
1:D:81:PHE:O	1:D:83:GLY:N	2.53	0.42
1:D:380:LEU:O	1:D:580:VAL:HG22	2.19	0.42
1:F:205:PHE:O	1:F:289:CYS:HB3	2.20	0.42
1:A:144:VAL:O	1:A:144:VAL:HG12	2.19	0.42
1:A:160:PHE:CE1	1:A:162:ILE:CG2	3.03	0.42
1:A:240:ILE:HD11	1:A:289:CYS:SG	2.60	0.42
1:B:152:ASP:OD1	1:B:152:ASP:N	2.52	0.42
1:C:160:PHE:CD1	1:C:161:PRO:O	2.70	0.42
1:C:272:ASP:N	1:C:272:ASP:OD1	2.51	0.42
1:D:451:PHE:O	1:D:452:ARG:C	2.61	0.42
1:E:381:ALA:HA	1:E:578:VAL:O	2.20	0.42
1:B:19:THR:HG22	1:B:22:VAL:HB	2.01	0.42
1:B:110:ARG:NH2	1:B:151:LEU:HD11	2.34	0.42
1:B:151:LEU:C	1:B:152:ASP:CG	2.86	0.42
1:B:176:HIS:NE2	1:B:177:GLU:CD	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:PHE:O	1:C:83:GLY:N	2.53	0.42
1:D:10:ILE:HG22	1:D:11:ILE:N	2.33	0.42
1:A:81:PHE:O	1:A:83:GLY:N	2.53	0.42
1:A:451:PHE:O	1:A:452:ARG:C	2.62	0.42
1:B:205:PHE:CE1	1:B:231:VAL:CG2	3.03	0.42
1:B:307:VAL:N	1:B:388:ILE:HG13	2.35	0.42
1:B:380:LEU:O	1:B:580:VAL:HG22	2.19	0.42
1:C:156:GLU:CA	1:C:157:GLN:HB2	2.49	0.42
1:C:380:LEU:O	1:C:580:VAL:HG22	2.19	0.42
1:D:144:VAL:HG12	1:D:144:VAL:O	2.19	0.42
1:D:444:PRO:O	1:D:445:SER:C	2.62	0.42
1:E:307:VAL:O	1:E:359:SER:HA	2.20	0.42
1:F:290:ASP:C	1:F:292:GLN:H	2.27	0.42
1:A:444:PRO:O	1:A:445:SER:C	2.62	0.41
1:B:451:PHE:O	1:B:452:ARG:C	2.62	0.41
1:C:50:LYS:CD	1:C:51:GLU:HB2	2.49	0.41
1:C:205:PHE:CE1	1:C:231:VAL:CG2	3.03	0.41
1:E:50:LYS:CE	1:E:51:GLU:HG3	2.47	0.41
1:F:444:PRO:O	1:F:445:SER:C	2.63	0.41
1:A:184:THR:HA	1:A:187:TYR:HD2	1.85	0.41
1:B:51:GLU:HB3	1:B:52:ARG:H	1.69	0.41
1:B:381:ALA:HA	1:B:578:VAL:O	2.20	0.41
1:B:422:ARG:NH1	1:B:447:GLY:O	2.48	0.41
1:A:237:VAL:CA	1:A:291:THR:CG2	2.98	0.41
1:A:348:GLU:HB2	1:A:357:ARG:HB3	2.02	0.41
1:D:187:TYR:O	1:D:191:VAL:HG23	2.20	0.41
1:D:381:ALA:HA	1:D:578:VAL:O	2.20	0.41
1:E:175:ASP:HB2	1:E:176:HIS:H	1.71	0.41
1:F:10:ILE:HG22	1:F:11:ILE:N	2.35	0.41
1:F:381:ALA:HA	1:F:578:VAL:O	2.20	0.41
1:A:19:THR:HG22	1:A:22:VAL:HB	2.01	0.41
1:A:68:TYR:CZ	1:A:191:VAL:HG11	2.55	0.41
1:A:205:PHE:CE1	1:A:231:VAL:CG2	3.03	0.41
1:C:151:LEU:C	1:C:152:ASP:CG	2.86	0.41
1:C:310:PHE:CG	1:C:383:SER:HB3	2.55	0.41
1:D:160:PHE:CE1	1:D:162:ILE:CG2	3.03	0.41
1:D:169:ASN:ND2	1:D:182:ASP:N	2.64	0.41
1:E:237:VAL:C	1:E:291:THR:HG22	2.46	0.41
1:A:156:GLU:CA	1:A:157:GLN:HB2	2.49	0.41
1:A:444:PRO:O	1:A:447:GLY:N	2.54	0.41
1:B:81:PHE:O	1:B:83:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:TYR:O	1:C:191:VAL:HG23	2.21	0.41
1:D:19:THR:HG22	1:D:22:VAL:HB	2.01	0.41
1:D:68:TYR:CZ	1:D:191:VAL:HG11	2.55	0.41
1:D:169:ASN:ND2	1:D:182:ASP:HB3	2.32	0.41
1:E:444:PRO:O	1:E:447:GLY:N	2.54	0.41
1:F:68:TYR:CZ	1:F:191:VAL:HG11	2.55	0.41
1:F:160:PHE:CE2	1:F:162:ILE:CD1	2.86	0.41
1:A:157:GLN:HB3	1:A:158:LEU:H	1.70	0.41
1:B:68:TYR:CZ	1:B:191:VAL:HG11	2.56	0.41
1:C:307:VAL:H	1:C:388:ILE:HD12	1.85	0.41
1:E:81:PHE:O	1:E:83:GLY:N	2.53	0.41
1:E:205:PHE:CE1	1:E:231:VAL:CG2	3.03	0.41
1:E:240:ILE:CD1	1:E:287:THR:OG1	2.67	0.41
1:F:336:ASN:HA	1:F:339:LEU:HB2	2.03	0.41
1:B:251:VAL:HG12	1:B:273:ILE:HB	2.03	0.41
1:C:444:PRO:O	1:C:445:SER:C	2.63	0.41
1:C:576:GLU:HG2	1:C:589:LYS:HD3	2.03	0.41
1:E:174:LEU:O	1:E:178:ASP:HB3	2.20	0.41
1:F:290:ASP:O	1:F:294:VAL:HG21	2.21	0.41
1:F:444:PRO:O	1:F:447:GLY:N	2.54	0.41
1:B:240:ILE:CD1	1:B:296:ALA:HB1	2.50	0.41
1:C:152:ASP:OD1	1:C:152:ASP:N	2.52	0.41
1:D:310:PHE:HB2	1:D:357:ARG:HH22	1.85	0.41
1:D:336:ASN:HA	1:D:339:LEU:HB2	2.02	0.41
1:E:68:TYR:CZ	1:E:191:VAL:HG11	2.55	0.41
1:E:164:TYR:H	1:E:164:TYR:HD1	1.69	0.41
1:E:287:THR:HB	1:E:297:LEU:CG	2.51	0.41
1:E:295:GLU:HA	1:E:296:ALA:HA	1.81	0.41
1:F:156:GLU:CG	1:F:159:ASP:CB	2.86	0.41
1:F:205:PHE:CE1	1:F:231:VAL:CG2	3.03	0.41
1:A:52:ARG:CB	1:A:53:GLY:HA3	2.50	0.41
1:A:381:ALA:HA	1:A:578:VAL:O	2.21	0.41
1:B:306:THR:CA	1:B:388:ILE:CD1	2.82	0.41
1:B:576:GLU:HG2	1:B:589:LYS:HD3	2.03	0.41
1:C:10:ILE:HG22	1:C:11:ILE:N	2.36	0.41
1:C:381:ALA:HA	1:C:578:VAL:O	2.20	0.41
1:D:148:PHE:O	1:D:151:LEU:HD22	2.21	0.41
1:F:81:PHE:O	1:F:83:GLY:N	2.53	0.41
1:B:123:PRO:O	1:B:124:ILE:HD13	2.21	0.40
1:B:287:THR:HG22	1:B:297:LEU:HD12	1.91	0.40
1:A:24:LYS:HG2	1:A:183:MET:HE3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:LEU:CG	1:D:599:ARG:NH1	2.83	0.40
1:D:177:GLU:CB	1:D:178:ASP:CA	2.96	0.40
1:D:445:SER:O	1:D:446:ARG:C	2.65	0.40
1:F:174:LEU:N	1:F:174:LEU:CD2	2.84	0.40
1:B:176:HIS:CD2	1:B:177:GLU:HA	2.55	0.40
1:B:230:LYS:HG2	1:B:266:ASP:HB3	2.04	0.40
1:B:336:ASN:HA	1:B:339:LEU:HB2	2.03	0.40
1:D:149:VAL:C	1:D:151:LEU:H	2.30	0.40
1:F:148:PHE:CE1	1:F:156:GLU:OE1	2.75	0.40
1:F:175:ASP:HB2	1:F:176:HIS:H	1.70	0.40
1:F:187:TYR:O	1:F:191:VAL:HG23	2.21	0.40
1:B:310:PHE:HB2	1:B:357:ARG:HH22	1.86	0.40
1:C:19:THR:HG21	1:C:52:ARG:O	2.22	0.40
1:C:174:LEU:N	1:C:174:LEU:CD2	2.84	0.40
1:C:336:ASN:HA	1:C:339:LEU:HB2	2.03	0.40
1:C:379:GLU:HG2	1:C:581:THR:HA	2.04	0.40
1:F:50:LYS:CE	1:F:51:GLU:HG3	2.48	0.40
1:A:237:VAL:CA	1:A:291:THR:HG23	2.45	0.40
1:A:336:ASN:HA	1:A:339:LEU:HB2	2.02	0.40
1:B:379:GLU:HG2	1:B:581:THR:HA	2.04	0.40
1:D:300:LEU:HG	1:D:304:GLU:OE1	2.21	0.40
1:E:22:VAL:CG1	1:E:56:ILE:HD13	2.52	0.40
1:E:187:TYR:O	1:E:191:VAL:HG23	2.22	0.40
1:F:123:PRO:O	1:F:124:ILE:HD13	2.22	0.40

There are no symmetry-related clashes.

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	543/607 (90%)	421 (78%)	85 (16%)	37 (7%)	1 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	543/607 (90%)	420 (77%)	89 (16%)	34 (6%)	1	8
1	C	543/607 (90%)	418 (77%)	89 (16%)	36 (7%)	1	7
1	D	543/607 (90%)	419 (77%)	87 (16%)	37 (7%)	1	7
1	E	543/607 (90%)	425 (78%)	86 (16%)	32 (6%)	1	9
1	F	543/607 (90%)	424 (78%)	85 (16%)	34 (6%)	1	8
All	All	3258/3642 (90%)	2527 (78%)	521 (16%)	210 (6%)	1	8

All (210) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	PRO
1	A	181	GLU
1	A	182	ASP
1	A	223	ILE
1	A	393	ASP
1	A	477	PRO
1	B	161	PRO
1	B	182	ASP
1	B	302	VAL
1	B	393	ASP
1	B	477	PRO
1	C	161	PRO
1	C	181	GLU
1	C	182	ASP
1	C	223	ILE
1	C	302	VAL
1	C	393	ASP
1	C	477	PRO
1	D	161	PRO
1	D	181	GLU
1	D	182	ASP
1	D	223	ILE
1	D	302	VAL
1	D	393	ASP
1	D	477	PRO
1	E	161	PRO
1	E	181	GLU
1	E	182	ASP
1	E	393	ASP
1	E	477	PRO

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Mol	Chain	Res	Type
1	F	161	PRO
1	F	181	GLU
1	F	182	ASP
1	F	393	ASP
1	F	477	PRO
1	A	18	LYS
1	A	20	THR
1	A	80	ASP
1	A	148	PHE
1	A	179	MET
1	A	180	ALA
1	A	286	ASP
1	A	294	VAL
1	A	396	LYS
1	A	433	GLY
1	B	18	LYS
1	B	20	THR
1	B	51	GLU
1	B	56	ILE
1	B	80	ASP
1	B	148	PHE
1	B	181	GLU
1	B	286	ASP
1	B	396	LYS
1	B	433	GLY
1	C	18	LYS
1	C	20	THR
1	C	80	ASP
1	C	148	PHE
1	C	396	LYS
1	C	433	GLY
1	D	18	LYS
1	D	20	THR
1	D	51	GLU
1	D	180	ALA
1	D	286	ASP
1	D	396	LYS
1	D	433	GLY
1	E	18	LYS
1	E	20	THR
1	E	51	GLU
1	E	56	ILE

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Mol	Chain	Res	Type
1	E	80	ASP
1	E	148	PHE
1	E	294	VAL
1	E	396	LYS
1	E	433	GLY
1	F	18	LYS
1	F	20	THR
1	F	51	GLU
1	F	80	ASP
1	F	148	PHE
1	F	286	ASP
1	F	294	VAL
1	F	302	VAL
1	F	396	LYS
1	F	433	GLY
1	A	51	GLU
1	A	83	GLY
1	A	175	ASP
1	A	257	HIS
1	A	275	ALA
1	A	298	PRO
1	A	302	VAL
1	A	412	GLN
1	B	83	GLY
1	B	160	PHE
1	B	175	ASP
1	B	183	MET
1	B	257	HIS
1	B	275	ALA
1	B	298	PRO
1	B	412	GLN
1	C	51	GLU
1	C	83	GLY
1	C	102	PHE
1	C	160	PHE
1	C	183	MET
1	C	257	HIS
1	C	275	ALA
1	C	298	PRO
1	C	412	GLN
1	D	80	ASP
1	D	83	GLY

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Mol	Chain	Res	Type
1	D	150	ASN
1	D	175	ASP
1	D	183	MET
1	D	257	HIS
1	D	275	ALA
1	D	298	PRO
1	D	412	GLN
1	E	83	GLY
1	E	160	PHE
1	E	183	MET
1	E	257	HIS
1	E	275	ALA
1	E	412	GLN
1	F	56	ILE
1	F	83	GLY
1	F	102	PHE
1	F	183	MET
1	F	257	HIS
1	F	275	ALA
1	F	298	PRO
1	F	412	GLN
1	A	102	PHE
1	A	155	ASP
1	A	160	PHE
1	A	289	CYS
1	A	339	LEU
1	B	102	PHE
1	B	155	ASP
1	B	156	GLU
1	B	290	ASP
1	B	339	LEU
1	C	155	ASP
1	C	156	GLU
1	C	290	ASP
1	C	339	LEU
1	D	102	PHE
1	D	160	PHE
1	D	290	ASP
1	D	339	LEU
1	E	102	PHE
1	E	155	ASP
1	E	157	GLN

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Mol	Chain	Res	Type
1	E	299	ALA
1	E	339	LEU
1	F	160	PHE
1	F	339	LEU
1	A	157	GLN
1	A	241	ASP
1	A	499	PHE
1	A	560	PRO
1	B	157	GLN
1	B	235	GLN
1	B	499	PHE
1	B	560	PRO
1	C	56	ILE
1	C	157	GLN
1	C	175	ASP
1	C	235	GLN
1	C	499	PHE
1	C	560	PRO
1	D	56	ILE
1	D	157	GLN
1	D	499	PHE
1	D	560	PRO
1	E	175	ASP
1	E	235	GLN
1	E	298	PRO
1	E	499	PHE
1	E	560	PRO
1	F	155	ASP
1	F	157	GLN
1	F	175	ASP
1	F	499	PHE
1	F	560	PRO
1	A	56	ILE
1	A	235	GLN
1	C	241	ASP
1	D	155	ASP
1	D	235	GLN
1	D	241	ASP
1	D	299	ALA
1	F	235	GLN
1	B	307	VAL
1	C	307	VAL

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Mol	Chain	Res	Type
1	A	14	VAL
1	B	14	VAL
1	C	14	VAL
1	D	14	VAL
1	E	14	VAL
1	F	14	VAL
1	D	120	GLY
1	E	120	GLY
1	F	120	GLY
1	A	120	GLY
1	C	120	GLY
1	F	162	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	447/519 (86%)	379 (85%)	68 (15%)	3	13
1	B	448/519 (86%)	376 (84%)	72 (16%)	2	12
1	C	447/519 (86%)	378 (85%)	69 (15%)	2	13
1	D	445/519 (86%)	378 (85%)	67 (15%)	3	13
1	E	449/519 (86%)	383 (85%)	66 (15%)	3	14
1	F	450/519 (87%)	376 (84%)	74 (16%)	2	11
All	All	2686/3114 (86%)	2270 (84%)	416 (16%)	2	12

All (416) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	10	ILE
1	A	11	ILE
1	A	21	LEU
1	A	50	LYS
1	A	51	GLU

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Mol	Chain	Res	Type
1	A	59	LYS
1	A	75	THR
1	A	96	LEU
1	A	102	PHE
1	A	122	LYS
1	A	150	ASN
1	A	151	LEU
1	A	157	GLN
1	A	160	PHE
1	A	169	ASN
1	A	175	ASP
1	A	181	GLU
1	A	182	ASP
1	A	183	MET
1	A	184	THR
1	A	186	LEU
1	A	199	VAL
1	A	216	SER
1	A	223	ILE
1	A	225	ARG
1	A	231	VAL
1	A	235	GLN
1	A	236	GLN
1	A	240	ILE
1	A	241	ASP
1	A	250	LYS
1	A	257	HIS
1	A	262	ARG
1	A	265	THR
1	A	272	ASP
1	A	273	ILE
1	A	274	VAL
1	A	289	CYS
1	A	294	VAL
1	A	297	LEU
1	A	300	LEU
1	A	302	VAL
1	A	303	ASP
1	A	308	SER
1	A	312	CYS
1	A	326	VAL
1	A	328	SER

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Mol	Chain	Res	Type
1	A	339	LEU
1	A	357	ARG
1	A	359	SER
1	A	361	ARG
1	A	364	LEU
1	A	365	HIS
1	A	379	GLU
1	A	392	ILE
1	A	398	GLU
1	A	417	GLN
1	A	429	MET
1	A	443	ILE
1	A	448	LEU
1	A	465	LEU
1	A	470	SER
1	A	480	VAL
1	A	482	GLN
1	A	539	THR
1	A	566	GLU
1	A	583	THR
1	B	1	MET
1	B	10	ILE
1	B	11	ILE
1	B	21	LEU
1	B	50	LYS
1	B	51	GLU
1	B	59	LYS
1	B	75	THR
1	B	96	LEU
1	B	102	PHE
1	B	122	LYS
1	B	151	LEU
1	B	152	ASP
1	B	156	GLU
1	B	157	GLN
1	B	158	LEU
1	B	160	PHE
1	B	169	ASN
1	B	175	ASP
1	B	177	GLU
1	B	181	GLU
1	B	183	MET

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Mol	Chain	Res	Type
1	B	184	THR
1	B	186	LEU
1	B	199	VAL
1	B	216	SER
1	B	223	ILE
1	B	225	ARG
1	B	231	VAL
1	B	235	GLN
1	B	236	GLN
1	B	240	ILE
1	B	241	ASP
1	B	250	LYS
1	B	257	HIS
1	B	262	ARG
1	B	265	THR
1	B	272	ASP
1	B	273	ILE
1	B	274	VAL
1	B	292	GLN
1	B	295	GLU
1	B	297	LEU
1	B	300	LEU
1	B	302	VAL
1	B	303	ASP
1	B	308	SER
1	B	312	CYS
1	B	326	VAL
1	B	328	SER
1	B	339	LEU
1	B	357	ARG
1	B	359	SER
1	B	361	ARG
1	B	364	LEU
1	B	365	HIS
1	B	392	ILE
1	B	398	GLU
1	B	405	LEU
1	B	417	GLN
1	B	425	ASP
1	B	429	MET
1	B	439	LEU
1	B	443	ILE

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Mol	Chain	Res	Type
1	B	448	LEU
1	B	465	LEU
1	B	470	SER
1	B	480	VAL
1	B	507	ARG
1	B	539	THR
1	B	566	GLU
1	B	583	THR
1	C	1	MET
1	C	10	ILE
1	C	11	ILE
1	C	21	LEU
1	C	50	LYS
1	C	51	GLU
1	C	59	LYS
1	C	75	THR
1	C	96	LEU
1	C	102	PHE
1	C	122	LYS
1	C	151	LEU
1	C	152	ASP
1	C	156	GLU
1	C	157	GLN
1	C	158	LEU
1	C	160	PHE
1	C	169	ASN
1	C	175	ASP
1	C	181	GLU
1	C	182	ASP
1	C	183	MET
1	C	184	THR
1	C	186	LEU
1	C	199	VAL
1	C	216	SER
1	C	223	ILE
1	C	225	ARG
1	C	231	VAL
1	C	235	GLN
1	C	236	GLN
1	C	240	ILE
1	C	241	ASP
1	C	250	LYS

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Mol	Chain	Res	Type
1	C	257	HIS
1	C	262	ARG
1	C	265	THR
1	C	272	ASP
1	C	273	ILE
1	C	274	VAL
1	C	292	GLN
1	C	295	GLU
1	C	297	LEU
1	C	300	LEU
1	C	302	VAL
1	C	303	ASP
1	C	308	SER
1	C	312	CYS
1	C	326	VAL
1	C	328	SER
1	C	339	LEU
1	C	357	ARG
1	C	359	SER
1	C	361	ARG
1	C	364	LEU
1	C	365	HIS
1	C	392	ILE
1	C	398	GLU
1	C	405	LEU
1	C	417	GLN
1	C	429	MET
1	C	443	ILE
1	C	448	LEU
1	C	465	LEU
1	C	470	SER
1	C	480	VAL
1	C	539	THR
1	C	566	GLU
1	C	583	THR
1	D	1	MET
1	D	10	ILE
1	D	11	ILE
1	D	21	LEU
1	D	50	LYS
1	D	51	GLU
1	D	59	LYS

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Mol	Chain	Res	Type
1	D	75	THR
1	D	96	LEU
1	D	102	PHE
1	D	122	LYS
1	D	148	PHE
1	D	150	ASN
1	D	151	LEU
1	D	158	LEU
1	D	160	PHE
1	D	169	ASN
1	D	175	ASP
1	D	177	GLU
1	D	181	GLU
1	D	182	ASP
1	D	183	MET
1	D	184	THR
1	D	186	LEU
1	D	199	VAL
1	D	216	SER
1	D	223	ILE
1	D	225	ARG
1	D	231	VAL
1	D	235	GLN
1	D	236	GLN
1	D	240	ILE
1	D	241	ASP
1	D	250	LYS
1	D	257	HIS
1	D	262	ARG
1	D	265	THR
1	D	272	ASP
1	D	273	ILE
1	D	274	VAL
1	D	288	VAL
1	D	294	VAL
1	D	297	LEU
1	D	300	LEU
1	D	302	VAL
1	D	308	SER
1	D	312	CYS
1	D	326	VAL
1	D	328	SER

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Mol	Chain	Res	Type
1	D	339	LEU
1	D	357	ARG
1	D	359	SER
1	D	361	ARG
1	D	364	LEU
1	D	365	HIS
1	D	392	ILE
1	D	398	GLU
1	D	417	GLN
1	D	429	MET
1	D	443	ILE
1	D	448	LEU
1	D	465	LEU
1	D	470	SER
1	D	480	VAL
1	D	539	THR
1	D	566	GLU
1	D	583	THR
1	E	1	MET
1	E	10	ILE
1	E	11	ILE
1	E	21	LEU
1	E	50	LYS
1	E	51	GLU
1	E	59	LYS
1	E	75	THR
1	E	102	PHE
1	E	122	LYS
1	E	150	ASN
1	E	152	ASP
1	E	156	GLU
1	E	157	GLN
1	E	160	PHE
1	E	164	TYR
1	E	169	ASN
1	E	175	ASP
1	E	181	GLU
1	E	182	ASP
1	E	183	MET
1	E	184	THR
1	E	186	LEU
1	E	199	VAL

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Mol	Chain	Res	Type
1	E	216	SER
1	E	223	ILE
1	E	225	ARG
1	E	231	VAL
1	E	235	GLN
1	E	236	GLN
1	E	240	ILE
1	E	241	ASP
1	E	250	LYS
1	E	257	HIS
1	E	262	ARG
1	E	265	THR
1	E	272	ASP
1	E	273	ILE
1	E	274	VAL
1	E	292	GLN
1	E	295	GLU
1	E	297	LEU
1	E	308	SER
1	E	312	CYS
1	E	326	VAL
1	E	328	SER
1	E	339	LEU
1	E	357	ARG
1	E	359	SER
1	E	361	ARG
1	E	364	LEU
1	E	365	HIS
1	E	392	ILE
1	E	398	GLU
1	E	405	LEU
1	E	417	GLN
1	E	429	MET
1	E	439	LEU
1	E	443	ILE
1	E	448	LEU
1	E	465	LEU
1	E	470	SER
1	E	480	VAL
1	E	539	THR
1	E	566	GLU
1	E	583	THR

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Mol	Chain	Res	Type
1	F	1	MET
1	F	10	ILE
1	F	11	ILE
1	F	21	LEU
1	F	50	LYS
1	F	51	GLU
1	F	59	LYS
1	F	75	THR
1	F	96	LEU
1	F	102	PHE
1	F	122	LYS
1	F	150	ASN
1	F	152	ASP
1	F	154	THR
1	F	156	GLU
1	F	157	GLN
1	F	158	LEU
1	F	160	PHE
1	F	164	TYR
1	F	169	ASN
1	F	175	ASP
1	F	181	GLU
1	F	182	ASP
1	F	183	MET
1	F	184	THR
1	F	186	LEU
1	F	199	VAL
1	F	216	SER
1	F	223	ILE
1	F	225	ARG
1	F	231	VAL
1	F	235	GLN
1	F	236	GLN
1	F	240	ILE
1	F	241	ASP
1	F	250	LYS
1	F	257	HIS
1	F	262	ARG
1	F	265	THR
1	F	272	ASP
1	F	273	ILE
1	F	274	VAL

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Mol	Chain	Res	Type
1	F	289	CYS
1	F	292	GLN
1	F	295	GLU
1	F	297	LEU
1	F	300	LEU
1	F	302	VAL
1	F	303	ASP
1	F	308	SER
1	F	312	CYS
1	F	326	VAL
1	F	328	SER
1	F	339	LEU
1	F	357	ARG
1	F	359	SER
1	F	361	ARG
1	F	364	LEU
1	F	365	HIS
1	F	392	ILE
1	F	398	GLU
1	F	405	LEU
1	F	417	GLN
1	F	429	MET
1	F	439	LEU
1	F	443	ILE
1	F	448	LEU
1	F	465	LEU
1	F	470	SER
1	F	480	VAL
1	F	539	THR
1	F	563	MET
1	F	566	GLU
1	F	583	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	169	ASN
1	A	193	HIS
1	A	208	GLN
1	A	211	GLN
1	A	292	GLN

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Mol	Chain	Res	Type
1	A	482	GLN
1	B	16	HIS
1	B	60	ASN
1	B	169	ASN
1	B	292	GLN
1	B	428	ASN
1	C	16	HIS
1	C	169	ASN
1	C	211	GLN
1	C	292	GLN
1	D	16	HIS
1	D	157	GLN
1	D	169	ASN
1	D	193	HIS
1	D	211	GLN
1	E	16	HIS
1	E	157	GLN
1	E	169	ASN
1	E	292	GLN
1	E	428	ASN
1	E	482	GLN
1	F	16	HIS
1	F	157	GLN
1	F	169	ASN
1	F	235	GLN
1	F	292	GLN

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 [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	555/607 (91%)	-1.13	0 100 100	79, 130, 184, 219	0
1	B	555/607 (91%)	-1.14	1 (0%) 91 86	80, 129, 184, 220	0
1	C	555/607 (91%)	-1.12	1 (0%) 91 86	82, 130, 183, 216	0
1	D	555/607 (91%)	-1.16	0 100 100	85, 131, 183, 218	0
1	E	555/607 (91%)	-1.10	0 100 100	83, 131, 183, 225	0
1	F	555/607 (91%)	-1.16	0 100 100	83, 131, 182, 218	0
All	All	3330/3642 (91%)	-1.13	2 (0%) 92 91	79, 131, 184, 225	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	77	GLY	4.0
1	C	556	VAL	2.7

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 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.