



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:39 AM UTC

PDB ID : 2W6I / pdb_00002w6i
Title : Low resolution structures of bovine mitochondrial F1-ATPase during controlled dehydration: Hydration State 4B.
Authors : Sanchez-Weatherby, J.; Felisaz, F.; Gobbo, A.; Huet, J.; Ravelli, R.B.G.; Bowler, M.W.; Cipriani, F.
Deposited on : 2008-12-18
Resolution : 4.00 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

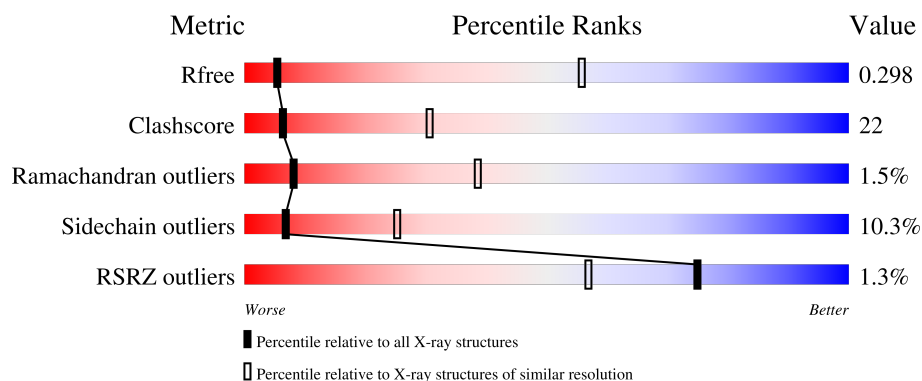
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	553	2% 42% 35% 9% 12%
1	B	553	% 41% 37% 8% 13%
1	C	553	2% 44% 35% 8% 11%
2	D	528	50% 30% 7% 12%
2	E	528	37% 39% 11% 12%

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Mol	Chain	Length	Quality of chain
2	F	528	2%49%32%6%12%
3	G	298	%53%29%6%12%
4	H	168	9%9%82%
5	I	51	33%18%45%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24216 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 ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	B	479	Total	C	N	O	S	0	0	0
			3656	2303	647	694	12			
1	C	492	Total	C	N	O	S	0	0	0
			3748	2360	661	715	12			

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	E	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	263	Total	C	N	O	S	0	0	0
			2051	1291	354	398	8			

- Molecule 4 is a protein called F1-ATPASE DELTA SUBUNIT.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	31	Total	C	N	O	0	0	0
			235	147	39	49			

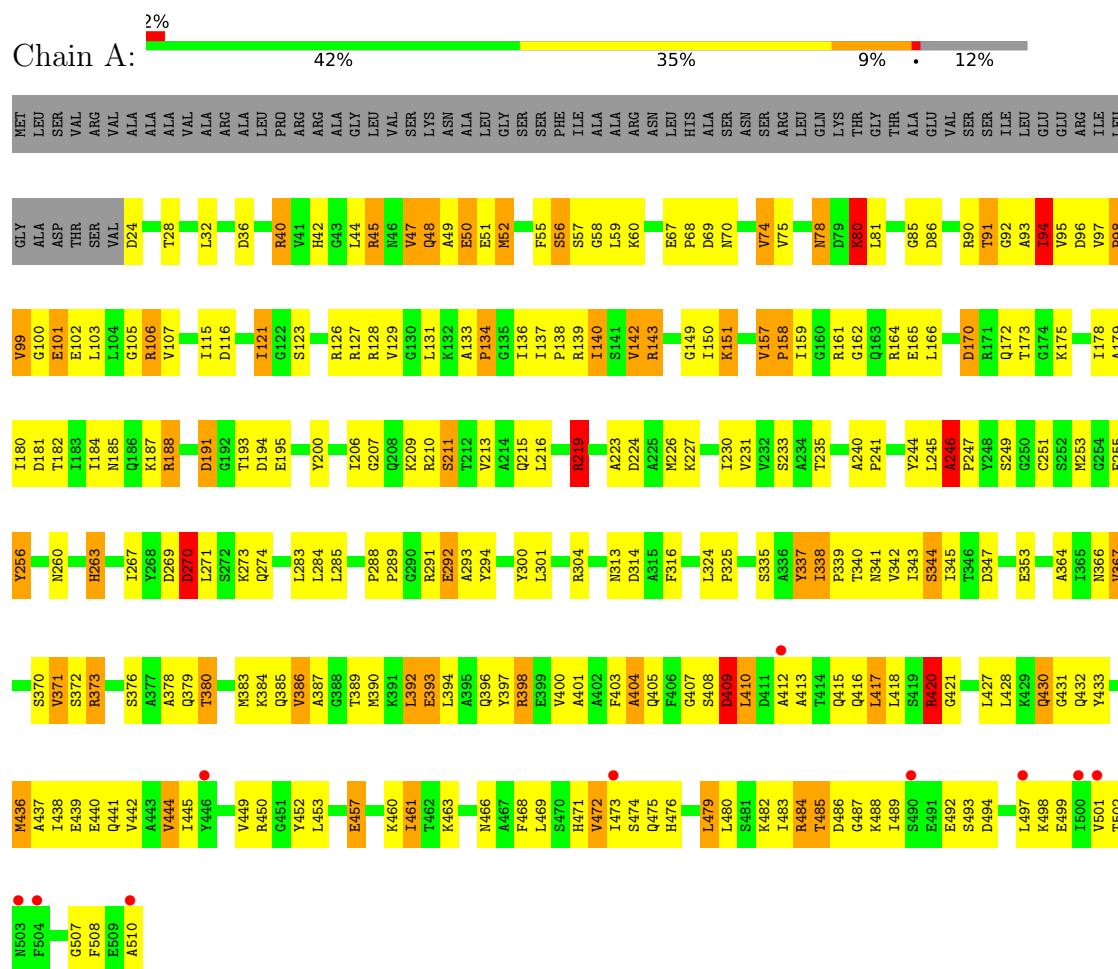
- Molecule 5 is a protein called ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	28	Total	C	N	O	S	0	0	0
			212	135	39	37	1			

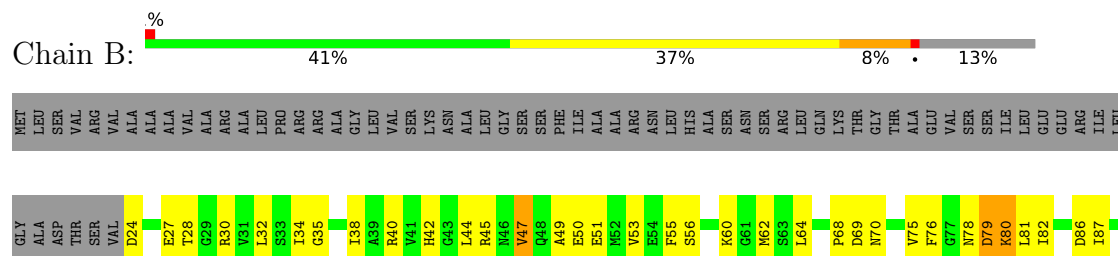
3 Residue-property plots

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: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL



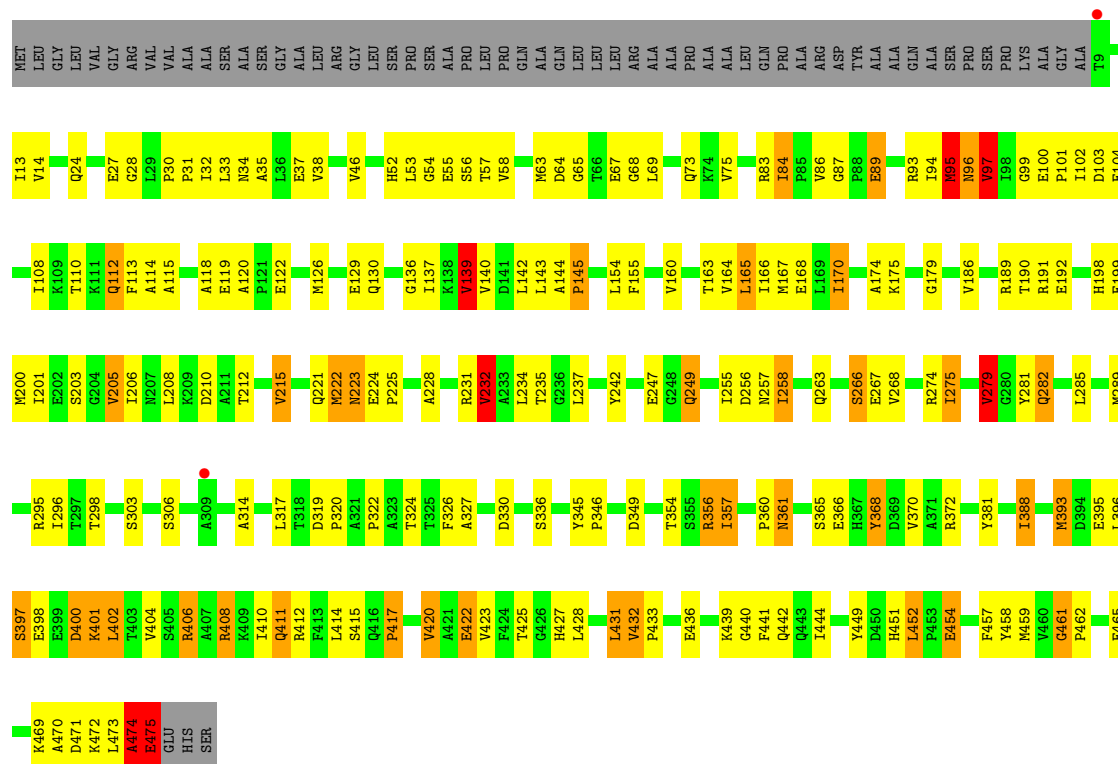
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL

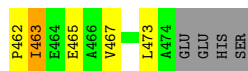




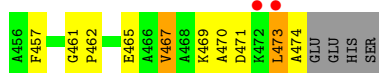
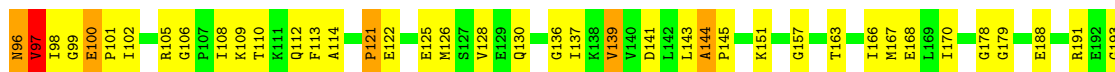
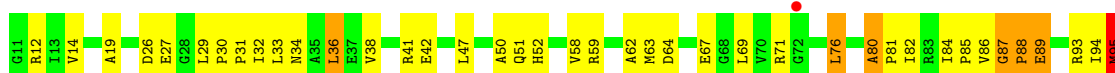
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain D:  50% 30% 7% 12%

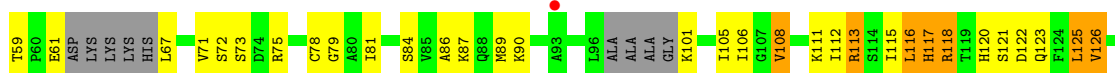
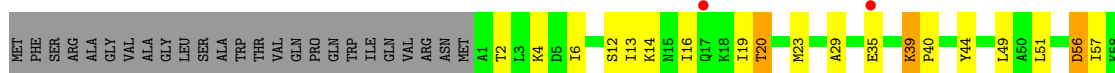




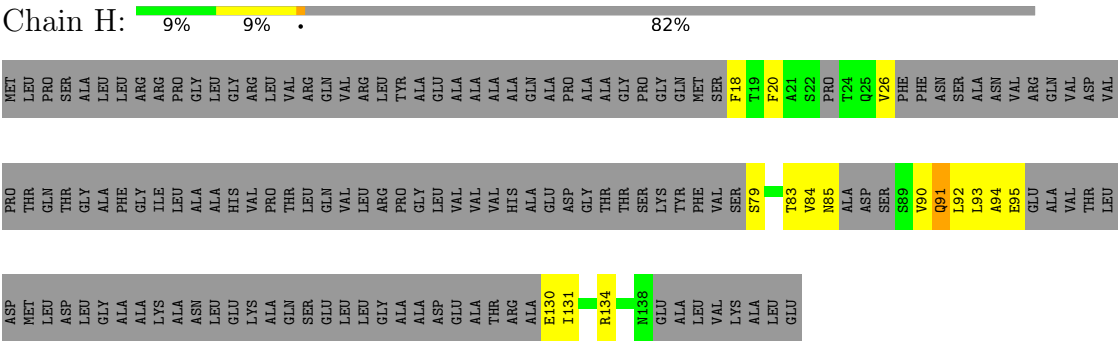
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



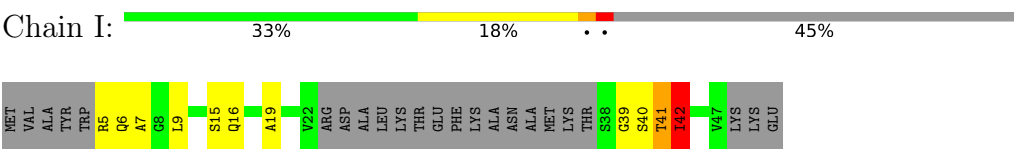
• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL



● Molecule 4: F1-ATPASE DELTA SUBUNIT



● Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.92Å 131.33Å 267.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 4.00 30.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	92.8 (30.00-4.00) 92.5 (30.00-4.00)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 4.01Å)	Xtriage
Refinement program	REFMAC 5.5.0038	Depositor
R, R_{free}	0.299 , 0.300 0.303 , 0.298	Depositor DCC
R_{free} test set	1557 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	92.8	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 3.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	24216	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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	0.77	0/3766	1.74	66/5080 (1.3%)
1	B	0.77	0/3704	1.76	69/4995 (1.4%)
1	C	0.80	0/3799	1.80	76/5126 (1.5%)
2	D	0.82	1/3596 (0.0%)	1.78	70/4879 (1.4%)
2	E	0.78	0/3587	1.78	89/4867 (1.8%)
2	F	0.80	1/3587 (0.0%)	1.79	93/4867 (1.9%)
3	G	0.45	0/2074	1.02	5/2785 (0.2%)
4	H	0.34	0/232	0.87	0/308
5	I	0.43	0/212	0.98	0/281
All	All	0.76	2/24557 (0.0%)	1.71	468/33188 (1.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	96	ASN	CA-CB	5.45	1.62	1.53
2	D	96	ASN	CA-CB	5.29	1.61	1.53

All (468) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	408	ARG	CD-NE-CZ	22.81	156.33	124.40
2	F	282	GLN	CB-CG-CD	15.22	138.48	112.60
2	E	408	ARG	CD-NE-CZ	13.33	143.07	124.40
1	B	351	PHE	CA-CB-CG	11.14	124.94	113.80
1	A	270	ASP	CA-CB-CG	10.97	123.57	112.60
2	F	139	VAL	CB-CA-C	-10.79	98.07	111.88
1	B	270	ASP	CA-CB-CG	10.59	123.19	112.60
1	B	375	GLY	N-CA-C	9.77	125.41	114.67
1	B	40	ARG	CD-NE-CZ	9.25	137.35	124.40
2	F	97	VAL	CB-CA-C	-9.14	99.80	112.14
2	D	96	ASN	CA-CB-CG	-8.67	103.93	112.60
2	D	95	MET	CA-C-N	8.65	138.37	122.02
2	D	95	MET	C-N-CA	8.65	138.37	122.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	139	VAL	CB-CA-C	-8.56	100.74	111.70
1	C	503	ASN	CA-CB-CG	-8.54	104.06	112.60
2	E	307	VAL	N-CA-CB	8.46	121.98	111.41
1	C	113	ASN	CA-CB-CG	-8.42	104.18	112.60
2	F	96	ASN	CB-CA-C	-8.28	93.27	110.40
2	F	427	HIS	CA-CB-CG	8.21	122.01	113.80
1	A	269	ASP	CA-C-N	8.08	136.24	121.70
1	A	269	ASP	C-N-CA	8.08	136.24	121.70
2	F	95	MET	CA-C-N	8.02	138.62	121.45
2	F	95	MET	C-N-CA	8.02	138.62	121.45
1	C	74	VAL	N-CA-CB	-8.02	101.98	110.72
1	C	476	HIS	N-CA-C	7.93	127.69	110.80
1	A	123	SER	N-CA-C	7.91	121.35	109.25
2	D	474	ALA	CA-C-N	7.80	135.73	121.70
2	D	474	ALA	C-N-CA	7.80	135.73	121.70
2	D	349	ASP	CA-C-N	7.75	127.47	119.56
2	D	349	ASP	C-N-CA	7.75	127.47	119.56
1	C	409	ASP	CA-CB-CG	7.75	120.35	112.60
2	E	349	ASP	CA-C-O	7.65	124.26	119.29
1	B	270	ASP	CB-CA-C	-7.60	95.66	110.10
2	F	221	GLN	N-CA-C	7.58	120.81	110.35
1	B	475	GLN	N-CA-C	7.50	119.53	111.36
2	E	95	MET	CA-C-O	7.44	129.82	121.11
1	A	91	THR	N-CA-C	-7.41	104.77	113.88
2	E	276	PRO	CA-C-O	-7.37	112.65	122.08
1	A	270	ASP	CB-CA-C	-7.36	96.11	110.10
1	C	429	LYS	CA-C-O	-7.35	113.35	121.87
2	F	95	MET	CA-CB-CG	7.33	128.77	114.10
1	A	170	ASP	CA-CB-CG	7.30	119.90	112.60
1	C	501	VAL	N-CA-CB	7.27	118.54	110.62
2	D	417	PRO	N-CA-CB	7.26	106.98	102.92
1	B	309	ALA	N-CA-C	-7.20	99.63	110.28
1	B	53	VAL	CA-C-O	-7.19	114.33	121.67
1	A	392	LEU	N-CA-C	7.18	119.19	111.36
2	E	395	GLU	N-CA-C	-7.14	104.69	113.19
2	D	393	MET	N-CA-C	7.12	122.14	113.38
2	F	256	ASP	CA-CB-CG	7.11	119.71	112.60
3	G	179	PHE	CA-CB-CG	7.10	120.90	113.80
2	F	232	VAL	CB-CA-C	-7.10	101.69	112.05
2	E	129	GLU	N-CA-C	7.05	120.16	109.23
2	E	343	GLY	N-CA-C	-7.03	106.71	115.08
2	D	97	VAL	CB-CA-C	-7.03	102.53	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	249	GLN	N-CA-C	7.01	119.58	110.53
2	D	406	ARG	NE-CZ-NH1	-7.00	114.50	121.50
1	A	210	ARG	CA-C-O	-7.00	112.19	120.10
1	C	476	HIS	CA-CB-CG	-6.98	106.82	113.80
1	A	431	GLY	N-CA-C	-6.97	101.62	112.85
1	A	260	ASN	CA-CB-CG	-6.97	105.63	112.60
2	F	312	VAL	CA-C-N	6.96	127.35	119.83
2	F	312	VAL	C-N-CA	6.96	127.35	119.83
1	A	149	GLY	N-CA-C	-6.94	105.48	115.27
1	B	349	GLN	CA-CB-CG	6.93	127.96	114.10
1	B	219	ARG	NE-CZ-NH2	6.91	125.42	119.20
2	E	160	VAL	N-CA-C	-6.91	98.64	108.58
2	E	95	MET	CA-CB-CG	6.90	127.90	114.10
2	E	261	PHE	CA-C-N	6.87	129.37	120.44
2	E	261	PHE	C-N-CA	6.87	129.37	120.44
2	F	59	ARG	NE-CZ-NH1	-6.86	114.64	121.50
2	F	179	GLY	N-CA-C	-6.85	103.75	111.63
1	A	476	HIS	N-CA-C	6.82	121.52	112.25
2	E	22	ASP	CA-CB-CG	6.79	119.39	112.60
2	E	87	GLY	CA-C-N	6.75	126.54	119.05
2	E	87	GLY	C-N-CA	6.75	126.54	119.05
2	D	96	ASN	CB-CA-C	-6.75	96.94	111.78
2	E	306	SER	N-CA-C	6.75	119.93	109.07
1	A	314	ASP	CA-CB-CG	-6.73	105.87	112.60
2	E	342	LEU	N-CA-C	-6.69	105.10	113.20
1	C	149	GLY	N-CA-C	-6.69	105.37	115.00
2	F	349	ASP	CA-C-N	6.67	126.30	119.56
2	F	349	ASP	C-N-CA	6.67	126.30	119.56
1	B	258	ARG	CD-NE-CZ	6.66	133.73	124.40
1	A	285	LEU	CA-C-O	6.63	127.31	119.28
1	B	209	LYS	CA-C-O	-6.62	113.45	120.80
2	D	400	ASP	CA-CB-CG	6.61	119.21	112.60
2	F	385	GLN	N-CA-C	6.61	120.22	111.75
2	E	141	ASP	CA-CB-CG	6.60	119.20	112.60
2	D	101	PRO	N-CA-CB	6.60	109.09	103.35
1	A	78	ASN	CA-CB-CG	6.59	119.19	112.60
2	E	432	VAL	CA-C-N	6.59	127.12	120.14
2	E	432	VAL	C-N-CA	6.59	127.12	120.14
2	F	313	PRO	N-CA-CB	6.58	109.19	103.27
2	E	156	GLY	N-CA-C	-6.55	104.56	112.48
1	A	80	LYS	N-CA-C	-6.54	104.33	112.90
2	E	41	ARG	CD-NE-CZ	6.54	133.56	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	328	GLU	CB-CG-CD	-6.54	101.48	112.60
1	C	47	VAL	CB-CA-C	-6.53	104.14	111.45
1	C	164	ARG	CD-NE-CZ	-6.53	115.27	124.40
1	C	235	THR	N-CA-C	6.51	118.93	110.53
2	D	420	VAL	N-CA-CB	-6.50	103.88	112.26
2	E	394	ASP	CA-CB-CG	-6.49	106.11	112.60
1	A	172	GLN	N-CA-CB	-6.49	102.34	111.62
2	D	113	PHE	CA-CB-CG	-6.47	107.33	113.80
2	F	143	LEU	N-CA-C	6.47	121.37	112.90
1	B	119	GLY	CA-C-N	6.45	126.47	119.89
1	B	119	GLY	C-N-CA	6.45	126.47	119.89
2	E	125	GLU	N-CA-C	-6.45	105.72	113.97
1	A	337	TYR	CA-C-N	6.44	124.30	120.24
1	A	337	TYR	C-N-CA	6.44	124.30	120.24
2	F	225	PRO	CA-C-N	6.43	127.88	119.84
2	F	225	PRO	C-N-CA	6.43	127.88	119.84
1	C	215	GLN	OE1-CD-NE2	6.43	129.03	122.60
2	E	394	ASP	N-CA-C	6.43	123.71	114.39
2	D	84	ILE	N-CA-C	6.42	114.96	107.84
2	F	275	ILE	N-CA-C	-6.41	102.67	108.95
1	A	230	ILE	CA-C-N	-6.38	114.61	123.10
1	A	230	ILE	C-N-CA	-6.38	114.61	123.10
1	B	279	ARG	CD-NE-CZ	6.35	133.29	124.40
2	D	144	ALA	CA-C-N	6.35	126.38	119.90
2	D	144	ALA	C-N-CA	6.35	126.38	119.90
2	D	221	GLN	N-CA-C	6.35	118.22	110.41
1	B	299	PHE	N-CA-C	-6.33	104.46	111.36
2	F	193	GLY	N-CA-C	-6.33	105.16	112.50
2	F	403	THR	N-CA-C	-6.32	104.32	111.14
1	A	157	VAL	CA-C-N	6.31	126.68	119.93
1	A	157	VAL	C-N-CA	6.31	126.68	119.93
1	A	231	VAL	CA-C-N	-6.29	115.00	122.93
1	A	231	VAL	C-N-CA	-6.29	115.00	122.93
1	A	371	VAL	CB-CA-C	-6.29	99.15	110.48
2	F	59	ARG	NE-CZ-NH2	6.29	124.86	119.20
2	F	26	ASP	CA-CB-CG	-6.28	106.32	112.60
2	F	64	ASP	CA-C-O	-6.26	114.76	121.45
1	C	288	PRO	N-CA-CB	6.24	109.13	103.08
1	C	291	ARG	NE-CZ-NH2	-6.23	113.59	119.20
2	E	416	GLN	CA-C-N	6.23	127.17	120.13
2	E	416	GLN	C-N-CA	6.23	127.17	120.13
1	C	164	ARG	NE-CZ-NH1	-6.22	115.28	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	PRO	N-CA-CB	6.21	108.78	103.19
2	D	120	ALA	CA-C-N	6.19	126.21	119.90
2	D	120	ALA	C-N-CA	6.19	126.21	119.90
2	E	106	GLY	CA-C-N	6.18	126.13	119.76
2	E	106	GLY	C-N-CA	6.18	126.13	119.76
1	B	142	VAL	N-CA-CB	6.18	118.42	110.13
1	C	70	ASN	CA-C-O	-6.18	114.83	121.38
1	A	292	GLU	CB-CG-CD	6.15	123.06	112.60
2	E	145	PRO	N-CA-CB	6.14	108.72	103.19
2	D	422	GLU	N-CA-C	-6.14	104.69	111.82
2	E	225	PRO	N-CA-CB	6.14	109.03	103.08
1	B	93	ALA	N-CA-C	6.12	118.39	108.41
1	B	374	VAL	N-CA-C	6.12	120.10	113.43
1	B	210	ARG	N-CA-CB	6.11	118.86	110.01
1	A	94	ILE	CB-CA-C	6.10	119.92	111.38
1	C	45	ARG	N-CA-C	6.09	118.71	111.71
2	F	80	ALA	CA-C-N	6.08	126.27	120.31
2	F	80	ALA	C-N-CA	6.08	126.27	120.31
2	E	94	ILE	N-CA-CB	6.08	119.52	111.25
2	E	90	THR	N-CA-C	-6.06	106.02	113.41
1	B	287	ARG	CB-CA-C	6.05	118.16	109.26
2	D	139	VAL	N-CA-CB	6.04	116.96	110.62
2	D	247	GLU	N-CA-C	-6.04	106.55	114.04
2	F	432	VAL	CB-CA-C	-6.04	104.13	110.53
2	E	422	GLU	N-CA-C	-6.02	105.97	113.55
1	C	336	ALA	O-C-N	-6.02	115.90	123.12
2	F	342	LEU	N-CA-C	-6.00	105.92	113.18
1	C	162	GLY	N-CA-C	-6.00	107.12	114.92
2	F	144	ALA	CA-C-N	5.99	126.01	119.90
2	F	144	ALA	C-N-CA	5.99	126.01	119.90
1	C	405	GLN	CA-C-N	5.99	132.98	121.54
1	C	405	GLN	C-N-CA	5.99	132.98	121.54
1	C	507	GLY	N-CA-C	-5.99	105.55	112.73
1	A	162	GLY	N-CA-C	-5.98	106.83	114.37
1	A	67	GLU	CA-C-N	5.98	125.46	119.24
1	A	67	GLU	C-N-CA	5.98	125.46	119.24
1	C	400	VAL	N-CA-CB	5.97	117.93	110.47
2	F	229	ARG	NE-CZ-NH1	-5.97	115.53	121.50
2	F	206	ILE	N-CA-CB	5.96	118.97	111.46
2	F	236	GLY	N-CA-C	-5.96	105.58	112.73
1	B	371	VAL	CB-CA-C	-5.95	99.76	110.48
1	B	167	ILE	N-CA-CB	5.95	118.17	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	157	VAL	CA-C-N	5.95	125.97	119.90
1	C	157	VAL	C-N-CA	5.95	125.97	119.90
1	C	341	ASN	CA-C-O	-5.94	114.54	120.90
2	F	261	PHE	CA-C-O	5.93	126.84	120.55
1	A	98	PRO	N-CA-CB	5.93	108.96	103.39
1	A	75	VAL	N-CA-C	5.92	116.70	109.30
1	B	423	ARG	CD-NE-CZ	5.91	132.68	124.40
1	C	46	ASN	CA-CB-CG	5.91	118.51	112.60
2	D	402	LEU	N-CA-C	-5.91	105.16	112.90
2	F	96	ASN	N-CA-CB	-5.91	101.99	110.44
1	B	162	GLY	N-CA-C	-5.90	106.84	115.63
2	D	143	LEU	N-CA-C	5.90	120.60	113.41
1	C	109	ASP	CA-CB-CG	5.89	118.49	112.60
2	F	370	VAL	N-CA-C	-5.89	105.00	110.53
1	A	106	ARG	CD-NE-CZ	5.88	132.63	124.40
1	C	379	GLN	N-CA-C	5.88	119.06	109.59
1	C	422	VAL	CB-CA-C	-5.88	104.20	112.14
1	A	373	ARG	NE-CZ-NH2	5.87	124.48	119.20
2	F	461	GLY	CA-C-N	5.87	126.20	119.92
2	F	461	GLY	C-N-CA	5.87	126.20	119.92
2	F	221	GLN	CA-C-N	5.87	130.07	120.63
2	F	221	GLN	C-N-CA	5.87	130.07	120.63
1	C	100	GLY	N-CA-C	5.85	117.99	112.08
1	C	406	PHE	CA-CB-CG	5.85	119.65	113.80
1	C	241	PRO	N-CA-CB	5.85	109.71	103.39
2	F	210	ASP	CB-CA-C	-5.84	100.32	111.48
1	C	91	THR	N-CA-C	-5.84	107.15	114.56
1	C	345	ILE	N-CA-C	-5.84	107.01	111.62
1	C	93	ALA	N-CA-C	5.83	118.45	109.07
1	B	136	ILE	CA-C-N	5.81	124.98	120.33
1	B	136	ILE	C-N-CA	5.81	124.98	120.33
2	D	454	GLU	CA-CB-CG	5.81	125.72	114.10
2	E	461	GLY	CA-C-N	5.81	125.72	119.85
2	E	461	GLY	C-N-CA	5.81	125.72	119.85
1	B	109	ASP	CA-CB-CG	5.81	118.41	112.60
1	B	45	ARG	CB-CG-CD	-5.80	97.95	111.30
2	E	133	LEU	CA-C-O	-5.80	114.15	120.36
1	C	69	ASP	CA-CB-CG	-5.80	106.80	112.60
1	B	351	PHE	N-CA-CB	5.78	119.84	110.42
1	B	79	ASP	CA-CB-CG	5.78	118.38	112.60
2	F	426	GLY	N-CA-C	-5.78	107.27	115.30
1	B	304	ARG	NE-CZ-NH1	-5.77	115.73	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	389	ALA	N-CA-C	5.77	118.35	111.71
1	C	341	ASN	O-C-N	5.77	128.09	122.09
2	E	349	ASP	CA-C-N	5.77	125.87	119.87
2	E	349	ASP	C-N-CA	5.77	125.87	119.87
1	A	370	SER	CA-C-O	-5.76	115.01	121.81
2	F	229	ARG	NE-CZ-NH2	5.75	124.38	119.20
2	F	113	PHE	CA-CB-CG	-5.74	108.06	113.80
1	B	245	LEU	N-CA-C	5.73	117.21	111.07
1	A	194	ASP	CA-CB-CG	5.73	118.33	112.60
1	B	304	ARG	NE-CZ-NH2	5.73	124.36	119.20
2	E	229	ARG	N-CA-C	-5.73	106.14	113.01
2	F	157	GLY	CA-C-O	-5.73	115.48	122.75
2	D	163	THR	N-CA-C	5.70	117.50	111.28
2	D	96	ASN	N-CA-CB	-5.70	101.77	110.49
2	E	36	LEU	CA-C-O	-5.70	114.72	121.16
1	C	230	ILE	CA-C-N	-5.68	115.27	123.11
1	C	230	ILE	C-N-CA	-5.68	115.27	123.11
2	D	368	TYR	N-CA-C	5.68	117.48	111.28
2	E	97	VAL	CB-CA-C	-5.68	102.90	112.16
2	F	84	ILE	N-CA-C	5.68	113.84	109.19
1	A	335	SER	CB-CA-C	-5.67	99.80	110.01
1	A	420	ARG	NE-CZ-NH1	-5.67	115.83	121.50
1	C	303	SER	CA-C-N	5.67	129.32	120.82
1	C	303	SER	C-N-CA	5.67	129.32	120.82
2	D	145	PRO	N-CA-CB	5.64	108.21	103.25
1	C	366	ASN	CA-C-O	5.62	126.77	120.92
1	C	362	ARG	NE-CZ-NH2	5.62	124.26	119.20
2	E	120	ALA	CA-C-N	5.62	126.86	119.84
2	E	120	ALA	C-N-CA	5.62	126.86	119.84
1	C	381	ARG	CD-NE-CZ	5.62	132.26	124.40
1	B	151	LYS	N-CA-C	5.61	117.84	111.11
1	B	91	THR	N-CA-C	-5.61	105.40	114.09
2	E	95	MET	CA-C-N	5.60	132.23	121.54
2	E	95	MET	C-N-CA	5.60	132.23	121.54
2	E	336	SER	N-CA-C	5.59	118.02	108.90
2	D	225	PRO	N-CA-CB	5.59	106.13	103.22
1	C	120	PRO	N-CA-CB	5.59	108.64	103.39
1	B	127	ARG	CD-NE-CZ	5.58	132.22	124.40
2	F	95	MET	O-C-N	-5.58	116.41	123.17
2	D	145	PRO	CA-C-O	-5.58	115.05	121.36
2	D	225	PRO	CA-C-N	5.58	126.82	119.84
2	D	225	PRO	C-N-CA	5.58	126.82	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	LEU	CA-C-O	5.58	125.80	119.27
1	B	103	LEU	N-CA-C	-5.58	106.61	113.41
1	B	477	GLN	CA-C-N	5.57	128.20	120.29
1	B	477	GLN	C-N-CA	5.57	128.20	120.29
2	D	356	ARG	CD-NE-CZ	-5.57	116.60	124.40
1	B	433	TYR	CA-C-N	-5.56	116.42	122.59
1	B	433	TYR	C-N-CA	-5.56	116.42	122.59
1	A	92	GLY	N-CA-C	-5.55	108.37	115.42
2	E	96	ASN	CA-CB-CG	5.55	118.15	112.60
1	A	367	VAL	CB-CA-C	5.55	119.63	112.14
1	A	200	TYR	CA-CB-CG	-5.55	103.92	113.90
1	A	164	ARG	CA-C-O	-5.53	113.60	120.57
2	E	219	TYR	N-CA-C	5.52	118.40	109.40
1	A	235	THR	N-CA-C	5.51	118.58	110.59
1	A	263	HIS	CA-CB-CG	-5.51	108.29	113.80
1	C	423	ARG	CD-NE-CZ	5.50	132.10	124.40
2	F	473	LEU	N-CA-C	-5.50	106.07	112.89
1	C	74	VAL	CB-CA-C	5.50	117.72	110.91
2	E	216	ALA	CA-C-N	-5.49	115.42	123.00
2	E	216	ALA	C-N-CA	-5.49	115.42	123.00
2	E	260	ARG	NE-CZ-NH1	-5.49	116.01	121.50
2	D	179	GLY	CA-C-O	-5.49	116.23	121.83
1	A	398	ARG	NE-CZ-NH1	-5.48	116.02	121.50
2	E	282	GLN	CA-C-N	5.48	125.13	119.05
2	E	282	GLN	C-N-CA	5.48	125.13	119.05
2	F	215	VAL	N-CA-C	5.48	116.01	108.12
2	D	30	PRO	N-CA-CB	5.47	108.39	103.08
2	E	137	ILE	CA-C-O	5.47	127.08	120.74
2	F	88	PRO	N-CA-CB	5.46	108.75	103.51
2	E	127	SER	N-CA-C	-5.46	101.63	110.32
2	E	257	ASN	CA-CB-CG	5.46	118.06	112.60
2	F	96	ASN	N-CA-C	5.46	117.57	110.53
2	E	239	VAL	N-CA-CB	-5.45	104.89	110.62
2	E	272	LEU	N-CA-C	-5.45	106.94	113.21
1	A	172	GLN	N-CA-C	5.45	118.71	111.30
1	C	33	SER	CA-C-O	-5.45	115.40	121.23
1	C	309	ALA	N-CA-C	-5.45	101.79	109.96
2	D	164	VAL	N-CA-C	-5.45	105.19	110.42
1	A	233	SER	N-CA-CB	-5.44	102.23	110.77
1	A	466	ASN	OD1-CG-ND2	5.44	128.04	122.60
1	C	106	ARG	CA-CB-CG	-5.43	103.23	114.10
2	E	83	ARG	NE-CZ-NH1	-5.43	116.07	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	200	MET	N-CA-C	-5.43	105.01	111.69
2	D	215	VAL	CA-C-O	-5.43	113.99	120.78
1	B	141	SER	CA-C-O	-5.42	115.05	120.96
2	D	198	HIS	CA-CB-CG	-5.42	108.38	113.80
3	G	39	LYS	CA-C-N	5.42	124.60	118.97
3	G	39	LYS	C-N-CA	5.42	124.60	118.97
2	F	282	GLN	OE1-CD-NE2	-5.41	117.19	122.60
1	C	48	GLN	CA-C-O	-5.41	115.05	121.16
1	A	134	PRO	N-CA-C	-5.41	102.71	111.14
2	D	232	VAL	N-CA-CB	5.40	120.15	111.23
2	E	83	ARG	CD-NE-CZ	-5.40	116.84	124.40
1	C	285	LEU	N-CA-C	-5.37	106.50	113.16
2	F	76	LEU	N-CA-C	5.36	117.26	108.52
2	E	417	PRO	CB-CA-C	-5.36	104.84	111.11
2	E	297	THR	CB-CA-C	-5.36	101.18	111.78
2	F	393	MET	N-CA-C	5.36	119.87	113.23
1	B	40	ARG	NE-CZ-NH1	5.35	126.85	121.50
2	F	388	ILE	CB-CA-C	-5.35	104.23	112.05
2	F	12	ARG	CD-NE-CZ	-5.35	116.91	124.40
2	F	408	ARG	NE-CZ-NH2	5.35	124.01	119.20
2	F	423	VAL	CB-CA-C	-5.35	101.58	111.79
2	E	171	ASN	OD1-CG-ND2	5.34	127.94	122.60
2	E	196	LEU	N-CA-C	-5.34	105.12	111.69
1	A	372	SER	N-CA-CB	5.34	120.19	110.95
1	C	304	ARG	NE-CZ-NH2	5.34	124.01	119.20
2	D	268	VAL	CA-C-O	5.34	123.60	118.90
2	F	41	ARG	CG-CD-NE	5.34	123.75	112.00
2	D	119	GLU	CA-C-O	-5.34	115.74	121.56
1	C	123	SER	N-CA-C	5.34	117.97	109.96
2	E	96	ASN	N-CA-CB	-5.34	101.47	110.49
1	A	93	ALA	CA-C-N	-5.33	114.92	122.34
1	A	93	ALA	C-N-CA	-5.33	114.92	122.34
1	C	411	ASP	CA-CB-CG	5.33	117.93	112.60
2	E	393	MET	N-CA-C	5.32	122.14	110.80
2	D	327	ALA	CA-C-O	-5.31	113.06	119.49
1	B	318	GLY	N-CA-C	-5.30	108.52	115.47
1	C	75	VAL	N-CA-C	5.30	115.73	107.99
1	C	336	ALA	N-CA-C	5.30	117.77	110.35
1	A	74	VAL	N-CA-CB	-5.30	105.62	111.66
2	D	222	MET	CB-CA-C	-5.30	98.61	110.21
2	E	122	GLU	CA-CB-CG	5.30	124.69	114.10
2	F	366	GLU	N-CA-C	-5.30	105.40	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	MET	CA-C-N	-5.29	115.30	122.92
1	A	52	MET	C-N-CA	-5.29	115.30	122.92
1	B	149	GLY	N-CA-C	-5.29	108.33	115.21
1	C	405	GLN	CA-C-O	5.29	128.07	120.51
1	B	287	ARG	CA-C-N	5.29	125.83	120.38
1	B	287	ARG	C-N-CA	5.29	125.83	120.38
2	F	19	ALA	CA-C-N	-5.29	115.92	123.11
2	F	19	ALA	C-N-CA	-5.29	115.92	123.11
1	C	299	PHE	N-CA-C	-5.28	105.21	110.97
2	D	155	PHE	CA-CB-CG	5.28	119.08	113.80
2	D	432	VAL	CA-C-N	5.27	125.18	119.85
2	D	432	VAL	C-N-CA	5.27	125.18	119.85
1	B	116	ASP	N-CA-C	-5.27	106.63	113.16
1	B	259	ASP	CA-CB-CG	-5.26	107.34	112.60
2	D	322	PRO	N-CA-C	-5.26	105.95	113.47
2	E	398	GLU	N-CA-C	-5.26	105.50	112.34
1	B	130	GLY	O-C-N	-5.25	115.88	122.70
1	C	127	ARG	NE-CZ-NH1	-5.25	116.25	121.50
2	F	330	ASP	CA-CB-CG	-5.25	107.36	112.60
2	E	331	ALA	CA-C-O	5.24	128.01	120.51
2	F	121	PRO	N-CA-CB	5.24	107.86	103.25
1	B	478	ALA	N-CA-C	5.24	117.07	111.36
2	E	173	VAL	N-CA-C	-5.24	105.29	111.00
2	D	354	THR	CA-C-O	-5.23	115.49	121.40
2	D	411	GLN	CA-C-O	5.23	126.28	120.63
2	D	160	VAL	N-CA-CB	5.22	117.95	112.21
1	C	336	ALA	CA-C-O	5.21	126.70	121.07
1	B	279	ARG	NE-CZ-NH1	5.21	126.71	121.50
2	F	257	ASN	OD1-CG-ND2	5.21	127.81	122.60
1	C	296	GLY	N-CA-C	-5.21	108.94	114.67
2	F	87	GLY	CA-C-N	5.20	124.82	119.56
2	F	87	GLY	C-N-CA	5.20	124.82	119.56
2	F	387	ILE	CB-CA-C	-5.20	105.20	112.02
2	E	250	ASP	CA-CB-CG	-5.19	107.41	112.60
2	F	59	ARG	CD-NE-CZ	-5.18	117.14	124.40
2	D	118	ALA	CA-C-O	-5.17	115.69	121.23
2	F	225	PRO	N-CA-C	-5.17	104.39	110.70
2	F	418	PHE	CA-CB-CG	5.17	118.97	113.80
2	D	224	GLU	CA-C-N	5.17	123.38	119.66
2	D	224	GLU	C-N-CA	5.17	123.38	119.66
1	C	136	ILE	CA-C-N	5.16	124.46	120.33
1	C	136	ILE	C-N-CA	5.16	124.46	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	165	LEU	N-CA-CB	5.16	117.71	110.12
2	D	175	LYS	N-CA-C	5.16	116.90	111.28
2	F	281	TYR	CA-C-N	5.14	127.79	120.49
2	F	281	TYR	C-N-CA	5.14	127.79	120.49
1	A	338	ILE	N-CA-CB	5.14	113.74	110.50
1	B	397	TYR	N-CA-C	-5.14	107.56	113.88
2	E	125	GLU	CA-C-O	5.14	124.47	118.97
2	E	439	LYS	O-C-N	5.14	127.36	122.07
1	A	219	ARG	CD-NE-CZ	5.13	131.59	124.40
2	D	361	ASN	CA-CB-CG	-5.13	107.47	112.60
2	F	178	GLY	CA-C-N	-5.13	114.40	122.92
2	F	178	GLY	C-N-CA	-5.13	114.40	122.92
2	E	358	MET	N-CA-CB	5.13	116.79	110.53
2	E	330	ASP	CA-CB-CG	-5.13	107.47	112.60
3	G	136	PRO	N-CA-CB	5.12	107.81	103.35
2	E	251	VAL	CB-CA-C	-5.11	105.97	111.59
2	F	200	MET	N-CA-CB	-5.11	102.59	110.16
2	E	72	GLY	N-CA-C	-5.11	108.61	114.69
1	C	270	ASP	CA-CB-CG	5.11	117.71	112.60
2	D	475	GLU	N-CA-CB	5.11	119.18	110.50
2	F	417	PRO	CB-CA-C	-5.10	105.14	111.11
2	E	56	SER	CA-C-N	-5.10	115.29	122.94
2	E	56	SER	C-N-CA	-5.10	115.29	122.94
1	B	391	LYS	N-CA-C	-5.10	105.90	111.82
1	B	338	ILE	N-CA-CB	5.09	114.42	110.45
2	F	200	MET	CA-C-O	5.08	125.81	120.42
2	E	400	ASP	CA-CB-CG	-5.08	107.52	112.60
2	D	357	ILE	N-CA-CB	5.07	119.61	112.15
2	F	330	ASP	N-CA-C	-5.07	107.22	113.41
1	B	295	PRO	N-CA-CB	5.07	107.76	103.35
1	B	349	GLN	N-CA-CB	5.07	120.50	111.69
2	E	226	PRO	CA-C-N	5.07	125.70	120.03
2	E	226	PRO	C-N-CA	5.07	125.70	120.03
2	F	85	PRO	N-CA-CB	5.06	107.67	103.17
2	F	101	PRO	N-CA-CB	5.06	107.75	103.35
1	B	222	ASP	CA-C-N	-5.06	114.19	122.54
1	B	222	ASP	C-N-CA	-5.06	114.19	122.54
2	D	454	GLU	CB-CA-C	-5.06	102.88	110.92
3	G	117	HIS	CA-CB-CG	-5.05	108.75	113.80
1	C	438	ILE	N-CA-C	5.05	115.67	110.36
1	B	374	VAL	CB-CA-C	-5.05	104.53	110.84
1	C	23	VAL	CA-C-N	5.05	128.87	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	23	VAL	C-N-CA	5.05	128.87	120.94
1	A	178	ILE	CB-CA-C	-5.05	105.42	111.88
1	C	145	PRO	N-CA-CB	5.05	108.13	103.39
1	C	269	ASP	CA-C-O	-5.05	114.95	120.70
2	E	435	LYS	O-C-N	5.05	127.47	122.12
2	F	416	GLN	CA-C-N	5.04	125.83	120.13
2	F	416	GLN	C-N-CA	5.04	125.83	120.13
2	F	170	ILE	N-CA-C	-5.04	105.48	110.62
1	A	101	GLU	N-CA-C	5.04	118.89	112.34
2	E	107	PRO	N-CA-CB	5.04	107.79	103.31
1	B	210	ARG	O-C-N	5.04	127.26	122.07
1	B	230	ILE	CA-C-O	-5.04	116.03	121.92
2	E	236	GLY	N-CA-C	-5.04	106.69	112.73
2	F	419	GLN	N-CA-C	-5.04	105.48	110.97
1	C	209	LYS	N-CA-CB	-5.03	102.67	110.57
1	B	141	SER	CB-CA-C	-5.03	102.29	109.84
2	D	275	ILE	N-CA-C	-5.03	104.02	108.95
2	F	198	HIS	CA-CB-CG	-5.03	108.78	113.80
1	B	487	GLY	N-CA-C	-5.02	108.39	115.32
1	C	132	LYS	CA-CB-CG	5.02	124.14	114.10
2	D	170	ILE	N-CA-C	-5.02	105.65	110.72
1	C	445	ILE	O-C-N	5.01	126.73	121.87
2	F	100	GLU	CA-C-O	-5.01	115.98	120.19
2	E	161	GLY	N-CA-C	5.01	125.05	113.18
1	A	246	ALA	CA-C-N	5.01	124.79	119.28
1	A	246	ALA	C-N-CA	5.01	124.79	119.28
2	D	461	GLY	CA-C-N	5.01	124.91	119.85
2	D	461	GLY	C-N-CA	5.01	124.91	119.85
2	F	305	THR	N-CA-C	-5.00	101.00	108.96
1	B	420	ARG	N-CA-C	-5.00	105.47	111.03
1	A	191	ASP	N-CA-C	-5.00	107.23	113.38
1	B	94	ILE	N-CA-C	-5.00	102.62	109.37
1	B	325	PRO	CA-C-N	-5.00	116.65	123.10
1	B	325	PRO	C-N-CA	-5.00	116.65	123.10
2	E	415	SER	CA-C-O	-5.00	116.04	121.89

There are no chirality outliers.

There are no planarity outliers.

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	3715	0	3813	172	3
1	B	3656	0	3764	160	52
1	C	3748	0	3843	171	53
2	D	3539	0	3593	157	0
2	E	3530	0	3587	214	0
2	F	3530	0	3587	129	2
3	G	2051	0	2115	123	0
4	H	235	0	230	18	0
5	I	212	0	232	14	0
All	All	24216	0	24764	1080	55

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 22.

All (1080) 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:C:127:ARG:HH12	1:C:255:GLU:HB2	1.00	1.16
1:A:291:ARG:HA	3:G:262:LEU:HD22	1.25	1.11
1:C:215:GLN:HG3	2:F:356:ARG:HH22	1.11	1.07
3:G:90:LYS:HB3	3:G:116:LEU:HD11	1.38	1.04
1:A:215:GLN:HG3	2:D:356:ARG:NH1	1.73	1.03
1:C:404:ALA:C	1:C:406:PHE:H	1.64	1.00
2:E:223:ASN:HD22	2:E:223:ASN:H	1.00	0.96
4:H:85:ASN:HD21	4:H:91:GLN:HE22	1.13	0.96
2:F:223:ASN:HD22	2:F:223:ASN:H	1.08	0.95
1:A:215:GLN:HG3	2:D:356:ARG:HH12	1.30	0.94
1:C:127:ARG:NH1	1:C:255:GLU:HB2	1.84	0.93
2:F:394:ASP:CG	3:G:79:GLY:HA2	1.93	0.93
3:G:19:ILE:HG22	3:G:23:MET:HE2	1.49	0.92
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.48	0.91
4:H:79:SER:OG	5:I:15:SER:HA	1.72	0.90
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.52	0.89
1:C:30:ARG:HE	1:C:87:ILE:HD11	1.37	0.88
4:H:130:GLU:HG2	5:I:9:LEU:HD21	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:89:GLU:HG2	2:E:110:THR:HG22	1.56	0.87
3:G:20:THR:HG22	3:G:236:SER:HB3	1.57	0.86
1:C:215:GLN:HG3	2:F:356:ARG:NH2	1.91	0.86
2:E:223:ASN:H	2:E:223:ASN:ND2	1.72	0.86
2:D:84:ILE:HD12	2:D:95:MET:HE1	1.57	0.85
1:B:456:LEU:HD12	1:B:457:GLU:H	1.42	0.84
2:D:275:ILE:HG23	3:G:269:ALA:HB2	1.60	0.84
2:E:132:ILE:HD12	2:E:145:PRO:HB3	1.61	0.83
1:A:400:VAL:HG12	1:A:418:LEU:HD21	1.60	0.82
3:G:137:THR:HG21	5:I:39:GLY:H	1.46	0.80
3:G:89:MET:HE1	3:G:112:ILE:HG23	1.63	0.80
1:A:291:ARG:CA	3:G:262:LEU:HD22	2.08	0.80
3:G:178:ILE:HG22	3:G:180:SER:HB2	1.64	0.79
3:G:161:ILE:HG12	3:G:175:GLU:HG2	1.63	0.79
3:G:89:MET:HB3	3:G:116:LEU:HD22	1.63	0.78
2:D:136:GLY:HA3	2:D:431:LEU:HD13	1.66	0.78
1:C:344:SER:O	2:D:222:MET:HE1	1.83	0.78
1:B:141:SER:O	1:B:143:ARG:HD2	1.83	0.78
2:D:139:VAL:HG13	2:D:414:LEU:HD22	1.65	0.77
2:E:370:VAL:HG21	2:E:438:ILE:HG22	1.65	0.77
3:G:121:SER:C	3:G:123:GLN:H	1.91	0.77
1:A:392:LEU:HG	1:A:396:GLN:HE21	1.50	0.77
2:F:130:GLN:HB3	2:F:357:ILE:HD11	1.67	0.77
1:B:186:GLN:HG3	1:B:199:LEU:HB3	1.65	0.76
2:D:53:LEU:HD12	2:D:57:THR:HG22	1.66	0.76
2:D:282:GLN:H	2:D:282:GLN:HE21	1.30	0.76
2:D:404:VAL:O	2:D:408:ARG:HG3	1.84	0.76
3:G:117:HIS:ND1	3:G:118:ARG:N	2.34	0.76
2:D:223:ASN:H	2:D:223:ASN:HD22	1.34	0.75
3:G:86:ALA:HA	3:G:89:MET:HE3	1.67	0.75
1:C:52:MET:HE3	1:C:95:VAL:HG22	1.68	0.75
2:E:391:LEU:HD22	3:G:29:ALA:HB2	1.68	0.75
2:D:395:GLU:OE2	3:G:75:ARG:NE	2.19	0.74
2:E:89:GLU:HG3	2:E:109:LYS:O	1.87	0.74
2:E:390:ILE:HG22	2:E:391:LEU:HD23	1.70	0.74
1:B:379:GLN:HB3	1:B:384:LYS:HE2	1.68	0.73
2:E:345:TYR:HA	2:E:346:PRO:C	2.13	0.73
2:F:89:GLU:HG3	2:F:109:LYS:O	1.89	0.73
1:B:180:ILE:HD11	1:B:216:LEU:HD21	1.72	0.72
2:D:433:PRO:HG2	2:D:436:GLU:HG2	1.69	0.72
2:E:96:ASN:HB3	2:E:100:GLU:H	1.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ARG:HA	3:G:262:LEU:CD2	2.13	0.72
2:E:394:ASP:C	2:E:396:LEU:H	1.93	0.72
2:E:38:VAL:HG21	2:E:45:LEU:HD23	1.71	0.72
2:E:139:VAL:HG13	2:E:414:LEU:HD22	1.71	0.72
3:G:57:ILE:CG2	3:G:184:ILE:HD12	2.19	0.71
4:H:84:VAL:HG12	4:H:90:VAL:HG22	1.72	0.71
1:C:34:ILE:HD11	1:C:79:ASP:HB2	1.71	0.71
2:E:388:ILE:HG23	2:E:393:MET:HG3	1.73	0.71
1:B:452:TYR:OH	1:B:498:LYS:HG3	1.92	0.70
2:D:96:ASN:HB2	2:D:100:GLU:H	1.56	0.70
1:A:407:GLY:HA2	1:A:410:LEU:HD21	1.73	0.70
1:A:479:LEU:HA	1:A:482:LYS:HE3	1.73	0.70
2:E:183:PHE:HB3	2:E:217:LEU:HD22	1.73	0.70
4:H:85:ASN:HD21	4:H:91:GLN:NE2	1.87	0.70
2:D:200:MET:HE3	2:D:215:VAL:HG21	1.74	0.70
1:A:97:VAL:HA	1:A:126:ARG:HH21	1.56	0.69
1:C:211:SER:O	1:C:215:GLN:HG2	1.91	0.69
2:E:433:PRO:HD2	2:E:436:GLU:HB2	1.74	0.69
2:F:252:LEU:HD23	2:F:305:THR:HB	1.75	0.69
2:E:105:ARG:CZ	2:E:208:LEU:HD23	2.23	0.69
1:C:385:GLN:OE1	1:C:488:LYS:HG2	1.93	0.68
2:E:321:ALA:HB3	2:E:322:PRO:HD3	1.75	0.68
2:F:89:GLU:HG2	2:F:110:THR:HG22	1.75	0.68
3:G:115:ILE:C	3:G:117:HIS:H	2.01	0.68
3:G:14:LYS:HG3	3:G:243:ILE:HD12	1.76	0.68
2:E:313:PRO:HD2	2:E:322:PRO:HG3	1.76	0.68
2:F:223:ASN:H	2:F:223:ASN:ND2	1.85	0.68
2:F:314:ALA:O	2:F:315:ASP:HB2	1.95	0.67
1:A:440:GLU:O	1:A:444:VAL:HG13	1.94	0.67
1:B:156:LEU:HD22	1:B:391:LYS:HD2	1.77	0.67
1:A:97:VAL:HB	1:A:98:PRO:HD2	1.76	0.67
2:E:136:GLY:HA3	2:E:431:LEU:HD13	1.77	0.67
4:H:130:GLU:CG	5:I:9:LEU:HD21	2.23	0.67
1:A:44:LEU:O	1:A:47:VAL:HG22	1.94	0.67
1:A:134:PRO:O	1:A:139:ARG:NH2	2.27	0.66
1:C:59:LEU:HD23	1:C:82:ILE:HD11	1.77	0.66
1:B:289:PRO:HG2	3:G:263:ILE:HD12	1.78	0.66
1:C:99:VAL:HG22	1:C:253:MET:HA	1.78	0.66
2:D:223:ASN:H	2:D:223:ASN:ND2	1.93	0.66
2:F:409:LYS:HD3	2:F:457:PHE:CE2	2.30	0.66
1:A:383:MET:HE2	1:A:438:ILE:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:LEU:O	1:C:422:VAL:HG23	1.94	0.66
2:D:223:ASN:HD22	2:D:223:ASN:N	1.89	0.66
1:C:362:ARG:HA	1:C:363:PRO:C	2.21	0.66
2:E:394:ASP:C	2:E:396:LEU:N	2.54	0.66
3:G:137:THR:HG22	3:G:139:GLY:H	1.60	0.66
1:A:136:ILE:HD11	2:E:219:TYR:HE2	1.60	0.66
1:A:376:SER:HB3	1:A:384:LYS:HE2	1.78	0.66
1:B:44:LEU:HB3	1:B:47:VAL:HG22	1.76	0.66
2:F:80:ALA:HB1	2:F:81:PRO:CD	2.26	0.66
2:F:136:GLY:HA3	2:F:431:LEU:CD1	2.26	0.66
1:A:376:SER:C	1:A:378:ALA:H	2.03	0.65
1:C:173:THR:HG22	1:C:354:THR:HG22	1.77	0.65
2:D:167:MET:HB3	2:D:420:VAL:HG11	1.79	0.65
2:F:344:ILE:HG23	2:F:415:SER:HB3	1.78	0.65
1:B:188:ARG:HH21	1:B:437:ALA:HB2	1.62	0.65
1:C:436:MET:HE3	1:C:469:LEU:HD21	1.79	0.65
1:B:362:ARG:HA	1:B:363:PRO:C	2.21	0.64
1:C:44:LEU:O	1:C:47:VAL:HG22	1.96	0.64
2:F:200:MET:HG3	2:F:205:VAL:CG2	2.27	0.64
2:E:359:ASP:OD2	2:E:361:ASN:HB2	1.97	0.64
1:C:188:ARG:HH21	1:C:437:ALA:HB2	1.62	0.64
1:B:389:THR:HA	1:B:392:LEU:CD1	2.28	0.64
2:F:94:ILE:HG22	2:F:102:ILE:HD11	1.80	0.64
1:C:419:SER:O	1:C:423:ARG:HG2	1.98	0.63
3:G:178:ILE:C	3:G:180:SER:H	2.04	0.63
2:E:139:VAL:CG1	2:E:414:LEU:HD22	2.28	0.63
2:E:443:GLN:HG2	2:E:448:GLU:OE2	1.98	0.63
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.63	0.63
1:A:471:HIS:CE1	1:A:475:GLN:HG3	2.33	0.63
1:C:202:ILE:HG12	1:C:230:ILE:HD12	1.80	0.63
1:C:488:LYS:HG2	1:C:489:ILE:H	1.63	0.63
2:E:346:PRO:HG3	2:E:418:PHE:CZ	2.33	0.63
1:B:437:ALA:O	1:B:440:GLU:N	2.30	0.63
2:D:54:GLY:O	2:D:55:GLU:HB2	1.96	0.63
1:B:184:ILE:HG22	1:B:435:PRO:HG2	1.81	0.63
2:E:138:LYS:HE2	2:E:432:VAL:HG21	1.80	0.63
2:E:400:ASP:O	2:E:404:VAL:HG23	1.98	0.63
2:E:425:THR:O	2:E:427:HIS:ND1	2.20	0.63
1:C:52:MET:HE2	1:C:76:PHE:HE2	1.62	0.63
2:D:200:MET:HB3	2:D:206:ILE:HG13	1.79	0.63
2:E:298:THR:HG23	2:E:303:SER:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:136:GLY:HA3	2:F:431:LEU:HD12	1.80	0.63
3:G:61:GLU:OE1	3:G:101:LYS:HG2	1.99	0.63
3:G:141:ALA:HB1	3:G:213:ILE:HG23	1.81	0.63
5:I:5:ARG:C	5:I:7:ALA:H	2.06	0.63
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.34	0.62
1:C:52:MET:O	1:C:91:THR:HB	1.98	0.62
4:H:79:SER:OG	5:I:15:SER:CA	2.46	0.62
1:A:394:LEU:HD11	1:A:428:LEU:HD11	1.82	0.62
2:E:158:ALA:C	2:E:160:VAL:H	2.08	0.62
2:E:204:GLY:O	2:E:206:ILE:N	2.32	0.62
1:A:211:SER:N	2:D:126:MET:HE2	2.13	0.62
1:B:390:MET:HE1	1:B:428:LEU:HD21	1.80	0.62
3:G:39:LYS:HB3	3:G:40:PRO:HD3	1.80	0.62
1:A:341:ASN:O	1:A:345:ILE:HG13	1.99	0.62
2:F:390:ILE:HD11	3:G:242:MET:CE	2.30	0.62
2:F:200:MET:HG3	2:F:205:VAL:HG23	1.80	0.62
1:B:102:GLU:HG3	1:B:122:GLY:O	2.00	0.62
1:B:389:THR:HA	1:B:392:LEU:HD12	1.81	0.61
2:E:422:GLU:HG2	2:E:427:HIS:O	1.99	0.61
1:B:422:VAL:O	1:B:426:GLU:HG2	2.00	0.61
2:F:363:VAL:HG23	2:F:367:HIS:HB3	1.81	0.61
1:B:214:ALA:HA	2:E:123:PHE:CZ	2.35	0.61
1:C:151:LYS:HE3	1:C:430:GLN:HG3	1.82	0.61
2:D:396:LEU:HD22	2:D:400:ASP:CB	2.30	0.61
2:E:391:LEU:CD2	3:G:29:ALA:HB2	2.28	0.61
2:E:201:ILE:HD13	2:E:208:LEU:HD11	1.81	0.61
1:A:121:ILE:HD13	1:A:121:ILE:H	1.66	0.61
2:E:397:SER:H	2:E:400:ASP:HB2	1.66	0.61
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.34	0.61
3:G:184:ILE:C	3:G:186:SER:H	2.08	0.61
1:A:376:SER:C	1:A:378:ALA:N	2.55	0.61
1:C:408:SER:O	1:C:409:ASP:C	2.44	0.61
2:D:473:LEU:C	2:D:475:GLU:H	2.08	0.61
1:A:439:GLU:HG2	1:A:484:ARG:HB2	1.83	0.61
1:A:52:MET:O	1:A:91:THR:HG23	2.01	0.60
1:C:99:VAL:HG13	1:C:256:TYR:HB2	1.83	0.60
1:C:433:TYR:C	1:C:435:PRO:HD3	2.26	0.60
2:E:149:GLY:HA2	2:E:304:ILE:O	2.01	0.60
1:A:40:ARG:HH11	1:A:40:ARG:HG3	1.66	0.60
1:A:270:ASP:OD1	1:A:273:LYS:HG3	2.00	0.60
1:A:283:LEU:HD21	1:A:289:PRO:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:GLU:HA	1:B:94:ILE:HA	1.83	0.60
2:D:393:MET:HE3	2:D:404:VAL:HG21	1.83	0.60
1:A:457:GLU:CB	1:A:460:LYS:HD3	2.32	0.60
1:C:313:ASN:OD1	1:C:316:PHE:HD1	1.85	0.60
2:F:122:GLU:HB2	2:F:125:GLU:HG3	1.84	0.60
1:C:404:ALA:C	1:C:406:PHE:N	2.44	0.60
1:C:403:PHE:CZ	2:D:408:ARG:HD2	2.37	0.60
2:D:93:ARG:HG3	2:D:93:ARG:HH11	1.66	0.60
2:F:63:MET:HE1	2:F:97:VAL:HG11	1.82	0.60
1:A:166:LEU:HA	1:A:325:PRO:HD2	1.83	0.60
1:A:432:GLN:HB3	1:A:433:TYR:CD2	2.37	0.60
2:E:224:GLU:O	2:E:229:ARG:NH1	2.32	0.60
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.37	0.59
1:C:210:ARG:NH1	2:F:121:PRO:O	2.35	0.59
1:B:411:ASP:HB3	1:B:414:THR:OG1	2.02	0.59
1:B:499:GLU:O	1:B:502:THR:HB	2.02	0.59
2:D:89:GLU:HG2	2:D:110:THR:HG22	1.83	0.59
2:E:419:GLN:HG3	2:E:429:GLY:HA3	1.84	0.59
1:A:157:VAL:N	1:A:158:PRO:CD	2.65	0.59
1:B:438:ILE:O	1:B:442:VAL:HG22	2.02	0.59
2:E:32:ILE:O	2:E:33:LEU:HB2	2.02	0.59
2:D:317:LEU:HD22	2:D:326:PHE:HZ	1.67	0.59
1:B:452:TYR:O	1:B:453:LEU:HD23	2.03	0.59
1:B:479:LEU:HD11	1:B:497:LEU:HD13	1.83	0.59
1:C:102:GLU:OE2	1:C:123:SER:HA	2.03	0.59
3:G:156:ASP:HA	3:G:181:LEU:HD13	1.85	0.59
1:B:170:ASP:O	1:B:175:LYS:HE2	2.03	0.59
1:C:140:ILE:HD11	1:C:143:ARG:NH2	2.17	0.59
2:D:63:MET:HE3	2:D:228:ALA:HA	1.83	0.59
2:E:200:MET:HB3	2:E:205:VAL:HG23	1.84	0.59
2:E:397:SER:C	2:E:399:GLU:N	2.57	0.59
2:E:408:ARG:O	2:E:412:ARG:HG3	2.03	0.59
2:F:105:ARG:NH1	2:F:208:LEU:HD23	2.18	0.59
1:C:292:GLU:O	1:C:293:ALA:HB3	2.00	0.59
1:C:407:GLY:HA2	1:C:410:LEU:HD11	1.84	0.59
2:D:263:GLN:O	2:D:267:GLU:HG3	2.03	0.59
1:B:391:LYS:O	1:B:395:ALA:N	2.36	0.58
1:C:335:SER:O	2:D:314:ALA:HA	2.02	0.58
1:C:405:GLN:C	1:C:406:PHE:HD1	2.11	0.58
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.85	0.58
1:A:472:VAL:HG23	1:A:480:LEU:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:122:GLU:N	2:E:125:GLU:OE2	2.37	0.58
2:E:226:PRO:HB3	2:E:267:GLU:HB2	1.84	0.58
2:F:29:LEU:HD12	2:F:30:PRO:HD2	1.85	0.58
3:G:57:ILE:CG2	3:G:184:ILE:CD1	2.81	0.58
1:B:283:LEU:CD1	2:E:277:SER:HB3	2.32	0.58
2:E:85:PRO:HD2	2:E:95:MET:HE2	1.85	0.58
1:B:358:TYR:C	1:B:360:GLY:H	2.12	0.58
2:D:186:VAL:HG13	2:D:232:VAL:HG23	1.85	0.58
3:G:87:LYS:O	3:G:90:LYS:HG2	2.04	0.58
2:E:246:GLN:HA	2:E:246:GLN:NE2	2.18	0.58
1:C:406:PHE:O	1:C:408:SER:N	2.36	0.58
2:E:126:MET:HE1	2:E:297:THR:HG21	1.86	0.58
2:D:431:LEU:C	2:D:431:LEU:HD12	2.29	0.58
1:B:434:SER:N	1:B:435:PRO:HD3	2.18	0.58
1:A:219:ARG:HH11	1:A:219:ARG:HB2	1.69	0.58
1:C:396:GLN:HG3	2:D:458:TYR:CE2	2.38	0.58
1:C:404:ALA:O	1:C:406:PHE:N	2.37	0.58
2:E:267:GLU:O	2:E:271:LEU:HG	2.04	0.58
4:H:95:GLU:OE2	5:I:16:GLN:HA	2.04	0.58
1:B:214:ALA:HB2	2:E:123:PHE:CE1	2.38	0.57
1:C:374:VAL:HG11	1:C:378:ALA:HB2	1.85	0.57
1:B:62:MET:HE3	1:B:64:LEU:HD13	1.86	0.57
2:E:95:MET:CG	2:E:99:GLY:HA2	2.34	0.57
2:E:223:ASN:ND2	2:E:223:ASN:N	2.46	0.57
2:F:96:ASN:HD22	2:F:100:GLU:HB2	1.68	0.57
2:F:440:GLY:O	2:F:444:ILE:HG13	2.04	0.57
2:F:14:VAL:O	2:F:71:ARG:HG2	2.05	0.57
3:G:57:ILE:HG23	3:G:184:ILE:CD1	2.35	0.57
1:B:51:GLU:OE2	1:B:90:ARG:HB3	2.05	0.57
2:E:433:PRO:HG2	2:E:436:GLU:HG2	1.86	0.57
1:C:464:PHE:CE1	1:C:505:LEU:HD23	2.38	0.57
1:A:136:ILE:HD11	2:E:219:TYR:CE2	2.39	0.57
1:B:400:VAL:HB	1:B:418:LEU:HD21	1.85	0.57
1:C:107:VAL:HG12	1:C:115:ILE:HD11	1.86	0.57
2:E:77:ASP:OD1	2:E:79:GLY:N	2.34	0.57
2:E:138:LYS:O	2:E:142:LEU:HB3	2.04	0.57
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.86	0.57
1:B:352:LEU:HA	1:B:364:ALA:O	2.04	0.57
2:E:92:GLY:N	2:E:215:VAL:O	2.29	0.57
1:A:107:VAL:HG12	1:A:115:ILE:HD11	1.87	0.57
2:F:324:THR:O	2:F:324:THR:HG22	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:180:SER:O	3:G:205:GLN:HG3	2.04	0.57
3:G:209:LEU:O	3:G:213:ILE:HG22	2.05	0.57
2:F:223:ASN:HD22	2:F:223:ASN:N	1.85	0.56
3:G:164:ARG:NH2	3:G:166:ARG:HD3	2.20	0.56
1:C:78:ASN:ND2	1:C:80:LYS:HD3	2.19	0.56
2:F:394:ASP:CB	3:G:79:GLY:HA2	2.34	0.56
1:A:159:ILE:HD12	1:A:165:GLU:HG2	1.88	0.56
1:A:347:ASP:OD1	2:E:191:ARG:NH1	2.38	0.56
1:B:283:LEU:HD12	2:E:277:SER:HB3	1.87	0.56
1:B:357:PHE:CE1	1:B:362:ARG:HD3	2.40	0.56
1:C:173:THR:CG2	1:C:354:THR:HG22	2.35	0.56
1:C:102:GLU:HG2	1:C:122:GLY:O	2.06	0.56
1:C:156:LEU:HD13	1:C:367:VAL:HG22	1.86	0.56
2:D:275:ILE:HG23	3:G:269:ALA:CB	2.33	0.56
2:E:105:ARG:NH2	2:E:208:LEU:HA	2.20	0.56
2:E:174:ALA:CB	2:E:214:LYS:HD3	2.35	0.56
1:A:224:ASP:CG	1:A:227:LYS:HE3	2.31	0.56
1:A:450:ARG:NH2	1:A:494:ASP:OD2	2.38	0.56
2:E:155:PHE:CE1	2:E:310:ILE:HD12	2.40	0.56
3:G:71:VAL:HG13	3:G:108:VAL:HG22	1.88	0.56
1:C:219:ARG:HD3	1:C:433:TYR:CE1	2.41	0.56
1:A:185:ASN:O	1:A:188:ARG:HG3	2.05	0.56
1:C:187:LYS:HE2	1:C:191:ASP:OD2	2.05	0.56
1:B:423:ARG:HE	1:B:458:PRO:HD3	1.71	0.56
2:E:396:LEU:HB3	2:E:401:LYS:HG2	1.88	0.56
1:B:393:GLU:OE1	1:B:424:LEU:HD11	2.05	0.55
2:E:138:LYS:HG3	2:E:416:GLN:OE1	2.06	0.55
2:F:98:ILE:HG13	2:F:100:GLU:HG3	1.88	0.55
1:A:291:ARG:N	3:G:262:LEU:HD21	2.21	0.55
1:B:180:ILE:O	1:B:181:ASP:C	2.47	0.55
1:B:351:PHE:CE1	1:B:369:LEU:HB3	2.41	0.55
1:C:442:VAL:CG1	1:C:489:ILE:HD11	2.37	0.55
1:B:80:LYS:HG3	1:B:81:LEU:HD23	1.88	0.55
1:A:99:VAL:CG2	1:A:253:MET:HA	2.36	0.55
2:D:84:ILE:CD1	2:D:95:MET:HE1	2.34	0.55
2:D:87:GLY:HA2	2:D:242:TYR:CE2	2.42	0.55
2:D:451:HIS:CD2	2:D:452:LEU:HD23	2.42	0.55
2:D:471:ASP:O	2:D:474:ALA:N	2.39	0.55
3:G:164:ARG:HD3	3:G:174:GLU:OE2	2.06	0.55
1:C:184:ILE:HG22	1:C:435:PRO:HG2	1.87	0.55
1:C:390:MET:HE3	1:C:424:LEU:HD22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:LEU:HD22	1:C:398:ARG:HH21	1.71	0.55
2:E:244:ARG:HG3	2:E:303:SER:N	2.22	0.55
1:A:479:LEU:HD21	1:A:493:SER:HB3	1.89	0.55
1:C:211:SER:HB3	2:F:126:MET:HE2	1.87	0.55
2:D:255:ILE:HG21	2:D:258:ILE:HD13	1.87	0.55
2:D:366:GLU:HG3	2:D:442:GLN:HE22	1.71	0.55
2:E:263:GLN:O	2:E:267:GLU:HG3	2.07	0.55
2:F:32:ILE:O	2:F:33:LEU:HB2	2.06	0.55
3:G:117:HIS:O	3:G:120:HIS:N	2.35	0.55
2:F:63:MET:CE	2:F:97:VAL:HG11	2.36	0.55
1:A:100:GLY:HA2	1:A:256:TYR:CE1	2.42	0.55
2:F:10:THR:HG23	2:F:76:LEU:HD12	1.88	0.55
1:A:209:LYS:HE3	1:A:211:SER:HB2	1.88	0.54
1:C:91:THR:HG22	1:C:93:ALA:H	1.72	0.54
2:D:473:LEU:O	2:D:475:GLU:N	2.40	0.54
2:F:390:ILE:HD11	3:G:242:MET:HE1	1.89	0.54
3:G:57:ILE:HG22	3:G:184:ILE:HD12	1.87	0.54
1:B:423:ARG:HE	1:B:458:PRO:HG3	1.71	0.54
2:D:142:LEU:HD22	2:D:441:PHE:CD2	2.42	0.54
2:E:174:ALA:HB2	2:E:214:LYS:HD3	1.89	0.54
3:G:144:ILE:HD13	3:G:213:ILE:HD11	1.90	0.54
3:G:160:ILE:CG2	3:G:176:LYS:HB2	2.37	0.54
1:B:347:ASP:HB3	1:B:374:VAL:HG22	1.88	0.54
2:D:83:ARG:HA	2:D:114:ALA:O	2.07	0.54
1:A:452:TYR:OH	1:A:498:LYS:HG3	2.08	0.54
1:C:52:MET:HE2	1:C:76:PHE:CE2	2.40	0.54
2:D:122:GLU:OE1	2:D:122:GLU:HA	2.07	0.54
2:E:218:VAL:HG11	2:E:235:THR:CG2	2.38	0.54
3:G:39:LYS:HB3	3:G:40:PRO:CD	2.38	0.54
3:G:117:HIS:CE1	3:G:121:SER:HB2	2.42	0.54
3:G:181:LEU:HB3	3:G:184:ILE:HG22	1.89	0.54
3:G:181:LEU:HG	3:G:183:THR:HB	1.89	0.54
1:A:373:ARG:HG3	1:A:373:ARG:HH11	1.72	0.54
2:D:282:GLN:H	2:D:282:GLN:NE2	2.01	0.54
1:A:161:ARG:HH11	1:A:263:HIS:CG	2.26	0.54
1:C:239:ALA:HB1	1:C:241:PRO:HD2	1.90	0.54
1:C:52:MET:HG3	1:C:61:GLY:O	2.07	0.54
1:C:218:LYS:HD2	2:F:128:VAL:HG21	1.88	0.54
1:B:218:LYS:HB2	2:E:128:VAL:HG12	1.89	0.54
1:B:446:TYR:CD2	1:B:497:LEU:HD23	2.43	0.54
1:A:468:PHE:CE1	1:A:501:VAL:HG12	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:LEU:HA	1:B:482:LYS:HE3	1.89	0.54
2:D:167:MET:CB	2:D:420:VAL:HG11	2.38	0.54
2:F:439:LYS:HE3	2:F:443:GLN:HE22	1.73	0.54
1:A:463:LYS:HD3	1:A:508:PHE:HZ	1.73	0.53
1:B:270:ASP:OD1	1:B:273:LYS:HG3	2.07	0.53
1:C:190:ASN:HA	1:C:198:LYS:HG2	1.90	0.53
1:A:150:ILE:HA	1:A:430:GLN:OE1	2.08	0.53
1:B:44:LEU:O	1:B:47:VAL:HG22	2.09	0.53
1:B:69:ASP:O	1:B:70:ASN:HB3	2.09	0.53
2:D:396:LEU:HD22	2:D:400:ASP:HB3	1.89	0.53
2:E:220:GLY:HA3	2:E:232:VAL:HG21	1.91	0.53
1:B:482:LYS:O	1:B:486:ASP:N	2.37	0.53
2:D:381:TYR:HE2	2:D:411:GLN:HE22	1.56	0.53
1:A:48:GLN:HB3	2:E:68:GLY:O	2.07	0.53
1:A:207:GLY:HA3	1:A:273:LYS:HD3	1.89	0.53
1:A:436:MET:HG3	1:A:441:GLN:HG2	1.90	0.53
2:D:388:ILE:HD12	2:D:393:MET:SD	2.48	0.53
2:D:412:ARG:HH11	2:D:412:ARG:HG3	1.73	0.53
2:F:292:MET:CE	2:F:296:ILE:HD11	2.38	0.53
3:G:249:THR:HA	3:G:252:ARG:NH1	2.24	0.53
1:A:170:ASP:O	1:A:175:LYS:HE2	2.08	0.53
1:C:140:ILE:HD11	1:C:143:ARG:HH22	1.74	0.53
2:D:136:GLY:CA	2:D:431:LEU:HD13	2.37	0.53
2:E:81:PRO:HG2	2:E:115:ALA:HB1	1.91	0.53
1:B:441:GLN:O	1:B:445:ILE:HG12	2.08	0.53
2:D:422:GLU:HG2	2:D:427:HIS:O	2.09	0.53
1:A:291:ARG:HG3	3:G:258:ILE:CG2	2.38	0.53
1:A:457:GLU:HB3	1:A:460:LYS:HD3	1.89	0.53
1:C:48:GLN:HB3	2:D:68:GLY:HA2	1.90	0.53
2:E:97:VAL:HG13	2:E:232:VAL:CG1	2.39	0.53
2:E:397:SER:O	2:E:401:LYS:HG3	2.07	0.53
3:G:117:HIS:ND1	3:G:118:ARG:HA	2.22	0.53
1:B:114:ALA:HB2	1:B:121:ILE:HD11	1.90	0.53
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.89	0.53
2:D:31:PRO:HD2	2:D:34:ASN:ND2	2.24	0.53
2:D:96:ASN:CB	2:D:100:GLU:H	2.22	0.53
2:E:9:THR:HG21	2:E:28:GLY:O	2.09	0.53
1:B:386:VAL:HG22	1:B:442:VAL:HG12	1.91	0.53
1:C:180:ILE:CD1	1:C:216:LEU:HD21	2.34	0.53
2:E:201:ILE:CD1	2:E:208:LEU:HD11	2.37	0.53
1:A:140:ILE:HG21	1:A:313:ASN:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:279:VAL:HG12	2:E:279:VAL:O	2.10	0.52
1:C:64:LEU:HD23	1:C:74:VAL:HG21	1.91	0.52
2:F:96:ASN:HB2	2:F:100:GLU:H	1.73	0.52
2:E:391:LEU:HD22	3:G:29:ALA:CB	2.36	0.52
3:G:137:THR:HG22	3:G:138:PHE:N	2.24	0.52
1:C:270:ASP:OD1	1:C:273:LYS:HG3	2.09	0.52
3:G:117:HIS:ND1	3:G:117:HIS:C	2.67	0.52
3:G:179:PHE:C	3:G:181:LEU:N	2.66	0.52
1:A:179:ALA:HB1	1:A:267:ILE:HG12	1.91	0.52
1:C:156:LEU:HD11	1:C:428:LEU:HD13	1.91	0.52
2:D:412:ARG:HD2	2:D:454:GLU:HB3	1.90	0.52
2:D:473:LEU:C	2:D:475:GLU:N	2.62	0.52
2:E:316:ASP:OD2	3:G:255:GLN:NE2	2.30	0.52
1:C:267:ILE:N	1:C:267:ILE:HD12	2.25	0.52
2:D:366:GLU:CG	2:D:442:GLN:HE22	2.23	0.52
3:G:140:ASP:HB3	5:I:42:ILE:HG13	1.92	0.52
3:G:181:LEU:O	3:G:184:ILE:HG22	2.08	0.52
1:B:383:MET:O	1:B:384:LYS:C	2.52	0.52
1:B:423:ARG:HD2	1:B:461:ILE:HD11	1.92	0.52
1:A:245:LEU:O	1:A:246:ALA:C	2.51	0.52
2:E:377:ILE:HG21	2:E:410:ILE:HD12	1.92	0.52
1:A:136:ILE:O	2:E:194:ASN:HB2	2.10	0.52
3:G:115:ILE:C	3:G:117:HIS:N	2.68	0.52
4:H:83:THR:HB	4:H:91:GLN:HE21	1.75	0.52
2:E:25:PHE:O	2:E:56:SER:HB3	2.10	0.52
2:E:80:ALA:HB1	2:E:81:PRO:HD2	1.91	0.52
2:F:210:ASP:HB2	2:F:212:THR:HG23	1.91	0.52
1:A:140:ILE:HD11	1:A:143:ARG:NE	2.25	0.51
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.75	0.51
2:E:204:GLY:C	2:E:206:ILE:N	2.68	0.51
2:E:254:PHE:CD1	2:E:307:VAL:HB	2.45	0.51
2:E:377:ILE:HG21	2:E:410:ILE:CD1	2.40	0.51
3:G:117:HIS:ND1	3:G:118:ARG:CA	2.74	0.51
1:B:157:VAL:N	1:B:158:PRO:CD	2.73	0.51
1:B:386:VAL:CG2	1:B:442:VAL:HG12	2.41	0.51
1:C:215:GLN:HE22	2:F:128:VAL:HA	1.75	0.51
2:D:356:ARG:O	2:D:356:ARG:HG2	2.09	0.51
2:E:218:VAL:HG11	2:E:235:THR:HG22	1.92	0.51
2:F:234:LEU:O	2:F:237:LEU:HB3	2.11	0.51
2:F:360:PRO:HD3	2:F:368:TYR:CD2	2.45	0.51
1:A:245:LEU:C	1:A:247:PRO:HD2	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:41:ARG:O	2:E:42:GLU:C	2.53	0.51
1:C:45:ARG:NH2	1:C:68:PRO:O	2.44	0.51
1:C:436:MET:CE	1:C:469:LEU:HD21	2.40	0.51
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.40	0.51
2:E:382:LYS:O	2:E:385:GLN:HB2	2.11	0.51
1:B:140:ILE:HG23	1:B:311:LYS:HG3	1.92	0.51
1:C:102:GLU:HG2	1:C:122:GLY:C	2.36	0.51
2:D:154:LEU:HD22	2:D:165:LEU:HD23	1.92	0.51
2:E:444:ILE:HD11	2:E:463:ILE:HD11	1.93	0.51
3:G:190:MET:HE3	3:G:190:MET:HA	1.92	0.51
5:I:5:ARG:O	5:I:6:GLN:HB3	2.10	0.51
1:B:157:VAL:N	1:B:158:PRO:HD3	2.26	0.51
1:C:406:PHE:N	1:C:406:PHE:CD1	2.79	0.51
2:E:142:LEU:HD21	2:E:374:VAL:HG21	1.93	0.51
2:E:293:GLN:HG3	2:E:328:HIS:CG	2.46	0.51
1:C:443:ALA:O	1:C:446:TYR:HB3	2.10	0.51
1:B:180:ILE:CD1	1:B:216:LEU:HD21	2.39	0.51
1:C:164:ARG:HD2	1:C:306:LEU:O	2.11	0.51
1:B:456:LEU:HD12	1:B:457:GLU:N	2.20	0.51
1:B:489:ILE:HG22	1:B:494:ASP:HB2	1.93	0.51
2:E:204:GLY:O	2:E:205:VAL:C	2.54	0.51
2:F:345:TYR:HA	2:F:346:PRO:C	2.36	0.51
2:F:421:ALA:O	2:F:425:THR:HG23	2.11	0.51
1:A:457:GLU:HB2	1:A:460:LYS:HD3	1.92	0.51
1:C:105:GLY:HA2	1:C:226:MET:HE3	1.93	0.51
1:C:244:TYR:O	1:C:247:PRO:HD2	2.11	0.51
2:E:443:GLN:O	2:E:446:ALA:HB3	2.10	0.51
1:A:137:ILE:N	1:A:138:PRO:CD	2.74	0.50
1:C:23:VAL:HG12	1:C:23:VAL:O	2.11	0.50
2:D:84:ILE:HD13	2:D:235:THR:HG23	1.92	0.50
2:E:82:ILE:HB	2:E:116:ILE:HD13	1.92	0.50
2:F:96:ASN:ND2	2:F:100:GLU:HB2	2.26	0.50
2:F:242:TYR:CD1	2:F:246:GLN:HG3	2.46	0.50
3:G:23:MET:SD	3:G:232:MET:HE2	2.50	0.50
2:F:390:ILE:HD11	3:G:242:MET:SD	2.51	0.50
2:F:455:GLN:H	2:F:455:GLN:CD	2.18	0.50
1:A:187:LYS:HE2	1:A:191:ASP:OD2	2.11	0.50
1:A:240:ALA:N	1:A:241:PRO:HD2	2.27	0.50
1:B:358:TYR:C	1:B:360:GLY:N	2.69	0.50
1:C:331:ALA:O	1:C:333:ASP:N	2.44	0.50
2:D:93:ARG:HG3	2:D:93:ARG:NH1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:241:GLU:HA	2:E:304:ILE:HD11	1.93	0.50
2:E:334:VAL:HG23	2:E:353:SER:HA	1.92	0.50
3:G:49:LEU:HD21	3:G:212:ILE:CD1	2.41	0.50
1:B:210:ARG:O	1:B:211:SER:C	2.54	0.50
2:D:406:ARG:O	2:D:410:ILE:HG13	2.11	0.50
2:E:155:PHE:HE1	2:E:310:ILE:HD12	1.77	0.50
2:F:386:ASP:O	2:F:389:ALA:HB3	2.11	0.50
4:H:79:SER:CB	5:I:15:SER:HA	2.41	0.50
1:A:291:ARG:CA	3:G:262:LEU:CD2	2.81	0.50
1:B:390:MET:CE	1:B:428:LEU:HD21	2.42	0.50
1:C:338:ILE:O	1:C:339:PRO:C	2.51	0.50
2:E:462:PRO:HD2	2:E:465:GLU:HG3	1.94	0.50
2:E:463:ILE:O	2:E:467:VAL:HG23	2.12	0.50
2:F:257:ASN:HB3	2:F:260:ARG:HG2	1.93	0.50
1:A:380:THR:O	1:A:384:LYS:HG3	2.12	0.50
1:C:359:LYS:O	2:F:376:LYS:HE2	2.12	0.50
2:D:136:GLY:HA2	2:D:432:VAL:O	2.12	0.50
2:E:221:GLN:N	2:E:224:GLU:OE1	2.44	0.50
1:A:94:ILE:HG12	1:A:95:VAL:N	2.27	0.50
1:C:30:ARG:HE	1:C:87:ILE:CD1	2.18	0.50
1:C:402:ALA:O	1:C:405:GLN:HG3	2.12	0.50
1:B:49:ALA:O	1:B:50:GLU:HB2	2.12	0.49
3:G:178:ILE:C	3:G:180:SER:N	2.69	0.49
1:B:107:VAL:HG12	1:B:115:ILE:CG1	2.43	0.49
1:B:423:ARG:HE	1:B:458:PRO:CD	2.25	0.49
2:E:275:ILE:O	2:E:283:PRO:HG3	2.12	0.49
2:F:168:GLU:OE1	2:F:418:PHE:HB3	2.12	0.49
4:H:18:PHE:CZ	4:H:20:PHE:HB2	2.46	0.49
4:H:130:GLU:HG3	5:I:9:LEU:HD11	1.93	0.49
1:A:294:TYR:HB2	1:A:337:TYR:HE2	1.76	0.49
2:E:242:TYR:C	2:E:244:ARG:H	2.18	0.49
1:A:417:LEU:HD23	1:A:417:LEU:H	1.77	0.49
1:B:27:GLU:O	1:B:90:ARG:HG3	2.12	0.49
2:D:345:TYR:HA	2:D:346:PRO:C	2.37	0.49
2:F:339:ILE:HG22	2:F:344:ILE:HB	1.94	0.49
3:G:197:ASP:O	3:G:200:VAL:HG12	2.13	0.49
1:B:151:LYS:NZ	1:B:429:LYS:O	2.45	0.49
2:F:360:PRO:HD3	2:F:368:TYR:CE2	2.48	0.49
1:B:96:ASP:HB2	1:B:127:ARG:O	2.13	0.49
1:B:437:ALA:O	1:B:438:ILE:C	2.54	0.49
2:F:394:ASP:HB3	3:G:79:GLY:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:121:SER:C	3:G:123:GLN:N	2.60	0.49
1:C:96:ASP:O	1:C:97:VAL:HG13	2.12	0.49
1:C:225:ALA:HA	1:C:228:TYR:CE1	2.47	0.49
2:D:84:ILE:N	2:D:114:ALA:O	2.42	0.49
2:E:54:GLY:O	2:E:55:GLU:HB2	2.13	0.49
2:E:444:ILE:HD11	2:E:463:ILE:CD1	2.43	0.49
1:A:300:TYR:O	1:A:304:ARG:HG2	2.13	0.49
1:C:30:ARG:HA	1:C:86:ASP:O	2.13	0.49
1:C:83:LYS:HB3	2:F:52:HIS:CE1	2.48	0.49
1:C:245:LEU:O	1:C:246:ALA:C	2.56	0.49
2:E:393:MET:HE3	2:E:396:LEU:HD12	1.95	0.49
2:F:80:ALA:HB1	2:F:81:PRO:HD2	1.95	0.49
2:F:163:THR:O	2:F:167:MET:HG2	2.12	0.49
1:B:24:ASP:O	1:B:28:THR:HB	2.12	0.49
1:B:211:SER:O	1:B:215:GLN:HG3	2.13	0.49
1:B:463:LYS:HE2	1:B:508:PHE:CZ	2.48	0.49
1:B:427:LEU:HD11	1:B:448:GLY:HA3	1.95	0.48
1:C:362:ARG:HG3	1:C:362:ARG:NH1	2.27	0.48
2:D:83:ARG:HA	2:D:115:ALA:HA	1.95	0.48
2:F:86:VAL:HG11	2:F:114:ALA:HB3	1.94	0.48
3:G:71:VAL:HG13	3:G:108:VAL:CG2	2.43	0.48
1:A:209:LYS:HZ1	2:D:330:ASP:CG	2.20	0.48
2:F:82:ILE:HD13	2:F:98:ILE:HG22	1.95	0.48
3:G:156:ASP:O	3:G:181:LEU:HB2	2.13	0.48
1:B:99:VAL:HG21	1:B:127:ARG:HB3	1.94	0.48
1:B:300:TYR:O	1:B:304:ARG:HG2	2.13	0.48
2:D:168:GLU:HG3	2:D:168:GLU:O	2.11	0.48
2:D:360:PRO:HD3	2:D:368:TYR:CE2	2.48	0.48
2:E:134:VAL:HG13	2:E:141:ASP:OD2	2.13	0.48
2:E:227:GLY:O	2:E:230:ALA:HB3	2.13	0.48
3:G:160:ILE:HG22	3:G:176:LYS:HB2	1.96	0.48
1:C:164:ARG:HD2	1:C:164:ARG:HH11	1.41	0.48
2:F:357:ILE:HD12	2:F:362:ILE:HG21	1.95	0.48
3:G:39:LYS:N	3:G:40:PRO:HD2	2.28	0.48
1:C:434:SER:N	1:C:435:PRO:HD3	2.27	0.48
1:C:488:LYS:HG2	1:C:489:ILE:N	2.28	0.48
2:E:223:ASN:HD22	2:E:223:ASN:N	1.84	0.48
3:G:136:PRO:HD3	3:G:221:THR:HG21	1.95	0.48
1:A:85:GLY:O	1:A:86:ASP:C	2.53	0.48
1:A:127:ARG:HE	1:A:131:LEU:CD1	2.27	0.48
1:C:334:VAL:HG13	1:C:351:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:PHE:CD2	2:D:408:ARG:CZ	2.97	0.48
2:D:319:ASP:O	2:D:320:PRO:C	2.55	0.48
2:E:374:VAL:O	2:E:377:ILE:HG22	2.14	0.48
2:E:404:VAL:O	2:E:408:ARG:HG3	2.14	0.48
1:C:485:THR:O	1:C:486:ASP:C	2.57	0.48
2:F:321:ALA:HB3	2:F:322:PRO:HD3	1.94	0.48
3:G:180:SER:O	3:G:181:LEU:C	2.56	0.48
1:A:40:ARG:HH11	1:A:40:ARG:CG	2.27	0.48
1:A:373:ARG:HG3	1:A:373:ARG:NH1	2.28	0.48
2:E:416:GLN:HG3	2:E:417:PRO:HD2	1.96	0.48
2:F:63:MET:HE1	2:F:231:ARG:HB2	1.95	0.48
2:F:221:GLN:HE21	2:F:221:GLN:HA	1.78	0.48
1:A:453:LEU:HD13	1:A:461:ILE:HG23	1.96	0.48
1:C:44:LEU:HB3	1:C:47:VAL:HG22	1.95	0.48
3:G:129:LYS:HG2	3:G:130:GLU:OE1	2.14	0.48
1:A:389:THR:O	1:A:393:GLU:HG2	2.13	0.48
1:B:481:SER:O	1:B:485:THR:HB	2.14	0.48
2:D:393:MET:HE1	2:D:404:VAL:HG11	1.95	0.48
2:D:425:THR:HB	2:D:459:MET:HE2	1.96	0.48
2:F:319:ASP:O	2:F:322:PRO:HD2	2.14	0.48
3:G:179:PHE:HB3	3:G:184:ILE:HG21	1.96	0.48
1:C:481:SER:O	1:C:485:THR:HB	2.14	0.47
2:D:32:ILE:O	2:D:33:LEU:HB2	2.14	0.47
2:E:397:SER:C	2:E:399:GLU:H	2.20	0.47
3:G:89:MET:CB	3:G:116:LEU:HD22	2.38	0.47
1:A:100:GLY:HA2	1:A:256:TYR:CD1	2.49	0.47
1:C:313:ASN:OD1	1:C:315:ALA:HB3	2.14	0.47
1:C:441:GLN:O	1:C:445:ILE:HG12	2.14	0.47
2:D:14:VAL:HG11	2:D:24:GLN:HB2	1.95	0.47
2:E:253:LEU:O	2:E:306:SER:HA	2.14	0.47
1:A:136:ILE:CD1	2:E:219:TYR:CE2	2.97	0.47
1:A:209:LYS:HE3	1:A:211:SER:CB	2.44	0.47
1:B:225:ALA:HA	1:B:228:TYR:CE2	2.49	0.47
1:C:180:ILE:HG22	1:C:184:ILE:HD12	1.97	0.47
2:E:360:PRO:HD3	2:E:368:TYR:CD1	2.49	0.47
2:E:388:ILE:HG23	2:E:393:MET:CG	2.43	0.47
1:A:49:ALA:O	1:A:50:GLU:HB2	2.13	0.47
1:A:444:VAL:CG1	1:A:469:LEU:HD13	2.44	0.47
1:B:443:ALA:O	1:B:446:TYR:HB3	2.14	0.47
2:E:116:ILE:HA	2:E:238:THR:OG1	2.14	0.47
2:F:93:ARG:NH2	2:F:106:GLY:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ILE:O	1:A:181:ASP:C	2.56	0.47
1:A:291:ARG:HG3	3:G:258:ILE:HG23	1.96	0.47
1:B:179:ALA:O	1:B:182:THR:HB	2.14	0.47
1:B:311:LYS:HD2	1:B:312:MET:O	2.13	0.47
2:D:129:GLU:OE1	2:D:129:GLU:HA	2.15	0.47
2:E:161:GLY:O	2:E:162:LYS:C	2.57	0.47
2:F:88:PRO:HD2	2:F:89:GLU:OE2	2.14	0.47
3:G:144:ILE:HG21	3:G:213:ILE:HD13	1.97	0.47
1:B:351:PHE:HE1	1:B:369:LEU:O	1.97	0.47
2:E:82:ILE:HB	2:E:116:ILE:CD1	2.45	0.47
2:F:467:VAL:O	2:F:470:ALA:HB3	2.14	0.47
1:A:188:ARG:HE	1:A:437:ALA:HB2	1.79	0.47
1:A:291:ARG:N	3:G:262:LEU:CD2	2.78	0.47
1:A:485:THR:C	1:A:487:GLY:H	2.23	0.47
1:B:151:LYS:NZ	1:B:427:LEU:O	2.47	0.47
1:B:171:ARG:HG3	1:B:171:ARG:HH11	1.79	0.47
1:C:59:LEU:HD23	1:C:82:ILE:CD1	2.44	0.47
1:C:445:ILE:HG22	1:C:449:VAL:CG2	2.44	0.47
2:D:368:TYR:CE1	2:D:372:ARG:HG3	2.50	0.47
2:E:33:LEU:HD13	2:E:117:HIS:CG	2.50	0.47
2:E:158:ALA:C	2:E:160:VAL:N	2.72	0.47
2:F:36:LEU:N	2:F:36:LEU:HD23	2.30	0.47
2:F:346:PRO:HG3	2:F:418:PHE:HZ	1.79	0.47
2:F:462:PRO:HG2	2:F:465:GLU:HG3	1.96	0.47
3:G:125:LEU:HD11	3:G:151:SER:HB2	1.96	0.47
1:A:107:VAL:HB	1:A:116:ASP:HB3	1.97	0.47
1:A:166:LEU:HD13	1:A:342:VAL:HG12	1.95	0.47
1:C:219:ARG:HD3	1:C:433:TYR:HE1	1.80	0.47
2:D:471:ASP:O	2:D:472:LYS:C	2.57	0.47
1:A:52:MET:HE1	1:A:60:LYS:HD3	1.97	0.47
2:E:431:LEU:HD12	2:E:431:LEU:O	2.15	0.47
2:F:409:LYS:HD3	2:F:457:PHE:HE2	1.78	0.47
3:G:78:CYS:O	3:G:81:ILE:HD13	2.15	0.47
1:A:78:ASN:OD1	1:A:80:LYS:HB3	2.15	0.47
1:B:240:ALA:N	1:B:241:PRO:CD	2.77	0.47
2:D:412:ARG:O	2:D:415:SER:OG	2.33	0.47
2:F:151:LYS:HD3	2:F:328:HIS:O	2.15	0.47
1:B:400:VAL:HB	1:B:418:LEU:CD2	2.45	0.46
1:C:34:ILE:HD11	1:C:79:ASP:CB	2.41	0.46
2:D:469:LYS:O	2:D:473:LEU:HG	2.15	0.46
1:B:271:LEU:HD12	1:B:325:PRO:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:259:PHE:CE2	2:E:263:GLN:HG2	2.50	0.46
2:E:438:ILE:O	2:E:442:GLN:HB2	2.15	0.46
2:F:200:MET:CG	2:F:206:ILE:HG12	2.46	0.46
3:G:179:PHE:O	3:G:181:LEU:N	2.48	0.46
1:B:389:THR:HA	1:B:392:LEU:HG	1.96	0.46
1:B:433:TYR:C	1:B:435:PRO:HD3	2.40	0.46
1:C:403:PHE:CG	2:D:408:ARG:CZ	2.99	0.46
2:E:61:ILE:HG13	2:E:61:ILE:O	2.14	0.46
2:E:409:LYS:NZ	2:E:450:ASP:HA	2.30	0.46
2:F:205:VAL:HG23	2:F:215:VAL:HG21	1.96	0.46
1:A:313:ASN:OD1	1:A:316:PHE:HD2	1.98	0.46
1:A:376:SER:O	1:A:378:ALA:N	2.48	0.46
1:B:353:GLU:HG3	1:B:366:ASN:HB2	1.98	0.46
1:B:485:THR:O	1:B:486:ASP:C	2.58	0.46
2:D:201:ILE:HD13	2:D:208:LEU:HD11	1.98	0.46
2:F:89:GLU:HG2	2:F:110:THR:CG2	2.44	0.46
1:A:139:ARG:C	1:A:140:ILE:HG22	2.41	0.46
1:A:240:ALA:HB3	1:A:241:PRO:HD3	1.97	0.46
1:A:353:GLU:CD	1:A:366:ASN:HD22	2.23	0.46
1:C:187:LYS:HE3	1:C:224:ASP:HB3	1.97	0.46
2:D:96:ASN:HB2	2:D:100:GLU:N	2.27	0.46
2:D:289:MET:SD	2:D:324:THR:HG22	2.56	0.46
2:E:120:ALA:HB1	2:E:121:PRO:HD2	1.98	0.46
2:F:81:PRO:O	2:F:82:ILE:C	2.58	0.46
1:A:339:PRO:O	1:A:343:ILE:HG13	2.16	0.46
2:E:146:TYR:O	2:E:357:ILE:HD11	2.16	0.46
1:A:36:ASP:O	1:A:284:LEU:HD13	2.16	0.46
1:B:27:GLU:OE1	1:B:90:ARG:HD3	2.16	0.46
1:C:26:GLU:HB3	1:C:46:ASN:ND2	2.31	0.46
1:C:156:LEU:HD11	1:C:428:LEU:CD1	2.46	0.46
2:D:154:LEU:HD13	2:D:165:LEU:HD23	1.96	0.46
2:D:417:PRO:HA	2:D:459:MET:HE1	1.96	0.46
2:F:469:LYS:O	2:F:473:LEU:HG	2.16	0.46
3:G:56:ASP:C	3:G:57:ILE:HG12	2.41	0.46
1:B:284:LEU:CD2	2:E:274:ARG:HD3	2.46	0.46
1:B:381:ARG:HG2	1:B:488:LYS:HG3	1.98	0.46
2:D:298:THR:HG23	2:D:303:SER:HA	1.98	0.46
2:E:189:ARG:O	2:E:190:THR:C	2.58	0.46
2:F:29:LEU:HD11	2:F:58:VAL:HG13	1.98	0.46
2:F:339:ILE:CG2	2:F:344:ILE:HB	2.46	0.46
1:A:213:VAL:O	1:A:216:LEU:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:PHE:O	1:A:404:ALA:C	2.59	0.46
1:C:45:ARG:HA	1:C:45:ARG:HD3	1.29	0.46
1:C:91:THR:HG22	1:C:93:ALA:HB3	1.97	0.46
1:C:251:CYS:O	1:C:255:GLU:HG3	2.16	0.46
2:D:432:VAL:HG13	2:D:433:PRO:HD2	1.97	0.46
2:D:440:GLY:O	2:D:444:ILE:HG13	2.16	0.46
2:D:461:GLY:HA3	2:D:462:PRO:HD3	1.74	0.46
2:E:77:ASP:C	2:E:79:GLY:H	2.24	0.46
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.97	0.46
1:B:469:LEU:HG	1:B:473:ILE:HD11	1.97	0.45
1:C:292:GLU:O	1:C:293:ALA:CB	2.63	0.45
2:D:397:SER:O	2:D:398:GLU:C	2.58	0.45
2:E:63:MET:CE	2:E:228:ALA:HA	2.45	0.45
2:F:96:ASN:HD22	2:F:100:GLU:CB	2.27	0.45
2:F:243:PHE:O	2:F:249:GLN:HB2	2.16	0.45
2:F:390:ILE:CD1	3:G:242:MET:CE	2.94	0.45
1:A:48:GLN:HA	2:E:69:LEU:O	2.16	0.45
1:A:142:VAL:HG22	1:A:161:ARG:O	2.16	0.45
1:A:485:THR:HG22	1:A:486:ASP:N	2.29	0.45
1:B:141:SER:HB2	1:B:143:ARG:NH1	2.31	0.45
1:C:67:GLU:HB3	1:C:68:PRO:HD2	1.98	0.45
2:F:275:ILE:HD13	3:G:271:ALA:HB1	1.98	0.45
1:B:496:LYS:O	1:B:500:ILE:HG13	2.15	0.45
1:C:158:PRO:HB3	1:C:379:GLN:HG3	1.99	0.45
2:D:237:LEU:HD21	2:D:295:ARG:HB2	1.97	0.45
2:D:274:ARG:HH11	2:D:274:ARG:HD2	1.49	0.45
2:E:77:ASP:CG	2:E:79:GLY:H	2.24	0.45
2:E:147:ALA:HB2	2:E:357:ILE:HD13	1.99	0.45
2:E:405:SER:OG	2:E:406:ARG:N	2.49	0.45
2:F:221:GLN:HA	2:F:221:GLN:NE2	2.31	0.45
3:G:259:THR:O	3:G:263:ILE:HG12	2.17	0.45
1:C:476:HIS:ND1	1:C:476:HIS:N	2.64	0.45
2:E:112:GLN:NE2	2:E:242:TYR:HE2	2.14	0.45
2:F:96:ASN:HB2	2:F:100:GLU:N	2.31	0.45
1:A:313:ASN:O	1:A:316:PHE:N	2.37	0.45
1:B:465:GLU:O	1:B:469:LEU:HB2	2.16	0.45
1:C:116:ASP:O	1:C:117:GLY:C	2.60	0.45
1:C:390:MET:HE1	1:C:428:LEU:HD21	1.99	0.45
1:C:432:GLN:O	1:C:433:TYR:HB2	2.16	0.45
1:C:474:SER:OG	1:C:475:GLN:N	2.49	0.45
2:D:412:ARG:C	2:D:414:LEU:N	2.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:425:THR:C	2:E:427:HIS:N	2.71	0.45
2:E:85:PRO:HD2	2:E:95:MET:CE	2.46	0.45
2:E:321:ALA:N	2:E:322:PRO:HD2	2.32	0.45
2:E:343:GLY:O	2:E:345:TYR:HD1	1.99	0.45
2:E:402:LEU:O	2:E:406:ARG:HG3	2.16	0.45
3:G:44:TYR:CD2	4:H:93:LEU:HD22	2.52	0.45
1:A:51:GLU:OE2	1:A:90:ARG:HB3	2.16	0.45
1:A:59:LEU:HD11	1:A:81:LEU:HD12	1.99	0.45
1:B:140:ILE:HG13	1:B:143:ARG:NH1	2.32	0.45
1:B:269:ASP:HA	1:B:270:ASP:HA	1.78	0.45
1:B:400:VAL:CG1	1:B:418:LEU:HD11	2.47	0.45
2:D:452:LEU:HD12	2:D:457:PHE:CZ	2.52	0.45
1:A:74:VAL:HG13	1:A:241:PRO:HG3	1.99	0.45
1:A:133:ALA:HB1	1:A:134:PRO:HD2	1.99	0.45
1:A:179:ALA:O	1:A:182:THR:HB	2.17	0.45
1:A:485:THR:C	1:A:487:GLY:N	2.73	0.45
1:B:300:TYR:HA	1:B:303:SER:OG	2.17	0.45
2:D:35:ALA:HB1	2:D:46:VAL:CG1	2.47	0.45
2:E:95:MET:HE2	2:E:99:GLY:CA	2.45	0.45
2:F:346:PRO:HG3	2:F:418:PHE:CZ	2.52	0.45
3:G:40:PRO:HB3	4:H:26:VAL:HG12	1.99	0.45
2:F:105:ARG:CZ	2:F:208:LEU:HD23	2.47	0.45
2:F:348:VAL:O	2:F:350:PRO:HD3	2.17	0.45
1:A:24:ASP:OD1	1:A:24:ASP:C	2.60	0.45
1:A:413:ALA:O	1:A:416:GLN:HB3	2.17	0.45
2:D:130:GLN:HE22	2:D:356:ARG:HD3	1.81	0.45
2:D:170:ILE:O	2:D:174:ALA:HB3	2.17	0.45
2:D:425:THR:HG21	2:D:459:MET:HE1	1.99	0.45
2:F:310:ILE:HD13	2:F:325:THR:HG21	1.98	0.45
3:G:13:ILE:HD13	3:G:242:MET:SD	2.57	0.45
3:G:84:SER:HB3	3:G:173:THR:OG1	2.17	0.45
1:A:412:ALA:HA	1:A:415:GLN:HB3	1.98	0.44
1:A:463:LYS:HD3	1:A:508:PHE:CZ	2.52	0.44
1:C:340:THR:O	1:C:341:ASN:C	2.58	0.44
1:A:166:LEU:HD13	1:A:342:VAL:CG1	2.47	0.44
1:A:244:TYR:HE1	1:A:301:LEU:HD11	1.83	0.44
1:A:461:ILE:H	1:A:461:ILE:HG12	1.60	0.44
1:A:482:LYS:O	1:A:483:ILE:C	2.61	0.44
1:B:76:PHE:HB3	1:B:242:LEU:HD21	1.98	0.44
2:D:190:THR:O	2:D:191:ARG:C	2.59	0.44
2:D:400:ASP:O	2:D:404:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:PHE:O	1:A:56:SER:C	2.61	0.44
1:A:140:ILE:CG2	1:A:313:ASN:HA	2.47	0.44
1:C:311:LYS:HE3	1:C:318:GLY:O	2.18	0.44
2:D:366:GLU:O	2:D:370:VAL:HG23	2.17	0.44
2:D:433:PRO:HG2	2:D:436:GLU:CG	2.44	0.44
2:F:359:ASP:OD1	2:F:360:PRO:HD2	2.18	0.44
1:A:471:HIS:ND1	1:A:475:GLN:HG3	2.33	0.44
2:E:282:GLN:HA	2:E:283:PRO:HD3	1.88	0.44
2:E:443:GLN:HA	2:E:446:ALA:HB3	1.99	0.44
2:F:257:ASN:OD1	2:F:259:PHE:HB3	2.18	0.44
3:G:86:ALA:O	3:G:116:LEU:HD13	2.18	0.44
1:A:392:LEU:O	1:A:396:GLN:HG3	2.18	0.44
1:A:492:GLU:C	1:A:494:ASP:N	2.73	0.44
1:B:34:ILE:HD12	1:B:35:GLY:H	1.81	0.44
2:D:95:MET:HG2	2:D:99:GLY:HA2	1.99	0.44
2:D:108:ILE:HG22	2:D:110:THR:HG23	1.99	0.44
2:D:231:ARG:O	2:D:232:VAL:C	2.60	0.44
2:E:114:ALA:HB3	2:E:238:THR:CG2	2.48	0.44
2:E:281:TYR:CZ	2:E:321:ALA:HB2	2.52	0.44
2:E:320:PRO:HD3	3:G:255:GLN:OE1	2.18	0.44
2:D:103:ASP:O	2:D:104:GLU:HB2	2.18	0.44
2:E:89:GLU:HG2	2:E:110:THR:CG2	2.39	0.44
2:E:433:PRO:HG2	2:E:436:GLU:CG	2.48	0.44
3:G:2:THR:C	3:G:4:LYS:N	2.74	0.44
1:A:97:VAL:HG11	1:A:249:SER:HB2	1.99	0.44
1:A:379:GLN:HB2	1:A:384:LYS:HE3	2.00	0.44
1:A:460:LYS:N	1:A:460:LYS:HD2	2.32	0.44
2:E:72:GLY:O	2:E:73:GLN:C	2.60	0.44
2:E:136:GLY:HA2	2:E:432:VAL:O	2.18	0.44
3:G:239:ALA:O	3:G:243:ILE:HG12	2.18	0.44
1:A:398:ARG:HH11	1:A:398:ARG:HD2	1.53	0.44
1:B:32:LEU:HD21	1:B:42:HIS:HB2	2.00	0.44
1:B:212:THR:O	1:B:216:LEU:HB2	2.18	0.44
1:B:400:VAL:HG12	1:B:418:LEU:HD11	2.00	0.44
1:C:83:LYS:HB3	2:F:52:HIS:HE1	1.83	0.44
1:C:404:ALA:HB1	1:C:410:LEU:HD11	1.99	0.44
2:D:397:SER:O	2:D:400:ASP:N	2.45	0.44
2:D:417:PRO:HB3	2:D:459:MET:HE3	1.99	0.44
2:E:166:ILE:O	2:E:170:ILE:HG13	2.18	0.44
2:F:188:GLU:H	2:F:221:GLN:NE2	2.15	0.44
2:F:407:ALA:O	2:F:411:GLN:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:VAL:O	1:B:217:VAL:HG13	2.18	0.44
1:C:209:LYS:HE3	1:C:211:SER:OG	2.18	0.44
2:D:470:ALA:O	2:D:474:ALA:N	2.50	0.44
2:F:136:GLY:HA3	2:F:431:LEU:HD11	1.99	0.44
3:G:105:ILE:HG22	3:G:106:ILE:N	2.32	0.44
1:A:151:LYS:HE2	1:A:427:LEU:O	2.17	0.43
1:A:385:GLN:OE1	1:A:488:LYS:HB2	2.17	0.43
1:B:389:THR:HA	1:B:392:LEU:CG	2.48	0.43
1:C:193:THR:O	1:C:195:GLU:OE1	2.36	0.43
2:D:63:MET:HE1	2:D:231:ARG:HB2	1.99	0.43
3:G:228:ARG:O	3:G:232:MET:HG2	2.17	0.43
1:A:251:CYS:O	1:A:255:GLU:HG3	2.18	0.43
2:D:412:ARG:HG3	2:D:412:ARG:NH1	2.33	0.43
2:E:310:ILE:HD11	2:E:329:LEU:HD11	2.00	0.43
2:F:289:MET:HE3	2:F:289:MET:HB2	1.73	0.43
2:F:439:LYS:HG2	2:F:443:GLN:NE2	2.33	0.43
2:F:50:ALA:O	2:F:51:GLN:HB3	2.16	0.43
1:A:99:VAL:HG23	1:A:253:MET:HA	2.00	0.43
1:B:55:PHE:O	1:B:56:SER:C	2.61	0.43
1:B:94:ILE:O	1:B:95:VAL:C	2.61	0.43
1:B:289:PRO:CG	3:G:263:ILE:HD12	2.47	0.43
1:B:450:ARG:HD3	1:B:450:ARG:HA	1.87	0.43
1:C:285:LEU:C	1:C:286:ARG:HG2	2.43	0.43
2:D:38:VAL:HG11	2:D:69:LEU:CD2	2.49	0.43
3:G:117:HIS:O	3:G:118:ARG:C	2.60	0.43
3:G:117:HIS:CE1	3:G:118:ARG:NE	2.86	0.43
1:A:45:ARG:HA	1:A:45:ARG:HD3	1.66	0.43
1:C:177:SER:O	1:C:178:ILE:C	2.60	0.43
1:C:180:ILE:O	1:C:181:ASP:C	2.61	0.43
1:C:290:GLY:O	1:C:291:ARG:C	2.61	0.43
2:E:242:TYR:C	2:E:242:TYR:CD1	2.96	0.43
1:A:283:LEU:HD11	1:A:293:ALA:HB1	1.98	0.43
1:C:49:ALA:N	1:C:66:LEU:HD11	2.34	0.43
2:D:93:ARG:NH1	2:D:108:ILE:HG12	2.33	0.43
2:E:105:ARG:NE	2:E:208:LEU:HD23	2.33	0.43
2:F:144:ALA:N	2:F:145:PRO:CD	2.82	0.43
1:A:383:MET:HE2	1:A:438:ILE:CD1	2.47	0.43
1:B:294:TYR:CE2	1:B:338:ILE:HD13	2.53	0.43
1:C:32:LEU:HD21	1:C:42:HIS:HB2	2.00	0.43
1:C:51:GLU:HG2	1:C:52:MET:N	2.33	0.43
1:C:147:GLN:OE1	1:C:438:ILE:HD13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:PHE:CD2	2:D:408:ARG:NH1	2.86	0.43
2:E:461:GLY:HA3	2:E:462:PRO:HD3	1.73	0.43
2:F:95:MET:HG3	2:F:99:GLY:HA2	2.00	0.43
2:F:122:GLU:OE1	2:F:122:GLU:HA	2.19	0.43
1:A:52:MET:CG	1:A:95:VAL:HG22	2.48	0.43
1:A:397:TYR:CD1	1:A:421:GLY:HA3	2.53	0.43
1:B:107:VAL:HG12	1:B:115:ILE:HD11	2.00	0.43
1:C:49:ALA:O	1:C:50:GLU:HB2	2.19	0.43
1:C:353:GLU:O	1:C:364:ALA:HB1	2.19	0.43
1:C:423:ARG:CD	1:C:461:ILE:HD11	2.49	0.43
2:D:231:ARG:O	2:D:234:LEU:N	2.50	0.43
2:E:439:LYS:O	2:E:440:GLY:C	2.61	0.43
2:F:141:ASP:HB3	2:F:434:LEU:HD13	2.01	0.43
2:F:196:LEU:O	2:F:200:MET:HB2	2.19	0.43
2:F:357:ILE:O	2:F:359:ASP:N	2.48	0.43
3:G:89:MET:HE1	3:G:112:ILE:CG2	2.43	0.43
4:H:79:SER:O	4:H:94:ALA:HA	2.18	0.43
1:A:78:ASN:ND2	1:A:80:LYS:HD2	2.34	0.43
1:B:423:ARG:HE	1:B:458:PRO:CG	2.31	0.43
2:F:31:PRO:O	2:F:34:ASN:HB2	2.18	0.43
2:F:319:ASP:O	2:F:320:PRO:C	2.60	0.43
3:G:113:ARG:O	3:G:117:HIS:HB2	2.18	0.43
1:A:96:ASP:HA	1:A:128:ARG:HA	2.01	0.43
1:B:434:SER:N	1:B:435:PRO:CD	2.82	0.43
2:D:94:ILE:HG22	2:D:102:ILE:HD11	2.01	0.43
2:D:189:ARG:O	2:D:192:GLU:HB2	2.18	0.43
2:E:35:ALA:HB2	2:E:82:ILE:HG13	1.99	0.43
2:E:242:TYR:C	2:E:244:ARG:N	2.77	0.43
2:E:397:SER:O	2:E:398:GLU:C	2.62	0.43
2:F:452:LEU:HD22	2:F:470:ALA:CB	2.49	0.43
3:G:106:ILE:HG12	3:G:126:VAL:HG23	2.01	0.43
1:C:107:VAL:O	1:C:115:ILE:HG12	2.18	0.42
1:C:269:ASP:HA	1:C:270:ASP:HA	1.79	0.42
2:E:376:LYS:O	2:E:379:GLN:HB2	2.19	0.42
3:G:179:PHE:C	3:G:181:LEU:H	2.27	0.42
1:C:187:LYS:O	1:C:188:ARG:C	2.61	0.42
2:E:422:GLU:C	2:E:424:PHE:N	2.74	0.42
2:F:400:ASP:O	2:F:404:VAL:HG23	2.19	0.42
1:A:340:THR:O	1:A:344:SER:HB3	2.19	0.42
1:C:185:ASN:HB2	1:C:435:PRO:HB3	2.00	0.42
2:D:95:MET:HE2	2:D:235:THR:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:258:ILE:HD12	2:D:258:ILE:HA	1.94	0.42
2:E:189:ARG:HB2	2:E:192:GLU:HG3	2.01	0.42
2:E:387:ILE:HG22	2:E:388:ILE:HD13	2.01	0.42
1:B:165:GLU:O	1:B:325:PRO:HD2	2.19	0.42
1:B:284:LEU:HD21	2:E:274:ARG:HD3	2.00	0.42
1:C:485:THR:C	1:C:487:GLY:N	2.75	0.42
2:D:35:ALA:HB1	2:D:46:VAL:HG13	2.02	0.42
2:D:266:SER:CB	2:D:282:GLN:NE2	2.82	0.42
2:E:95:MET:HE2	2:E:99:GLY:HA2	2.01	0.42
3:G:180:SER:O	3:G:182:ASP:N	2.52	0.42
1:B:385:GLN:NE2	1:B:489:ILE:HB	2.34	0.42
2:E:231:ARG:O	2:E:232:VAL:C	2.60	0.42
2:E:441:PHE:O	2:E:445:LEU:HG	2.19	0.42
2:E:425:THR:C	2:E:427:HIS:H	2.28	0.42
2:F:385:GLN:HA	2:F:388:ILE:HG12	2.01	0.42
2:F:471:ASP:O	2:F:474:ALA:N	2.53	0.42
3:G:6:ILE:HG21	3:G:250:PHE:HB2	2.00	0.42
5:I:5:ARG:O	5:I:6:GLN:CB	2.68	0.42
5:I:41:THR:O	5:I:42:ILE:C	2.62	0.42
1:A:383:MET:O	1:A:386:VAL:HG23	2.19	0.42
1:B:99:VAL:HG13	1:B:256:TYR:HB2	2.02	0.42
1:B:353:GLU:OE2	1:B:366:ASN:ND2	2.50	0.42
1:C:169:GLY:O	1:C:175:LYS:HE2	2.18	0.42
1:C:489:ILE:HG22	1:C:494:ASP:HB2	1.99	0.42
2:D:396:LEU:HD22	2:D:400:ASP:HB2	2.00	0.42
2:E:388:ILE:HD12	2:E:396:LEU:HD11	2.01	0.42
1:A:184:ILE:HD12	1:A:223:ALA:CB	2.49	0.42
1:B:255:GLU:HG2	1:B:258:ARG:CZ	2.50	0.42
2:D:279:VAL:HG12	2:D:279:VAL:O	2.20	0.42
2:E:88:PRO:C	2:E:90:THR:H	2.28	0.42
2:E:97:VAL:HG13	2:E:232:VAL:HG12	2.02	0.42
2:E:410:ILE:O	2:E:411:GLN:C	2.63	0.42
2:E:412:ARG:NH1	2:E:454:GLU:OE1	2.53	0.42
2:F:47:LEU:HD23	2:F:62:ALA:HA	2.01	0.42
3:G:12:SER:O	3:G:16:ILE:HD12	2.20	0.42
4:H:20:PHE:CD1	4:H:92:LEU:HD23	2.54	0.42
1:A:247:PRO:HG2	1:A:274:GLN:NE2	2.35	0.42
1:A:267:ILE:HA	1:A:324:LEU:O	2.20	0.42
1:A:294:TYR:HB2	1:A:337:TYR:CE2	2.54	0.42
1:B:381:ARG:HA	1:B:384:LYS:HB2	2.01	0.42
1:C:129:VAL:HG21	1:C:245:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:ASP:OD1	1:C:227:LYS:HE3	2.19	0.42
1:C:299:PHE:O	1:C:300:TYR:C	2.62	0.42
1:C:392:LEU:HD11	2:D:425:THR:HA	2.01	0.42
2:D:64:ASP:CG	2:D:65:GLY:H	2.28	0.42
2:D:112:GLN:NE2	2:D:242:TYR:HE1	2.18	0.42
2:D:201:ILE:CD1	2:D:208:LEU:HD11	2.50	0.42
2:D:462:PRO:HD2	2:D:465:GLU:HG3	2.01	0.42
2:E:95:MET:HA	2:E:100:GLU:O	2.20	0.42
2:E:185:GLY:HA3	2:E:188:GLU:HG3	2.02	0.42
2:E:316:ASP:CG	3:G:251:ASN:HB3	2.45	0.42
2:E:346:PRO:HG3	2:E:418:PHE:HZ	1.83	0.42
2:F:423:VAL:O	2:F:423:VAL:HG12	2.20	0.42
3:G:234:ASN:O	3:G:235:ALA:C	2.62	0.42
1:A:56:SER:O	1:A:58:GLY:N	2.53	0.42
1:B:249:SER:O	1:B:250:GLY:C	2.61	0.42
1:B:420:ARG:O	1:B:423:ARG:N	2.50	0.42
1:C:78:ASN:HD21	1:C:80:LYS:HD3	1.85	0.42
2:D:112:GLN:NE2	2:D:242:TYR:CE1	2.88	0.42
2:D:139:VAL:O	2:D:140:VAL:C	2.63	0.42
2:D:410:ILE:HG23	2:D:441:PHE:CE1	2.54	0.42
2:D:475:GLU:OE1	2:D:475:GLU:HA	2.20	0.42
4:H:95:GLU:HB3	5:I:19:ALA:HB2	2.01	0.42
1:A:68:PRO:HD3	2:E:15:ALA:HB2	2.02	0.41
1:B:78:ASN:ND2	1:B:80:LYS:HE2	2.35	0.41
1:C:105:GLY:N	1:C:229:THR:O	2.41	0.41
1:C:457:GLU:O	1:C:458:PRO:C	2.61	0.41
2:D:95:MET:HE3	2:D:99:GLY:HA2	2.02	0.41
2:F:252:LEU:HD23	2:F:252:LEU:HA	1.81	0.41
2:F:357:ILE:HD13	2:F:357:ILE:HA	1.80	0.41
1:A:206:ILE:O	1:A:273:LYS:HD2	2.20	0.41
1:B:75:VAL:HG21	1:B:82:ILE:HD12	2.02	0.41
1:B:389:THR:HG22	1:B:392:LEU:HD12	2.00	0.41
1:C:467:ALA:O	1:C:470:SER:HB2	2.20	0.41
2:D:145:PRO:HB2	2:D:357:ILE:HD11	2.01	0.41
2:E:340:ALA:O	2:E:343:GLY:N	2.42	0.41
2:E:396:LEU:CB	2:E:401:LYS:HG2	2.50	0.41
1:A:105:GLY:HA2	1:A:226:MET:O	2.21	0.41
1:A:338:ILE:N	1:A:339:PRO:CD	2.83	0.41
1:A:390:MET:HE1	1:A:428:LEU:HD21	2.02	0.41
1:B:107:VAL:O	1:B:115:ILE:HG12	2.20	0.41
1:C:139:ARG:HB3	1:C:311:LYS:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:LYS:HE2	1:C:436:MET:SD	2.60	0.41
2:D:84:ILE:HB	2:D:95:MET:HE3	2.02	0.41
2:E:122:GLU:HB2	2:E:125:GLU:HG3	2.01	0.41
2:D:63:MET:CE	2:D:97:VAL:HG11	2.51	0.41
2:D:398:GLU:HA	2:D:401:LYS:CG	2.51	0.41
2:E:29:LEU:HA	2:E:30:PRO:HD2	1.92	0.41
2:E:139:VAL:HG21	2:E:348:VAL:HB	2.02	0.41
2:E:165:LEU:HD22	2:E:335:LEU:HD21	2.02	0.41
2:E:182:VAL:HG21	2:E:240:ALA:HB2	2.01	0.41
2:E:282:GLN:H	2:E:282:GLN:NE2	2.19	0.41
2:E:434:LEU:O	2:E:437:THR:HB	2.21	0.41
2:F:95:MET:HE3	2:F:108:ILE:HD13	2.02	0.41
4:H:131:ILE:HG23	4:H:134:ARG:HH21	1.84	0.41
1:A:288:PRO:HA	1:A:289:PRO:HD3	1.88	0.41
1:B:366:ASN:ND2	1:B:369:LEU:HG	2.35	0.41
1:B:461:ILE:H	1:B:461:ILE:HG12	1.75	0.41
1:C:405:GLN:C	1:C:406:PHE:CD1	2.96	0.41
2:D:449:TYR:C	2:D:451:HIS:H	2.28	0.41
2:E:12:ARG:NH2	2:E:24:GLN:OE1	2.50	0.41
1:B:62:MET:HE3	1:B:64:LEU:CD1	2.51	0.41
1:B:340:THR:O	1:B:341:ASN:C	2.63	0.41
1:B:361:ILE:HD13	1:B:429:LYS:HE2	2.02	0.41
2:D:52:HIS:CD2	2:D:58:VAL:HG12	2.56	0.41
2:D:86:VAL:HG11	2:D:114:ALA:HB3	2.02	0.41
2:E:32:ILE:O	2:E:33:LEU:CB	2.68	0.41
2:E:35:ALA:C	2:E:36:LEU:HD23	2.46	0.41
2:E:345:TYR:CA	2:E:346:PRO:C	2.89	0.41
2:F:38:VAL:HG11	2:F:69:LEU:CD2	2.50	0.41
1:A:441:GLN:O	1:A:445:ILE:HG12	2.21	0.41
1:B:382:ALA:HB1	1:B:442:VAL:HG11	2.02	0.41
1:C:104:LEU:HD21	1:C:257:PHE:CZ	2.56	0.41
1:C:331:ALA:O	1:C:332:GLY:C	2.63	0.41
2:D:281:TYR:HB3	2:D:285:LEU:HD12	2.03	0.41
2:D:281:TYR:CD2	2:D:320:PRO:HG2	2.56	0.41
2:E:387:ILE:HG22	2:E:388:ILE:N	2.36	0.41
2:F:80:ALA:HB1	2:F:81:PRO:HD3	2.03	0.41
2:F:445:LEU:HD23	2:F:445:LEU:HA	1.92	0.41
3:G:129:LYS:O	3:G:130:GLU:HB2	2.21	0.41
3:G:181:LEU:C	3:G:183:THR:N	2.78	0.41
1:A:103:LEU:O	1:A:106:ARG:HB2	2.20	0.41
1:B:423:ARG:O	1:B:426:GLU:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:LYS:HG3	1:C:430:GLN:OE1	2.21	0.41
1:C:280:GLN:OE1	2:F:287:THR:HG23	2.20	0.41
2:D:402:LEU:O	2:D:406:ARG:HG3	2.21	0.41
2:F:251:VAL:HG12	2:F:252:LEU:N	2.35	0.41
1:A:408:SER:O	1:A:409:ASP:HB2	2.21	0.41
1:A:420:ARG:HA	1:A:420:ARG:HD3	1.78	0.41
1:A:498:LYS:O	1:A:502:THR:HG23	2.21	0.41
1:B:44:LEU:HB3	1:B:47:VAL:CG2	2.47	0.41
1:B:103:LEU:O	1:B:104:LEU:C	2.63	0.41
1:B:138:PRO:HB2	1:B:312:MET:HE1	2.03	0.41
1:B:221:THR:HG22	1:B:222:ASP:N	2.36	0.41
1:B:423:ARG:NE	1:B:458:PRO:HD3	2.35	0.41
2:D:256:ASP:HA	2:D:257:ASN:HA	1.87	0.41
2:E:82:ILE:CG2	2:E:116:ILE:HD13	2.51	0.41
2:E:97:VAL:HG13	2:E:232:VAL:HG13	2.03	0.41
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.48	0.41
2:E:167:MET:SD	2:E:200:MET:HA	2.61	0.41
2:E:296:ILE:HD13	2:E:306:SER:HB2	2.02	0.41
2:E:360:PRO:HD3	2:E:368:TYR:CG	2.56	0.41
2:E:397:SER:O	2:E:399:GLU:N	2.54	0.41
3:G:73:SER:O	3:G:111:LYS:HB2	2.21	0.41
3:G:120:HIS:HB3	3:G:123:GLN:HB2	2.03	0.41
1:A:32:LEU:HD21	1:A:42:HIS:HB2	2.03	0.41
1:A:347:ASP:C	1:A:373:ARG:HH11	2.28	0.41
1:A:485:THR:O	1:A:487:GLY:N	2.54	0.41
1:B:201:CYS:O	1:B:229:THR:HA	2.21	0.41
1:B:206:ILE:HA	1:B:234:ALA:O	2.21	0.41
1:B:452:TYR:CD2	1:B:501:VAL:HG21	2.56	0.41
2:D:38:VAL:HG22	2:D:75:VAL:HG22	2.02	0.41
2:D:97:VAL:HG11	2:D:231:ARG:HB2	2.03	0.41
2:D:210:ASP:CG	2:D:212:THR:HG23	2.46	0.41
2:E:430:LYS:HA	2:E:430:LYS:HD3	1.97	0.41
3:G:19:ILE:CG2	3:G:23:MET:HE2	2.34	0.41
3:G:184:ILE:C	3:G:186:SER:N	2.72	0.41
1:A:74:VAL:CG1	1:A:241:PRO:HG3	2.51	0.40
1:A:400:VAL:O	1:A:401:ALA:C	2.64	0.40
1:C:44:LEU:HD23	1:C:44:LEU:HA	1.92	0.40
1:C:442:VAL:HG11	1:C:489:ILE:HD11	2.01	0.40
1:C:465:GLU:O	1:C:465:GLU:HG2	2.21	0.40
1:C:465:GLU:O	1:C:469:LEU:HB2	2.21	0.40
2:D:203:SER:OG	2:D:205:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:231:ARG:O	2:E:234:LEU:N	2.50	0.40
3:G:87:LYS:HA	3:G:90:LYS:HE2	2.02	0.40
1:A:129:VAL:HG12	1:A:249:SER:HA	2.03	0.40
1:B:187:LYS:HE3	1:B:227:LYS:NZ	2.37	0.40
1:B:297:ASP:OD1	1:B:297:ASP:N	2.52	0.40
1:C:206:ILE:C	1:C:208:GLN:H	2.29	0.40
1:C:390:MET:HE2	1:C:428:LEU:HD11	2.02	0.40
2:E:227:GLY:O	2:E:231:ARG:HG2	2.21	0.40
2:E:439:LYS:O	2:E:442:GLN:HB3	2.22	0.40
3:G:179:PHE:O	3:G:180:SER:C	2.64	0.40
1:A:69:ASP:O	1:A:70:ASN:HB3	2.21	0.40
1:A:292:GLU:HB2	1:A:294:TYR:HD2	1.86	0.40
1:A:383:MET:HG3	1:A:387:ALA:HB2	2.02	0.40
1:B:30:ARG:HA	1:B:86:ASP:O	2.21	0.40
1:B:209:LYS:HG2	2:E:294:GLU:OE2	2.21	0.40
1:B:239:ALA:HB1	1:B:241:PRO:HD2	2.03	0.40
1:B:300:TYR:O	1:B:301:LEU:C	2.64	0.40
1:B:336:ALA:HB3	1:B:339:PRO:HD2	2.02	0.40
1:B:382:ALA:O	1:B:385:GLN:HB2	2.22	0.40
1:B:423:ARG:HH21	1:B:458:PRO:HD3	1.86	0.40
1:C:30:ARG:HG2	1:C:87:ILE:HD12	2.04	0.40
1:C:342:VAL:HA	1:C:345:ILE:HD12	2.03	0.40
2:E:329:LEU:O	2:E:356:ARG:CZ	2.70	0.40
2:E:366:GLU:O	2:E:367:HIS:C	2.63	0.40
2:F:200:MET:HE2	2:F:205:VAL:CG2	2.51	0.40
3:G:2:THR:HG22	3:G:4:LYS:H	1.86	0.40
1:C:142:VAL:C	1:C:143:ARG:HG3	2.46	0.40
1:C:469:LEU:HD12	1:C:469:LEU:HA	1.96	0.40
2:D:13:ILE:HD12	2:D:73:GLN:HB3	2.03	0.40
2:D:406:ARG:HH11	2:D:406:ARG:HD2	1.60	0.40
2:D:449:TYR:C	2:D:451:HIS:N	2.78	0.40
2:E:413:PHE:HE2	2:E:440:GLY:HA3	1.87	0.40
2:D:360:PRO:HD3	2:D:368:TYR:CD2	2.56	0.40
2:E:84:ILE:HD13	2:E:235:THR:HG23	2.03	0.40
2:F:94:ILE:CG2	2:F:102:ILE:HD11	2.50	0.40
2:F:442:GLN:O	2:F:445:LEU:HB2	2.20	0.40
3:G:115:ILE:O	3:G:117:HIS:N	2.54	0.40

All (55) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:GLY:O	1:C:20:ASP:OD2[4_555]	0.43	1.77
1:B:314:ASP:N	1:C:21:THR:C[4_555]	0.83	1.37
1:B:318:GLY:N	1:C:22:SER:OG[4_555]	0.92	1.28
1:B:313:ASN:O	1:C:22:SER:CA[4_555]	0.99	1.21
1:B:314:ASP:O	1:C:22:SER:O[4_555]	1.06	1.14
1:B:313:ASN:O	1:C:22:SER:CB[4_555]	1.08	1.12
1:B:124:LYS:NZ	2:F:31:PRO:CB[4_555]	1.10	1.10
1:B:311:LYS:NZ	1:C:20:ASP:CB[4_555]	1.14	1.06
1:B:314:ASP:O	1:C:22:SER:C[4_555]	1.18	1.02
1:B:314:ASP:CA	1:C:21:THR:C[4_555]	1.23	0.97
1:B:314:ASP:CA	1:C:21:THR:O[4_555]	1.26	0.94
1:B:314:ASP:N	1:C:21:THR:O[4_555]	1.28	0.92
1:B:318:GLY:CA	1:C:20:ASP:OD1[4_555]	1.29	0.91
1:B:314:ASP:N	1:C:22:SER:N[4_555]	1.30	0.90
1:B:317:GLY:CA	1:C:23:VAL:CG2[4_555]	1.31	0.89
1:B:318:GLY:O	1:C:20:ASP:CG[4_555]	1.31	0.89
1:B:318:GLY:C	1:C:20:ASP:OD2[4_555]	1.47	0.73
1:B:314:ASP:OD1	1:C:21:THR:CA[4_555]	1.49	0.71
1:B:313:ASN:C	1:C:22:SER:N[4_555]	1.50	0.70
1:B:143:ARG:CG	1:C:19:ALA:N[4_555]	1.52	0.68
1:B:314:ASP:CB	1:C:21:THR:O[4_555]	1.53	0.67
1:B:314:ASP:CG	1:C:21:THR:CA[4_555]	1.59	0.61
1:B:313:ASN:C	1:C:22:SER:CA[4_555]	1.60	0.60
1:B:314:ASP:CA	1:C:22:SER:N[4_555]	1.60	0.60
1:B:314:ASP:C	1:C:22:SER:C[4_555]	1.69	0.51
1:B:311:LYS:NZ	1:C:20:ASP:CA[4_555]	1.76	0.44
1:A:510:ALA:CB	1:C:508:PHE:CD1[3_444]	1.83	0.37
1:B:311:LYS:NZ	1:C:20:ASP:CG[4_555]	1.84	0.36
1:B:314:ASP:O	1:C:23:VAL:N[4_555]	1.84	0.36
1:B:314:ASP:CB	1:C:21:THR:C[4_555]	1.84	0.36
1:B:318:GLY:C	1:C:20:ASP:CG[4_555]	1.85	0.35
1:B:318:GLY:CA	1:C:22:SER:OG[4_555]	1.88	0.32
1:B:317:GLY:C	1:C:23:VAL:CG2[4_555]	1.89	0.31
1:B:313:ASN:O	1:C:22:SER:N[4_555]	1.90	0.30
1:B:317:GLY:N	1:C:22:SER:O[4_555]	1.94	0.26
1:B:314:ASP:C	1:C:22:SER:O[4_555]	1.97	0.23
1:B:316:PHE:N	1:C:22:SER:O[4_555]	1.98	0.22
1:B:314:ASP:CA	1:C:22:SER:CA[4_555]	1.99	0.21
1:B:318:GLY:C	1:C:20:ASP:OD1[4_555]	2.00	0.20
1:B:314:ASP:N	1:C:22:SER:CA[4_555]	2.02	0.18
1:B:313:ASN:C	1:C:21:THR:C[4_555]	2.04	0.16
1:B:317:GLY:O	1:C:23:VAL:CG2[4_555]	2.04	0.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:ALA:O	1:C:508:PHE:CE1[3_444]	2.05	0.15
1:B:314:ASP:C	1:C:22:SER:CA[4_555]	2.05	0.15
1:B:317:GLY:C	1:C:22:SER:OG[4_555]	2.05	0.15
1:B:318:GLY:N	1:C:22:SER:CB[4_555]	2.06	0.14
1:B:318:GLY:CA	1:C:20:ASP:CG[4_555]	2.07	0.13
1:B:314:ASP:OD1	1:C:20:ASP:O[4_555]	2.09	0.11
1:B:314:ASP:CG	1:C:21:THR:C[4_555]	2.11	0.09
1:B:317:GLY:N	1:C:22:SER:C[4_555]	2.11	0.09
1:B:124:LYS:CE	2:F:31:PRO:CB[4_555]	2.13	0.07
1:B:314:ASP:C	1:C:21:THR:O[4_555]	2.14	0.06
1:B:314:ASP:N	1:C:21:THR:CA[4_555]	2.15	0.05
1:A:507:GLY:CA	1:C:504:PHE:O[3_444]	2.17	0.03
1:B:314:ASP:OD1	1:C:21:THR:C[4_555]	2.19	0.01

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	485/553 (88%)	443 (91%)	35 (7%)	7 (1%)	9	39
1	B	475/553 (86%)	427 (90%)	41 (9%)	7 (2%)	8	38
1	C	490/553 (89%)	444 (91%)	38 (8%)	8 (2%)	7	37
2	D	465/528 (88%)	419 (90%)	43 (9%)	3 (1%)	21	57
2	E	464/528 (88%)	407 (88%)	47 (10%)	10 (2%)	5	31
2	F	464/528 (88%)	433 (93%)	29 (6%)	2 (0%)	30	65
3	G	257/298 (86%)	223 (87%)	26 (10%)	8 (3%)	3	25
4	H	21/168 (12%)	21 (100%)	0	0	100	100
5	I	24/51 (47%)	20 (83%)	2 (8%)	2 (8%)	0	11
All	All	3145/3760 (84%)	2837 (90%)	261 (8%)	47 (2%)	8	38

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	407	GLY
2	E	393	MET
1	A	57	SER
1	A	405	GLN
1	A	409	ASP
1	B	364	ALA
1	C	332	GLY
1	C	408	SER
1	C	411	ASP
1	C	476	HIS
2	D	28	GLY
2	E	161	GLY
2	E	205	VAL
3	G	51	LEU
3	G	56	ASP
1	A	364	ALA
1	A	404	ALA
1	B	236	ALA
1	B	452	TYR
2	E	121	PRO
2	E	455	GLN
3	G	72	SER
3	G	180	SER
1	B	411	ASP
1	C	405	GLN
1	C	475	GLN
2	D	474	ALA
2	E	122	GLU
2	F	327	ALA
3	G	122	ASP
5	I	40	SER
1	A	484	ARG
1	B	359	LYS
1	C	409	ASP
2	E	33	LEU
3	G	116	LEU
3	G	179	PHE
3	G	185	SER
5	I	42	ILE
1	B	458	PRO
2	E	28	GLY
2	E	243	PHE
2	E	279	VAL

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Mol	Chain	Res	Type
1	B	68	PRO
2	F	279	VAL
2	D	279	VAL
1	A	246	ALA

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	393/444 (88%)	343 (87%)	50 (13%)	4	20
1	B	388/444 (87%)	335 (86%)	53 (14%)	3	17
1	C	397/444 (89%)	359 (90%)	38 (10%)	8	28
2	D	377/417 (90%)	344 (91%)	33 (9%)	9	32
2	E	376/417 (90%)	336 (89%)	40 (11%)	6	24
2	F	376/417 (90%)	343 (91%)	33 (9%)	9	32
3	G	225/251 (90%)	208 (92%)	17 (8%)	12	36
4	H	27/128 (21%)	26 (96%)	1 (4%)	30	52
5	I	23/42 (55%)	21 (91%)	2 (9%)	9	32
All	All	2582/3004 (86%)	2315 (90%)	267 (10%)	7	25

All (267) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	40	ARG
1	A	45	ARG
1	A	47	VAL
1	A	48	GLN
1	A	50	GLU
1	A	56	SER
1	A	80	LYS
1	A	94	ILE
1	A	99	VAL

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Mol	Chain	Res	Type
1	A	101	GLU
1	A	102	GLU
1	A	121	ILE
1	A	140	ILE
1	A	142	VAL
1	A	143	ARG
1	A	151	LYS
1	A	173	THR
1	A	188	ARG
1	A	193	THR
1	A	195	GLU
1	A	211	SER
1	A	219	ARG
1	A	256	TYR
1	A	270	ASP
1	A	344	SER
1	A	367	VAL
1	A	371	VAL
1	A	380	THR
1	A	386	VAL
1	A	393	GLU
1	A	409	ASP
1	A	410	LEU
1	A	417	LEU
1	A	420	ARG
1	A	430	GLN
1	A	436	MET
1	A	442	VAL
1	A	444	VAL
1	A	449	VAL
1	A	457	GLU
1	A	461	ILE
1	A	472	VAL
1	A	473	ILE
1	A	474	SER
1	A	479	LEU
1	A	485	THR
1	A	489	ILE
1	A	497	LEU
1	A	499	GLU
1	B	38	ILE
1	B	47	VAL

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Mol	Chain	Res	Type
1	B	60	LYS
1	B	79	ASP
1	B	80	LYS
1	B	87	ILE
1	B	99	VAL
1	B	102	GLU
1	B	121	ILE
1	B	123	SER
1	B	141	SER
1	B	143	ARG
1	B	173	THR
1	B	186	GLN
1	B	188	ARG
1	B	193	THR
1	B	211	SER
1	B	216	LEU
1	B	217	VAL
1	B	218	LYS
1	B	221	THR
1	B	227	LYS
1	B	233	SER
1	B	270	ASP
1	B	298	VAL
1	B	327	ILE
1	B	334	VAL
1	B	335	SER
1	B	349	GLN
1	B	351	PHE
1	B	361	ILE
1	B	371	VAL
1	B	374	VAL
1	B	376	SER
1	B	380	THR
1	B	381	ARG
1	B	398	ARG
1	B	399	GLU
1	B	400	VAL
1	B	416	GLN
1	B	423	ARG
1	B	430	GLN
1	B	442	VAL
1	B	444	VAL

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Mol	Chain	Res	Type
1	B	454	ASP
1	B	472	VAL
1	B	474	SER
1	B	479	LEU
1	B	482	LYS
1	B	484	ARG
1	B	485	THR
1	B	490	SER
1	B	505	LEU
1	C	45	ARG
1	C	47	VAL
1	C	56	SER
1	C	63	SER
1	C	64	LEU
1	C	74	VAL
1	C	87	ILE
1	C	91	THR
1	C	99	VAL
1	C	101	GLU
1	C	164	ARG
1	C	184	ILE
1	C	195	GLU
1	C	208	GLN
1	C	216	LEU
1	C	217	VAL
1	C	227	LYS
1	C	267	ILE
1	C	270	ASP
1	C	282	SER
1	C	298	VAL
1	C	334	VAL
1	C	338	ILE
1	C	339	PRO
1	C	349	GLN
1	C	399	GLU
1	C	400	VAL
1	C	406	PHE
1	C	440	GLU
1	C	444	VAL
1	C	469	LEU
1	C	474	SER
1	C	477	GLN

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Mol	Chain	Res	Type
1	C	479	LEU
1	C	485	THR
1	C	501	VAL
1	C	502	THR
1	C	505	LEU
2	D	27	GLU
2	D	37	GLU
2	D	56	SER
2	D	67	GLU
2	D	89	GLU
2	D	95	MET
2	D	97	VAL
2	D	112	GLN
2	D	137	ILE
2	D	139	VAL
2	D	166	ILE
2	D	199	GLU
2	D	205	VAL
2	D	223	ASN
2	D	232	VAL
2	D	249	GLN
2	D	258	ILE
2	D	266	SER
2	D	279	VAL
2	D	282	GLN
2	D	306	SER
2	D	336	SER
2	D	361	ASN
2	D	365	SER
2	D	388	ILE
2	D	397	SER
2	D	401	LYS
2	D	423	VAL
2	D	428	LEU
2	D	431	LEU
2	D	439	LYS
2	D	452	LEU
2	D	475	GLU
2	E	9	THR
2	E	67	GLU
2	E	89	GLU
2	E	95	MET

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Mol	Chain	Res	Type
2	E	97	VAL
2	E	119	GLU
2	E	127	SER
2	E	128	VAL
2	E	132	ILE
2	E	133	LEU
2	E	139	VAL
2	E	142	LEU
2	E	148	LYS
2	E	164	VAL
2	E	182	VAL
2	E	188	GLU
2	E	194	ASN
2	E	213	SER
2	E	215	VAL
2	E	223	ASN
2	E	257	ASN
2	E	282	GLN
2	E	293	GLN
2	E	297	THR
2	E	333	THR
2	E	358	MET
2	E	365	SER
2	E	385	GLN
2	E	387	ILE
2	E	391	LEU
2	E	393	MET
2	E	394	ASP
2	E	395	GLU
2	E	402	LEU
2	E	412	ARG
2	E	431	LEU
2	E	438	ILE
2	E	452	LEU
2	E	463	ILE
2	E	473	LEU
2	F	10	THR
2	F	27	GLU
2	F	36	LEU
2	F	42	GLU
2	F	67	GLU
2	F	89	GLU

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Mol	Chain	Res	Type
2	F	95	MET
2	F	97	VAL
2	F	112	GLN
2	F	137	ILE
2	F	139	VAL
2	F	166	ILE
2	F	191	ARG
2	F	200	MET
2	F	201	ILE
2	F	210	ASP
2	F	223	ASN
2	F	232	VAL
2	F	279	VAL
2	F	292	MET
2	F	357	ILE
2	F	386	ASP
2	F	387	ILE
2	F	393	MET
2	F	397	SER
2	F	405	SER
2	F	410	ILE
2	F	423	VAL
2	F	428	LEU
2	F	435	LYS
2	F	438	ILE
2	F	455	GLN
2	F	467	VAL
3	G	20	THR
3	G	35	GLU
3	G	59	THR
3	G	67	LEU
3	G	108	VAL
3	G	113	ARG
3	G	118	ARG
3	G	125	LEU
3	G	126	VAL
3	G	130	GLU
3	G	180	SER
3	G	184	ILE
3	G	190	MET
3	G	205	GLN
3	G	212	ILE

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Mol	Chain	Res	Type
3	G	213	ILE
3	G	262	LEU
4	H	91	GLN
5	I	41	THR
5	I	42	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	396	GLN
1	A	476	HIS
1	B	42	HIS
1	B	330	GLN
1	B	415	GLN
1	B	466	ASN
1	C	48	GLN
1	C	208	GLN
1	C	215	GLN
1	C	260	ASN
1	C	396	GLN
1	C	416	GLN
1	C	432	GLN
2	D	24	GLN
2	D	130	GLN
2	D	171	ASN
2	D	221	GLN
2	D	223	ASN
2	D	282	GLN
2	D	328	HIS
2	D	411	GLN
2	D	442	GLN
2	D	455	GLN
2	E	130	GLN
2	E	223	ASN
2	E	246	GLN
2	E	282	GLN
2	E	367	HIS
2	F	51	GLN
2	F	96	ASN
2	F	194	ASN
2	F	198	HIS
2	F	221	GLN

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Mol	Chain	Res	Type
2	F	223	ASN
2	F	282	GLN
2	F	293	GLN
2	F	308	GLN
2	F	361	ASN
2	F	443	GLN
3	G	82	HIS
3	G	88	GLN
3	G	234	ASN
4	H	91	GLN
5	I	16	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	487/553 (88%)	0.28	10 (2%) 63 47	20, 20, 20, 20	0
1	B	479/553 (86%)	0.13	4 (0%) 82 65	20, 20, 20, 20	0
1	C	492/553 (88%)	0.31	10 (2%) 65 48	20, 20, 20, 20	0
2	D	467/528 (88%)	0.24	2 (0%) 88 75	20, 20, 20, 20	0
2	E	466/528 (88%)	0.04	0 100 100	20, 20, 20, 20	0
2	F	466/528 (88%)	0.19	10 (2%) 63 47	20, 20, 20, 20	0
3	G	263/298 (88%)	0.26	4 (1%) 72 54	20, 20, 20, 20	0
4	H	31/168 (18%)	0.17	0 100 100	20, 20, 20, 20	0
5	I	28/51 (54%)	0.33	0 100 100	20, 20, 20, 20	0
All	All	3179/3760 (84%)	0.21	40 (1%) 75 57	20, 20, 20, 20	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	21	THR	5.1
1	C	23	VAL	5.0
1	C	19	ALA	4.9
1	A	510	ALA	4.7
1	C	20	ASP	4.3
1	C	122	GLY	3.7
1	A	412	ALA	3.6
1	B	314	ASP	3.5
2	F	220	GLY	3.3
1	A	504	PHE	3.3
2	F	360	PRO	3.3
1	C	22	SER	3.1
1	A	497	LEU	3.0
1	A	503	ASN	3.0
2	F	227	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	309	ALA	2.8
2	F	305	THR	2.8
1	C	24	ASP	2.8
1	A	501	VAL	2.7
2	D	9	THR	2.6
2	F	283	PRO	2.5
1	A	473	ILE	2.5
1	C	461	ILE	2.5
1	B	448	GLY	2.3
2	F	228	ALA	2.3
3	G	35	GLU	2.3
1	A	446	TYR	2.3
2	F	72	GLY	2.3
1	C	510	ALA	2.2
2	F	472	LYS	2.2
2	D	309	ALA	2.2
1	A	490	SER	2.2
1	B	313	ASN	2.2
3	G	17	GLN	2.1
1	C	471	HIS	2.1
1	B	254	GLY	2.1
3	G	93	ALA	2.1
2	F	473	LEU	2.0
3	G	149	LEU	2.0
1	A	500	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.