



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:07 PM UTC

PDB ID : 2W6H / pdb_00002w6h
Title : Low resolution structures of bovine mitochondrial F1-ATPase during controlled dehydration: Hydration State 4A.
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 : 5.00 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:

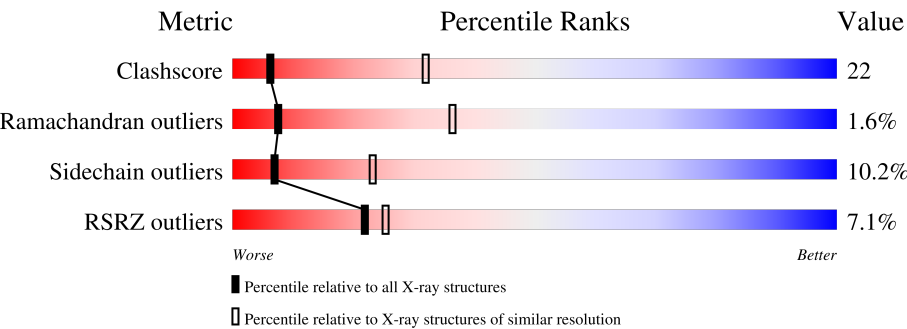
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 5.00 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))
Clashscore	190562	1040 (6.00-4.00)
Ramachandran outliers	187476	1015 (6.06-3.92)
Sidechain outliers	187428	1136 (6.10-3.90)
RSRZ outliers	180081	1004 (6.02-3.98)

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	
1	B	553	
1	C	553	
2	D	528	
2	E	528	
2	F	528	
3	G	298	

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Mol	Chain	Length	Quality of chain
4	H	168	7% 38% 35% 5% 22%
5	I	51	4% 53% 29% 8% • 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25108 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 ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	131	Total	C	N	O	S	0	0	0
			970	609	164	195	2			

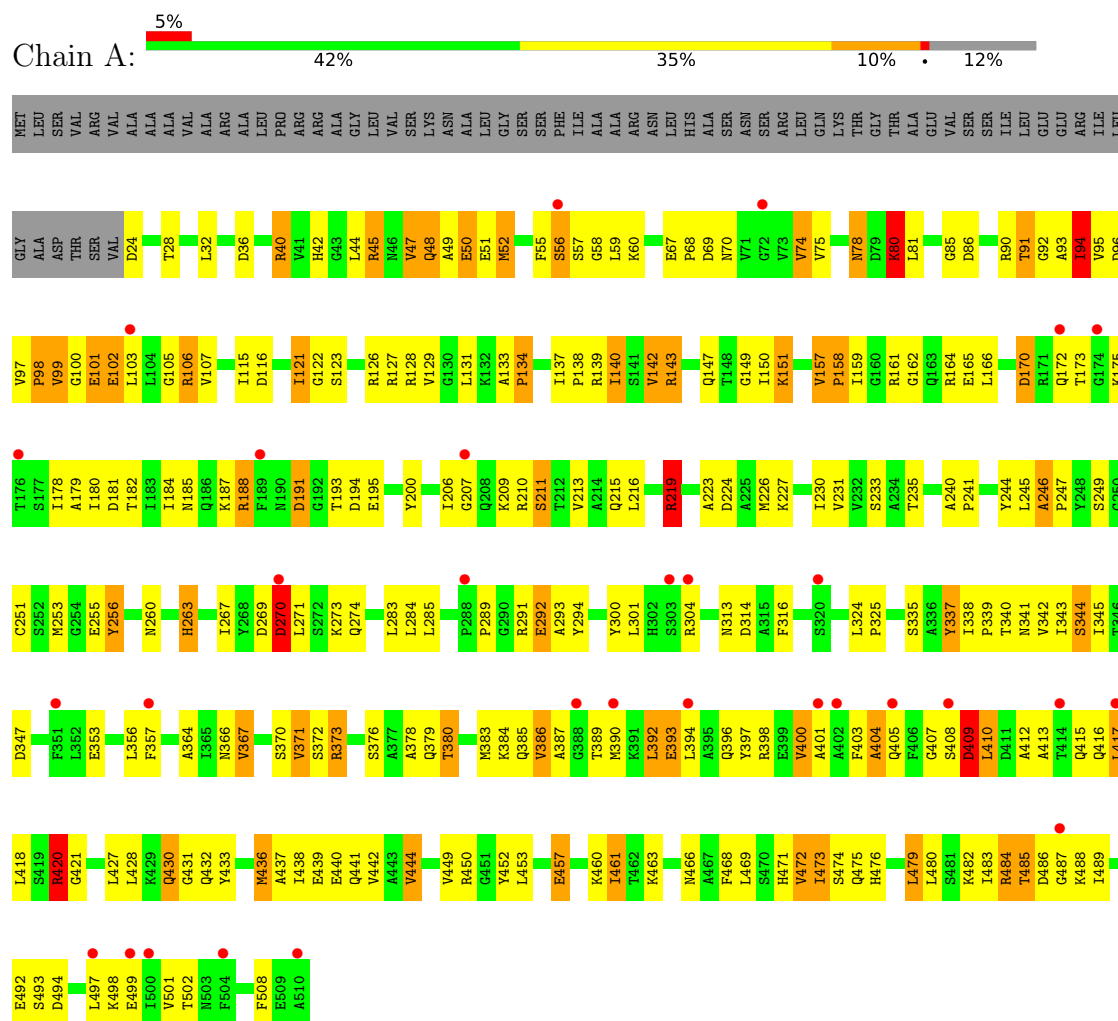
- Molecule 5 is a protein called ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	47	Total 369	C 237	N 66	O 64	S 2	0	0	0

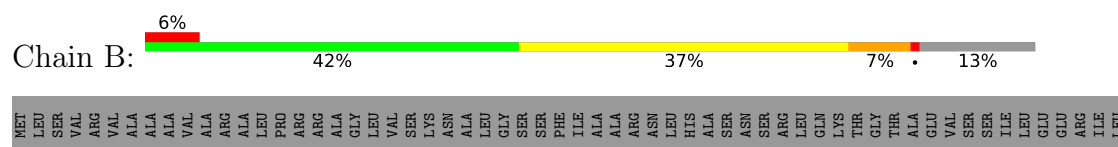
3 Residue-property plots

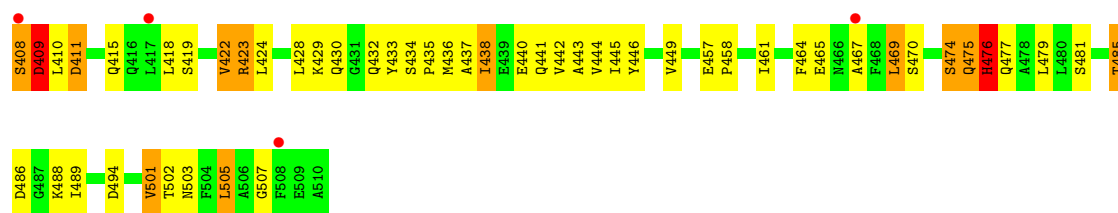
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

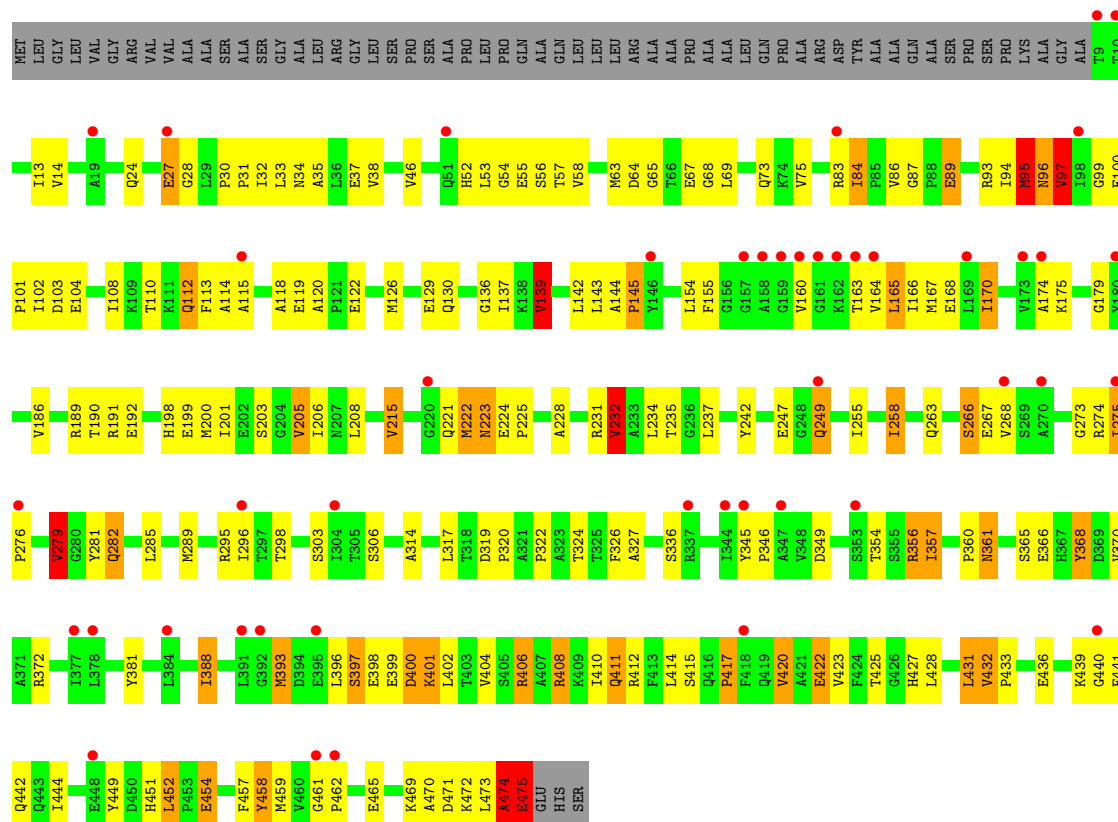


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL

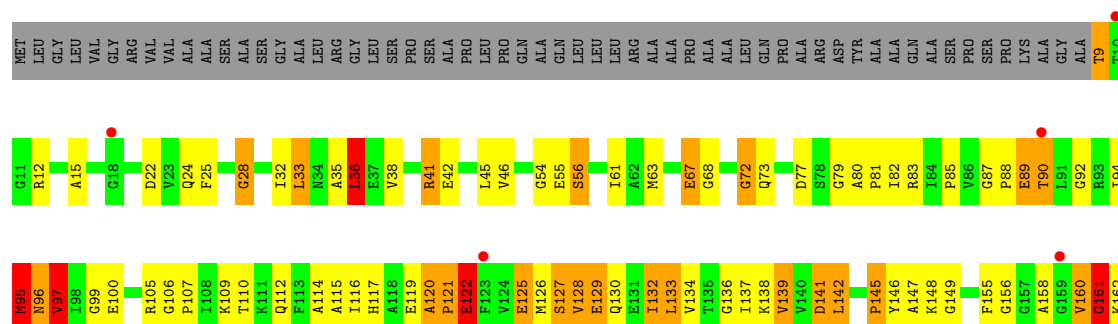


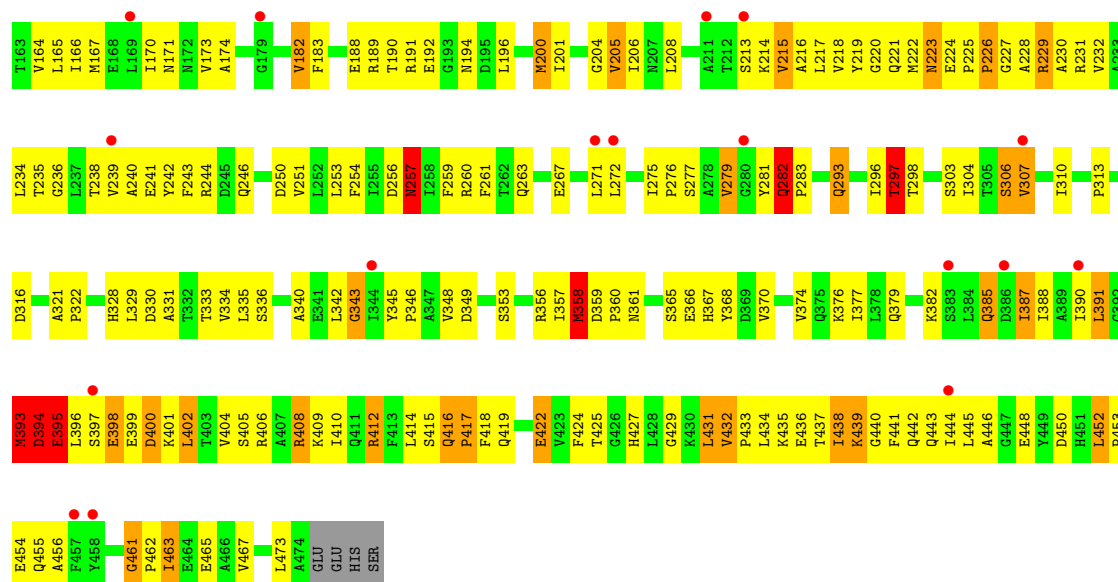


- Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

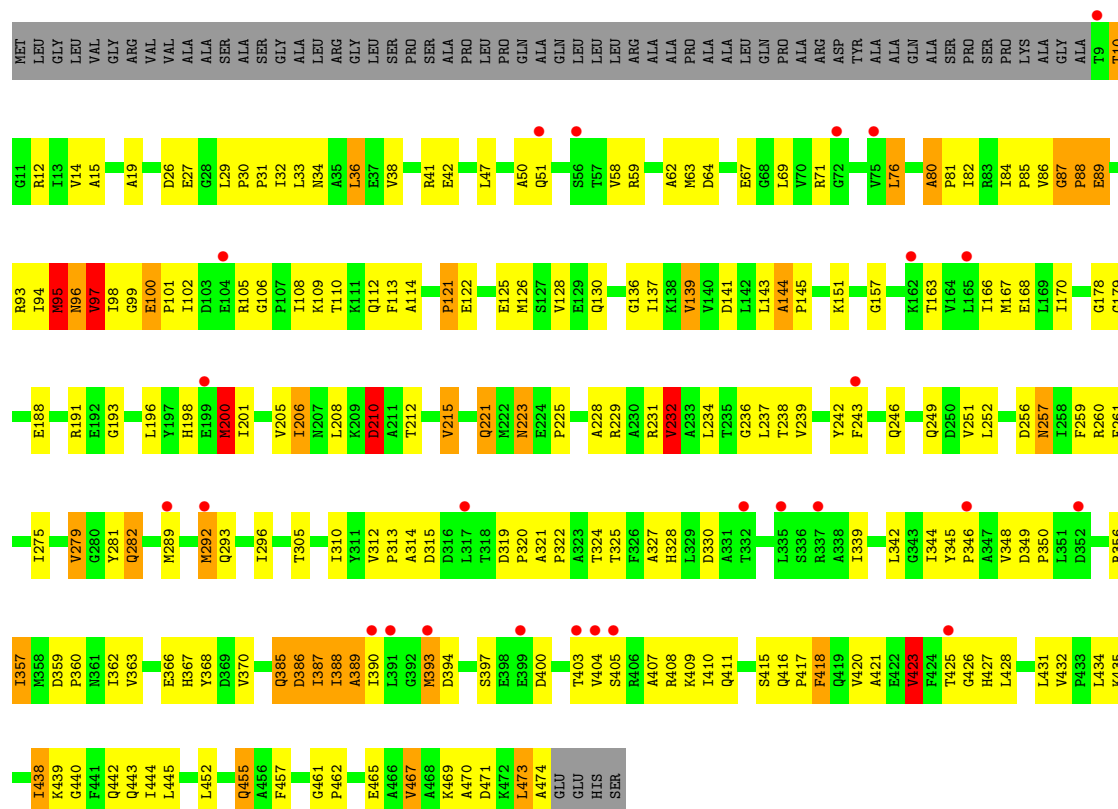


- Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



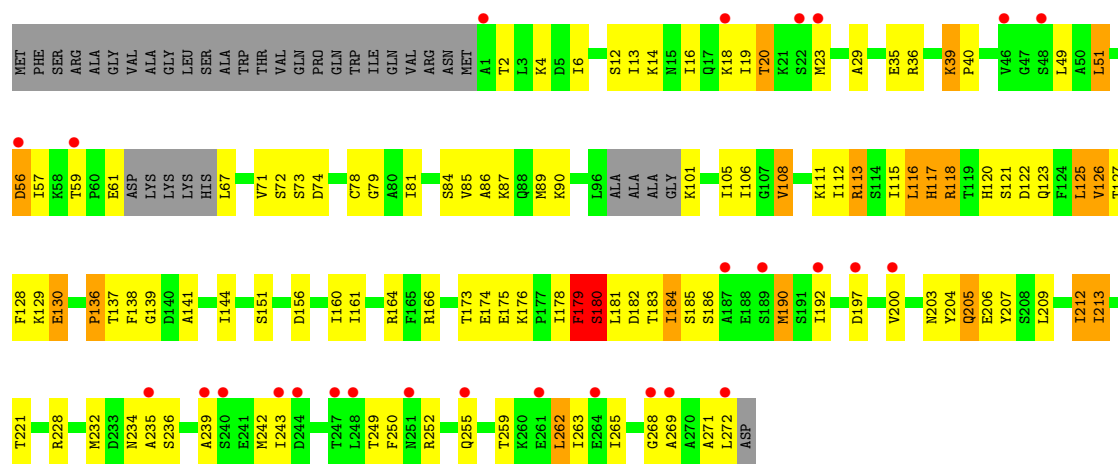


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL





• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL



• 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	107.90Å 140.24Å 268.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.14 – 5.00 62.14 – 5.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.14-5.00) 97.1 (62.14-5.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 5.11Å)	Xtriage
Refinement program	REFMAC 5.5.0038	Depositor
R, R_{free}	0.296 , (Not available) 0.305 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	88.5	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 82.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	25108	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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	64/5080 (1.3%)
1	B	0.77	0/3704	1.76	66/4995 (1.3%)
1	C	0.80	0/3799	1.80	74/5126 (1.4%)
2	D	0.81	1/3596 (0.0%)	1.78	72/4879 (1.5%)
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	6/2785 (0.2%)
4	H	0.41	0/982	0.98	2/1337 (0.1%)
5	I	0.44	0/374	0.96	0/501
All	All	0.75	2/25469 (0.0%)	1.69	466/34437 (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	5.44	1.62	1.53
2	D	96	ASN	CA-CB	5.25	1.61	1.53

All (466) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	408	ARG	CD-NE-CZ	22.76	156.26	124.40
2	F	282	GLN	CB-CG-CD	15.19	138.42	112.60
2	E	408	ARG	CD-NE-CZ	13.39	143.15	124.40
1	B	351	PHE	CA-CB-CG	11.07	124.87	113.80
1	A	270	ASP	CA-CB-CG	10.99	123.59	112.60
2	F	139	VAL	CB-CA-C	-10.87	97.96	111.88
1	B	270	ASP	CA-CB-CG	10.55	123.15	112.60
1	B	375	GLY	N-CA-C	9.83	125.48	114.67
1	B	40	ARG	CD-NE-CZ	9.30	137.42	124.40
2	F	97	VAL	CB-CA-C	-9.12	99.83	112.14
2	D	96	ASN	CA-CB-CG	-8.68	103.92	112.60
2	D	95	MET	CA-C-N	8.67	138.40	122.02
2	D	95	MET	C-N-CA	8.67	138.40	122.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	139	VAL	CB-CA-C	-8.62	100.67	111.70
1	C	503	ASN	CA-CB-CG	-8.51	104.09	112.60
2	E	307	VAL	N-CA-CB	8.45	121.97	111.41
1	C	113	ASN	CA-CB-CG	-8.45	104.15	112.60
2	F	96	ASN	CB-CA-C	-8.26	93.30	110.40
2	F	427	HIS	CA-CB-CG	8.19	121.99	113.80
1	A	269	ASP	CA-C-N	8.11	136.29	121.70
1	A	269	ASP	C-N-CA	8.11	136.29	121.70
1	C	74	VAL	N-CA-CB	-8.04	101.96	110.72
2	F	95	MET	CA-C-N	8.00	138.58	121.45
2	F	95	MET	C-N-CA	8.00	138.58	121.45
1	C	476	HIS	N-CA-C	7.90	127.63	110.80
1	A	123	SER	N-CA-C	7.87	121.29	109.25
2	D	474	ALA	CA-C-N	7.79	135.72	121.70
2	D	474	ALA	C-N-CA	7.79	135.72	121.70
2	D	349	ASP	CA-C-N	7.76	127.48	119.56
2	D	349	ASP	C-N-CA	7.76	127.48	119.56
1	C	409	ASP	CA-CB-CG	7.72	120.32	112.60
1	B	270	ASP	CB-CA-C	-7.61	95.64	110.10
2	E	349	ASP	CA-C-O	7.58	124.22	119.29
2	F	221	GLN	N-CA-C	7.56	120.79	110.35
2	E	95	MET	CA-C-O	7.51	129.90	121.11
1	B	475	GLN	N-CA-C	7.46	119.49	111.36
1	A	91	THR	N-CA-C	-7.41	104.77	113.88
2	F	95	MET	CA-CB-CG	7.36	128.82	114.10
2	E	276	PRO	CA-C-O	-7.35	112.68	122.08
1	A	270	ASP	CB-CA-C	-7.33	96.17	110.10
1	C	429	LYS	CA-C-O	-7.32	113.37	121.87
2	D	417	PRO	N-CA-CB	7.30	107.01	102.92
1	A	170	ASP	CA-CB-CG	7.26	119.86	112.60
1	A	392	LEU	N-CA-C	7.22	119.23	111.36
1	B	53	VAL	CA-C-O	-7.19	114.33	121.67
1	B	309	ALA	N-CA-C	-7.18	99.65	110.28
1	C	501	VAL	N-CA-CB	7.17	118.44	110.62
2	D	393	MET	N-CA-C	7.17	122.20	113.38
2	E	395	GLU	N-CA-C	-7.13	104.71	113.19
3	G	179	PHE	CA-CB-CG	7.11	120.91	113.80
2	E	343	GLY	N-CA-C	-7.10	106.64	115.08
2	F	256	ASP	CA-CB-CG	7.09	119.69	112.60
2	E	129	GLU	N-CA-C	7.08	120.20	109.23
2	D	249	GLN	N-CA-C	7.04	119.61	110.53
2	F	232	VAL	CB-CA-C	-7.03	101.79	112.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	97	VAL	CB-CA-C	-7.02	102.53	112.22
1	A	260	ASN	CA-CB-CG	-7.01	105.59	112.60
1	A	431	GLY	N-CA-C	-6.99	101.59	112.85
1	A	210	ARG	CA-C-O	-6.99	112.20	120.10
1	B	219	ARG	NE-CZ-NH2	6.98	125.48	119.20
2	D	406	ARG	NE-CZ-NH1	-6.98	114.52	121.50
2	E	160	VAL	N-CA-C	-6.98	98.53	108.58
1	C	476	HIS	CA-CB-CG	-6.93	106.87	113.80
1	B	349	GLN	CA-CB-CG	6.92	127.93	114.10
2	F	312	VAL	CA-C-N	6.92	127.30	119.83
2	F	312	VAL	C-N-CA	6.92	127.30	119.83
2	F	59	ARG	NE-CZ-NH1	-6.89	114.61	121.50
2	E	261	PHE	CA-C-N	6.88	129.38	120.44
2	E	261	PHE	C-N-CA	6.88	129.38	120.44
1	A	149	GLY	N-CA-C	-6.87	105.59	115.27
2	F	179	GLY	N-CA-C	-6.87	103.73	111.63
2	E	95	MET	CA-CB-CG	6.84	127.77	114.10
1	A	476	HIS	N-CA-C	6.83	121.54	112.25
2	E	22	ASP	CA-CB-CG	6.81	119.41	112.60
2	E	306	SER	N-CA-C	6.76	119.96	109.07
1	A	314	ASP	CA-CB-CG	-6.75	105.86	112.60
2	D	96	ASN	CB-CA-C	-6.68	97.08	111.78
2	E	342	LEU	N-CA-C	-6.68	105.12	113.20
2	D	101	PRO	N-CA-CB	6.68	109.16	103.35
1	C	149	GLY	N-CA-C	-6.66	105.41	115.00
2	D	400	ASP	CA-CB-CG	6.66	119.26	112.60
1	B	209	LYS	CA-C-O	-6.66	113.41	120.80
2	E	87	GLY	CA-C-N	6.65	126.43	119.05
2	E	87	GLY	C-N-CA	6.65	126.43	119.05
2	F	349	ASP	CA-C-N	6.63	126.26	119.56
2	F	349	ASP	C-N-CA	6.63	126.26	119.56
1	A	285	LEU	CA-C-O	6.63	127.30	119.28
2	F	385	GLN	N-CA-C	6.62	120.22	111.75
1	B	258	ARG	CD-NE-CZ	6.61	133.66	124.40
2	E	141	ASP	CA-CB-CG	6.60	119.20	112.60
4	H	69	ASP	N-CA-C	6.57	118.54	109.54
1	C	328	GLU	CB-CG-CD	-6.57	101.44	112.60
2	E	41	ARG	CD-NE-CZ	6.57	133.59	124.40
1	C	215	GLN	OE1-CD-NE2	6.56	129.16	122.60
2	E	156	GLY	N-CA-C	-6.55	104.55	112.48
1	C	164	ARG	CD-NE-CZ	-6.55	115.24	124.40
1	A	80	LYS	N-CA-C	-6.53	104.34	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	313	PRO	N-CA-CB	6.53	109.14	103.27
1	C	47	VAL	CB-CA-C	-6.51	104.16	111.45
1	C	235	THR	N-CA-C	6.51	118.92	110.53
2	E	432	VAL	CA-C-N	6.50	127.03	120.14
2	E	432	VAL	C-N-CA	6.50	127.03	120.14
2	E	394	ASP	CA-CB-CG	-6.50	106.10	112.60
1	A	78	ASN	CA-CB-CG	6.50	119.09	112.60
1	A	172	GLN	N-CA-CB	-6.48	102.36	111.62
2	E	394	ASP	N-CA-C	6.47	123.77	114.39
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
2	F	275	ILE	N-CA-C	-6.44	102.64	108.95
2	D	420	VAL	N-CA-CB	-6.44	103.95	112.26
2	D	113	PHE	CA-CB-CG	-6.42	107.38	113.80
2	F	143	LEU	N-CA-C	6.42	121.31	112.90
2	F	225	PRO	CA-C-N	6.41	127.85	119.84
2	F	225	PRO	C-N-CA	6.41	127.85	119.84
1	A	230	ILE	CA-C-N	-6.40	114.58	123.10
1	A	230	ILE	C-N-CA	-6.40	114.58	123.10
1	B	279	ARG	CD-NE-CZ	6.38	133.33	124.40
2	D	84	ILE	N-CA-C	6.37	114.91	107.84
2	F	193	GLY	N-CA-C	-6.37	105.11	112.50
2	D	144	ALA	CA-C-N	6.37	126.39	119.90
2	D	144	ALA	C-N-CA	6.37	126.39	119.90
2	D	221	GLN	N-CA-C	6.35	118.22	110.41
1	A	157	VAL	CA-C-N	6.34	126.71	119.93
1	A	157	VAL	C-N-CA	6.34	126.71	119.93
2	F	26	ASP	CA-CB-CG	-6.34	106.26	112.60
2	F	59	ARG	NE-CZ-NH2	6.32	124.89	119.20
1	C	288	PRO	N-CA-CB	6.29	109.18	103.08
1	A	337	TYR	CA-C-N	6.28	124.20	120.24
1	A	337	TYR	C-N-CA	6.28	124.20	120.24
1	B	299	PHE	N-CA-C	-6.28	104.52	111.36
2	F	403	THR	N-CA-C	-6.27	104.37	111.14
1	A	231	VAL	CA-C-N	-6.27	115.03	122.93
1	A	231	VAL	C-N-CA	-6.27	115.03	122.93
1	C	291	ARG	NE-CZ-NH2	-6.26	113.56	119.20
1	A	371	VAL	CB-CA-C	-6.26	99.22	110.48
2	F	64	ASP	CA-C-O	-6.24	114.78	121.45
1	C	70	ASN	CA-C-O	-6.23	114.77	121.38
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(°)
2	E	416	GLN	CA-C-N	6.21	127.15	120.13
2	E	416	GLN	C-N-CA	6.21	127.15	120.13
2	E	145	PRO	N-CA-CB	6.20	108.77	103.19
1	A	158	PRO	N-CA-CB	6.19	108.76	103.19
1	B	93	ALA	N-CA-C	6.17	118.46	108.41
1	A	292	GLU	CB-CG-CD	6.16	123.07	112.60
2	E	225	PRO	N-CA-CB	6.15	109.05	103.08
4	H	39	PRO	N-CA-CB	6.15	107.35	103.23
1	B	142	VAL	N-CA-CB	6.15	118.37	110.13
2	D	422	GLU	N-CA-C	-6.13	104.71	111.82
2	D	120	ALA	CA-C-N	6.12	126.14	119.90
2	D	120	ALA	C-N-CA	6.12	126.14	119.90
2	E	106	GLY	CA-C-N	6.12	126.06	119.76
2	E	106	GLY	C-N-CA	6.12	126.06	119.76
2	E	94	ILE	N-CA-CB	6.10	119.55	111.25
2	E	90	THR	N-CA-C	-6.09	105.98	113.41
1	B	374	VAL	N-CA-C	6.08	120.06	113.43
1	B	287	ARG	CB-CA-C	6.08	118.19	109.26
1	B	210	ARG	N-CA-CB	6.07	118.82	110.01
1	A	94	ILE	CB-CA-C	6.06	119.87	111.38
2	F	144	ALA	CA-C-N	6.06	126.08	119.90
2	F	144	ALA	C-N-CA	6.06	126.08	119.90
2	D	139	VAL	N-CA-CB	6.06	116.98	110.62
2	F	432	VAL	CB-CA-C	-6.06	104.11	110.53
2	E	422	GLU	N-CA-C	-6.04	105.94	113.55
1	A	162	GLY	N-CA-C	-6.02	106.78	114.37
1	C	507	GLY	N-CA-C	-6.02	105.50	112.73
1	A	67	GLU	CA-C-N	6.01	125.49	119.24
1	A	67	GLU	C-N-CA	6.01	125.49	119.24
1	C	405	GLN	CA-C-N	6.00	133.01	121.54
1	C	405	GLN	C-N-CA	6.00	133.01	121.54
1	C	157	VAL	CA-C-N	6.00	126.02	119.90
1	C	157	VAL	C-N-CA	6.00	126.02	119.90
1	C	400	VAL	N-CA-CB	6.00	117.97	110.47
1	C	45	ARG	N-CA-C	6.00	118.61	111.71
2	F	261	PHE	CA-C-O	5.99	126.90	120.55
2	F	80	ALA	CA-C-N	5.98	126.17	120.31
2	F	80	ALA	C-N-CA	5.98	126.17	120.31
2	F	229	ARG	NE-CZ-NH1	-5.98	115.52	121.50
1	C	162	GLY	N-CA-C	-5.97	107.15	114.92
1	B	167	ILE	N-CA-CB	5.97	118.19	111.21
1	B	423	ARG	CD-NE-CZ	5.97	132.76	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	341	ASN	CA-C-O	-5.97	114.52	120.90
2	F	342	LEU	N-CA-C	-5.97	105.96	113.18
1	B	371	VAL	CB-CA-C	-5.96	99.75	110.48
1	C	336	ALA	O-C-N	-5.96	115.97	123.12
2	F	96	ASN	N-CA-CB	-5.96	101.92	110.44
2	D	247	GLU	N-CA-C	-5.96	106.65	114.04
1	A	373	ARG	NE-CZ-NH2	5.95	124.56	119.20
1	B	91	THR	N-CA-C	-5.95	105.36	114.16
2	D	402	LEU	N-CA-C	-5.95	105.11	112.90
2	F	206	ILE	N-CA-CB	5.94	118.94	111.46
2	F	388	ILE	CB-CA-C	-5.93	104.27	112.04
1	A	98	PRO	N-CA-CB	5.91	108.94	103.39
1	C	422	VAL	CB-CA-C	-5.91	104.16	112.14
1	B	162	GLY	N-CA-C	-5.91	106.83	115.63
1	A	106	ARG	CD-NE-CZ	5.90	132.66	124.40
2	F	221	GLN	CA-C-N	5.89	130.12	120.63
2	F	221	GLN	C-N-CA	5.89	130.12	120.63
1	A	75	VAL	N-CA-C	5.89	116.66	109.30
2	D	143	LEU	N-CA-C	5.89	120.59	113.41
1	C	109	ASP	CA-CB-CG	5.89	118.49	112.60
2	F	236	GLY	N-CA-C	-5.89	105.67	112.73
2	E	461	GLY	CA-C-N	5.88	125.79	119.85
2	E	461	GLY	C-N-CA	5.88	125.79	119.85
1	C	379	GLN	N-CA-C	5.87	119.04	109.59
1	C	91	THR	N-CA-C	-5.86	107.11	114.56
1	C	69	ASP	CA-CB-CG	-5.86	106.74	112.60
1	B	477	GLN	CA-C-N	5.85	128.12	120.28
1	B	477	GLN	C-N-CA	5.85	128.12	120.28
1	C	406	PHE	CA-CB-CG	5.85	119.65	113.80
2	F	461	GLY	CA-C-N	5.85	126.18	119.92
2	F	461	GLY	C-N-CA	5.85	126.18	119.92
1	C	46	ASN	CA-CB-CG	5.84	118.44	112.60
2	F	370	VAL	N-CA-C	-5.84	105.04	110.53
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	45	ARG	CB-CG-CD	-5.83	97.90	111.30
1	B	351	PHE	N-CA-CB	5.82	119.91	110.42
2	F	210	ASP	CB-CA-C	-5.82	100.36	111.48
2	F	426	GLY	N-CA-C	-5.82	107.21	115.30
1	C	241	PRO	N-CA-CB	5.80	109.66	103.39
2	E	349	ASP	CA-C-N	5.80	125.90	119.87
2	E	349	ASP	C-N-CA	5.80	125.90	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	ASP	CA-CB-CG	5.79	118.39	112.60
1	B	136	ILE	CA-C-N	5.79	124.96	120.33
1	B	136	ILE	C-N-CA	5.79	124.96	120.33
1	C	100	GLY	N-CA-C	5.78	117.92	112.08
2	D	454	GLU	CA-CB-CG	5.77	125.64	114.10
1	C	341	ASN	O-C-N	5.76	128.08	122.09
1	B	79	ASP	CA-CB-CG	5.75	118.35	112.60
2	E	229	ARG	N-CA-C	-5.75	106.11	113.01
1	A	370	SER	CA-C-O	-5.73	115.04	121.81
1	B	304	ARG	NE-CZ-NH1	-5.73	115.77	121.50
2	D	96	ASN	N-CA-CB	-5.73	101.73	110.49
2	F	157	GLY	CA-C-O	-5.71	115.50	122.75
2	F	389	ALA	N-CA-C	5.70	118.27	111.71
1	A	194	ASP	CA-CB-CG	5.70	118.30	112.60
2	D	163	THR	N-CA-C	5.70	117.49	111.28
2	D	368	TYR	N-CA-C	5.69	117.48	111.28
1	C	303	SER	CA-C-N	5.69	129.35	120.82
1	C	303	SER	C-N-CA	5.69	129.35	120.82
2	F	113	PHE	CA-CB-CG	-5.68	108.12	113.80
1	A	335	SER	CB-CA-C	-5.68	99.79	110.01
2	E	133	LEU	CA-C-O	-5.68	114.28	120.36
2	F	229	ARG	NE-CZ-NH2	5.67	124.31	119.20
2	E	36	LEU	CA-C-O	-5.67	114.75	121.16
2	E	97	VAL	CB-CA-C	-5.66	102.93	112.16
1	B	245	LEU	N-CA-C	5.66	117.12	111.07
1	C	230	ILE	CA-C-N	-5.66	115.30	123.11
1	C	230	ILE	C-N-CA	-5.66	115.30	123.11
2	D	225	PRO	N-CA-CB	5.65	106.16	103.22
1	B	127	ARG	CD-NE-CZ	5.65	132.31	124.40
1	C	362	ARG	NE-CZ-NH2	5.65	124.29	119.20
2	D	145	PRO	N-CA-CB	5.64	108.22	103.25
2	D	356	ARG	CD-NE-CZ	-5.64	116.50	124.40
2	F	84	ILE	N-CA-C	5.63	113.81	109.19
2	D	145	PRO	CA-C-O	-5.63	115.00	121.36
1	A	420	ARG	NE-CZ-NH1	-5.63	115.87	121.50
1	B	103	LEU	N-CA-C	-5.62	106.55	113.41
1	B	304	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	C	120	PRO	N-CA-CB	5.62	108.67	103.39
1	C	381	ARG	CD-NE-CZ	5.61	132.25	124.40
1	B	433	TYR	CA-C-N	-5.60	116.37	122.59
1	B	433	TYR	C-N-CA	-5.60	116.37	122.59
1	A	200	TYR	CA-CB-CG	-5.58	103.85	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	95	MET	O-C-N	-5.58	116.42	123.17
1	A	164	ARG	CA-C-O	-5.58	113.54	120.57
1	B	151	LYS	N-CA-C	5.58	117.81	111.11
2	E	95	MET	CA-C-N	5.58	132.19	121.54
2	E	95	MET	C-N-CA	5.58	132.19	121.54
2	D	30	PRO	N-CA-CB	5.57	108.49	103.08
2	D	225	PRO	CA-C-N	5.57	126.81	119.84
2	D	225	PRO	C-N-CA	5.57	126.81	119.84
2	E	120	ALA	CA-C-N	5.57	126.81	119.84
2	E	120	ALA	C-N-CA	5.57	126.81	119.84
2	E	336	SER	N-CA-C	5.56	117.96	108.90
1	A	367	VAL	CB-CA-C	5.54	119.62	112.14
1	A	263	HIS	CA-CB-CG	-5.54	108.26	113.80
2	E	216	ALA	CA-C-N	-5.53	115.36	123.00
2	E	216	ALA	C-N-CA	-5.53	115.36	123.00
1	C	74	VAL	CB-CA-C	5.53	117.77	110.91
1	C	366	ASN	CA-C-O	5.53	126.67	120.92
2	E	219	TYR	N-CA-C	5.53	118.41	109.40
2	D	164	VAL	N-CA-C	-5.53	105.11	110.42
1	A	235	THR	N-CA-C	5.52	118.59	110.59
1	A	271	LEU	CA-C-O	5.52	125.72	119.27
2	F	473	LEU	N-CA-C	-5.51	106.05	112.89
2	E	96	ASN	CA-CB-CG	5.51	118.11	112.60
1	A	92	GLY	N-CA-C	-5.51	108.42	115.42
1	B	141	SER	CA-C-O	-5.51	114.95	120.96
2	F	96	ASN	N-CA-C	5.51	117.64	110.53
2	E	260	ARG	NE-CZ-NH1	-5.48	116.02	121.50
2	D	215	VAL	CA-C-O	-5.47	113.94	120.78
2	E	127	SER	N-CA-C	-5.47	101.63	110.32
1	C	285	LEU	N-CA-C	-5.46	106.39	113.16
1	A	398	ARG	NE-CZ-NH1	-5.46	116.04	121.50
1	C	423	ARG	CD-NE-CZ	5.46	132.04	124.40
2	E	272	LEU	N-CA-C	-5.45	106.94	113.21
2	F	215	VAL	N-CA-C	5.45	115.97	108.12
2	E	83	ARG	NE-CZ-NH1	-5.44	116.06	121.50
2	E	282	GLN	CA-C-N	5.44	125.09	119.05
2	E	282	GLN	C-N-CA	5.44	125.09	119.05
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
2	F	88	PRO	N-CA-CB	5.44	108.73	103.51
2	F	282	GLN	OE1-CD-NE2	-5.43	117.17	122.60
2	D	198	HIS	CA-CB-CG	-5.43	108.37	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	239	VAL	N-CA-CB	-5.43	104.92	110.62
2	D	119	GLU	CA-C-O	-5.43	115.64	121.56
2	D	179	GLY	CA-C-O	-5.42	116.30	121.83
1	A	172	GLN	N-CA-C	5.42	118.67	111.30
1	C	33	SER	CA-C-O	-5.42	115.44	121.23
2	F	408	ARG	NE-CZ-NH2	5.42	124.07	119.20
1	C	106	ARG	CA-CB-CG	-5.41	103.28	114.10
2	F	12	ARG	CD-NE-CZ	-5.41	116.82	124.40
1	C	309	ALA	N-CA-C	-5.41	101.85	109.96
1	A	93	ALA	CA-C-N	-5.40	114.83	122.34
1	A	93	ALA	C-N-CA	-5.40	114.83	122.34
2	E	137	ILE	CA-C-O	5.40	127.00	120.74
2	F	121	PRO	N-CA-CB	5.40	108.00	103.25
1	A	74	VAL	N-CA-CB	-5.39	105.52	111.66
2	E	200	MET	N-CA-C	-5.38	105.08	111.69
1	C	48	GLN	CA-C-O	-5.38	115.09	121.16
2	D	232	VAL	N-CA-CB	5.37	120.09	111.23
2	E	83	ARG	CD-NE-CZ	-5.37	116.88	124.40
1	A	134	PRO	N-CA-C	-5.36	102.78	111.14
2	E	257	ASN	CA-CB-CG	5.36	117.96	112.60
2	E	297	THR	CB-CA-C	-5.36	101.17	111.78
2	F	41	ARG	CG-CD-NE	5.35	123.76	112.00
1	B	478	ALA	N-CA-C	5.35	117.11	111.28
2	E	417	PRO	CB-CA-C	-5.34	104.86	111.11
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
2	D	155	PHE	CA-CB-CG	5.34	119.14	113.80
1	B	40	ARG	NE-CZ-NH1	5.33	126.83	121.50
2	F	366	GLU	N-CA-C	-5.33	105.36	111.07
2	E	393	MET	N-CA-C	5.33	122.16	110.80
2	F	423	VAL	CB-CA-C	-5.33	101.61	111.79
2	D	222	MET	CB-CA-C	-5.33	98.54	110.21
2	E	196	LEU	N-CA-C	-5.33	105.14	111.69
2	E	398	GLU	N-CA-C	-5.33	105.41	112.34
1	B	148	THR	N-CA-C	-5.33	106.91	113.41
2	E	331	ALA	CA-C-O	5.32	128.12	120.51
3	G	39	LYS	CA-C-N	5.32	124.50	118.97
3	G	39	LYS	C-N-CA	5.32	124.50	118.97
1	A	52	MET	CA-C-N	-5.32	115.27	122.92
1	A	52	MET	C-N-CA	-5.32	115.27	122.92
1	C	304	ARG	NE-CZ-NH2	5.32	123.98	119.20
1	C	75	VAL	N-CA-C	5.30	115.73	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	ARG	CA-C-N	5.30	125.84	120.38
1	B	287	ARG	C-N-CA	5.30	125.84	120.38
2	D	322	PRO	N-CA-C	-5.30	105.90	113.47
1	A	372	SER	N-CA-CB	5.29	120.11	110.95
2	F	387	ILE	CB-CA-C	-5.29	105.09	112.02
1	B	259	ASP	CA-CB-CG	-5.29	107.31	112.60
2	F	393	MET	N-CA-C	5.28	119.78	113.23
2	F	76	LEU	N-CA-C	5.28	117.13	108.52
1	C	411	ASP	CA-CB-CG	5.27	117.87	112.60
1	B	318	GLY	N-CA-C	-5.27	108.56	115.47
2	F	330	ASP	CA-CB-CG	-5.27	107.33	112.60
1	C	127	ARG	NE-CZ-NH1	-5.26	116.24	121.50
1	C	299	PHE	N-CA-C	-5.26	105.23	110.97
2	D	327	ALA	CA-C-O	-5.26	113.12	119.49
2	D	411	GLN	CA-C-O	5.26	126.31	120.63
1	B	116	ASP	N-CA-C	-5.26	106.64	113.16
2	E	122	GLU	CA-CB-CG	5.25	124.61	114.10
1	B	149	GLY	N-CA-C	-5.24	108.39	115.21
2	D	268	VAL	CA-C-O	5.24	123.51	118.90
2	F	19	ALA	CA-C-N	-5.24	115.98	123.11
2	F	19	ALA	C-N-CA	-5.24	115.98	123.11
1	C	405	GLN	CA-C-O	5.24	128.00	120.51
2	D	432	VAL	CA-C-N	5.24	125.14	119.85
2	D	432	VAL	C-N-CA	5.24	125.14	119.85
1	B	279	ARG	NE-CZ-NH1	5.22	126.72	121.50
1	C	336	ALA	N-CA-C	5.22	117.65	110.35
2	F	87	GLY	CA-C-N	5.21	124.82	119.56
2	F	87	GLY	C-N-CA	5.21	124.82	119.56
1	B	130	GLY	O-C-N	-5.21	115.93	122.70
1	C	296	GLY	N-CA-C	-5.20	108.95	114.67
2	E	173	VAL	N-CA-C	-5.20	105.33	111.00
2	D	160	VAL	N-CA-CB	5.20	117.93	112.21
2	E	171	ASN	OD1-CG-ND2	5.20	127.80	122.60
2	E	330	ASP	CA-CB-CG	-5.19	107.41	112.60
2	F	200	MET	CA-C-O	5.19	125.92	120.42
2	F	225	PRO	N-CA-C	-5.19	104.37	110.70
2	D	118	ALA	CA-C-O	-5.18	115.68	121.23
1	C	336	ALA	CA-C-O	5.18	126.66	121.07
2	F	418	PHE	CA-CB-CG	5.18	118.98	113.80
2	E	439	LYS	O-C-N	5.17	127.40	122.07
2	D	354	THR	CA-C-O	-5.17	115.56	121.40
2	F	257	ASN	OD1-CG-ND2	5.17	127.77	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	358	MET	N-CA-CB	5.16	116.83	110.53
2	F	59	ARG	CD-NE-CZ	-5.16	117.17	124.40
2	D	165	LEU	N-CA-CB	5.16	117.70	110.12
2	F	200	MET	N-CA-CB	-5.16	102.53	110.16
1	C	136	ILE	CA-C-N	5.16	124.45	120.33
1	C	136	ILE	C-N-CA	5.16	124.45	120.33
2	E	250	ASP	CA-CB-CG	-5.15	107.45	112.60
2	D	224	GLU	CA-C-N	5.14	123.36	119.66
2	D	224	GLU	C-N-CA	5.14	123.36	119.66
2	E	251	VAL	CB-CA-C	-5.13	105.94	111.59
2	D	175	LYS	N-CA-C	5.13	116.87	111.28
1	B	397	TYR	N-CA-C	-5.13	107.57	113.88
2	D	361	ASN	CA-CB-CG	-5.12	107.48	112.60
2	D	475	GLU	N-CA-CB	5.12	119.20	110.50
2	F	178	GLY	CA-C-N	-5.11	114.43	122.92
2	F	178	GLY	C-N-CA	-5.11	114.43	122.92
2	F	281	TYR	CA-C-N	5.11	127.75	120.49
2	F	281	TYR	C-N-CA	5.11	127.75	120.49
2	F	416	GLN	CA-C-N	5.11	125.90	120.13
2	F	416	GLN	C-N-CA	5.11	125.90	120.13
3	G	136	PRO	N-CA-CB	5.11	107.79	103.35
1	A	219	ARG	CD-NE-CZ	5.10	131.55	124.40
1	B	230	ILE	CA-C-O	-5.10	115.95	121.92
2	E	72	GLY	N-CA-C	-5.10	108.62	114.69
2	F	330	ASP	N-CA-C	-5.10	107.19	113.41
1	C	270	ASP	CA-CB-CG	5.10	117.70	112.60
2	D	454	GLU	CB-CA-C	-5.10	102.81	110.92
2	E	56	SER	CA-C-N	-5.10	115.30	122.94
2	E	56	SER	C-N-CA	-5.10	115.30	122.94
2	F	388	ILE	N-CA-CB	5.09	116.83	110.47
2	E	400	ASP	CA-CB-CG	-5.08	107.52	112.60
2	E	125	GLU	CA-C-O	5.08	124.41	118.97
2	E	415	SER	CA-C-O	-5.07	115.95	121.89
1	A	400	VAL	N-CA-C	5.07	119.50	112.35
2	D	357	ILE	N-CA-CB	5.07	119.60	112.15
2	E	107	PRO	N-CA-CB	5.07	107.82	103.31
2	F	101	PRO	N-CA-CB	5.07	107.76	103.35
1	B	349	GLN	N-CA-CB	5.06	120.50	111.69
3	G	117	HIS	CA-CB-CG	-5.06	108.74	113.80
1	B	141	SER	CB-CA-C	-5.06	102.25	109.84
1	B	391	LYS	N-CA-C	-5.06	105.95	111.82
1	B	374	VAL	CB-CA-C	-5.05	104.52	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	219	ARG	NE-CZ-NH1	-5.05	116.45	121.50
1	A	178	ILE	CB-CA-C	-5.05	105.41	111.88
2	E	435	LYS	O-C-N	5.05	127.47	122.12
2	F	198	HIS	CA-CB-CG	-5.05	108.75	113.80
1	B	487	GLY	N-CA-C	-5.04	108.36	115.32
2	F	100	GLU	CA-C-O	-5.04	115.95	120.19
2	F	417	PRO	CB-CA-C	-5.04	105.21	111.11
1	A	101	GLU	N-CA-C	5.04	118.89	112.34
1	C	438	ILE	N-CA-C	5.04	115.65	110.36
1	B	94	ILE	N-CA-C	-5.04	102.57	109.37
1	A	191	ASP	N-CA-C	-5.03	107.19	113.38
3	G	74	ASP	CA-CB-CG	5.03	117.63	112.60
1	B	222	ASP	CA-C-N	-5.03	114.24	122.54
1	B	222	ASP	C-N-CA	-5.03	114.24	122.54
1	C	269	ASP	CA-C-O	-5.03	114.97	120.70
2	F	170	ILE	N-CA-C	-5.03	105.49	110.62
1	C	145	PRO	N-CA-CB	5.03	108.11	103.39
2	E	161	GLY	N-CA-C	5.02	125.08	113.18
2	D	461	GLY	CA-C-N	5.02	124.92	119.85
2	D	461	GLY	C-N-CA	5.02	124.92	119.85
2	D	170	ILE	N-CA-C	-5.01	105.66	110.72
2	D	275	ILE	N-CA-C	-5.01	104.03	108.95
2	E	226	PRO	CA-C-N	5.01	125.64	120.03
2	E	226	PRO	C-N-CA	5.01	125.64	120.03
1	B	457	GLU	N-CA-C	5.01	116.21	109.24
2	E	236	GLY	N-CA-C	-5.01	106.72	112.73
2	F	85	PRO	N-CA-CB	5.01	107.63	103.17
2	D	458	TYR	CA-C-N	5.01	130.39	122.78
2	D	458	TYR	C-N-CA	5.01	130.39	122.78
2	F	293	GLN	CA-C-O	-5.01	115.24	120.55
1	C	209	LYS	N-CA-CB	-5.00	102.72	110.57
1	C	415	GLN	N-CA-C	-5.00	105.93	112.23
1	C	136	ILE	N-CA-C	5.00	115.23	110.53

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	168	0
1	B	3656	0	3764	161	5
1	C	3748	0	3843	164	0
2	D	3539	0	3593	157	0
2	E	3530	0	3587	209	0
2	F	3530	0	3587	131	0
3	G	2051	0	2115	140	0
4	H	970	0	972	62	5
5	I	369	0	395	20	0
All	All	25108	0	25669	1132	5

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 (1132) 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)
2:D:275:ILE:HG23	3:G:269:ALA:HB2	1.25	1.18
1:C:127:ARG:HH12	1:C:255:GLU:HB2	1.00	1.15
1:A:291:ARG:HA	3:G:262:LEU:HD22	1.17	1.14
2:E:391:LEU:HD22	3:G:29:ALA:HB2	1.32	1.11
1:C:215:GLN:HG3	2:F:356:ARG:HH22	1.17	1.09
2:D:274:ARG:C	3:G:272:LEU:HD11	1.78	1.07
2:D:275:ILE:HG23	3:G:269:ALA:CB	1.86	1.05
3:G:90:LYS:HB3	3:G:116:LEU:HD11	1.38	1.04
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	0.99
1:A:215:GLN:HG3	2:D:356:ARG:NH1	1.77	0.99
2:F:223:ASN:HD22	2:F:223:ASN:H	1.08	0.97
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.48	0.95
3:G:19:ILE:HG22	3:G:23:MET:HE2	1.49	0.95
1:A:215:GLN:HG3	2:D:356:ARG:HH12	1.33	0.93
1:A:291:ARG:HA	3:G:262:LEU:CD2	2.00	0.92
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.52	0.92
4:H:62:LEU:HD11	4:H:144:ALA:HB2	1.49	0.91
4:H:85:ASN:HD21	4:H:91:GLN:HE22	1.13	0.91
1:C:127:ARG:NH1	1:C:255:GLU:HB2	1.84	0.91
1:A:291:ARG:CA	3:G:262:LEU:HD22	2.00	0.90
1:C:30:ARG:HE	1:C:87:ILE:HD11	1.37	0.88

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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
2:D:276:PRO:HG3	3:G:268:GLY:HA3	1.54	0.86
2:D:275:ILE:CG2	3:G:269:ALA:HB2	2.04	0.86
2:D:84:ILE:HD12	2:D:95:MET:HE1	1.57	0.86
1:B:456:LEU:HD12	1:B:457:GLU:H	1.42	0.84
1:A:400:VAL:HG12	1:A:418:LEU:HD21	1.60	0.84
3:G:20:THR:HG22	3:G:236:SER:HB3	1.57	0.83
2:F:394:ASP:CG	3:G:79:GLY:HA2	2.04	0.82
2:E:132:ILE:HD12	2:E:145:PRO:HB3	1.61	0.81
3:G:161:ILE:HG12	3:G:175:GLU:HG2	1.63	0.81
3:G:89:MET:HB3	3:G:116:LEU:HD22	1.63	0.80
1:C:215:GLN:HG3	2:F:356:ARG:NH2	1.95	0.79
1:B:141:SER:O	1:B:143:ARG:HD2	1.83	0.79
2:D:139:VAL:HG13	2:D:414:LEU:HD22	1.65	0.79
2:D:282:GLN:H	2:D:282:GLN:HE21	1.30	0.79
2:E:223:ASN:H	2:E:223:ASN:ND2	1.72	0.79
2:D:136:GLY:HA3	2:D:431:LEU:HD13	1.66	0.78
2:F:390:ILE:HD11	3:G:242:MET:CE	2.14	0.78
1:B:186:GLN:HG3	1:B:199:LEU:HB3	1.65	0.78
2:E:370:VAL:HG21	2:E:438:ILE:HG22	1.65	0.78
3:G:89:MET:HE1	3:G:112:ILE:HG23	1.63	0.78
4:H:105:LEU:HD22	4:H:109:LYS:HE3	1.63	0.78
3:G:178:ILE:HG22	3:G:180:SER:HB2	1.65	0.78
2:D:404:VAL:O	2:D:408:ARG:HG3	1.84	0.78
3:G:121:SER:C	3:G:123:GLN:H	1.91	0.77
3:G:137:THR:HG21	5:I:39:GLY:H	1.47	0.77
2:D:53:LEU:HD12	2:D:57:THR:HG22	1.66	0.77
3:G:86:ALA:HA	3:G:89:MET:HE3	1.67	0.77
4:H:138:ASN:HA	4:H:141:LEU:HD12	1.68	0.76
2:E:394:ASP:C	2:E:396:LEU:H	1.93	0.76
1:C:52:MET:HE3	1:C:95:VAL:HG22	1.68	0.76
1:A:392:LEU:HG	1:A:396:GLN:HE21	1.50	0.75
1:B:379:GLN:HB3	1:B:384:LYS:HE2	1.68	0.75
3:G:117:HIS:ND1	3:G:118:ARG:N	2.34	0.75
2:F:390:ILE:HD11	3:G:242:MET:HE1	1.69	0.75
2:E:391:LEU:CD2	3:G:29:ALA:HB2	2.14	0.75
2:D:433:PRO:HG2	2:D:436:GLU:HG2	1.69	0.74
2:F:130:GLN:HB3	2:F:357:ILE:HD11	1.67	0.74
1:C:288:PRO:HB3	3:G:271:ALA:HB3	1.69	0.74
2:E:345:TYR:HA	2:E:346:PRO:C	2.13	0.74
2:E:89:GLU:HG3	2:E:109:LYS:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:223:ASN:H	2:D:223:ASN:HD22	1.34	0.73
2:E:139:VAL:HG13	2:E:414:LEU:HD22	1.71	0.73
2:E:390:ILE:HG22	2:E:391:LEU:HD23	1.70	0.73
3:G:57:ILE:CG2	3:G:184:ILE:HD12	2.19	0.73
4:H:85:ASN:HD21	4:H:91:GLN:NE2	1.87	0.73
2:E:96:ASN:HB3	2:E:100:GLU:H	1.52	0.72
2:D:273:GLY:HA2	3:G:272:LEU:HD22	1.71	0.72
2:F:89:GLU:HG3	2:F:109:LYS:O	1.89	0.72
4:H:34:ARG:HH22	4:H:70:GLY:HA2	1.52	0.72
2:D:274:ARG:O	3:G:272:LEU:HD11	1.89	0.72
2:F:223:ASN:HD22	2:F:223:ASN:N	1.85	0.72
2:E:38:VAL:HG21	2:E:45:LEU:HD23	1.71	0.71
2:E:183:PHE:HB3	2:E:217:LEU:HD22	1.73	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:A:479:LEU:HA	1:A:482:LYS:HE3	1.73	0.71
4:H:84:VAL:HG12	4:H:90:VAL:HG22	1.72	0.71
1:B:180:ILE:HD11	1:B:216:LEU:HD21	1.71	0.70
2:F:394:ASP:CB	3:G:79:GLY:HA2	2.21	0.70
1:A:97:VAL:HA	1:A:126:ARG:HH21	1.56	0.70
1:A:407:GLY:HA2	1:A:410:LEU:HD21	1.73	0.70
2:D:96:ASN:HB2	2:D:100:GLU:H	1.56	0.70
5:I:35:MET:C	5:I:37:THR:H	1.99	0.70
2:E:433:PRO:HD2	2:E:436:GLU:HB2	1.74	0.69
1:C:211:SER:O	1:C:215:GLN:HG2	1.91	0.69
2:D:200:MET:HE3	2:D:215:VAL:HG21	1.74	0.69
2:E:391:LEU:HD22	3:G:29:ALA:CB	2.19	0.69
2:E:105:ARG:CZ	2:E:208:LEU:HD23	2.23	0.69
4:H:133:ILE:HD11	5:I:4:TRP:HB3	1.73	0.69
1:B:452:TYR:OH	1:B:498:LYS:HG3	1.92	0.68
1:C:385:GLN:OE1	1:C:488:LYS:HG2	1.93	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
1:B:283:LEU:HD12	2:E:277:SER:HB3	1.75	0.68
2:D:223:ASN:HD22	2:D:223:ASN:N	1.89	0.68
2:E:321:ALA:HB3	2:E:322:PRO:HD3	1.75	0.68
1:A:44:LEU:O	1:A:47:VAL:HG22	1.94	0.68
1:A:440:GLU:O	1:A:444:VAL:HG13	1.94	0.68
1:B:283:LEU:CD1	2:E:277:SER:HB3	2.24	0.68
4:H:65:VAL:C	4:H:72:THR:HG23	2.19	0.68
1:A:383:MET:HE2	1:A:438:ILE:HD11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:252:LEU:HD23	2:F:305:THR:HB	1.75	0.67
1:B:44:LEU:HB3	1:B:47:VAL:HG22	1.77	0.67
1:C:418:LEU:O	1:C:422:VAL:HG23	1.94	0.67
3:G:137:THR:HG22	3:G:139:GLY:H	1.60	0.67
2:F:80:ALA:HB1	2:F:81:PRO:CD	2.26	0.66
3:G:14:LYS:HG3	3:G:243:ILE:HD12	1.76	0.66
1:B:156:LEU:HD22	1:B:391:LYS:HD2	1.77	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:376:SER:C	1:A:378:ALA:H	2.03	0.66
2:E:313:PRO:HD2	2:E:322:PRO:HG3	1.76	0.66
1:A:347:ASP:OD1	2:E:191:ARG:NH1	2.28	0.66
1:C:99:VAL:HG22	1:C:253:MET:HA	1.78	0.66
3:G:178:ILE:C	3:G:180:SER:H	2.04	0.66
1:A:97:VAL:HB	1:A:98:PRO:HD2	1.76	0.66
1:C:173:THR:HG22	1:C:354:THR:HG22	1.77	0.66
1:C:44:LEU:O	1:C:47:VAL:HG22	1.96	0.65
1:C:59:LEU:HD23	1:C:82:ILE:HD11	1.77	0.65
2:E:359:ASP:OD2	2:E:361:ASN:HB2	1.96	0.65
2:E:136:GLY:HA3	2:E:431:LEU:HD13	1.77	0.65
2:F:136:GLY:HA3	2:F:431:LEU:CD1	2.26	0.65
1:A:211:SER:N	2:D:126:MET:HE2	2.11	0.65
2:D:54:GLY:O	2:D:55:GLU:HB2	1.96	0.65
1:B:362:ARG:HA	1:B:363:PRO:C	2.21	0.65
2:D:200:MET:HB3	2:D:206:ILE:HG13	1.79	0.65
2:F:344:ILE:HG23	2:F:415:SER:HB3	1.79	0.65
2:E:394:ASP:C	2:E:396:LEU:N	2.54	0.65
1:C:362:ARG:HA	1:C:363:PRO:C	2.21	0.65
2:D:167:MET:HB3	2:D:420:VAL:HG11	1.79	0.65
2:F:200:MET:HG3	2:F:205:VAL:CG2	2.27	0.64
2:F:314:ALA:O	2:F:315:ASP:HB2	1.95	0.64
1:A:134:PRO:O	1:A:139:ARG:NH2	2.27	0.64
1:C:188:ARG:HH21	1:C:437:ALA:HB2	1.62	0.64
2:F:394:ASP:HB3	3:G:79:GLY:HA2	1.79	0.64
1:A:471:HIS:CE1	1:A:475:GLN:HG3	2.33	0.64
2:E:139:VAL:CG1	2:E:414:LEU:HD22	2.28	0.64
1:C:344:SER:O	2:D:222:MET:HE1	1.97	0.64
3:G:39:LYS:HB3	3:G:40:PRO:HD3	1.80	0.64
1:A:376:SER:C	1:A:378:ALA:N	2.55	0.64
1:A:376:SER:HB3	1:A:384:LYS:HE2	1.78	0.64
1:C:211:SER:HB3	2:F:126:MET:HE2	1.79	0.64

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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	0.64
1:B:188:ARG:HH21	1:B:437:ALA:HB2	1.62	0.64
1:C:52:MET:HE2	1:C:76:PHE:HE2	1.62	0.64
2:E:346:PRO:HG3	2:E:418:PHE:CZ	2.33	0.64
2:E:400:ASP:O	2:E:404:VAL:HG23	1.98	0.64
4:H:54:THR:N	4:H:84:VAL:HG23	2.13	0.64
1:B:389:THR:HA	1:B:392:LEU:CD1	2.28	0.63
1:C:488:LYS:HG2	1:C:489:ILE:H	1.63	0.63
1:C:202:ILE:HG12	1:C:230:ILE:HD12	1.80	0.63
2:F:200:MET:HG3	2:F:205:VAL:HG23	1.80	0.63
1:A:291:ARG:CA	3:G:262:LEU:CD2	2.70	0.63
2:F:363:VAL:HG23	2:F:367:HIS:HB3	1.81	0.63
1:A:341:ASN:O	1:A:345:ILE:HG13	1.99	0.63
1:B:390:MET:HE1	1:B:428:LEU:HD21	1.80	0.63
1:C:419:SER:O	1:C:423:ARG:HG2	1.98	0.63
2:E:298:THR:HG23	2:E:303:SER:HB3	1.81	0.62
2:E:443:GLN:HG2	2:E:448:GLU:OE2	1.98	0.62
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.34	0.62
2:F:94:ILE:HG22	2:F:102:ILE:HD11	1.80	0.62
1:B:437:ALA:O	1:B:440:GLU:N	2.30	0.62
1:C:436:MET:HE3	1:C:469:LEU:HD21	1.79	0.62
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.34	0.62
2:E:204:GLY:O	2:E:206:ILE:N	2.32	0.62
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.63	0.62
1:C:151:LYS:HE3	1:C:430:GLN:HG3	1.82	0.62
1:C:404:ALA:C	1:C:406:PHE:N	2.44	0.62
2:E:422:GLU:HG2	2:E:427:HIS:O	1.99	0.62
2:E:138:LYS:HE2	2:E:432:VAL:HG21	1.80	0.62
2:E:158:ALA:C	2:E:160:VAL:H	2.08	0.62
3:G:141:ALA:HB1	3:G:213:ILE:HG23	1.81	0.62
2:E:425:THR:O	2:E:427:HIS:ND1	2.20	0.62
5:I:5:ARG:C	5:I:7:ALA:H	2.06	0.62
1:A:394:LEU:HD11	1:A:428:LEU:HD11	1.82	0.61
1:B:422:VAL:O	1:B:426:GLU:HG2	2.00	0.61
1:A:283:LEU:HD21	1:A:289:PRO:HB3	1.82	0.61
1:B:102:GLU:HG3	1:B:122:GLY:O	2.00	0.61
1:C:52:MET:O	1:C:91:THR:HB	1.99	0.61
1:C:292:GLU:O	1:C:293:ALA:HB3	2.00	0.61
2:D:473:LEU:C	2:D:475:GLU:H	2.07	0.61
3:G:184:ILE:C	3:G:186:SER:H	2.08	0.61
2:D:396:LEU:HD22	2:D:400:ASP:CB	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:223:ASN:H	2:F:223:ASN:ND2	1.85	0.61
1:B:184:ILE:HG22	1:B:435:PRO:HG2	1.81	0.61
1:B:218:LYS:HB2	2:E:128:VAL:HG12	1.82	0.61
2:E:201:ILE:HD13	2:E:208:LEU:HD11	1.81	0.61
2:D:274:ARG:C	3:G:272:LEU:CD1	2.65	0.61
2:E:223:ASN:ND2	2:E:223:ASN:N	2.46	0.61
3:G:61:GLU:OE1	3:G:101:LYS:HG2	1.99	0.61
4:H:54:THR:H	4:H:84:VAL:HG23	1.65	0.61
1:A:166:LEU:HA	1:A:325:PRO:HD2	1.83	0.61
2:D:93:ARG:HG3	2:D:93:ARG:HH11	1.66	0.61
1:B:479:LEU:HD11	1:B:497:LEU:HD13	1.83	0.60
1:A:40:ARG:HH11	1:A:40:ARG:HG3	1.66	0.60
2:D:89:GLU:HG2	2:D:110:THR:HG22	1.83	0.60
1:A:457:GLU:CB	1:A:460:LYS:HD3	2.32	0.60
1:B:389:THR:HA	1:B:392:LEU:HD12	1.81	0.60
2:E:92:GLY:N	2:E:215:VAL:O	2.30	0.60
2:E:419:GLN:HG3	2:E:429:GLY:HA3	1.84	0.60
2:F:63:MET:HE1	2:F:97:VAL:HG11	1.82	0.60
1:A:52:MET:O	1:A:91:THR:HG23	2.01	0.60
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.37	0.60
2:E:149:GLY:HA2	2:E:304:ILE:O	2.01	0.60
2:E:397:SER:H	2:E:400:ASP:HB2	1.66	0.60
1:A:270:ASP:OD1	1:A:273:LYS:HG3	2.01	0.60
1:C:99:VAL:HG13	1:C:256:TYR:HB2	1.83	0.60
2:D:63:MET:HE3	2:D:228:ALA:HA	1.83	0.60
1:C:408:SER:O	1:C:409:ASP:C	2.44	0.60
1:C:433:TYR:C	1:C:435:PRO:HD3	2.26	0.60
1:A:121:ILE:HD13	1:A:121:ILE:H	1.66	0.59
1:B:51:GLU:HA	1:B:94:ILE:HA	1.83	0.59
3:G:207:TYR:HA	5:I:12:ILE:HD11	1.84	0.59
1:C:102:GLU:OE2	1:C:123:SER:HA	2.03	0.59
1:B:215:GLN:NE2	2:E:130:GLN:NE2	2.51	0.59
1:A:439:GLU:HG2	1:A:484:ARG:HB2	1.83	0.59
2:E:200:MET:HB3	2:E:205:VAL:HG23	1.84	0.59
1:A:432:GLN:HB3	1:A:433:TYR:CD2	2.37	0.59
1:B:411:ASP:HB3	1:B:414:THR:OG1	2.02	0.59
1:C:374:VAL:HG11	1:C:378:ALA:HB2	1.85	0.59
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.85	0.59
2:D:317:LEU:HD22	2:D:326:PHE:HZ	1.67	0.59
1:B:434:SER:N	1:B:435:PRO:HD3	2.18	0.59
1:C:407:GLY:HA2	1:C:410:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:393:MET:HE3	2:D:404:VAL:HG21	1.83	0.59
2:E:226:PRO:HB3	2:E:267:GLU:HB2	1.84	0.59
1:B:391:LYS:O	1:B:395:ALA:N	2.36	0.59
2:E:397:SER:C	2:E:399:GLU:N	2.57	0.59
1:A:157:VAL:N	1:A:158:PRO:CD	2.65	0.58
1:B:438:ILE:O	1:B:442:VAL:HG22	2.02	0.58
1:C:140:ILE:HD11	1:C:143:ARG:NH2	2.18	0.58
2:F:122:GLU:HB2	2:F:125:GLU:HG3	1.84	0.58
1:B:400:VAL:HB	1:B:418:LEU:HD21	1.85	0.58
1:B:452:TYR:O	1:B:453:LEU:HD23	2.03	0.58
2:D:186:VAL:HG13	2:D:232:VAL:HG23	1.85	0.58
2:F:105:ARG:NH1	2:F:208:LEU:HD23	2.18	0.58
1:B:170:ASP:O	1:B:175:LYS:HE2	2.03	0.58
1:C:405:GLN:C	1:C:406:PHE:HD1	2.11	0.58
1:C:406:PHE:O	1:C:408:SER:N	2.36	0.58
1:C:464:PHE:CE1	1:C:505:LEU:HD23	2.39	0.58
2:E:32:ILE:O	2:E:33:LEU:HB2	2.02	0.58
2:E:138:LYS:O	2:E:142:LEU:HB3	2.04	0.58
1:B:499:GLU:O	1:B:502:THR:HB	2.02	0.58
2:E:408:ARG:O	2:E:412:ARG:HG3	2.03	0.58
3:G:57:ILE:CG2	3:G:184:ILE:CD1	2.81	0.58
4:H:37:ASP:HB2	4:H:64:VAL:HB	1.85	0.58
2:D:263:GLN:O	2:D:267:GLU:HG3	2.03	0.58
2:E:95:MET:CG	2:E:99:GLY:HA2	2.34	0.58
1:C:313:ASN:OD1	1:C:316:PHE:HD1	1.85	0.58
2:E:122:GLU:N	2:E:125:GLU:OE2	2.37	0.58
1:B:352:LEU:HA	1:B:364:ALA:O	2.04	0.58
1:B:358:TYR:C	1:B:360:GLY:H	2.12	0.58
2:E:85:PRO:HD2	2:E:95:MET:HE2	1.85	0.58
2:F:29:LEU:HD12	2:F:30:PRO:HD2	1.85	0.58
2:F:440:GLY:O	2:F:444:ILE:HG13	2.04	0.58
1:A:472:VAL:HG23	1:A:480:LEU:HD11	1.85	0.58
2:E:246:GLN:HA	2:E:246:GLN:NE2	2.19	0.58
2:E:267:GLU:O	2:E:271:LEU:HG	2.04	0.58
2:E:433:PRO:HG2	2:E:436:GLU:HG2	1.86	0.58
2:F:96:ASN:HD22	2:F:100:GLU:HB2	1.68	0.58
3:G:156:ASP:HA	3:G:181:LEU:HD13	1.85	0.57
1:C:107:VAL:HG12	1:C:115:ILE:HD11	1.86	0.57
1:B:180:ILE:O	1:B:181:ASP:C	2.47	0.57
4:H:64:VAL:HG13	4:H:72:THR:HG21	1.85	0.57
1:B:215:GLN:HE22	2:E:130:GLN:NE2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:THR:CG2	1:C:354:THR:HG22	2.35	0.57
2:E:224:GLU:O	2:E:229:ARG:NH1	2.32	0.57
3:G:87:LYS:O	3:G:90:LYS:HG2	2.04	0.57
1:C:184:ILE:HG22	1:C:435:PRO:HG2	1.87	0.57
2:D:431:LEU:C	2:D:431:LEU:HD12	2.29	0.57
4:H:65:VAL:O	4:H:72:THR:HG23	2.05	0.57
1:A:219:ARG:HH11	1:A:219:ARG:HB2	1.69	0.57
1:A:450:ARG:NH2	1:A:494:ASP:OD2	2.38	0.57
1:C:78:ASN:ND2	1:C:80:LYS:HD3	2.19	0.57
2:E:155:PHE:CE1	2:E:310:ILE:HD12	2.40	0.57
4:H:96:GLU:OE2	5:I:23:ARG:NE	2.38	0.57
2:D:273:GLY:HA2	3:G:272:LEU:CD2	2.34	0.57
3:G:57:ILE:HG23	3:G:184:ILE:CD1	2.34	0.57
1:C:156:LEU:HD13	1:C:367:VAL:HG22	1.86	0.57
2:E:105:ARG:NH2	2:E:208:LEU:HA	2.20	0.57
1:A:107:VAL:HG12	1:A:115:ILE:HD11	1.87	0.56
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.86	0.56
1:C:187:LYS:HE2	1:C:191:ASP:OD2	2.05	0.56
1:B:51:GLU:OE2	1:B:90:ARG:HB3	2.05	0.56
1:C:52:MET:HE2	1:C:76:PHE:CE2	2.40	0.56
3:G:57:ILE:HG22	3:G:184:ILE:HD12	1.87	0.56
3:G:164:ARG:NH2	3:G:166:ARG:HD3	2.20	0.56
3:G:180:SER:O	3:G:205:GLN:HG3	2.04	0.56
3:G:209:LEU:O	3:G:213:ILE:HG22	2.05	0.56
1:B:347:ASP:HB3	1:B:374:VAL:HG22	1.88	0.56
1:B:357:PHE:CE1	1:B:362:ARG:HD3	2.40	0.56
2:D:255:ILE:HG21	2:D:258:ILE:HD13	1.87	0.56
1:A:209:LYS:HE3	1:A:211:SER:HB2	1.88	0.56
2:D:473:LEU:C	2:D:475:GLU:N	2.62	0.56
2:F:14:VAL:O	2:F:71:ARG:HG2	2.05	0.56
2:F:98:ILE:HG13	2:F:100:GLU:HG3	1.88	0.56
1:A:99:VAL:CG2	1:A:253:MET:HA	2.36	0.56
1:A:224:ASP:CG	1:A:227:LYS:HE3	2.31	0.56
1:B:62:MET:HE3	1:B:64:LEU:HD13	1.87	0.56
1:B:393:GLU:OE1	1:B:424:LEU:HD11	2.05	0.56
1:C:219:ARG:HD3	1:C:433:TYR:CE1	2.41	0.56
2:D:366:GLU:HG3	2:D:442:GLN:HE22	1.71	0.56
3:G:71:VAL:HG13	3:G:108:VAL:HG22	1.88	0.56
1:B:351:PHE:CE1	1:B:369:LEU:HB3	2.40	0.56
2:E:126:MET:HE1	2:E:297:THR:HG21	1.86	0.56
1:B:80:LYS:HG3	1:B:81:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:ARG:HE	1:B:458:PRO:HD3	1.72	0.55
1:B:423:ARG:HE	1:B:458:PRO:HG3	1.71	0.55
2:F:32:ILE:O	2:F:33:LEU:HB2	2.05	0.55
3:G:181:LEU:HG	3:G:183:THR:HB	1.89	0.55
1:A:291:ARG:N	3:G:262:LEU:HD21	2.21	0.55
2:E:244:ARG:HG3	2:E:303:SER:N	2.22	0.55
2:E:396:LEU:HB3	2:E:401:LYS:HG2	1.88	0.55
2:F:390:ILE:CD1	3:G:242:MET:CE	2.84	0.55
3:G:164:ARG:HD3	3:G:174:GLU:OE2	2.07	0.55
1:A:185:ASN:O	1:A:188:ARG:HG3	2.05	0.55
3:G:160:ILE:CG2	3:G:176:LYS:HB2	2.37	0.55
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.89	0.55
1:C:442:VAL:CG1	1:C:489:ILE:HD11	2.37	0.55
2:F:10:THR:HG23	2:F:76:LEU:HD12	1.88	0.55
2:F:63:MET:CE	2:F:97:VAL:HG11	2.36	0.55
4:H:22:SER:HB2	4:H:23:PRO:HD2	1.89	0.55
2:E:138:LYS:HG3	2:E:416:GLN:OE1	2.06	0.55
3:G:137:THR:HG21	5:I:39:GLY:N	2.19	0.55
1:C:404:ALA:O	1:C:406:PHE:N	2.37	0.55
2:D:471:ASP:O	2:D:474:ALA:N	2.39	0.55
2:F:324:THR:O	2:F:324:THR:HG22	2.05	0.55
1:A:207:GLY:HA3	1:A:273:LYS:HD3	1.89	0.55
3:G:117:HIS:CE1	3:G:121:SER:HB2	2.42	0.55
1:A:159:ILE:HD12	1:A:165:GLU:HG2	1.88	0.55
2:D:142:LEU:HD22	2:D:441:PHE:CD2	2.42	0.55
3:G:121:SER:C	3:G:123:GLN:N	2.60	0.55
3:G:181:LEU:HB3	3:G:184:ILE:HG22	1.89	0.55
1:C:394:LEU:HD22	1:C:398:ARG:HH21	1.71	0.55
2:E:174:ALA:CB	2:E:214:LYS:HD3	2.35	0.55
2:E:263:GLN:O	2:E:267:GLU:HG3	2.07	0.55
2:E:77:ASP:OD1	2:E:79:GLY:N	2.34	0.54
3:G:207:TYR:HA	5:I:12:ILE:CD1	2.37	0.54
1:A:100:GLY:HA2	1:A:256:TYR:CE1	2.42	0.54
1:B:441:GLN:O	1:B:445:ILE:HG12	2.08	0.54
1:C:52:MET:HG3	1:C:61:GLY:O	2.07	0.54
2:D:83:ARG:HA	2:D:114:ALA:O	2.07	0.54
2:D:87:GLY:HA2	2:D:242:TYR:CE2	2.42	0.54
2:E:397:SER:O	2:E:401:LYS:HG3	2.07	0.54
1:A:161:ARG:HH11	1:A:263:HIS:CG	2.25	0.54
1:A:457:GLU:HB3	1:A:460:LYS:HD3	1.89	0.54
1:B:114:ALA:HB2	1:B:121:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:396:LEU:HD22	2:D:400:ASP:HB3	1.89	0.54
1:A:479:LEU:HD21	1:A:493:SER:HB3	1.89	0.54
1:B:270:ASP:OD1	1:B:273:LYS:HG3	2.07	0.54
2:D:388:ILE:HD12	2:D:393:MET:SD	2.48	0.54
2:D:451:HIS:CD2	2:D:452:LEU:HD23	2.42	0.54
3:G:117:HIS:O	3:G:120:HIS:N	2.35	0.54
1:B:479:LEU:HA	1:B:482:LYS:HE3	1.89	0.54
2:D:473:LEU:O	2:D:475:GLU:N	2.40	0.54
1:C:102:GLU:HG2	1:C:122:GLY:O	2.06	0.54
2:D:282:GLN:H	2:D:282:GLN:NE2	2.01	0.54
1:A:373:ARG:HG3	1:A:373:ARG:HH11	1.72	0.54
2:D:275:ILE:CG2	3:G:269:ALA:CB	2.72	0.54
2:E:395:GLU:HG3	3:G:36:ARG:HH22	1.72	0.54
3:G:181:LEU:O	3:G:184:ILE:HG22	2.08	0.54
2:D:122:GLU:OE1	2:D:122:GLU:HA	2.07	0.54
5:I:28:THR:O	5:I:29:GLU:HB2	2.08	0.54
2:D:412:ARG:HH11	2:D:412:ARG:HG3	1.73	0.54
1:B:446:TYR:CD2	1:B:497:LEU:HD23	2.43	0.53
2:E:174:ALA:HB2	2:E:214:LYS:HD3	1.89	0.53
2:F:96:ASN:HB2	2:F:100:GLU:H	1.73	0.53
3:G:137:THR:HG22	3:G:138:PHE:N	2.24	0.53
3:G:144:ILE:HD13	3:G:213:ILE:HD11	1.90	0.53
3:G:249:THR:HA	3:G:252:ARG:NH1	2.24	0.53
2:F:292:MET:CE	2:F:296:ILE:HD11	2.38	0.53
1:A:245:LEU:O	1:A:246:ALA:C	2.51	0.53
1:A:452:TYR:OH	1:A:498:LYS:HG3	2.08	0.53
2:D:84:ILE:CD1	2:D:95:MET:HE1	2.34	0.53
3:G:117:HIS:ND1	3:G:118:ARG:HA	2.22	0.53
1:A:403:PHE:HE1	3:G:18:LYS:HB3	1.73	0.53
1:C:270:ASP:OD1	1:C:273:LYS:HG3	2.09	0.53
1:A:463:LYS:HD3	1:A:508:PHE:HZ	1.73	0.53
1:C:91:THR:HG22	1:C:93:ALA:H	1.72	0.53
2:D:167:MET:CB	2:D:420:VAL:HG11	2.38	0.53
2:E:81:PRO:HG2	2:E:115:ALA:HB1	1.91	0.53
2:E:201:ILE:CD1	2:E:208:LEU:HD11	2.37	0.53
2:F:210:ASP:HB2	2:F:212:THR:HG23	1.91	0.53
4:H:16:MET:HE2	4:H:18:PHE:HB2	1.91	0.53
2:D:422:GLU:HG2	2:D:427:HIS:O	2.09	0.53
2:F:439:LYS:HE3	2:F:443:GLN:HE22	1.73	0.53
3:G:39:LYS:HB3	3:G:40:PRO:CD	2.38	0.53
3:G:179:PHE:C	3:G:181:LEU:N	2.66	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ALA:HB1	1:A:267:ILE:HG12	1.91	0.53
1:B:69:ASP:O	1:B:70:ASN:HB3	2.08	0.53
1:C:156:LEU:HD11	1:C:428:LEU:HD13	1.91	0.53
1:C:239:ALA:HB1	1:C:241:PRO:HD2	1.90	0.53
1:C:390:MET:HE3	1:C:424:LEU:HD22	1.89	0.53
2:D:381:TYR:HE2	2:D:411:GLN:HE22	1.56	0.53
1:A:150:ILE:HA	1:A:430:GLN:OE1	2.08	0.53
1:B:456:LEU:HD12	1:B:457:GLU:N	2.20	0.53
2:D:96:ASN:CB	2:D:100:GLU:H	2.22	0.53
1:A:170:ASP:O	1:A:175:LYS:HE2	2.08	0.53
1:B:44:LEU:O	1:B:47:VAL:HG22	2.09	0.53
2:D:31:PRO:HD2	2:D:34:ASN:ND2	2.24	0.53
1:A:468:PHE:CE1	1:A:501:VAL:HG12	2.43	0.52
2:D:356:ARG:O	2:D:356:ARG:HG2	2.09	0.52
3:G:117:HIS:ND1	3:G:117:HIS:C	2.67	0.52
1:B:140:ILE:HG23	1:B:311:LYS:HG3	1.92	0.52
1:B:423:ARG:HD2	1:B:461:ILE:HD11	1.91	0.52
2:D:136:GLY:CA	2:D:431:LEU:HD13	2.37	0.52
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.75	0.52
2:E:254:PHE:CD1	2:E:307:VAL:HB	2.45	0.52
2:E:218:VAL:HG11	2:E:235:THR:CG2	2.38	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
2:E:220:GLY:HA3	2:E:232:VAL:HG21	1.91	0.52
2:E:334:VAL:HG23	2:E:353:SER:HA	1.92	0.52
1:C:140:ILE:HD11	1:C:143:ARG:HH22	1.74	0.52
2:E:80:ALA:HB1	2:E:81:PRO:HD2	1.91	0.52
2:E:82:ILE:HB	2:E:116:ILE:HD13	1.92	0.52
2:E:377:ILE:HG21	2:E:410:ILE:CD1	2.40	0.52
4:H:127:THR:O	4:H:131:ILE:HG12	2.10	0.52
1:A:436:MET:HG3	1:A:441:GLN:HG2	1.91	0.52
1:B:68:PRO:HD3	2:F:15:ALA:HB2	1.92	0.52
1:C:64:LEU:HD23	1:C:74:VAL:HG21	1.92	0.52
2:F:360:PRO:HD3	2:F:368:TYR:CD2	2.45	0.52
3:G:23:MET:SD	3:G:232:MET:HE2	2.50	0.52
4:H:34:ARG:HG2	4:H:66:HIS:O	2.10	0.52
1:C:338:ILE:O	1:C:339:PRO:C	2.51	0.52
2:E:97:VAL:HG13	2:E:232:VAL:CG1	2.39	0.52
4:H:40:THR:HG23	4:H:42:THR:H	1.75	0.52
5:I:5:ARG:O	5:I:6:GLN:HB3	2.10	0.52
2:E:9:THR:HG21	2:E:28:GLY:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:84:ILE:HD13	2:D:235:THR:HG23	1.92	0.51
2:E:25:PHE:O	2:E:56:SER:HB3	2.10	0.51
1:A:457:GLU:HB2	1:A:460:LYS:HD3	1.92	0.51
1:B:386:VAL:HG22	1:B:442:VAL:HG12	1.91	0.51
3:G:190:MET:HE3	3:G:190:MET:HA	1.92	0.51
5:I:35:MET:C	5:I:37:THR:N	2.68	0.51
1:C:436:MET:CE	1:C:469:LEU:HD21	2.41	0.51
2:D:412:ARG:HD2	2:D:454:GLU:HB3	1.90	0.51
2:E:204:GLY:C	2:E:206:ILE:N	2.68	0.51
2:E:443:GLN:O	2:E:446:ALA:HB3	2.11	0.51
2:F:257:ASN:HB3	2:F:260:ARG:HG2	1.93	0.51
1:C:190:ASN:HA	1:C:198:LYS:HG2	1.91	0.51
2:E:218:VAL:HG11	2:E:235:THR:HG22	1.92	0.51
2:E:242:TYR:C	2:E:244:ARG:H	2.18	0.51
3:G:89:MET:CB	3:G:116:LEU:HD22	2.38	0.51
4:H:18:PHE:CZ	4:H:20:PHE:HB2	2.46	0.51
1:B:489:ILE:HG22	1:B:494:ASP:HB2	1.92	0.51
2:E:444:ILE:HD11	2:E:463:ILE:HD11	1.93	0.51
3:G:117:HIS:ND1	3:G:118:ARG:CA	2.74	0.51
1:C:105:GLY:HA2	1:C:226:MET:HE3	1.93	0.51
2:E:293:GLN:HG3	2:E:328:HIS:CG	2.46	0.51
1:A:140:ILE:HG21	1:A:313:ASN:HA	1.91	0.51
1:B:157:VAL:N	1:B:158:PRO:CD	2.73	0.51
1:C:331:ALA:O	1:C:333:ASP:N	2.44	0.51
1:C:443:ALA:O	1:C:446:TYR:HB3	2.10	0.51
1:A:245:LEU:C	1:A:247:PRO:HD2	2.36	0.51
1:A:294:TYR:HB2	1:A:337:TYR:HE2	1.76	0.51
1:B:482:LYS:O	1:B:486:ASP:N	2.37	0.51
2:E:279:VAL:HG12	2:E:279:VAL:O	2.10	0.51
2:E:377:ILE:HG21	2:E:410:ILE:HD12	1.92	0.51
2:F:394:ASP:HB3	3:G:79:GLY:CA	2.40	0.51
1:A:85:GLY:O	1:A:86:ASP:C	2.53	0.51
1:C:23:VAL:HG12	1:C:23:VAL:O	2.11	0.51
1:C:48:GLN:HB3	2:D:68:GLY:HA2	1.93	0.51
2:D:406:ARG:O	2:D:410:ILE:HG13	2.11	0.51
2:F:242:TYR:CD1	2:F:246:GLN:HG3	2.47	0.51
4:H:70:GLY:O	4:H:71:THR:C	2.53	0.51
2:F:234:LEU:O	2:F:237:LEU:HB3	2.10	0.50
1:A:48:GLN:HB3	2:E:68:GLY:O	2.10	0.50
1:B:157:VAL:N	1:B:158:PRO:HD3	2.26	0.50
1:C:362:ARG:HG3	1:C:362:ARG:NH1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:154:LEU:HD22	2:D:165:LEU:HD23	1.92	0.50
1:A:140:ILE:HD11	1:A:143:ARG:NE	2.26	0.50
1:B:437:ALA:O	1:B:438:ILE:C	2.54	0.50
1:C:45:ARG:NH2	1:C:68:PRO:O	2.44	0.50
1:C:102:GLU:HG2	1:C:122:GLY:C	2.36	0.50
2:F:455:GLN:H	2:F:455:GLN:CD	2.18	0.50
1:B:151:LYS:NZ	1:B:429:LYS:O	2.45	0.50
1:B:386:VAL:CG2	1:B:442:VAL:HG12	2.41	0.50
1:C:215:GLN:HE22	2:F:128:VAL:HA	1.77	0.50
2:D:168:GLU:HG3	2:D:168:GLU:O	2.11	0.50
2:E:41:ARG:O	2:E:42:GLU:C	2.53	0.50
4:H:83:THR:HB	4:H:91:GLN:HE21	1.75	0.50
1:C:96:ASP:O	1:C:97:VAL:HG13	2.12	0.50
2:E:204:GLY:O	2:E:205:VAL:C	2.54	0.50
2:F:96:ASN:ND2	2:F:100:GLU:HB2	2.26	0.50
2:F:386:ASP:O	2:F:389:ALA:HB3	2.11	0.50
2:F:421:ALA:O	2:F:425:THR:HG23	2.11	0.50
3:G:49:LEU:HD21	3:G:212:ILE:CD1	2.41	0.50
2:E:142:LEU:HD21	2:E:374:VAL:HG21	1.93	0.50
2:E:241:GLU:HA	2:E:304:ILE:HD11	1.93	0.50
2:E:275:ILE:O	2:E:283:PRO:HG3	2.12	0.50
2:F:86:VAL:HG11	2:F:114:ALA:HB3	1.94	0.50
4:H:35:GLN:HB3	4:H:66:HIS:HD2	1.77	0.50
1:A:187:LYS:HE2	1:A:191:ASP:OD2	2.11	0.50
1:C:406:PHE:N	1:C:406:PHE:CD1	2.79	0.50
2:D:345:TYR:HA	2:D:346:PRO:C	2.37	0.50
2:E:382:LYS:O	2:E:385:GLN:HB2	2.11	0.50
3:G:115:ILE:C	3:G:117:HIS:N	2.68	0.50
4:H:58:LEU:HD13	4:H:77:VAL:HG11	1.92	0.50
1:A:313:ASN:O	1:A:316:PHE:N	2.37	0.50
1:C:34:ILE:HD11	1:C:79:ASP:CB	2.41	0.50
2:D:93:ARG:HG3	2:D:93:ARG:NH1	2.27	0.50
2:E:155:PHE:HE1	2:E:310:ILE:HD12	1.77	0.50
2:F:394:ASP:HB3	3:G:79:GLY:C	2.36	0.50
3:G:203:ASN:CB	4:H:57:VAL:HG21	2.42	0.50
1:B:27:GLU:O	1:B:90:ARG:HG3	2.12	0.50
1:C:164:ARG:HD2	1:C:306:LEU:O	2.11	0.50
1:C:244:TYR:O	1:C:247:PRO:HD2	2.11	0.50
1:C:225:ALA:HA	1:C:228:TYR:CE1	2.47	0.49
1:A:240:ALA:N	1:A:241:PRO:HD2	2.27	0.49
1:B:107:VAL:HG12	1:B:115:ILE:CG1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ARG:O	1:B:211:SER:C	2.54	0.49
1:B:390:MET:CE	1:B:428:LEU:HD21	2.42	0.49
1:C:434:SER:N	1:C:435:PRO:HD3	2.27	0.49
2:D:319:ASP:O	2:D:320:PRO:C	2.55	0.49
1:C:180:ILE:CD1	1:C:216:LEU:HD21	2.34	0.49
2:E:397:SER:C	2:E:399:GLU:H	2.20	0.49
2:F:168:GLU:OE1	2:F:418:PHE:HB3	2.12	0.49
1:B:300:TYR:O	1:B:304:ARG:HG2	2.13	0.49
2:F:80:ALA:HB1	2:F:81:PRO:HD2	1.95	0.49
1:B:383:MET:O	1:B:384:LYS:C	2.52	0.49
1:C:396:GLN:HG3	2:D:458:TYR:CE2	2.47	0.49
2:F:163:THR:O	2:F:167:MET:HG2	2.12	0.49
1:A:94:ILE:HG12	1:A:95:VAL:N	2.27	0.49
1:A:137:ILE:N	1:A:138:PRO:CD	2.75	0.49
2:D:83:ARG:HA	2:D:115:ALA:HA	1.95	0.49
2:D:136:GLY:HA2	2:D:432:VAL:O	2.12	0.49
2:E:227:GLY:O	2:E:230:ALA:HB3	2.13	0.49
1:B:99:VAL:HG21	1:B:127:ARG:HB3	1.94	0.49
1:B:463:LYS:HE2	1:B:508:PHE:CZ	2.48	0.49
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.40	0.49
2:E:462:PRO:HD2	2:E:465:GLU:HG3	1.94	0.49
3:G:197:ASP:O	3:G:200:VAL:HG12	2.13	0.49
4:H:138:ASN:O	4:H:141:LEU:HB2	2.12	0.49
1:B:24:ASP:O	1:B:28:THR:HB	2.13	0.49
1:B:180:ILE:CD1	1:B:216:LEU:HD21	2.39	0.49
2:D:14:VAL:HG11	2:D:24:GLN:HB2	1.95	0.49
2:F:321:ALA:HB3	2:F:322:PRO:HD3	1.95	0.49
3:G:180:SER:O	3:G:181:LEU:C	2.56	0.49
4:H:105:LEU:HG	4:H:145:LEU:HB3	1.94	0.49
1:C:402:ALA:O	1:C:405:GLN:HG3	2.12	0.49
2:D:360:PRO:HD3	2:D:368:TYR:CE2	2.48	0.49
2:F:339:ILE:HG22	2:F:344:ILE:HB	1.94	0.49
1:A:180:ILE:O	1:A:181:ASP:C	2.56	0.49
1:A:380:THR:O	1:A:384:LYS:HG3	2.12	0.49
1:C:334:VAL:HG13	1:C:351:PHE:CE1	2.48	0.49
2:E:221:GLN:N	2:E:224:GLU:OE1	2.44	0.49
2:E:463:ILE:O	2:E:467:VAL:HG23	2.12	0.49
2:F:345:TYR:HA	2:F:346:PRO:C	2.36	0.49
1:B:96:ASP:HB2	1:B:127:ARG:O	2.13	0.48
1:C:30:ARG:HA	1:C:86:ASP:O	2.13	0.48
2:E:444:ILE:HD11	2:E:463:ILE:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:71:VAL:HG13	3:G:108:VAL:CG2	2.43	0.48
3:G:136:PRO:HD3	3:G:221:THR:HG21	1.95	0.48
1:A:373:ARG:HG3	1:A:373:ARG:NH1	2.28	0.48
1:B:351:PHE:HE1	1:B:369:LEU:O	1.96	0.48
1:B:211:SER:O	1:B:215:GLN:HG3	2.13	0.48
1:B:430:GLN:HE21	1:B:430:GLN:HB3	1.50	0.48
2:F:82:ILE:HD13	2:F:98:ILE:HG22	1.95	0.48
2:F:88:PRO:HD2	2:F:89:GLU:OE2	2.14	0.48
2:F:360:PRO:HD3	2:F:368:TYR:CE2	2.48	0.48
1:B:209:LYS:NZ	2:E:356:ARG:NH1	2.62	0.48
2:E:134:VAL:HG13	2:E:141:ASP:OD2	2.13	0.48
2:E:360:PRO:HD3	2:E:368:TYR:CD1	2.49	0.48
2:F:221:GLN:HE21	2:F:221:GLN:HA	1.78	0.48
1:A:417:LEU:HD23	1:A:417:LEU:H	1.77	0.48
2:E:374:VAL:O	2:E:377:ILE:HG22	2.14	0.48
1:B:49:ALA:O	1:B:50:GLU:HB2	2.12	0.48
1:B:358:TYR:C	1:B:360:GLY:N	2.69	0.48
2:D:425:THR:HB	2:D:459:MET:HE2	1.96	0.48
3:G:125:LEU:HD11	3:G:151:SER:HB2	1.96	0.48
4:H:41:GLN:HG2	4:H:57:VAL:HG12	1.94	0.48
1:B:240:ALA:N	1:B:241:PRO:CD	2.77	0.48
1:B:311:LYS:HD2	1:B:312:MET:O	2.13	0.48
1:C:488:LYS:HG2	1:C:489:ILE:N	2.28	0.48
2:E:158:ALA:C	2:E:160:VAL:N	2.72	0.48
2:E:404:VAL:O	2:E:408:ARG:HG3	2.14	0.48
2:E:416:GLN:HG3	2:E:417:PRO:HD2	1.96	0.48
3:G:39:LYS:N	3:G:40:PRO:HD2	2.28	0.48
1:A:453:LEU:HD13	1:A:461:ILE:HG23	1.96	0.48
1:B:481:SER:O	1:B:485:THR:HB	2.14	0.48
1:C:481:SER:O	1:C:485:THR:HB	2.14	0.48
2:F:63:MET:HE1	2:F:231:ARG:HB2	1.95	0.48
1:A:49:ALA:O	1:A:50:GLU:HB2	2.13	0.48
1:A:389:THR:O	1:A:393:GLU:HG2	2.13	0.48
1:B:179:ALA:O	1:B:182:THR:HB	2.14	0.48
1:B:225:ALA:HA	1:B:228:TYR:CE2	2.49	0.48
2:E:253:LEU:O	2:E:306:SER:HA	2.14	0.48
1:B:151:LYS:NZ	1:B:427:LEU:O	2.47	0.48
2:D:32:ILE:O	2:D:33:LEU:HB2	2.14	0.48
2:F:467:VAL:O	2:F:470:ALA:HB3	2.14	0.48
3:G:160:ILE:HG22	3:G:176:LYS:HB2	1.95	0.48
5:I:37:THR:HG22	5:I:38:SER:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:TYR:O	1:A:304:ARG:HG2	2.13	0.47
1:A:444:VAL:CG1	1:A:469:LEU:HD13	2.44	0.47
3:G:156:ASP:O	3:G:181:LEU:HB2	2.14	0.47
1:B:423:ARG:HE	1:B:458:PRO:CD	2.26	0.47
1:C:59:LEU:HD23	1:C:82:ILE:CD1	2.44	0.47
1:A:344:SER:O	2:E:222:MET:HE1	2.13	0.47
1:C:485:THR:O	1:C:486:ASP:C	2.57	0.47
2:F:462:PRO:HG2	2:F:465:GLU:HG3	1.96	0.47
1:A:376:SER:O	1:A:378:ALA:N	2.48	0.47
1:B:427:LEU:HD11	1:B:448:GLY:HA3	1.95	0.47
2:D:417:PRO:HA	2:D:459:MET:HE1	1.96	0.47
2:E:54:GLY:O	2:E:55:GLU:HB2	2.13	0.47
2:E:438:ILE:O	2:E:442:GLN:HB2	2.15	0.47
1:A:52:MET:HE1	1:A:60:LYS:HD3	1.97	0.47
1:A:68:PRO:HD3	2:E:15:ALA:HB2	1.96	0.47
1:A:100:GLY:HA2	1:A:256:TYR:CD1	2.49	0.47
1:C:292:GLU:O	1:C:293:ALA:CB	2.63	0.47
2:E:61:ILE:HG13	2:E:61:ILE:O	2.14	0.47
2:E:259:PHE:CE2	2:E:263:GLN:HG2	2.50	0.47
2:F:93:ARG:NH2	2:F:106:GLY:O	2.48	0.47
2:F:205:VAL:HG23	2:F:215:VAL:HG21	1.96	0.47
2:F:346:PRO:HG3	2:F:418:PHE:HZ	1.79	0.47
1:A:127:ARG:HE	1:A:131:LEU:CD1	2.27	0.47
1:A:209:LYS:HE3	1:A:211:SER:CB	2.44	0.47
1:A:485:THR:C	1:A:487:GLY:H	2.23	0.47
1:B:171:ARG:HG3	1:B:171:ARG:HH11	1.79	0.47
1:B:433:TYR:C	1:B:435:PRO:HD3	2.40	0.47
1:C:187:LYS:HE3	1:C:224:ASP:HB3	1.97	0.47
2:E:388:ILE:HG23	2:E:393:MET:CG	2.43	0.47
2:E:393:MET:HE3	2:E:396:LEU:HD12	1.95	0.47
1:A:485:THR:HG22	1:A:486:ASP:N	2.29	0.47
1:C:44:LEU:HB3	1:C:47:VAL:HG22	1.95	0.47
1:C:313:ASN:OD1	1:C:315:ALA:HB3	2.14	0.47
2:E:425:THR:C	2:E:427:HIS:N	2.72	0.47
3:G:19:ILE:CG2	3:G:23:MET:HE2	2.35	0.47
4:H:57:VAL:HG13	5:I:11:TYR:CZ	2.50	0.47
1:A:166:LEU:HD13	1:A:342:VAL:HG12	1.95	0.47
1:B:389:THR:HA	1:B:392:LEU:HG	1.96	0.47
1:B:485:THR:O	1:B:486:ASP:C	2.58	0.47
2:F:357:ILE:HD12	2:F:362:ILE:HG21	1.95	0.47
2:F:390:ILE:CD1	3:G:242:MET:HE1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:47:ILE:HD12	4:H:47:ILE:H	1.79	0.47
1:B:218:LYS:NZ	2:E:129:GLU:OE2	2.48	0.47
1:C:91:THR:HG22	1:C:93:ALA:HB3	1.97	0.47
2:D:397:SER:O	2:D:398:GLU:C	2.58	0.47
2:F:96:ASN:HD22	2:F:100:GLU:CB	2.27	0.47
2:F:409:LYS:HD3	2:F:457:PHE:HE2	1.78	0.47
4:H:62:LEU:CD1	4:H:144:ALA:HB2	2.34	0.47
1:A:188:ARG:HE	1:A:437:ALA:HB2	1.79	0.47
1:B:400:VAL:HB	1:B:418:LEU:CD2	2.45	0.47
1:C:441:GLN:O	1:C:445:ILE:HG12	2.14	0.47
2:D:154:LEU:HD13	2:D:165:LEU:HD23	1.96	0.47
2:E:116:ILE:HA	2:E:238:THR:OG1	2.14	0.47
2:F:310:ILE:HD13	2:F:325:THR:HG21	1.97	0.47
3:G:144:ILE:HG21	3:G:213:ILE:HD13	1.97	0.47
3:G:179:PHE:HB3	3:G:184:ILE:HG21	1.96	0.47
3:G:207:TYR:CZ	4:H:80:GLY:HA2	2.50	0.47
1:B:209:LYS:NZ	2:E:356:ARG:HH12	2.13	0.46
1:B:443:ALA:O	1:B:446:TYR:HB3	2.14	0.46
1:C:180:ILE:HG22	1:C:184:ILE:HD12	1.97	0.46
2:D:368:TYR:CE1	2:D:372:ARG:HG3	2.50	0.46
2:D:471:ASP:O	2:D:472:LYS:C	2.57	0.46
2:F:289:MET:HE3	2:F:289:MET:HB2	1.73	0.46
2:E:63:MET:CE	2:E:228:ALA:HA	2.45	0.46
2:F:319:ASP:O	2:F:322:PRO:HD2	2.14	0.46
3:G:56:ASP:C	3:G:57:ILE:HG12	2.41	0.46
1:A:78:ASN:OD1	1:A:80:LYS:HB3	2.15	0.46
1:A:107:VAL:HB	1:A:116:ASP:HB3	1.97	0.46
1:A:293:ALA:HB2	3:G:265:ILE:HD13	1.98	0.46
1:C:340:THR:O	1:C:341:ASN:C	2.59	0.46
2:D:129:GLU:OE1	2:D:129:GLU:HA	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:C:30:ARG:HE	1:C:87:ILE:CD1	2.18	0.46
1:C:445:ILE:HG22	1:C:449:VAL:CG2	2.45	0.46
2:D:397:SER:O	2:D:400:ASP:N	2.45	0.46
2:D:412:ARG:O	2:D:415:SER:OG	2.33	0.46
2:E:343:GLY:O	2:E:345:TYR:HD1	1.99	0.46
2:E:431:LEU:HD12	2:E:431:LEU:O	2.15	0.46
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.98	0.46
2:F:339:ILE:CG2	2:F:344:ILE:HB	2.46	0.46
1:A:51:GLU:OE2	1:A:90:ARG:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:GLU:CD	1:A:366:ASN:HD22	2.23	0.46
1:B:496:LYS:O	1:B:500:ILE:HG13	2.15	0.46
1:C:156:LEU:HD11	1:C:428:LEU:CD1	2.45	0.46
2:D:393:MET:HE1	2:D:404:VAL:HG11	1.95	0.46
2:E:161:GLY:O	2:E:162:LYS:C	2.57	0.46
2:F:151:LYS:HD3	2:F:328:HIS:O	2.15	0.46
3:G:78:CYS:O	3:G:81:ILE:HD13	2.15	0.46
3:G:129:LYS:HG2	3:G:130:GLU:OE1	2.14	0.46
1:A:403:PHE:O	1:A:404:ALA:C	2.59	0.46
1:B:271:LEU:HD12	1:B:325:PRO:HB2	1.98	0.46
2:E:409:LYS:NZ	2:E:450:ASP:HA	2.30	0.46
4:H:35:GLN:HB3	4:H:66:HIS:CD2	2.50	0.46
2:D:469:LYS:O	2:D:473:LEU:HG	2.15	0.46
2:E:77:ASP:CG	2:E:79:GLY:H	2.24	0.46
2:F:36:LEU:N	2:F:36:LEU:HD23	2.30	0.46
3:G:51:LEU:HD13	4:H:55:LEU:HD21	1.97	0.46
1:A:240:ALA:HB3	1:A:241:PRO:HD3	1.97	0.46
1:A:313:ASN:OD1	1:A:316:PHE:HD2	1.98	0.46
1:B:27:GLU:OE1	1:B:90:ARG:HD3	2.16	0.46
1:B:469:LEU:HG	1:B:473:ILE:HD11	1.97	0.46
1:C:245:LEU:O	1:C:246:ALA:C	2.56	0.46
2:D:289:MET:SD	2:D:324:THR:HG22	2.56	0.46
2:D:412:ARG:C	2:D:414:LEU:N	2.73	0.46
2:E:67:GLU:H	2:E:67:GLU:HG3	1.16	0.46
2:E:95:MET:HE2	2:E:99:GLY:CA	2.45	0.46
1:A:36:ASP:O	1:A:284:LEU:HD13	2.16	0.46
1:A:139:ARG:C	1:A:140:ILE:HG22	2.40	0.46
1:C:45:ARG:HD3	1:C:45:ARG:HA	1.29	0.46
2:D:237:LEU:HD21	2:D:295:ARG:HB2	1.97	0.46
2:D:432:VAL:HG13	2:D:433:PRO:HD2	1.97	0.46
2:E:82:ILE:HB	2:E:116:ILE:CD1	2.45	0.46
2:E:112:GLN:NE2	2:E:242:TYR:HE2	2.14	0.46
2:E:405:SER:OG	2:E:406:ARG:N	2.49	0.46
2:F:243:PHE:O	2:F:249:GLN:HB2	2.16	0.46
1:A:213:VAL:O	1:A:216:LEU:HB3	2.16	0.46
1:A:492:GLU:C	1:A:494:ASP:N	2.74	0.46
2:F:50:ALA:O	2:F:51:GLN:HB3	2.16	0.46
2:F:96:ASN:HB2	2:F:100:GLU:N	2.31	0.46
2:D:130:GLN:HE22	2:D:356:ARG:HD3	1.81	0.45
2:E:85:PRO:HD2	2:E:95:MET:CE	2.46	0.45
2:E:120:ALA:HB1	2:E:121:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:340:ALA:O	2:E:343:GLY:N	2.42	0.45
4:H:99:THR:O	4:H:102:MET:HG2	2.15	0.45
1:B:34:ILE:HD12	1:B:35:GLY:H	1.81	0.45
1:C:26:GLU:HB3	1:C:46:ASN:ND2	2.31	0.45
2:E:189:ARG:O	2:E:190:THR:C	2.58	0.45
1:A:40:ARG:HH11	1:A:40:ARG:CG	2.27	0.45
1:A:166:LEU:HD13	1:A:342:VAL:CG1	2.47	0.45
1:B:353:GLU:HG3	1:B:366:ASN:HB2	1.98	0.45
1:C:158:PRO:HB3	1:C:379:GLN:HG3	1.99	0.45
2:D:35:ALA:HB1	2:D:46:VAL:CG1	2.47	0.45
2:D:417:PRO:HB3	2:D:459:MET:HE3	1.99	0.45
2:E:33:LEU:HD13	2:E:117:HIS:CG	2.50	0.45
2:E:443:GLN:HA	2:E:446:ALA:HB3	1.99	0.45
2:F:252:LEU:HD23	2:F:252:LEU:HA	1.81	0.45
3:G:259:THR:O	3:G:263:ILE:HG12	2.17	0.45
1:A:140:ILE:CG2	1:A:313:ASN:HA	2.47	0.45
1:C:432:GLN:O	1:C:433:TYR:HB2	2.16	0.45
2:F:221:GLN:HA	2:F:221:GLN:NE2	2.31	0.45
3:G:84:SER:HB3	3:G:173:THR:OG1	2.17	0.45
1:A:59:LEU:HD11	1:A:81:LEU:HD12	1.99	0.45
1:A:179:ALA:O	1:A:182:THR:HB	2.17	0.45
1:A:283:LEU:HD11	1:A:293:ALA:HB1	1.99	0.45
2:D:84:ILE:N	2:D:114:ALA:O	2.42	0.45
2:D:96:ASN:HB2	2:D:100:GLU:N	2.27	0.45
2:E:77:ASP:C	2:E:79:GLY:H	2.24	0.45
2:E:146:TYR:O	2:E:357:ILE:HD11	2.16	0.45
2:E:147:ALA:HB2	2:E:357:ILE:HD13	1.99	0.45
2:F:136:GLY:HA3	2:F:431:LEU:HD11	1.99	0.45
1:A:151:LYS:HE2	1:A:427:LEU:O	2.17	0.45
1:A:339:PRO:O	1:A:343:ILE:HG13	2.16	0.45
1:A:485:THR:C	1:A:487:GLY:N	2.73	0.45
1:B:381:ARG:HG2	1:B:488:LYS:HG3	1.97	0.45
2:F:390:ILE:HD11	3:G:242:MET:SD	2.56	0.45
1:A:142:VAL:HG22	1:A:161:ARG:O	2.16	0.45
1:B:465:GLU:O	1:B:469:LEU:HB2	2.17	0.45
2:D:201:ILE:HD13	2:D:208:LEU:HD11	1.98	0.45
2:D:452:LEU:HD12	2:D:457:PHE:CZ	2.52	0.45
2:E:231:ARG:O	2:E:232:VAL:C	2.60	0.45
2:F:346:PRO:HG3	2:F:418:PHE:CZ	2.52	0.45
1:B:76:PHE:HB3	1:B:242:LEU:HD21	1.99	0.45
1:C:474:SER:OG	1:C:475:GLN:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:95:MET:HG2	2:D:99:GLY:HA2	1.99	0.45
1:A:97:VAL:HG11	1:A:249:SER:HB2	1.99	0.45
1:A:385:GLN:OE1	1:A:488:LYS:HB2	2.17	0.45
1:C:67:GLU:HB3	1:C:68:PRO:HD2	1.98	0.45
2:D:440:GLY:O	2:D:444:ILE:HG13	2.16	0.45
3:G:13:ILE:HD13	3:G:242:MET:SD	2.57	0.45
1:A:55:PHE:O	1:A:56:SER:C	2.61	0.44
1:A:412:ALA:HA	1:A:415:GLN:HB3	1.98	0.44
1:C:251:CYS:O	1:C:255:GLU:HG3	2.16	0.44
1:C:476:HIS:ND1	1:C:476:HIS:N	2.64	0.44
2:D:298:THR:HG23	2:D:303:SER:HA	1.98	0.44
2:F:29:LEU:HD11	2:F:58:VAL:HG13	1.98	0.44
2:F:319:ASP:O	2:F:320:PRO:C	2.60	0.44
4:H:55:LEU:O	4:H:56:GLN:HG3	2.17	0.44
2:D:366:GLU:O	2:D:370:VAL:HG23	2.17	0.44
2:E:321:ALA:N	2:E:322:PRO:HD2	2.32	0.44
2:F:257:ASN:OD1	2:F:259:PHE:HB3	2.18	0.44
3:G:105:ILE:HG22	3:G:106:ILE:N	2.32	0.44
3:G:228:ARG:O	3:G:232:MET:HG2	2.17	0.44
4:H:34:ARG:HH22	4:H:70:GLY:CA	2.24	0.44
1:A:392:LEU:O	1:A:396:GLN:HG3	2.18	0.44
1:A:463:LYS:HD3	1:A:508:PHE:CZ	2.52	0.44
1:B:141:SER:HB2	1:B:143:ARG:NH1	2.31	0.44
1:B:300:TYR:HA	1:B:303:SER:OG	2.17	0.44
1:B:400:VAL:CG1	1:B:418:LEU:HD11	2.47	0.44
2:D:103:ASP:O	2:D:104:GLU:HB2	2.18	0.44
2:E:281:TYR:CZ	2:E:321:ALA:HB2	2.52	0.44
2:F:469:LYS:O	2:F:473:LEU:HG	2.16	0.44
4:H:33:VAL:HG11	4:H:65:VAL:HG13	1.99	0.44
1:A:379:GLN:HB2	1:A:384:LYS:HE3	2.00	0.44
1:B:140:ILE:HG13	1:B:143:ARG:NH1	2.32	0.44
1:C:219:ARG:HD3	1:C:433:TYR:HE1	1.80	0.44
2:D:63:MET:HE1	2:D:231:ARG:HB2	1.99	0.44
2:D:170:ILE:O	2:D:174:ALA:HB3	2.17	0.44
2:F:188:GLU:H	2:F:221:GLN:NE2	2.15	0.44
1:A:413:ALA:O	1:A:416:GLN:HB3	2.17	0.44
1:A:460:LYS:N	1:A:460:LYS:HD2	2.32	0.44
1:C:132:LYS:NZ	2:D:64:ASP:OD1	2.49	0.44
2:E:402:LEU:O	2:E:406:ARG:HG3	2.16	0.44
2:F:348:VAL:O	2:F:350:PRO:HD3	2.17	0.44
3:G:117:HIS:CE1	3:G:118:ARG:NE	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LEU:HD21	1:B:42:HIS:HB2	2.00	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	2.51	0.44
3:G:128:PHE:HB3	5:I:42:ILE:CD1	2.48	0.44
1:A:74:VAL:HG13	1:A:241:PRO:HG3	2.00	0.44
2:E:114:ALA:HB3	2:E:238:THR:CG2	2.47	0.44
3:G:184:ILE:C	3:G:186:SER:N	2.72	0.44
1:A:24:ASP:OD1	1:A:24:ASP:C	2.60	0.44
1:B:107:VAL:HG12	1:B:115:ILE:HD11	2.00	0.44
1:B:389:THR:HA	1:B:392:LEU:CG	2.48	0.44
1:C:169:GLY:O	1:C:175:LYS:HE2	2.18	0.44
1:C:311:LYS:HE3	1:C:318:GLY:O	2.18	0.44
2:D:189:ARG:O	2:D:192:GLU:HB2	2.18	0.44
2:F:105:ARG:CZ	2:F:208:LEU:HD23	2.47	0.44
3:G:206:GLU:O	5:I:12:ILE:HD11	2.17	0.44
1:A:244:TYR:HE1	1:A:301:LEU:HD11	1.82	0.44
1:A:420:ARG:HA	1:A:420:ARG:HD3	1.78	0.44
1:C:177:SER:O	1:C:178:ILE:C	2.60	0.44
1:C:208:GLN:HE21	1:C:208:GLN:HB2	1.37	0.44
1:C:489:ILE:HG22	1:C:494:ASP:HB2	1.99	0.44
2:D:231:ARG:O	2:D:234:LEU:N	2.50	0.44
2:E:316:ASP:OD2	3:G:255:GLN:NE2	2.39	0.44
2:F:357:ILE:O	2:F:359:ASP:N	2.48	0.44
3:G:113:ARG:O	3:G:117:HIS:HB2	2.18	0.44
3:G:117:HIS:O	3:G:118:ARG:C	2.61	0.44
4:H:38:VAL:HA	4:H:39:PRO:HD3	1.83	0.44
1:A:52:MET:CG	1:A:95:VAL:HG22	2.48	0.43
1:B:294:TYR:CE2	1:B:338:ILE:HD13	2.53	0.43
1:C:90:ARG:HE	1:C:90:ARG:HB3	1.61	0.43
1:C:335:SER:O	2:D:314:ALA:HA	2.18	0.43
2:D:425:THR:HG21	2:D:459:MET:HE1	1.99	0.43
2:E:72:GLY:O	2:E:73:GLN:C	2.60	0.43
2:F:31:PRO:O	2:F:34:ASN:HB2	2.18	0.43
2:F:359:ASP:OD1	2:F:360:PRO:HD2	2.17	0.43
3:G:2:THR:C	3:G:4:LYS:N	2.75	0.43
1:A:471:HIS:ND1	1:A:475:GLN:HG3	2.33	0.43
1:B:212:THR:O	1:B:216:LEU:HB2	2.18	0.43
1:B:423:ARG:HE	1:B:458:PRO:CG	2.31	0.43
2:D:231:ARG:O	2:D:232:VAL:C	2.60	0.43
2:D:400:ASP:O	2:D:404:VAL:HG23	2.18	0.43
3:G:178:ILE:C	3:G:180:SER:N	2.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:234:ASN:O	3:G:235:ALA:C	2.62	0.43
1:A:133:ALA:HB1	1:A:134:PRO:HD2	1.99	0.43
1:B:249:SER:O	1:B:250:GLY:C	2.61	0.43
1:B:269:ASP:HA	1:B:270:ASP:HA	1.78	0.43
1:B:423:ARG:O	1:B:426:GLU:N	2.51	0.43
1:C:32:LEU:HD21	1:C:42:HIS:HB2	2.00	0.43
1:C:116:ASP:O	1:C:117:GLY:C	2.60	0.43
1:C:285:LEU:C	1:C:286:ARG:HG2	2.43	0.43
2:E:35:ALA:HB2	2:E:82:ILE:HG13	1.99	0.43
2:E:136:GLY:HA2	2:E:432:VAL:O	2.18	0.43
2:E:166:ILE:O	2:E:170:ILE:HG13	2.18	0.43
2:E:376:LYS:O	2:E:379:GLN:HB2	2.18	0.43
1:B:400:VAL:HG12	1:B:418:LEU:HD11	2.00	0.43
1:C:180:ILE:O	1:C:181:ASP:C	2.61	0.43
1:C:390:MET:HE1	1:C:428:LEU:HD21	1.99	0.43
1:C:404:ALA:HB1	1:C:410:LEU:HD11	1.99	0.43
2:D:93:ARG:NH1	2:D:108:ILE:HG12	2.33	0.43
2:F:385:GLN:HA	2:F:388:ILE:HG12	2.01	0.43
4:H:41:GLN:CG	4:H:57:VAL:HG12	2.48	0.43
4:H:112:LEU:HD21	4:H:135:ILE:HG23	1.99	0.43
1:B:213:VAL:O	1:B:217:VAL:HG13	2.18	0.43
1:B:289:PRO:HG2	3:G:263:ILE:HD12	1.99	0.43
1:B:389:THR:HG22	1:B:392:LEU:HD12	2.00	0.43
1:C:144:GLU:H	1:C:144:GLU:HG3	1.65	0.43
1:C:187:LYS:O	1:C:188:ARG:C	2.62	0.43
2:D:275:ILE:HG23	3:G:269:ALA:CA	2.46	0.43
2:E:242:TYR:C	2:E:244:ARG:N	2.77	0.43
2:F:81:PRO:O	2:F:82:ILE:C	2.58	0.43
2:F:141:ASP:HB3	2:F:434:LEU:HD13	2.01	0.43
4:H:35:GLN:HG2	4:H:36:VAL:N	2.34	0.43
4:H:105:LEU:CD2	4:H:109:LYS:HE3	2.41	0.43
1:A:251:CYS:O	1:A:255:GLU:HG3	2.18	0.43
1:A:397:TYR:CD1	1:A:421:GLY:HA3	2.54	0.43
1:C:51:GLU:HG2	1:C:52:MET:N	2.33	0.43
1:C:185:ASN:HB2	1:C:435:PRO:HB3	2.00	0.43
2:E:439:LYS:O	2:E:440:GLY:C	2.61	0.43
1:C:193:THR:O	1:C:195:GLU:OE1	2.36	0.43
1:C:353:GLU:O	1:C:364:ALA:HB1	2.18	0.43
2:D:108:ILE:HG22	2:D:110:THR:HG23	1.99	0.43
2:D:274:ARG:HH11	2:D:274:ARG:HD2	1.50	0.43
2:F:407:ALA:O	2:F:411:GLN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:6:ILE:HG21	3:G:250:PHE:HB2	2.00	0.43
1:A:45:ARG:HD3	1:A:45:ARG:HA	1.67	0.43
2:F:89:GLU:HG2	2:F:110:THR:CG2	2.44	0.43
2:F:439:LYS:HG2	2:F:443:GLN:NE2	2.33	0.43
4:H:20:PHE:CD1	4:H:92:LEU:HD23	2.54	0.43
1:A:383:MET:O	1:A:386:VAL:HG23	2.19	0.43
1:C:83:LYS:HB2	1:C:83:LYS:HE3	1.83	0.43
2:E:432:VAL:HA	2:E:433:PRO:HD3	1.81	0.43
2:E:433:PRO:HG2	2:E:436:GLU:CG	2.48	0.43
2:F:144:ALA:N	2:F:145:PRO:CD	2.82	0.43
3:G:179:PHE:C	3:G:181:LEU:H	2.27	0.43
4:H:79:SER:O	4:H:94:ALA:HA	2.18	0.43
1:C:49:ALA:O	1:C:50:GLU:HB2	2.19	0.43
1:C:49:ALA:N	1:C:66:LEU:HD11	2.34	0.43
1:C:147:GLN:OE1	1:C:438:ILE:HD13	2.19	0.43
1:C:224:ASP:OD1	1:C:227:LYS:HE3	2.19	0.43
2:D:462:PRO:HD2	2:D:465:GLU:HG3	2.00	0.43
2:E:182:VAL:HG21	2:E:240:ALA:HB2	2.01	0.43
2:E:242:TYR:C	2:E:242:TYR:CD1	2.97	0.43
2:E:461:GLY:HA3	2:E:462:PRO:HD3	1.73	0.43
5:I:35:MET:O	5:I:37:THR:N	2.52	0.43
1:A:291:ARG:N	3:G:262:LEU:CD2	2.82	0.42
1:B:94:ILE:O	1:B:95:VAL:C	2.61	0.42
2:D:145:PRO:HB2	2:D:357:ILE:HD11	2.01	0.42
2:E:310:ILE:HD11	2:E:329:LEU:HD11	2.00	0.42
2:E:441:PHE:O	2:E:445:LEU:HG	2.19	0.42
3:G:192:ILE:HG22	4:H:53:PRO:HG2	2.00	0.42
3:G:239:ALA:O	3:G:243:ILE:HG12	2.18	0.42
1:A:99:VAL:HG23	1:A:253:MET:HA	2.01	0.42
1:A:340:THR:O	1:A:344:SER:HB3	2.19	0.42
1:A:482:LYS:O	1:A:483:ILE:C	2.61	0.42
1:C:107:VAL:O	1:C:115:ILE:HG12	2.18	0.42
1:C:139:ARG:HB3	1:C:311:LYS:O	2.19	0.42
2:D:95:MET:HE2	2:D:235:THR:CG2	2.49	0.42
2:D:410:ILE:HG23	2:D:441:PHE:CE1	2.54	0.42
2:F:357:ILE:HD13	2:F:357:ILE:HA	1.80	0.42
2:F:452:LEU:HD22	2:F:470:ALA:CB	2.49	0.42
3:G:203:ASN:HB3	4:H:57:VAL:HG21	2.01	0.42
4:H:131:ILE:HG23	4:H:134:ARG:HH21	1.84	0.42
1:A:96:ASP:HA	1:A:128:ARG:HA	2.01	0.42
1:B:385:GLN:NE2	1:B:489:ILE:HB	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:SER:N	1:B:435:PRO:CD	2.82	0.42
2:D:412:ARG:HG3	2:D:412:ARG:NH1	2.33	0.42
2:F:122:GLU:OE1	2:F:122:GLU:HA	2.19	0.42
2:F:400:ASP:O	2:F:404:VAL:HG23	2.19	0.42
1:A:184:ILE:HD12	1:A:223:ALA:CB	2.50	0.42
1:A:338:ILE:N	1:A:339:PRO:CD	2.83	0.42
2:F:95:MET:HG3	2:F:99:GLY:HA2	2.00	0.42
2:F:438:ILE:H	2:F:438:ILE:HG12	1.73	0.42
1:B:55:PHE:O	1:B:56:SER:C	2.61	0.42
1:C:137:ILE:HD13	1:C:137:ILE:HA	1.88	0.42
2:E:296:ILE:HD13	2:E:306:SER:HB2	2.02	0.42
3:G:180:SER:O	3:G:182:ASP:N	2.52	0.42
5:I:5:ARG:O	5:I:6:GLN:CB	2.68	0.42
1:C:423:ARG:CD	1:C:461:ILE:HD11	2.49	0.42
2:E:32:ILE:O	2:E:33:LEU:CB	2.68	0.42
2:E:397:SER:O	2:E:398:GLU:C	2.62	0.42
2:F:47:LEU:HD23	2:F:62:ALA:HA	2.01	0.42
3:G:86:ALA:O	3:G:116:LEU:HD13	2.18	0.42
1:B:165:GLU:O	1:B:325:PRO:HD2	2.19	0.42
2:D:38:VAL:HG22	2:D:75:VAL:HG22	2.02	0.42
2:D:266:SER:CB	2:D:282:GLN:NE2	2.82	0.42
2:E:12:ARG:NH2	2:E:24:GLN:OE1	2.50	0.42
2:E:95:MET:HA	2:E:100:GLU:O	2.20	0.42
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.48	0.42
2:E:282:GLN:HA	2:E:283:PRO:HD3	1.89	0.42
2:E:412:ARG:NH1	2:E:454:GLU:OE1	2.53	0.42
2:F:251:VAL:HG12	2:F:252:LEU:N	2.35	0.42
2:F:423:VAL:O	2:F:423:VAL:HG12	2.20	0.42
3:G:203:ASN:HB2	4:H:57:VAL:HG21	2.02	0.42
1:B:361:ILE:HD13	1:B:429:LYS:HE2	2.02	0.42
1:C:151:LYS:HE2	1:C:436:MET:SD	2.60	0.42
1:C:331:ALA:O	1:C:332:GLY:C	2.63	0.42
1:C:442:VAL:HG11	1:C:489:ILE:HD11	2.01	0.42
1:C:457:GLU:O	1:C:458:PRO:C	2.61	0.42
2:D:38:VAL:HG11	2:D:69:LEU:CD2	2.49	0.42
2:D:190:THR:O	2:D:191:ARG:C	2.59	0.42
2:E:422:GLU:C	2:E:424:PHE:N	2.74	0.42
5:I:41:THR:O	5:I:42:ILE:C	2.62	0.42
1:A:78:ASN:ND2	1:A:80:LYS:HD2	2.34	0.42
1:B:75:VAL:HG21	1:B:82:ILE:HD12	2.02	0.42
1:C:210:ARG:NH1	2:F:121:PRO:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:279:VAL:HG12	2:D:279:VAL:O	2.20	0.42
2:D:397:SER:C	2:D:399:GLU:N	2.77	0.42
2:D:475:GLU:OE1	2:D:475:GLU:HA	2.20	0.42
2:E:105:ARG:NE	2:E:208:LEU:HD23	2.33	0.42
4:H:54:THR:O	4:H:55:LEU:HD23	2.20	0.42
1:B:379:GLN:HB3	1:B:384:LYS:CE	2.46	0.42
1:C:290:GLY:O	1:C:291:ARG:C	2.61	0.42
2:E:95:MET:HE2	2:E:99:GLY:HA2	2.01	0.42
2:E:358:MET:HE3	2:E:358:MET:HB3	1.93	0.42
1:A:56:SER:O	1:A:58:GLY:N	2.53	0.41
1:C:467:ALA:O	1:C:470:SER:HB2	2.20	0.41
2:D:63:MET:CE	2:D:228:ALA:HA	2.50	0.41
2:E:396:LEU:CB	2:E:401:LYS:HG2	2.50	0.41
4:H:39:PRO:HG3	4:H:62:LEU:N	2.34	0.41
4:H:62:LEU:HD21	4:H:100:LEU:HD21	2.02	0.41
1:A:383:MET:HG3	1:A:387:ALA:HB2	2.02	0.41
1:B:255:GLU:HG2	1:B:258:ARG:CZ	2.50	0.41
1:B:381:ARG:HA	1:B:384:LYS:HB2	2.01	0.41
1:C:403:PHE:CZ	2:D:408:ARG:HD2	2.55	0.41
2:D:95:MET:HE3	2:D:99:GLY:HA2	2.02	0.41
2:D:201:ILE:CD1	2:D:208:LEU:HD11	2.50	0.41
2:E:360:PRO:HD3	2:E:368:TYR:CG	2.56	0.41
3:G:87:LYS:HA	3:G:90:LYS:HE2	2.02	0.41
1:A:103:LEU:O	1:A:106:ARG:HB2	2.20	0.41
1:B:382:ALA:HB1	1:B:442:VAL:HG11	2.02	0.41
2:D:35:ALA:HB1	2:D:46:VAL:HG13	2.02	0.41
2:E:88:PRO:C	2:E:90:THR:H	2.28	0.41
2:E:366:GLU:O	2:E:367:HIS:C	2.63	0.41
2:F:167:MET:HB2	2:F:420:VAL:HG11	2.02	0.41
3:G:106:ILE:HG12	3:G:126:VAL:HG23	2.01	0.41
4:H:64:VAL:CG1	4:H:72:THR:HG21	2.50	0.41
1:A:292:GLU:HB2	1:A:294:TYR:HD2	1.86	0.41
1:A:294:TYR:HB2	1:A:337:TYR:CE2	2.54	0.41
1:A:347:ASP:C	1:A:373:ARG:HH11	2.28	0.41
1:A:390:MET:HE1	1:A:428:LEU:HD21	2.02	0.41
1:A:400:VAL:O	1:A:401:ALA:C	2.64	0.41
1:B:304:ARG:HH11	1:B:304:ARG:HD3	1.64	0.41
2:E:189:ARG:HB2	2:E:192:GLU:HG3	2.02	0.41
1:B:44:LEU:HB3	1:B:47:VAL:CG2	2.47	0.41
1:B:366:ASN:ND2	1:B:369:LEU:HG	2.36	0.41
1:B:423:ARG:HH21	1:B:458:PRO:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:MET:HE2	1:C:428:LEU:HD11	2.02	0.41
2:D:84:ILE:HB	2:D:95:MET:HE3	2.02	0.41
2:D:449:TYR:C	2:D:451:HIS:N	2.78	0.41
2:E:35:ALA:C	2:E:36:LEU:HD23	2.46	0.41
2:E:282:GLN:H	2:E:282:GLN:NE2	2.19	0.41
2:E:388:ILE:HD12	2:E:396:LEU:HD11	2.01	0.41
2:F:196:LEU:O	2:F:200:MET:HB2	2.19	0.41
4:H:119:LEU:HD21	4:H:132:GLN:HE21	1.86	0.41
1:A:408:SER:O	1:A:409:ASP:HB2	2.20	0.41
1:B:290:GLY:O	1:B:291:ARG:C	2.64	0.41
1:C:151:LYS:HG3	1:C:430:GLN:OE1	2.21	0.41
2:D:52:HIS:CD2	2:D:58:VAL:HG12	2.56	0.41
2:D:63:MET:CE	2:D:97:VAL:HG11	2.51	0.41
2:D:396:LEU:HD22	2:D:400:ASP:HB2	2.00	0.41
2:E:231:ARG:O	2:E:234:LEU:N	2.50	0.41
2:F:94:ILE:CG2	2:F:102:ILE:HD11	2.50	0.41
2:F:442:GLN:O	2:F:445:LEU:HB2	2.20	0.41
1:A:206:ILE:O	1:A:273:LYS:HD2	2.20	0.41
1:B:78:ASN:ND2	1:B:80:LYS:HE2	2.35	0.41
1:B:206:ILE:HA	1:B:234:ALA:O	2.21	0.41
2:D:13:ILE:HD12	2:D:73:GLN:HB3	2.03	0.41
2:D:64:ASP:CG	2:D:65:GLY:H	2.28	0.41
2:D:360:PRO:HD3	2:D:368:TYR:CD2	2.56	0.41
2:E:82:ILE:CG2	2:E:116:ILE:HD13	2.51	0.41
2:E:167:MET:SD	2:E:200:MET:HA	2.61	0.41
2:F:282:GLN:H	2:F:282:GLN:HG2	1.07	0.41
2:F:471:ASP:O	2:F:474:ALA:N	2.53	0.41
3:G:120:HIS:HB3	3:G:123:GLN:HB2	2.03	0.41
4:H:58:LEU:HG	4:H:80:GLY:C	2.46	0.41
1:A:32:LEU:HD21	1:A:42:HIS:HB2	2.02	0.41
1:A:105:GLY:HA2	1:A:226:MET:O	2.21	0.41
1:A:129:VAL:HG12	1:A:249:SER:HA	2.03	0.41
1:A:498:LYS:O	1:A:502:THR:HG23	2.21	0.41
1:B:210:ARG:C	1:B:212:THR:N	2.79	0.41
1:C:19:ALA:O	1:C:21:THR:HG23	2.21	0.41
1:C:78:ASN:HD21	1:C:80:LYS:HD3	1.85	0.41
2:D:112:GLN:NE2	2:D:242:TYR:CE1	2.88	0.41
2:D:449:TYR:C	2:D:451:HIS:H	2.28	0.41
1:A:102:GLU:HG3	1:A:122:GLY:C	2.46	0.41
1:A:184:ILE:HD12	1:A:223:ALA:HB3	2.03	0.41
1:A:294:TYR:CE2	1:A:338:ILE:HD13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:MET:HE3	1:B:64:LEU:CD1	2.51	0.41
1:B:107:VAL:O	1:B:115:ILE:HG12	2.20	0.41
1:B:201:CYS:O	1:B:229:THR:HA	2.21	0.41
1:C:129:VAL:HG21	1:C:245:LEU:HD11	2.02	0.41
1:C:299:PHE:O	1:C:300:TYR:C	2.62	0.41
1:C:374:VAL:CG1	1:C:378:ALA:HB2	2.51	0.41
1:C:465:GLU:O	1:C:465:GLU:HG2	2.21	0.41
2:D:398:GLU:HA	2:D:401:LYS:CG	2.51	0.41
2:E:97:VAL:HG13	2:E:232:VAL:HG12	2.02	0.41
2:E:122:GLU:HB2	2:E:125:GLU:HG3	2.01	0.41
2:E:165:LEU:HD22	2:E:335:LEU:HD21	2.02	0.41
2:E:256:ASP:HA	2:E:257:ASN:HA	1.65	0.41
2:F:228:ALA:O	2:F:232:VAL:HG22	2.21	0.41
2:F:434:LEU:O	2:F:438:ILE:HG12	2.21	0.41
3:G:85:VAL:HG12	3:G:173:THR:HG23	2.03	0.41
3:G:180:SER:O	3:G:205:GLN:NE2	2.50	0.41
4:H:34:ARG:NH2	4:H:70:GLY:HA2	2.28	0.41
1:A:74:VAL:CG1	1:A:241:PRO:HG3	2.51	0.41
1:A:247:PRO:HG2	1:A:274:GLN:NE2	2.35	0.41
1:B:30:ARG:HA	1:B:86:ASP:O	2.21	0.41
1:B:138:PRO:HB2	1:B:312:MET:HE1	2.03	0.41
1:B:336:ALA:HB3	1:B:339:PRO:HD2	2.02	0.41
1:B:413:ALA:O	1:B:414:THR:C	2.64	0.41
1:B:423:ARG:NE	1:B:458:PRO:HD3	2.36	0.41
1:C:423:ARG:HD2	1:C:461:ILE:HD11	2.03	0.41
2:D:27:GLU:H	2:D:27:GLU:HG3	1.77	0.41
2:D:86:VAL:HG11	2:D:114:ALA:HB3	2.02	0.41
2:D:97:VAL:HG11	2:D:231:ARG:HB2	2.03	0.41
2:D:112:GLN:NE2	2:D:242:TYR:HE1	2.18	0.41
2:D:368:TYR:O	2:D:372:ARG:HG2	2.21	0.41
2:E:227:GLY:O	2:E:231:ARG:HG2	2.21	0.41
2:E:397:SER:O	2:E:399:GLU:N	2.54	0.41
2:E:452:LEU:HA	2:E:453:PRO:HD3	1.85	0.41
3:G:51:LEU:HD22	3:G:204:TYR:OH	2.21	0.41
4:H:48:LEU:C	4:H:50:ALA:N	2.78	0.41
1:A:147:GLN:OE1	1:A:438:ILE:HD13	2.21	0.40
1:A:440:GLU:HG2	1:A:473:ILE:HD11	2.03	0.40
1:B:45:ARG:HH11	1:B:45:ARG:HD3	1.53	0.40
1:B:99:VAL:HG13	1:B:256:TYR:HB2	2.02	0.40
1:B:340:THR:O	1:B:341:ASN:C	2.63	0.40
2:D:94:ILE:HG22	2:D:102:ILE:HD11	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:433:PRO:HG2	2:D:436:GLU:CG	2.44	0.40
2:E:105:ARG:NH1	2:E:208:LEU:HD23	2.36	0.40
2:E:434:LEU:O	2:E:437:THR:HB	2.21	0.40
3:G:12:SER:O	3:G:16:ILE:HD12	2.20	0.40
3:G:73:SER:O	3:G:111:LYS:HB2	2.21	0.40
4:H:78:SER:HB3	5:I:22:VAL:HG21	2.03	0.40
1:A:69:ASP:O	1:A:70:ASN:HB3	2.21	0.40
1:A:267:ILE:HA	1:A:324:LEU:O	2.20	0.40
1:A:356:LEU:O	1:A:357:PHE:C	2.63	0.40
1:A:479:LEU:O	1:A:482:LYS:HB2	2.22	0.40
1:C:192:GLY:O	1:C:198:LYS:NZ	2.53	0.40
1:C:465:GLU:O	1:C:469:LEU:HB2	2.21	0.40
2:D:281:TYR:HB3	2:D:285:LEU:HD12	2.03	0.40
2:E:96:ASN:OD1	2:E:97:VAL:N	2.54	0.40
2:E:387:ILE:HG22	2:E:388:ILE:HD13	2.02	0.40
2:E:454:GLU:C	2:E:456:ALA:H	2.29	0.40
3:G:2:THR:HG22	3:G:4:LYS:H	1.86	0.40
1:B:439:GLU:HA	1:B:442:VAL:CG2	2.52	0.40
1:B:452:TYR:CD2	1:B:501:VAL:HG21	2.56	0.40
1:C:240:ALA:N	1:C:241:PRO:CD	2.84	0.40
2:D:203:SER:OG	2:D:205:VAL:HG23	2.21	0.40
2:E:35:ALA:HB1	2:E:46:VAL:CG1	2.52	0.40
2:E:139:VAL:HG21	2:E:348:VAL:HB	2.02	0.40
2:E:200:MET:CB	2:E:206:ILE:HD12	2.52	0.40
2:E:454:GLU:C	2:E:456:ALA:N	2.79	0.40
2:F:95:MET:HE3	2:F:108:ILE:HD13	2.03	0.40
3:G:39:LYS:CB	3:G:40:PRO:CD	2.99	0.40
3:G:113:ARG:HG3	3:G:127:THR:HG21	2.03	0.40
4:H:82:VAL:HB	4:H:92:LEU:CD1	2.52	0.40
5:I:20:LYS:HA	5:I:23:ARG:NH1	2.36	0.40
1:B:376:SER:O	1:B:384:LYS:HE2	2.22	0.40
1:C:313:ASN:OD1	1:C:313:ASN:C	2.65	0.40
2:E:329:LEU:O	2:E:356:ARG:CZ	2.70	0.40
2:F:30:PRO:HA	2:F:31:PRO:HD3	1.98	0.40
2:F:238:THR:O	2:F:239:VAL:C	2.64	0.40
1:B:209:LYS:HZ3	2:E:356:ARG:NH1	2.18	0.40
1:B:362:ARG:HA	1:B:364:ALA:N	2.37	0.40
1:B:388:GLY:O	1:B:392:LEU:HG	2.22	0.40
1:C:206:ILE:C	1:C:208:GLN:H	2.29	0.40
2:E:425:THR:C	2:E:427:HIS:H	2.28	0.40
2:E:434:LEU:CD1	2:E:438:ILE:HD11	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:38:VAL:HG11	2:F:69:LEU:CD2	2.50	0.40
4:H:62:LEU:HD23	4:H:75:TYR:O	2.22	0.40
4:H:95:GLU:O	4:H:96:GLU:HG2	2.22	0.40

All (5) 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:45:ARG:NE	4:H:128:ARG:CZ[2_554]	1.86	0.34
1:B:45:ARG:CD	4:H:128:ARG:NH2[2_554]	2.04	0.16
1:B:45:ARG:NE	4:H:128:ARG:NH1[2_554]	2.15	0.05
1:B:45:ARG:NE	4:H:128:ARG:NH2[2_554]	2.15	0.05
1:B:26:GLU:OE2	4:H:122:ALA:O[2_554]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/553 (88%)	443 (91%)	35 (7%)	7 (1%)	9	38
1	B	475/553 (86%)	426 (90%)	42 (9%)	7 (2%)	8	38
1	C	490/553 (89%)	444 (91%)	38 (8%)	8 (2%)	7	36
2	D	465/528 (88%)	419 (90%)	43 (9%)	3 (1%)	21	58
2	E	464/528 (88%)	407 (88%)	47 (10%)	10 (2%)	5	28
2	F	464/528 (88%)	433 (93%)	29 (6%)	2 (0%)	30	67
3	G	257/298 (86%)	223 (87%)	26 (10%)	8 (3%)	3	21
4	H	129/168 (77%)	118 (92%)	8 (6%)	3 (2%)	5	27
5	I	45/51 (88%)	36 (80%)	4 (9%)	5 (11%)	0	6
All	All	3274/3760 (87%)	2949 (90%)	272 (8%)	53 (2%)	7	36

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	407	GLY
2	E	393	MET
4	H	71	THR
5	I	29	GLU
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
5	I	36	LYS
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
4	H	49	ALA

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Mol	Chain	Res	Type
4	H	79	SER
5	I	28	THR
5	I	42	ILE
1	B	458	PRO
2	E	28	GLY
2	E	243	PHE
2	E	279	VAL
2	F	279	VAL
1	B	68	PRO
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	17
1	B	388/444 (87%)	336 (87%)	52 (13%)	4	15
1	C	397/444 (89%)	359 (90%)	38 (10%)	8	25
2	D	377/417 (90%)	344 (91%)	33 (9%)	9	29
2	E	376/417 (90%)	335 (89%)	41 (11%)	6	21
2	F	376/417 (90%)	343 (91%)	33 (9%)	9	29
3	G	225/251 (90%)	208 (92%)	17 (8%)	12	33
4	H	104/128 (81%)	99 (95%)	5 (5%)	23	45
5	I	38/42 (90%)	34 (90%)	4 (10%)	6	22
All	All	2674/3004 (89%)	2401 (90%)	273 (10%)	7	23

All (273) 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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	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

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Mol	Chain	Res	Type
1	B	400	VAL
1	B	416	GLN
1	B	423	ARG
1	B	430	GLN
1	B	442	VAL
1	B	444	VAL
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

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Mol	Chain	Res	Type
1	C	406	PHE
1	C	440	GLU
1	C	444	VAL
1	C	469	LEU
1	C	474	SER
1	C	477	GLN
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

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Mol	Chain	Res	Type
2	D	452	LEU
2	D	475	GLU
2	E	9	THR
2	E	36	LEU
2	E	67	GLU
2	E	89	GLU
2	E	95	MET
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
3	G	213	ILE
3	G	262	LEU
4	H	54	THR
4	H	57	VAL
4	H	91	GLN
4	H	105	LEU
4	H	112	LEU
5	I	1	VAL
5	I	37	THR
5	I	41	THR
5	I	42	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	GLN
1	A	280	GLN
1	A	349	GLN
1	A	396	GLN
1	A	476	HIS
1	B	42	HIS
1	B	65	ASN
1	B	215	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
1	C	475	GLN
2	D	24	GLN
2	D	130	GLN

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Mol	Chain	Res	Type
2	D	171	ASN
2	D	221	GLN
2	D	223	ASN
2	D	282	GLN
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
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	225	GLN
3	G	234	ASN
4	H	91	GLN
4	H	111	ASN
5	I	16	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 [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%)	0.72	30 (6%) 26 29	70, 70, 70, 70	0
1	B	479/553 (86%)	0.77	35 (7%) 21 24	70, 70, 70, 70	0
1	C	492/553 (88%)	0.80	37 (7%) 20 24	70, 70, 70, 70	0
2	D	467/528 (88%)	0.84	45 (9%) 13 18	70, 70, 70, 70	0
2	E	466/528 (88%)	0.72	22 (4%) 36 34	70, 70, 70, 70	0
2	F	466/528 (88%)	0.70	26 (5%) 30 31	70, 70, 70, 70	0
3	G	263/298 (88%)	0.86	27 (10%) 12 17	36, 68, 116, 133	0
4	H	131/168 (77%)	0.94	11 (8%) 17 22	67, 97, 131, 136	0
5	I	47/51 (92%)	0.65	2 (4%) 40 36	58, 91, 127, 129	0
All	All	3298/3760 (87%)	0.77	235 (7%) 22 25	36, 70, 90, 136	0

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	510	ALA	5.2
3	G	22	SER	5.1
2	D	160	VAL	5.0
2	D	162	LYS	4.7
3	G	269	ALA	4.7
1	C	125	ALA	4.5
2	D	159	GLY	4.5
2	D	157	GLY	4.3
1	A	497	LEU	4.1
2	D	163	THR	3.9
3	G	251	ASN	3.7
4	H	122	ALA	3.7
1	C	417	LEU	3.7
2	D	378	LEU	3.6
2	E	280	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	180	TYR	3.6
2	F	162	LYS	3.6
1	A	487	GLY	3.6
1	C	205	ALA	3.6
2	D	249	GLN	3.5
1	A	417	LEU	3.4
1	A	408	SER	3.4
1	A	176	THR	3.4
1	A	402	ALA	3.3
2	D	337	ARG	3.3
4	H	115	ALA	3.3
1	C	408	SER	3.2
3	G	247	THR	3.2
2	E	457	PHE	3.2
1	C	398	ARG	3.2
2	F	317	LEU	3.2
2	E	390	ILE	3.2
2	D	115	ALA	3.2
1	A	414	THR	3.1
1	C	123	SER	3.1
1	C	282	SER	3.1
2	D	161	GLY	3.1
2	D	173	VAL	3.1
1	A	504	PHE	3.1
3	G	248	LEU	3.1
1	B	233	SER	3.1
1	B	274	GLN	3.0
1	C	104	LEU	3.0
3	G	243	ILE	3.0
1	B	510	ALA	3.0
1	A	394	LEU	3.0
1	A	405	GLN	3.0
3	G	239	ALA	2.9
2	E	169	LEU	2.9
3	G	1	ALA	2.9
2	D	448	GLU	2.9
2	D	174	ALA	2.9
2	F	165	LEU	2.9
1	B	101	GLU	2.9
1	B	182	THR	2.9
1	B	64	LEU	2.9
1	B	39	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
4	H	126	ALA	2.8
2	D	51	GLN	2.8
1	B	205	ALA	2.8
1	B	504	PHE	2.8
1	C	178	ILE	2.7
3	G	46	VAL	2.7
1	B	493	SER	2.7
2	F	390	ILE	2.7
1	C	208	GLN	2.7
2	D	462	PRO	2.7
1	B	296	GLY	2.7
2	D	392	GLY	2.7
1	B	239	ALA	2.7
2	D	270	ALA	2.7
2	D	98	ILE	2.7
2	F	425	THR	2.7
2	F	51	GLN	2.7
2	F	289	MET	2.7
3	G	235	ALA	2.6
2	E	307	VAL	2.6
3	G	264	GLU	2.6
2	D	158	ALA	2.6
1	C	265	LEU	2.6
1	C	176	THR	2.6
1	B	129	VAL	2.6
3	G	261	GLU	2.6
2	E	10	THR	2.6
1	A	499	GLU	2.6
1	A	388	GLY	2.6
2	F	335	LEU	2.6
1	B	178	ILE	2.6
1	C	364	ALA	2.6
1	A	500	ILE	2.6
2	D	461	GLY	2.5
2	D	296	ILE	2.5
1	A	357	PHE	2.5
2	D	9	THR	2.5
2	D	268	VAL	2.5
3	G	189	SER	2.5
1	C	271	LEU	2.5
2	E	272	LEU	2.5
1	B	412	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	384	LEU	2.5
2	D	220	GLY	2.5
1	B	264	ALA	2.5
2	F	403	THR	2.5
4	H	127	THR	2.5
1	B	257	PHE	2.5
2	F	346	PRO	2.5
2	F	404	VAL	2.5
1	A	401	ALA	2.5
2	E	211	ALA	2.5
1	C	324	LEU	2.4
1	C	183	ILE	2.4
1	C	292	GLU	2.4
2	F	104	GLU	2.4
2	F	405	SER	2.4
1	B	174	GLY	2.4
4	H	105	LEU	2.4
2	D	276	PRO	2.4
1	B	375	GLY	2.4
2	F	72	GLY	2.4
1	B	137	ILE	2.4
3	G	272	LEU	2.4
2	D	418	PHE	2.4
2	D	275	ILE	2.4
1	B	207	GLY	2.4
2	E	123	PHE	2.4
1	B	213	VAL	2.4
2	D	83	ARG	2.4
2	D	169	LEU	2.4
4	H	39	PRO	2.3
1	A	172	GLN	2.3
1	A	207	GLY	2.3
1	B	492	GLU	2.3
2	E	239	VAL	2.3
2	F	337	ARG	2.3
2	F	352	ASP	2.3
1	C	403	PHE	2.3
1	C	467	ALA	2.3
2	D	395	GLU	2.3
2	D	440	GLY	2.3
2	E	271	LEU	2.3
1	B	328	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	349	GLN	2.3
2	D	344	ILE	2.3
1	C	193	THR	2.3
1	A	304	ARG	2.3
1	A	56	SER	2.3
1	C	291	ARG	2.3
1	C	182	THR	2.3
2	D	353	SER	2.3
1	A	288	PRO	2.3
1	A	103	LEU	2.3
1	A	270	ASP	2.3
1	C	229	THR	2.2
2	F	9	THR	2.2
1	B	271	LEU	2.2
2	E	18	GLY	2.2
2	E	383	SER	2.2
5	I	1	VAL	2.2
3	G	255	GLN	2.2
1	C	343	ILE	2.2
2	E	344	ILE	2.2
2	F	56	SER	2.2
3	G	200	VAL	2.2
2	F	199	GLU	2.2
3	G	56	ASP	2.2
3	G	192	ILE	2.2
4	H	143	LYS	2.2
1	A	72	GLY	2.2
3	G	244	ASP	2.2
1	A	174	GLY	2.2
2	F	75	VAL	2.2
1	C	287	ARG	2.2
1	A	320	SER	2.2
1	B	304	ARG	2.2
4	H	97	ALA	2.2
2	D	345	TYR	2.2
2	D	164	VAL	2.2
1	B	234	ALA	2.2
3	G	268	GLY	2.2
1	C	257	PHE	2.2
1	A	390	MET	2.2
3	G	23	MET	2.2
1	B	270	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	19	ALA	2.1
1	B	175	LYS	2.1
1	C	56	SER	2.1
2	E	458	TYR	2.1
2	D	27	GLU	2.1
3	G	197	ASP	2.1
2	F	391	LEU	2.1
2	F	393	MET	2.1
3	G	48	SER	2.1
4	H	68	GLU	2.1
1	C	121	ILE	2.1
1	C	361	ILE	2.1
2	E	444	ILE	2.1
2	F	292	MET	2.1
2	F	332	THR	2.1
3	G	59	THR	2.1
1	C	233	SER	2.1
3	G	240	SER	2.1
2	D	391	LEU	2.1
1	A	303	SER	2.1
2	D	347	ALA	2.1
2	E	159	GLY	2.1
2	D	377	ILE	2.1
1	B	448	GLY	2.1
1	B	167	ILE	2.1
2	D	304	ILE	2.1
1	C	344	SER	2.1
2	E	397	SER	2.1
2	D	146	TYR	2.1
1	A	189	PHE	2.1
1	C	174	GLY	2.1
5	I	6	GLN	2.1
1	B	63	SER	2.1
2	F	399	GLU	2.1
2	E	386	ASP	2.0
3	G	187	ALA	2.0
4	H	131	ILE	2.0
1	B	416	GLN	2.0
4	H	54	THR	2.0
1	C	352	LEU	2.0
1	C	356	LEU	2.0
3	G	18	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	377	ALA	2.0
1	C	508	PHE	2.0
2	F	243	PHE	2.0
2	E	179	GLY	2.0
1	B	172	GLN	2.0
1	C	354	THR	2.0
2	D	10	THR	2.0
2	E	90	THR	2.0
2	E	213	SER	2.0
1	A	351	PHE	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.