



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:12 AM GMT

PDB ID : 2W6H
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

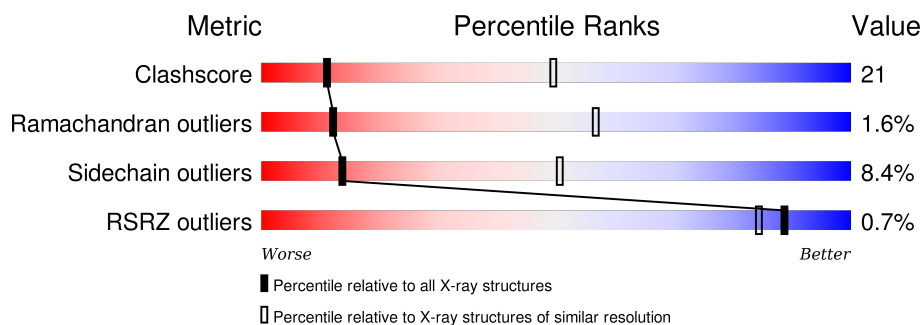
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	102246	1019 (6.22-3.66)
Ramachandran outliers	100387	1158 (6.22-3.60)
Sidechain outliers	100360	1136 (6.22-3.60)
RSRZ outliers	91569	1122 (6.22-3.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>47%</div> <div>33%</div> <div>7%</div> <div>•</div> <div>12%</div> </div>
1	B	553	<div> <div>48%</div> <div>32%</div> <div>6%</div> <div>•</div> <div>13%</div> </div>
1	C	553	<div> <div>53%</div> <div>32%</div> <div>•</div> <div>•</div> <div>11%</div> </div>
2	D	528	<div> <div>55%</div> <div>28%</div> <div>•</div> <div>•</div> <div>12%</div> </div>
2	E	528	<div> <div>%</div> <div>46%</div> <div>36%</div> <div>6%</div> <div>•</div> <div>12%</div> </div>
2	F	528	<div> <div>56%</div> <div>28%</div> <div>•</div> <div>•</div> <div>12%</div> </div>
3	G	298	<div> <div>%</div> <div>50%</div> <div>33%</div> <div>5%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
4	H	168	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>6%40%34%•22%</div></div>
5	I	51	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>55%29%6%•8%</div></div>

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			

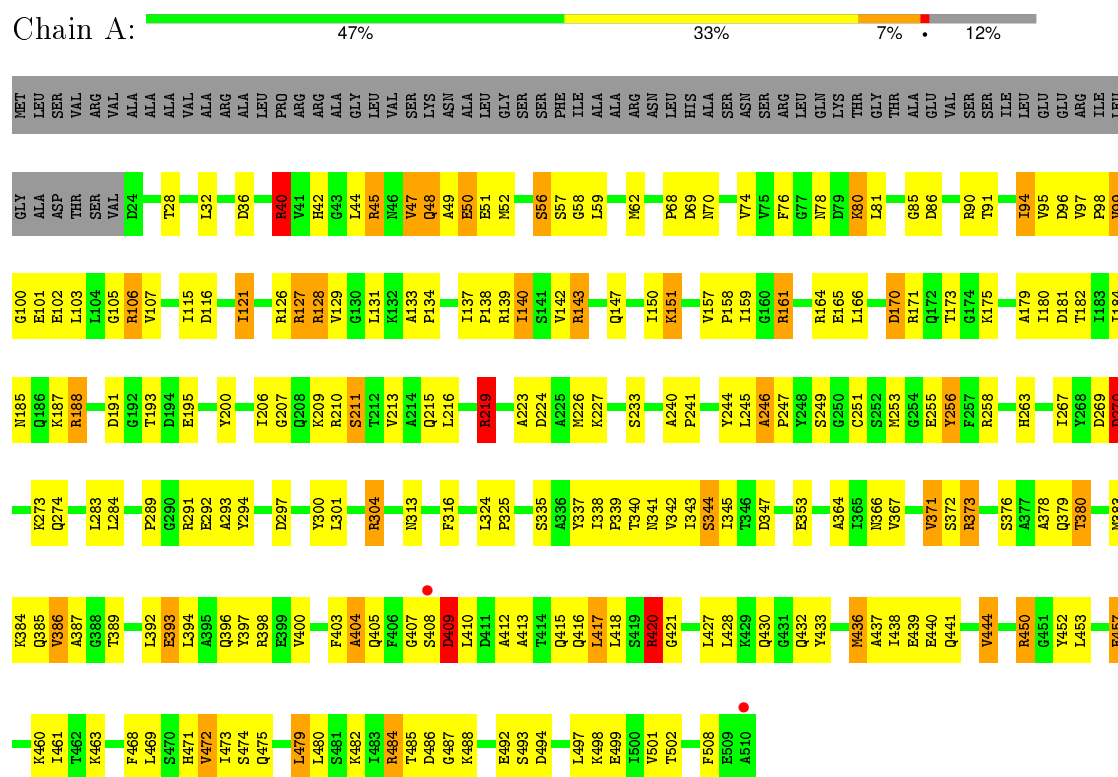
- Molecule 5 is a protein called ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL.

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

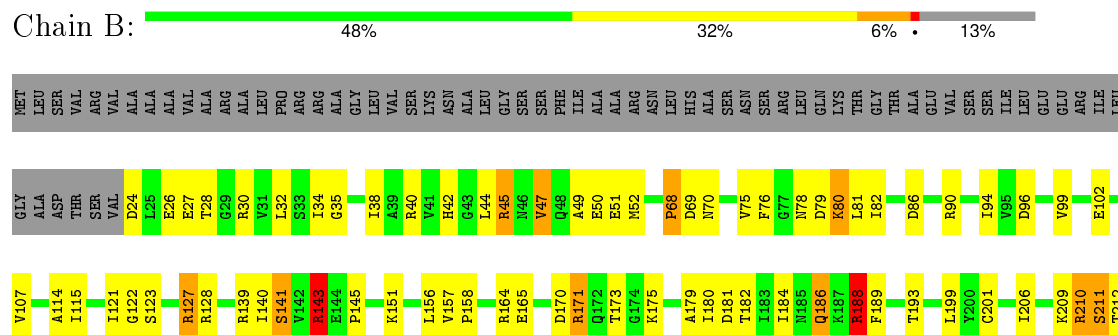
3 Residue-property plots

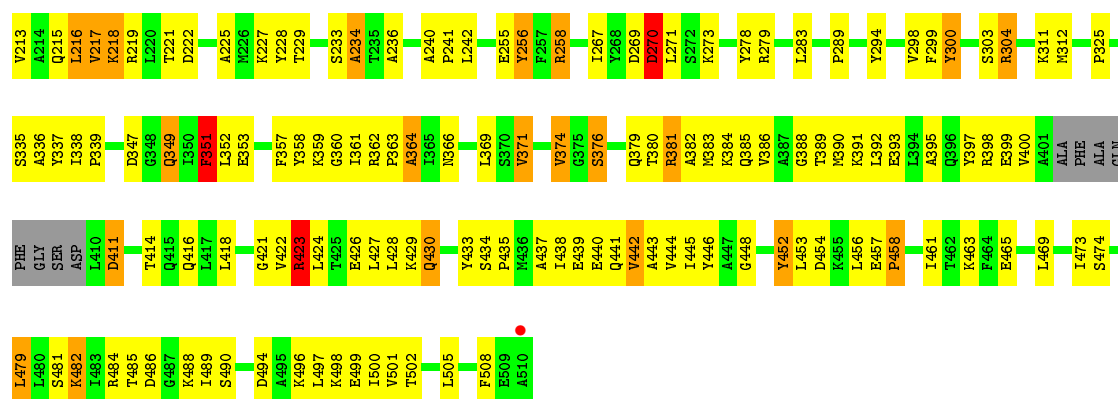
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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



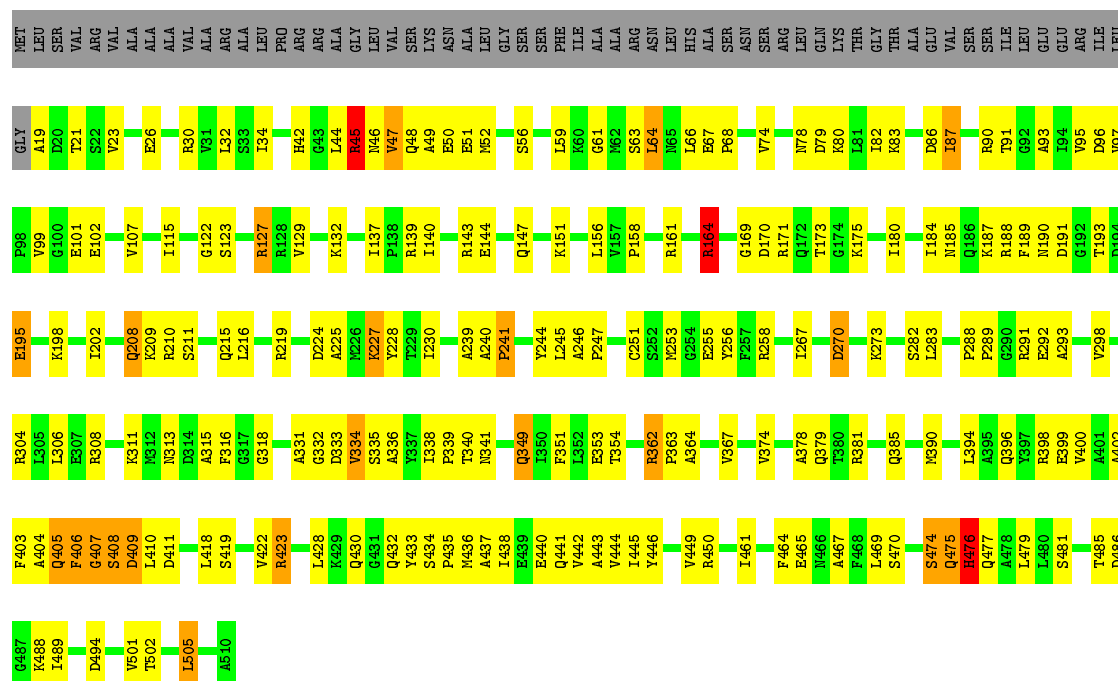
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL





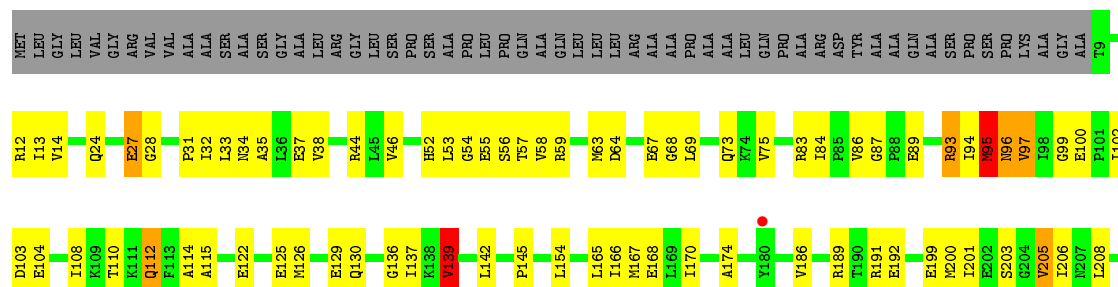
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL

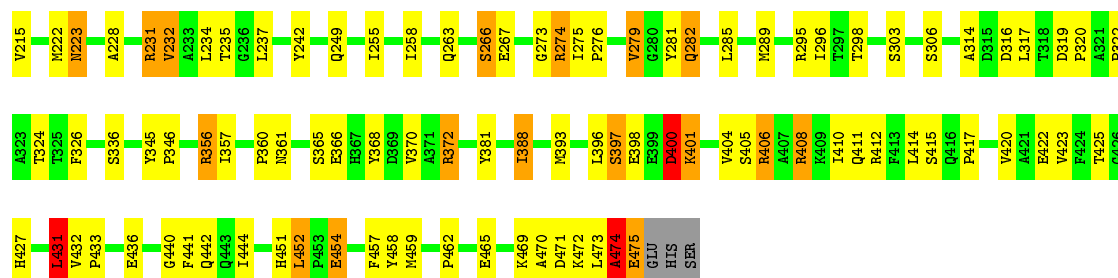
Chain C: 53% 32% 11%



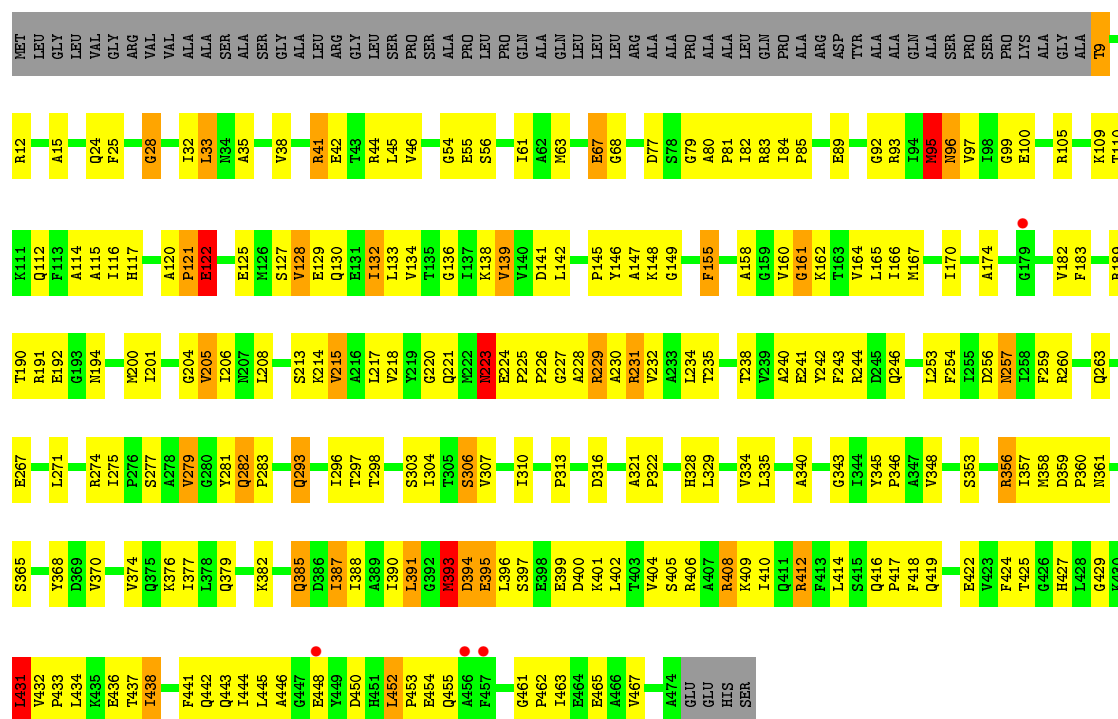
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain D: 55% 28% 12%

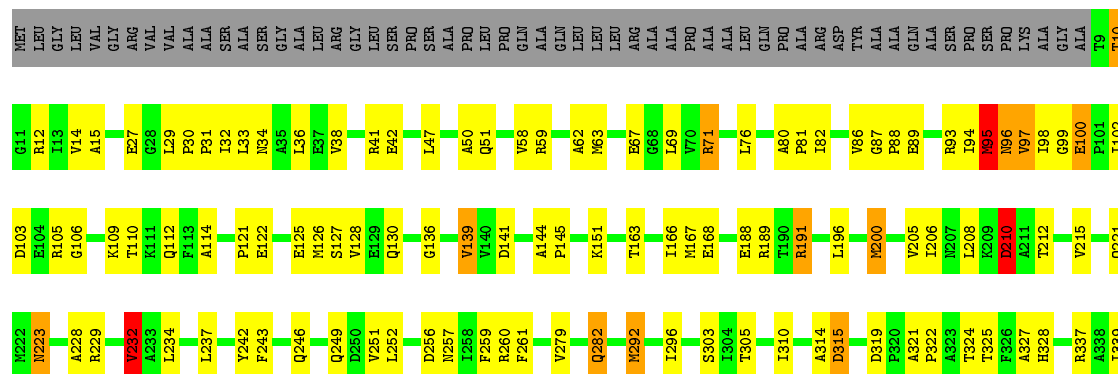


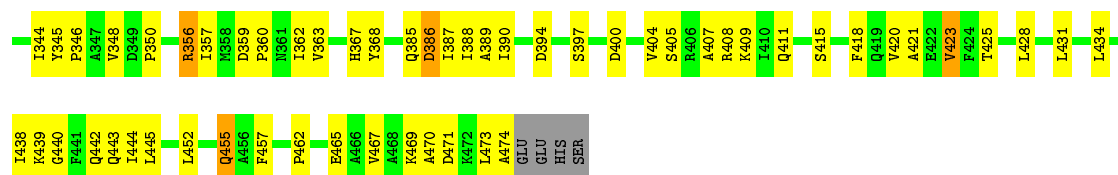


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

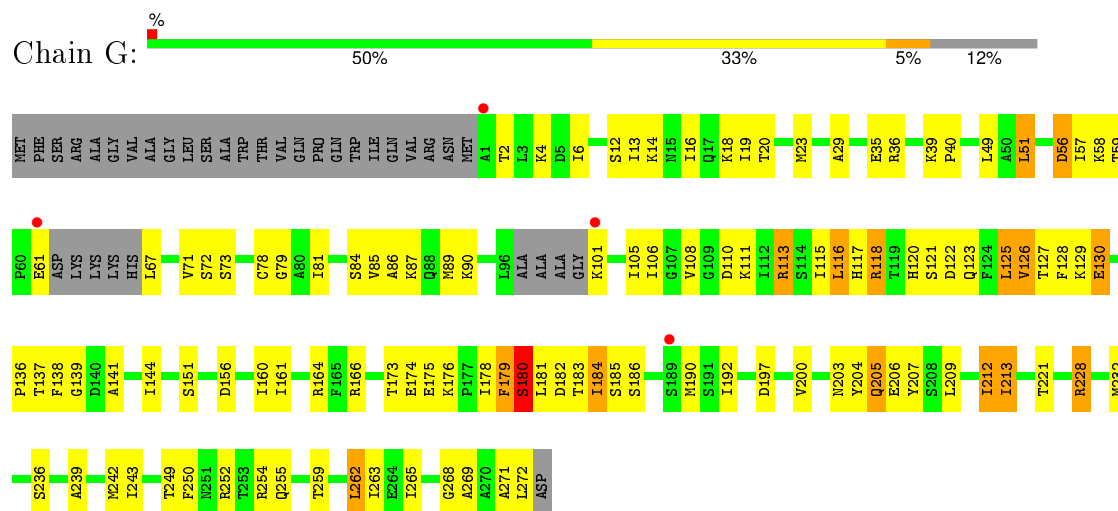


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

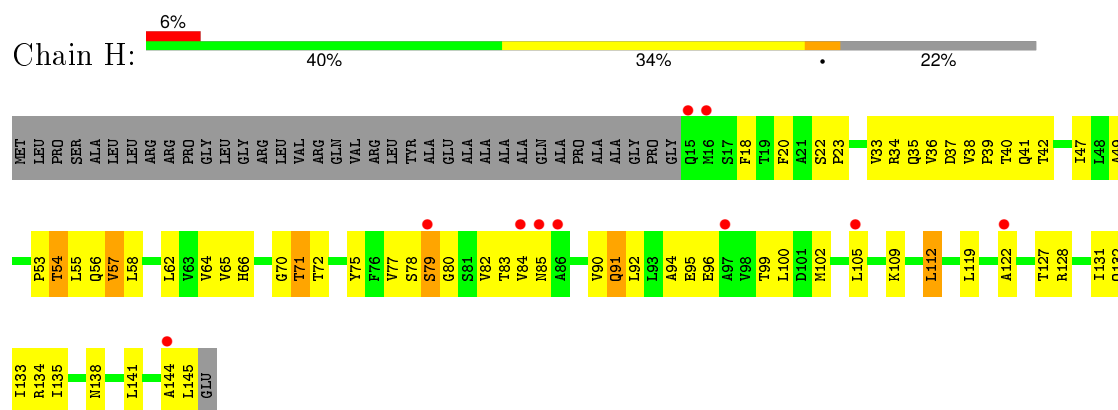




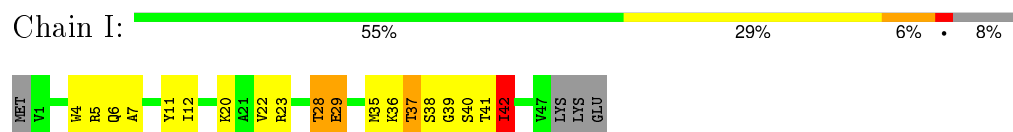
- Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL



- 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 61.85 – 5.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.14-5.00) 97.2 (61.85-5.00)	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.	DCC
Wilson B-factor (Å ²)	88.5	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 75.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 17754 reflections	Xtriage
F_o, F_c correlation	0.80	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.60	0/3766	1.31	28/5080 (0.6%)
1	B	0.60	0/3704	1.36	33/4995 (0.7%)
1	C	0.62	0/3799	1.38	24/5126 (0.5%)
2	D	0.62	0/3596	1.36	23/4879 (0.5%)
2	E	0.60	0/3587	1.32	18/4867 (0.4%)
2	F	0.62	0/3587	1.36	28/4867 (0.6%)
3	G	0.35	0/2074	0.72	3/2785 (0.1%)
4	H	0.33	0/982	0.67	0/1337
5	I	0.34	0/374	0.71	0/501
All	All	0.58	0/25469	1.28	157/34437 (0.5%)

There are no bond length outliers.

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	408	ARG	CD-NE-CZ	23.33	156.26	123.60
2	E	408	ARG	CD-NE-CZ	13.96	143.15	123.60
1	C	291	ARG	NE-CZ-NH2	-13.47	113.56	120.30
1	B	40	ARG	NE-CZ-NH1	13.07	126.83	120.30
1	B	279	ARG	NE-CZ-NH1	12.84	126.72	120.30
2	F	356	ARG	NE-CZ-NH1	11.65	126.12	120.30
2	D	406	ARG	NE-CZ-NH1	-11.56	114.52	120.30
2	F	59	ARG	NE-CZ-NH1	-11.38	114.61	120.30
2	D	408	ARG	NE-CZ-NH1	11.12	125.86	120.30
1	B	219	ARG	NE-CZ-NH2	10.37	125.48	120.30
2	F	282	GLN	CB-CG-CD	10.31	138.42	111.60
1	C	164	ARG	NE-CZ-NH1	-10.03	115.28	120.30
1	C	258	ARG	NE-CZ-NH1	9.95	125.27	120.30
1	B	40	ARG	CD-NE-CZ	9.87	137.42	123.60
2	F	229	ARG	NE-CZ-NH1	-9.55	115.52	120.30
2	F	356	ARG	NE-CZ-NH2	-9.40	115.60	120.30
2	F	59	ARG	NE-CZ-NH2	9.18	124.89	120.30
2	F	95	MET	CA-CB-CG	9.13	128.82	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	161	ARG	NE-CZ-NH1	9.11	124.86	120.30
2	D	44	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	B	304	ARG	NE-CZ-NH1	-9.07	115.77	120.30
1	A	420	ARG	NE-CZ-NH1	-8.85	115.87	120.30
2	E	260	ARG	NE-CZ-NH1	-8.57	116.02	120.30
2	F	96	ASN	CB-CA-C	-8.55	93.30	110.40
1	A	373	ARG	NE-CZ-NH2	8.51	124.56	120.30
1	A	398	ARG	NE-CZ-NH1	-8.51	116.04	120.30
2	E	95	MET	CA-CB-CG	8.51	127.77	113.30
2	E	83	ARG	NE-CZ-NH1	-8.49	116.06	120.30
1	C	450	ARG	NE-CZ-NH2	-8.43	116.09	120.30
1	A	450	ARG	NE-CZ-NH2	-8.27	116.16	120.30
1	C	127	ARG	NE-CZ-NH1	-8.13	116.24	120.30
2	F	229	ARG	NE-CZ-NH2	8.01	124.31	120.30
1	C	362	ARG	NE-CZ-NH2	7.97	124.29	120.30
2	D	125	GLU	OE1-CD-OE2	-7.93	113.79	123.30
1	B	304	ARG	NE-CZ-NH2	7.92	124.26	120.30
2	E	229	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	B	219	ARG	NE-CZ-NH1	-7.71	116.45	120.30
2	F	408	ARG	NE-CZ-NH2	7.55	124.07	120.30
1	B	279	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	C	450	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	B	270	ASP	CB-CA-C	-7.38	95.64	110.40
1	C	304	ARG	NE-CZ-NH2	7.37	123.98	120.30
1	C	161	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	B	258	ARG	CD-NE-CZ	7.19	133.66	123.60
2	E	356	ARG	NE-CZ-NH1	7.18	123.89	120.30
2	E	356	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	450	ARG	NE-CZ-NH1	7.17	123.89	120.30
2	D	93	ARG	NE-CZ-NH1	-7.17	116.71	120.30
2	E	41	ARG	CD-NE-CZ	7.14	133.59	123.60
1	A	270	ASP	CB-CA-C	-7.12	96.17	110.40
2	F	139	VAL	CB-CA-C	-7.07	97.96	111.40
1	B	279	ARG	CD-NE-CZ	6.95	133.33	123.60
1	C	45	ARG	NE-CZ-NH2	-6.92	116.84	120.30
2	F	95	MET	C-N-CA	6.75	138.58	121.70
2	D	95	MET	C-N-CA	6.68	138.40	121.70
2	D	96	ASN	CB-CA-C	-6.66	97.08	110.40
1	B	349	GLN	CA-CB-CG	6.61	127.93	113.40
1	C	308	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	B	423	ARG	CD-NE-CZ	6.54	132.76	123.60
1	A	127	ARG	NE-CZ-NH2	-6.52	117.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	191	ARG	NE-CZ-NH1	-6.51	117.05	120.30
2	D	231	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	B	270	ASP	CB-CG-OD1	6.48	124.13	118.30
1	A	106	ARG	CD-NE-CZ	6.47	132.66	123.60
2	D	274	ARG	NE-CZ-NH1	-6.46	117.07	120.30
2	F	256	ASP	CB-CG-OD1	6.46	124.11	118.30
2	F	189	ARG	NE-CZ-NH2	6.44	123.52	120.30
2	D	59	ARG	NE-CZ-NH1	-6.43	117.08	120.30
1	A	371	VAL	CB-CA-C	-6.41	99.22	111.40
1	A	372	SER	N-CA-CB	6.41	120.11	110.50
2	E	44	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	C	308	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	A	170	ASP	CB-CG-OD1	6.39	124.05	118.30
2	E	431	LEU	CA-CB-CG	6.37	129.95	115.30
1	A	398	ARG	NE-CZ-NH2	6.29	123.45	120.30
1	C	291	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	171	ARG	NE-CZ-NH2	6.27	123.44	120.30
2	F	12	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	210	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	B	127	ARG	CD-NE-CZ	6.22	132.31	123.60
2	D	372	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	C	381	ARG	CD-NE-CZ	6.18	132.25	123.60
1	C	476	HIS	N-CA-C	6.16	127.63	111.00
1	B	128	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	B	371	VAL	CB-CA-C	-6.13	99.75	111.40
1	B	300	TYR	CB-CG-CD2	-6.09	117.34	121.00
2	F	97	VAL	CB-CA-C	-6.09	99.83	111.40
1	C	423	ARG	CD-NE-CZ	6.03	132.04	123.60
2	E	274	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	C	164	ARG	CD-NE-CZ	-5.97	115.24	123.60
2	D	222	MET	CB-CA-C	-5.93	98.54	110.40
1	A	269	ASP	C-N-CA	5.84	136.29	121.70
3	G	254	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	B	398	ARG	NE-CZ-NH1	-5.81	117.39	120.30
1	A	40	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	B	337	TYR	CB-CG-CD1	5.74	124.45	121.00
1	B	139	ARG	NE-CZ-NH1	5.71	123.16	120.30
2	F	41	ARG	CG-CD-NE	5.70	123.76	111.80
1	A	219	ARG	CD-NE-CZ	5.68	131.55	123.60
2	F	103	ASP	CB-CG-OD2	-5.66	113.20	118.30
2	D	139	VAL	CB-CA-C	-5.65	100.67	111.40
2	D	474	ALA	C-N-CA	5.61	135.72	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	297	ASP	CB-CG-OD2	-5.58	113.28	118.30
2	D	431	LEU	CA-CB-CG	5.57	128.10	115.30
2	F	191	ARG	NE-CZ-NH2	-5.57	117.52	120.30
2	D	454	GLU	CA-CB-CG	5.56	125.64	113.40
1	A	233	SER	N-CA-CB	-5.51	102.23	110.50
1	B	349	GLN	N-CA-CB	5.50	120.50	110.60
1	B	210	ARG	NE-CZ-NH1	-5.50	117.55	120.30
2	D	372	ARG	NE-CZ-NH1	-5.45	117.58	120.30
1	B	143	ARG	NE-CZ-NH2	5.45	123.02	120.30
1	A	335	SER	CB-CA-C	-5.43	99.79	110.10
1	C	170	ASP	CB-CG-OD1	5.42	123.18	118.30
2	E	408	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	304	ARG	NE-CZ-NH1	-5.40	117.60	120.30
2	F	191	ARG	CD-NE-CZ	5.40	131.16	123.60
1	B	222	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	C	349	GLN	CB-CA-C	-5.36	99.68	110.40
3	G	254	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	B	423	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	C	171	ARG	NE-CZ-NH2	-5.34	117.63	120.30
2	F	71	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	C	241	PRO	N-CA-CB	5.30	109.66	103.30
1	B	45	ARG	CB-CG-CD	-5.27	97.90	111.60
2	F	100	GLU	OE1-CD-OE2	5.25	129.60	123.30
2	E	93	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	B	40	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	D	12	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	B	188	ARG	CG-CD-NE	5.23	122.78	111.80
2	E	260	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	C	127	ARG	NH1-CZ-NH2	5.20	125.12	119.40
1	B	351	PHE	N-CA-CB	5.17	119.91	110.60
1	C	336	ALA	N-CA-CB	-5.17	102.86	110.10
1	A	161	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	258	ARG	CD-NE-CZ	5.16	130.82	123.60
1	B	171	ARG	NE-CZ-NH2	-5.15	117.72	120.30
2	F	423	VAL	CB-CA-C	-5.15	101.61	111.40
1	A	270	ASP	CB-CG-OD1	5.13	122.91	118.30
2	D	400	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	278	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	A	128	ARG	NE-CZ-NH1	-5.10	117.75	120.30
2	E	122	GLU	CA-CB-CG	5.09	124.61	113.40
2	F	303	SER	N-CA-CB	-5.09	102.86	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	ARG	CG-CD-NE	5.09	122.48	111.80
2	D	316	ASP	CB-CG-OD2	-5.08	113.73	118.30
2	E	96	ASN	N-CA-CB	-5.07	101.47	110.60
2	D	356	ARG	CD-NE-CZ	-5.07	116.50	123.60
2	E	223	ASN	CB-CA-C	-5.06	100.28	110.40
2	F	337	ARG	CD-NE-CZ	5.06	130.69	123.60
2	F	232	VAL	CB-CA-C	-5.06	101.79	111.40
1	A	200	TYR	CA-CB-CG	-5.03	103.85	113.40
3	G	228	ARG	NE-CZ-NH1	5.03	122.81	120.30
2	E	231	ARG	NE-CZ-NH1	-5.02	117.79	120.30
2	F	210	ASP	CB-CA-C	-5.02	100.36	110.40
1	B	234	ALA	N-CA-C	-5.01	97.47	111.00
2	F	315	ASP	CB-CG-OD1	5.00	122.80	118.30

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	160	0
1	B	3656	0	3764	149	5
1	C	3748	0	3843	146	0
2	D	3539	0	3593	147	0
2	E	3530	0	3587	193	0
2	F	3530	0	3586	125	0
3	G	2051	0	2115	136	0
4	H	970	0	972	59	5
5	I	369	0	395	20	0
All	All	25108	0	25668	1057	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 21.

All (1057) 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: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
2:D:274:ARG:C	3:G:272:LEU:HD11	1.78	1.02
2:E:223:ASN:H	2:E:223:ASN:HD22	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
1:A:215:GLN:HG3	2:D:356:ARG:HH12	1.33	0.93
1:C:404:ALA:C	1:C:406:PHE:H	1.64	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:85:ASN:HD21	4:H:91:GLN:HE22	1.13	0.91
4:H:62:LEU:HD11	4:H:144:ALA:HB2	1.49	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
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
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
3:G:161:ILE:HG12	3:G:175:GLU:HG2	1.63	0.81
2:E:132:ILE:HD12	2:E:145:PRO:HB3	1.61	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
2:D:282:GLN:H	2:D:282:GLN:HE21	1.30	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:394:ASP:CG	3:G:79:GLY:HA2	2.04	0.77
4:H:138:ASN:HA	4:H:141:LEU:HD12	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: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:89:GLU:HG3	2:E:109:LYS:O	1.87	0.74
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
3:G:121:SER:C	3:G:123:GLN:H	1.91	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:N	2:F:223:ASN:HD22	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
2:E:388:ILE:HG23	2:E:393:MET:HG3	1.73	0.71
1:C:34:ILE:HD11	1:C:79:ASP:HB2	1.71	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
2:D:84:ILE:HB	2:D:95:MET:HE3	1.74	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
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:E:391:LEU:HD22	3:G:29:ALA:CB	2.19	0.69
2:E:394:ASP:C	2:E:396:LEU:H	1.93	0.69
2:E:105:ARG:CZ	2:E:208:LEU:HD23	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:133:ILE:HD11	5:I:4:TRP:HB3	1.73	0.69
2:E:345:TYR:HA	2:E:346:PRO:C	2.13	0.69
2:F:89:GLU:HG2	2:F:110:THR:HG22	1.75	0.68
1:C:385:GLN:OE1	1:C:488:LYS:HG2	1.93	0.68
1:B:452:TYR:OH	1:B:498:LYS:HG3	1.92	0.68
1:B:283:LEU:HD12	2:E:277:SER:HB3	1.75	0.68
2:D:223:ASN:N	2:D:223:ASN:HD22	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
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
2:D:223:ASN:ND2	2:D:223:ASN:H	1.93	0.66
2:F:409:LYS:HD3	2:F:457:PHE:CE2	2.30	0.66
1:B:156:LEU:HD22	1:B:391:LYS:HD2	1.77	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
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
2:D:54:GLY:O	2:D:55:GLU:HB2	1.96	0.65
5:I:35:MET:C	5:I:37:THR:H	1.99	0.65
2:F:344:ILE:HG23	2:F:415:SER:HB3	1.79	0.65
2:D:200:MET:HB3	2:D:206:ILE:HG13	1.79	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
2:F:394:ASP:HB3	3:G:79:GLY:HA2	1.79	0.64
1:C:188:ARG:HH21	1:C:437:ALA:HB2	1.62	0.64
1:A:471:HIS:CE1	1:A:475:GLN:HG3	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:139:VAL:CG1	2:E:414:LEU:HD22	2.28	0.64
1:C:404:ALA:C	1:C:406:PHE:N	2.44	0.64
3:G:115:ILE:C	3:G:117:HIS:H	2.01	0.64
3:G:39:LYS:HB3	3:G:40:PRO:HD3	1.80	0.64
2:F:136:GLY:HA3	2:F:431:LEU:HD12	1.80	0.64
1:A:376:SER:HB3	1:A:384:LYS:HE2	1.78	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
2:E:346:PRO:HG3	2:E:418:PHE:CZ	2.33	0.64
1:B:188:ARG:HH21	1:B:437:ALA:HB2	1.62	0.64
1:B:389:THR:HA	1:B:392:LEU:CD1	2.28	0.63
2:D:393:MET:HE3	2:D:404:VAL:HG21	1.79	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
4:H:65:VAL:C	4:H:72:THR:HG23	2.19	0.63
1:C:419:SER:O	1:C:423:ARG:HG2	1.98	0.63
1:A:341:ASN:O	1:A:345:ILE:HG13	1.99	0.63
2:F:94:ILE:HG22	2:F:102:ILE:HD11	1.80	0.62
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.34	0.62
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
1:B:437:ALA:O	1:B:440:GLU:N	2.30	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:C:151:LYS:HE3	1:C:430:GLN:HG3	1.82	0.62
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.63	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
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
1:B:422:VAL:O	1:B:426:GLU:HG2	2.00	0.61
1:A:394:LEU:HD11	1:A:428:LEU:HD11	1.82	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:292:GLU:O	1:C:293:ALA:HB3	2.00	0.61
1:C:52:MET:O	1:C:91:THR:HB	1.99	0.61
1:A:376:SER:C	1:A:378:ALA:H	2.03	0.61
2:F:223:ASN:ND2	2:F:223:ASN:H	1.85	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:396:LEU:HD22	2:D:400:ASP:CB	2.30	0.61
1:B:218:LYS:HB2	2:E:128:VAL:HG12	1.82	0.61
1:B:184:ILE:HG22	1:B:435:PRO:HG2	1.81	0.61
2:E:201:ILE:HD13	2:E:208:LEU:HD11	1.81	0.61
2:E:223:ASN:ND2	2:E:223:ASN:N	2.46	0.61
4:H:54:THR:H	4:H:84:VAL:HG23	1.65	0.61
3:G:61:GLU:OE1	3:G:101:LYS:HG2	1.99	0.61
1:A:166:LEU:HA	1:A:325:PRO:HD2	1.83	0.61
2:D:93:ARG:HH11	2:D:93:ARG:HG3	1.66	0.61
2:F:390:ILE:HD11	3:G:242:MET:HE1	1.83	0.60
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
2:E:394:ASP:C	2:E:396:LEU:N	2.54	0.60
1:B:389:THR:HA	1:B:392:LEU:HD12	1.81	0.60
1:A:457:GLU:CB	1:A:460:LYS:HD3	2.32	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:E:397:SER:H	2:E:400:ASP:HB2	1.66	0.60
1:A:376:SER:C	1:A:378:ALA:N	2.55	0.60
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.37	0.60
1:A:52:MET:O	1:A:91:THR:HG23	2.01	0.60
2:E:149:GLY:HA2	2:E:304:ILE:O	2.01	0.60
3:G:178:ILE:C	3:G:180:SER:H	2.04	0.60
1:A:270:ASP:OD1	1:A:273:LYS:HG3	2.01	0.60
1:B:362:ARG:HA	1:B:363:PRO:C	2.21	0.60
1:C:362:ARG:HA	1:C:363:PRO:C	2.21	0.60
1:C:99:VAL:HG13	1:C:256:TYR:HB2	1.83	0.60
2:E:32:ILE:O	2:E:33:LEU:HB2	2.02	0.60
1:B:51:GLU:HA	1:B:94:ILE:HA	1.83	0.59
1:A:121:ILE:H	1:A:121:ILE:HD13	1.66	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
2:E:200:MET:HB3	2:E:205:VAL:HG23	1.84	0.59
1:A:439:GLU:HG2	1:A:484:ARG:HB2	1.83	0.59
1:B:411:ASP:HB3	1:B:414:THR:OG1	2.02	0.59
1:A:432:GLN:HB3	1:A:433:TYR:CD2	2.37	0.59
1:C:374:VAL:HG11	1:C:378:ALA:HB2	1.85	0.59
2:D:317:LEU:HD22	2:D:326:PHE:HZ	1.67	0.59
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:GLY:HA2	1:C:410:LEU:HD11	1.84	0.59
1:B:434:SER:N	1:B:435:PRO:HD3	2.18	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
1:B:438:ILE:O	1:B:442:VAL:HG22	2.02	0.58
1:A:157:VAL:N	1:A:158:PRO:CD	2.65	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:452:TYR:O	1:B:453:LEU:HD23	2.03	0.58
1:B:400:VAL:HB	1:B:418:LEU:HD21	1.85	0.58
2:F:105:ARG:NH1	2:F:208:LEU:HD23	2.18	0.58
2:D:186:VAL:HG13	2:D:232:VAL:HG23	1.85	0.58
1:C:406:PHE:O	1:C:408:SER:N	2.36	0.58
2:E:138:LYS:O	2:E:142:LEU:HB3	2.04	0.58
1:C:464:PHE:CE1	1:C:505:LEU:HD23	2.39	0.58
1:B:170:ASP:O	1:B:175:LYS:HE2	2.03	0.58
3:G:57:ILE:CG2	3:G:184:ILE:CD1	2.81	0.58
2:E:408:ARG:O	2:E:412:ARG:HG3	2.03	0.58
4:H:37:ASP:HB2	4:H:64:VAL:HB	1.85	0.58
5:I:5:ARG:C	5:I:7:ALA:H	2.06	0.58
1:B:499:GLU:O	1:B:502:THR:HB	2.02	0.58
2:E:95:MET:CG	2:E:99:GLY:HA2	2.34	0.58
2:D:263:GLN:O	2:D:267:GLU:HG3	2.03	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
2:F:440:GLY:O	2:F:444:ILE:HG13	2.04	0.58
2:F:29:LEU:HD12	2:F:30:PRO:HD2	1.85	0.58
2:E:433:PRO:HG2	2:E:436:GLU:HG2	1.86	0.58
2:E:267:GLU:O	2:E:271:LEU:HG	2.04	0.58
1:A:472:VAL:HG23	1:A:480:LEU:HD11	1.85	0.58
2:F:96:ASN:HD22	2:F:100:GLU:HB2	1.68	0.58
2:E:246:GLN:NE2	2:E:246:GLN:HA	2.19	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
4:H:64:VAL:HG13	4:H:72:THR:HG21	1.85	0.57
3:G:87:LYS:O	3:G:90:LYS:HG2	2.04	0.57
1:C:173:THR:CG2	1:C:354:THR:HG22	2.35	0.57
1:B:215:GLN:HE22	2:E:130:GLN:NE2	2.03	0.57
2:E:224:GLU:O	2:E:229:ARG:NH1	2.32	0.57
1:C:184:ILE:HG22	1:C:435:PRO:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:158:ALA:C	2:E:160:VAL:H	2.08	0.57
2:E:397:SER:C	2:E:399:GLU:N	2.57	0.57
4:H:65:VAL:O	4:H:72:THR:HG23	2.05	0.57
1:C:78:ASN:ND2	1:C:80:LYS:HD3	2.19	0.57
2:D:63:MET:HE3	2:D:228:ALA:HA	1.86	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
1:A:450:ARG:NH2	1:A:494:ASP:OD2	2.38	0.57
1:A:219:ARG:HH11	1:A:219:ARG:HB2	1.69	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
2:D:84:ILE:HD12	2:D:95:MET:HE1	1.86	0.57
3:G:184:ILE:C	3:G:186:SER:H	2.08	0.57
2:E:105:ARG:NH2	2:E:208:LEU:HA	2.20	0.57
1:C:156:LEU:HD13	1:C:367:VAL:HG22	1.86	0.57
2:D:473:LEU:C	2:D:475:GLU:H	2.07	0.57
1:C:187:LYS:HE2	1:C:191:ASP:OD2	2.05	0.56
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.86	0.56
1:A:107:VAL:HG12	1:A:115:ILE:HD11	1.87	0.56
1:B:51:GLU:OE2	1:B:90:ARG:HB3	2.05	0.56
3:G:57:ILE:HG22	3:G:184:ILE:HD12	1.87	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
3:G:164:ARG:NH2	3:G:166:ARG:HD3	2.20	0.56
2:E:84:ILE:HB	2:E:95:MET:HE1	1.87	0.56
1:B:357:PHE:CE1	1:B:362:ARG:HD3	2.40	0.56
1:B:347:ASP:HB3	1:B:374:VAL:HG22	1.88	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:F:98:ILE:HG13	2:F:100:GLU:HG3	1.88	0.56
2:F:14:VAL:O	2:F:71:ARG:HG2	2.05	0.56
1:C:219:ARG:HD3	1:C:433:TYR:CE1	2.41	0.56
1:A:99:VAL:CG2	1:A:253:MET:HA	2.36	0.56
1:B:393:GLU:OE1	1:B:424:LEU:HD11	2.05	0.56
3:G:71:VAL:HG13	3:G:108:VAL:HG22	1.88	0.56
2:D:366:GLU:HG3	2:D:442:GLN:HE22	1.71	0.56
1:B:351:PHE:CE1	1:B:369:LEU:HB3	2.40	0.56
2:D:425:THR:HG21	2:D:459:MET:HE1	1.87	0.55
3:G:181:LEU:HG	3:G:183:THR:HB	1.89	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LYS:HG3	1:B:81:LEU:HD23	1.88	0.55
2:F:32:ILE:O	2:F:33:LEU:HB2	2.05	0.55
1:A:291:ARG:N	3:G:262:LEU:HD21	2.21	0.55
2:F:390:ILE:CD1	3:G:242:MET:CE	2.84	0.55
2:E:396:LEU:HB3	2:E:401:LYS:HG2	1.88	0.55
2:E:244:ARG:HG3	2:E:303:SER:N	2.22	0.55
3:G:164:ARG:HD3	3:G:174:GLU:OE2	2.07	0.55
3:G:160:ILE:CG2	3:G:176:LYS:HB2	2.37	0.55
1:A:185:ASN:O	1:A:188:ARG:HG3	2.05	0.55
1:C:408:SER:O	1:C:409:ASP:C	2.44	0.55
1:C:442:VAL:CG1	1:C:489:ILE:HD11	2.37	0.55
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.89	0.55
4:H:22:SER:HB2	4:H:23:PRO:HD2	1.89	0.55
2:F:63:MET:CE	2:F:97:VAL:HG11	2.36	0.55
2:F:10:THR:HG23	2:F:76:LEU:HD12	1.88	0.55
1:C:433:TYR:C	1:C:435:PRO:HD3	2.26	0.55
3:G:137:THR:HG21	5:I:39:GLY:N	2.19	0.55
2:E:138:LYS:HG3	2:E:416:GLN:OE1	2.06	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
3:G:117:HIS:CE1	3:G:121:SER:HB2	2.42	0.55
1:A:207:GLY:HA3	1:A:273:LYS:HD3	1.89	0.55
2:D:274:ARG:C	3:G:272:LEU:CD1	2.65	0.55
3:G:181:LEU:HB3	3:G:184:ILE:HG22	1.89	0.55
2:D:142:LEU:HD22	2:D:441:PHE:CD2	2.42	0.55
1:A:159:ILE:HD12	1:A:165:GLU:HG2	1.88	0.55
2:E:263:GLN:O	2:E:267:GLU:HG3	2.07	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
3:G:207:TYR:HA	5:I:12:ILE:CD1	2.37	0.54
2:E:77:ASP:OD1	2:E:79:GLY:N	2.34	0.54
2:E:397:SER:O	2:E:401:LYS:HG3	2.07	0.54
2:D:83:ARG:HA	2:D:114:ALA:O	2.07	0.54
1:C:52:MET:HG3	1:C:61:GLY:O	2.07	0.54
1:A:100:GLY:HA2	1:A:256:TYR:CE1	2.42	0.54
2:D:87:GLY:HA2	2:D:242:TYR:CE2	2.42	0.54
1:B:441:GLN:O	1:B:445:ILE:HG12	2.08	0.54
2:D:396:LEU:HD22	2:D:400:ASP:HB3	1.89	0.54
3:G:121:SER:C	3:G:123:GLN:N	2.60	0.54
1:A:457:GLU:HB3	1:A:460:LYS:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ARG:HH11	1:A:263:HIS:CG	2.25	0.54
1:B:114:ALA:HB2	1:B:121:ILE:HD11	1.89	0.54
2:D:388:ILE:HD12	2:D:393:MET:SD	2.48	0.54
3:G:117:HIS:O	3:G:120:HIS:N	2.35	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:451:HIS:CD2	2:D:452:LEU:HD23	2.42	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
3:G:86:ALA:HA	3:G:89:MET:HE2	1.90	0.54
2:D:282:GLN:H	2:D:282:GLN:NE2	2.01	0.54
1:C:102:GLU:HG2	1:C:122:GLY:O	2.06	0.54
2:D:275:ILE:CG2	3:G:269:ALA:CB	2.72	0.54
2:D:417:PRO:HB3	2:D:459:MET:HE3	1.90	0.54
2:E:395:GLU:HG3	3:G:36:ARG:HH22	1.72	0.54
1:A:373:ARG:HG3	1:A:373:ARG:HH11	1.72	0.54
3:G:181:LEU:O	3:G:184:ILE:HG22	2.08	0.54
5:I:28:THR:O	5:I:29:GLU:HB2	2.08	0.54
2:D:122:GLU:HA	2:D:122:GLU:OE1	2.07	0.54
1:C:405:GLN:C	1:C:406:PHE:HD1	2.11	0.54
2:D:412:ARG:HG3	2:D:412:ARG:HH11	1.73	0.54
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
1:B:446:TYR:CD2	1:B:497:LEU:HD23	2.43	0.53
2:F:96:ASN:HB2	2:F:100:GLU:H	1.73	0.53
2:E:174:ALA:HB2	2:E:214:LYS:HD3	1.89	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
3:G:117:HIS:ND1	3:G:118:ARG:HA	2.22	0.53
1:A:452:TYR:OH	1:A:498:LYS:HG3	2.08	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
2:E:201:ILE:CD1	2:E:208:LEU:HD11	2.37	0.53
2:D:167:MET:CB	2:D:420:VAL:HG11	2.38	0.53
1:C:91:THR:HG22	1:C:93:ALA:H	1.72	0.53
1:A:463:LYS:HD3	1:A:508:PHE:HZ	1.73	0.53
2:E:81:PRO:HG2	2:E:115:ALA:HB1	1.91	0.53
2:F:210:ASP:HB2	2:F:212:THR:HG23	1.91	0.53
3:G:39:LYS:HB3	3:G:40:PRO:CD	2.38	0.53
2:F:439:LYS:HE3	2:F:443:GLN:HE22	1.73	0.53
2:D:422:GLU:HG2	2:D:427:HIS:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:LEU:HD11	1:C:428:LEU:HD13	1.91	0.53
2:D:381:TYR:HE2	2:D:411:GLN:HE22	1.56	0.53
1:A:179:ALA:HB1	1:A:267:ILE:HG12	1.91	0.53
1:C:239:ALA:HB1	1:C:241:PRO:HD2	1.90	0.53
1:B:69:ASP:O	1:B:70:ASN:HB3	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:150:ILE:HA	1:A:430:GLN:OE1	2.08	0.53
1:B:180:ILE:O	1:B:181:ASP:C	2.47	0.53
1:B:44:LEU:O	1:B:47:VAL:HG22	2.09	0.53
1:A:170:ASP:O	1:A:175:LYS:HE2	2.08	0.53
2:D:31:PRO:HD2	2:D:34:ASN:ND2	2.24	0.53
2:D:356:ARG:HG2	2:D:356:ARG:O	2.09	0.52
1:A:468:PHE:CE1	1:A:501:VAL:HG12	2.43	0.52
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.75	0.52
1:B:140:ILE:HG23	1:B:311:LYS:HG3	1.92	0.52
2:D:136:GLY:CA	2:D:431:LEU:HD13	2.37	0.52
1:B:423:ARG:HD2	1:B:461:ILE:HD11	1.91	0.52
2:E:254:PHE:CD1	2:E:307:VAL:HB	2.45	0.52
2:D:431:LEU:C	2:D:431:LEU:HD12	2.29	0.52
2:E:218:VAL:HG11	2:E:235:THR:CG2	2.38	0.52
1:B:358:TYR:C	1:B:360:GLY:H	2.12	0.52
2:E:220:GLY:HA3	2:E:232:VAL:HG21	1.91	0.52
2:D:366:GLU:CG	2:D:442:GLN:HE22	2.23	0.52
2:E:334:VAL:HG23	2:E:353:SER:HA	1.92	0.52
1:C:267:ILE:N	1:C:267:ILE:HD12	2.25	0.52
2:E:377:ILE:HG21	2:E:410:ILE:CD1	2.40	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
4:H:127:THR:O	4:H:131:ILE:HG12	2.10	0.52
2:E:82:ILE:HB	2:E:116:ILE:HD13	1.92	0.52
2:F:360:PRO:HD3	2:F:368:TYR:CD2	2.45	0.52
4:H:34:ARG:HG2	4:H:66:HIS:O	2.10	0.52
3:G:23:MET:SD	3:G:232:MET:HE2	2.50	0.52
1:C:64:LEU:HD23	1:C:74:VAL:HG21	1.92	0.52
1:B:68:PRO:HD3	2:F:15:ALA:HB2	1.92	0.52
1:A:436:MET:HG3	1:A:441:GLN:HG2	1.91	0.52
2:E:97:VAL:HG13	2:E:232:VAL:CG1	2.39	0.52
5:I:5:ARG:O	5:I:6:GLN:HB3	2.10	0.52
4:H:40:THR:HG23	4:H:42:THR:H	1.75	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:B:386:VAL:HG22	1:B:442:VAL:HG12	1.91	0.51
1:A:457:GLU:HB2	1:A:460:LYS:HD3	1.92	0.51
2:D:412:ARG:HD2	2:D:454:GLU:HB3	1.90	0.51
2:E:443:GLN:O	2:E:446:ALA:HB3	2.11	0.51
1:C:436:MET:CE	1:C:469:LEU:HD21	2.41	0.51
2:F:257:ASN:HB3	2:F:260:ARG:HG2	1.93	0.51
3:G:89:MET:CB	3:G:116:LEU:HD22	2.38	0.51
1:C:52:MET:HE3	1:C:95:VAL:HG13	1.92	0.51
2:E:218:VAL:HG11	2:E:235:THR:HG22	1.92	0.51
1:C:190:ASN:HA	1:C:198:LYS:HG2	1.91	0.51
4:H:18:PHE:CZ	4:H:20:PHE:HB2	2.46	0.51
3:G:117:HIS:ND1	3:G:118:ARG:CA	2.74	0.51
2:D:473:LEU:C	2:D:475:GLU:N	2.62	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
2:E:293:GLN:HG3	2:E:328:HIS:CG	2.46	0.51
2:E:279:VAL:O	2:E:279:VAL:HG12	2.10	0.51
1:A:224:ASP:CG	1:A:227:LYS:HE3	2.31	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
3:G:19:ILE:HG22	3:G:23:MET:CE	2.40	0.51
1:C:443:ALA:O	1:C:446:TYR:HB3	2.10	0.51
2:F:394:ASP:HB3	3:G:79:GLY:CA	2.40	0.51
2:E:377:ILE:HG21	2:E:410:ILE:HD12	1.92	0.51
1:B:482:LYS:O	1:B:486:ASP:N	2.37	0.51
1:A:294:TYR:HB2	1:A:337:TYR:HE2	1.76	0.51
2:F:242:TYR:CD1	2:F:246:GLN:HG3	2.47	0.51
2:D:406:ARG:O	2:D:410:ILE:HG13	2.11	0.51
1:C:48:GLN:HB3	2:D:68:GLY:HA2	1.93	0.51
1:C:23:VAL:O	1:C:23:VAL:HG12	2.11	0.51
2:F:234:LEU:O	2:F:237:LEU:HB3	2.10	0.50
1:C:362:ARG:HG3	1:C:362:ARG:NH1	2.27	0.50
1:B:157:VAL:N	1:B:158:PRO:HD3	2.26	0.50
1:A:48:GLN:HB3	2:E:68:GLY:O	2.10	0.50
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
3:G:19:ILE:HG22	3:G:23:MET:HE2	1.93	0.50
1:C:45:ARG:NH2	1:C:68:PRO:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:GLN:HE22	2:F:128:VAL:HA	1.77	0.50
4:H:83:THR:HB	4:H:91:GLN:HE21	1.75	0.50
1:B:386:VAL:CG2	1:B:442:VAL:HG12	2.41	0.50
1:B:151:LYS:NZ	1:B:429:LYS:O	2.45	0.50
2:D:168:GLU:O	2:D:168:GLU:HG3	2.11	0.50
2:F:96:ASN:ND2	2:F:100:GLU:HB2	2.26	0.50
1:C:96:ASP:O	1:C:97:VAL:HG13	2.12	0.50
2:F:386:ASP:O	2:F:389:ALA:HB3	2.11	0.50
3:G:49:LEU:HD21	3:G:212:ILE:CD1	2.41	0.50
2:F:421:ALA:O	2:F:425:THR:HG23	2.11	0.50
4:H:35:GLN:HB3	4:H:66:HIS:HD2	1.77	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
1:C:406:PHE:N	1:C:406:PHE:CD1	2.79	0.50
2:E:382:LYS:O	2:E:385:GLN:HB2	2.11	0.50
1:A:187:LYS:HE2	1:A:191:ASP:OD2	2.11	0.50
1:B:390:MET:CE	1:B:428:LEU:HD21	2.42	0.50
4:H:58:LEU:HD13	4:H:77:VAL:HG11	1.92	0.50
1:C:34:ILE:HD11	1:C:79:ASP:CB	2.41	0.50
1:A:313:ASN:O	1:A:316:PHE:N	2.37	0.50
2:D:93:ARG:NH1	2:D:93:ARG:HG3	2.27	0.50
2:E:155:PHE:HE1	2:E:310:ILE:HD12	1.77	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:244:TYR:O	1:C:247:PRO:HD2	2.11	0.50
1:C:164:ARG:HD2	1:C:306:LEU:O	2.11	0.50
1:C:225:ALA:HA	1:C:228:TYR:CE1	2.47	0.49
1:C:434:SER:N	1:C:435:PRO:HD3	2.27	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
1:C:180:ILE:CD1	1:C:216:LEU:HD21	2.34	0.49
2:F:168:GLU:OE1	2:F:418:PHE:HB3	2.12	0.49
2:F:80:ALA:HB1	2:F:81:PRO:HD2	1.95	0.49
1:B:300:TYR:O	1:B:304:ARG:HG2	2.13	0.49
2:F:163:THR:O	2:F:167:MET:HG2	2.12	0.49
1:C:396:GLN:HG3	2:D:458:TYR:CE2	2.47	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
2:D:83:ARG:HA	2:D:115:ALA:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:H:138:ASN:O	4:H:141:LEU:HB2	2.12	0.49
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.40	0.49
1:B:99:VAL:HG21	1:B:127:ARG:HB3	1.94	0.49
2:E:462:PRO:HD2	2:E:465:GLU:HG3	1.94	0.49
1:B:463:LYS:HE2	1:B:508:PHE:CZ	2.48	0.49
3:G:197:ASP:O	3:G:200:VAL:HG12	2.13	0.49
4:H:105:LEU:HG	4:H:145:LEU:HB3	1.94	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
1:B:24:ASP:O	1:B:28:THR:HB	2.13	0.49
1:C:402:ALA:O	1:C:405:GLN:HG3	2.12	0.49
2:F:339:ILE:HG22	2:F:344:ILE:HB	1.94	0.49
2:D:360:PRO:HD3	2:D:368:TYR:CE2	2.48	0.49
1:A:380:THR:O	1:A:384:LYS:HG3	2.12	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
1:C:334:VAL:HG13	1:C:351:PHE:CE1	2.48	0.49
1:C:30:ARG:HA	1:C:86:ASP:O	2.13	0.48
3:G:71:VAL:HG13	3:G:108:VAL:CG2	2.43	0.48
2:E:444:ILE:HD11	2:E:463:ILE:CD1	2.43	0.48
1:B:96:ASP:HB2	1:B:127:ARG:O	2.13	0.48
1:A:245:LEU:O	1:A:246:ALA:C	2.51	0.48
3:G:136:PRO:HD3	3:G:221:THR:HG21	1.95	0.48
3:G:179:PHE:C	3:G:181:LEU:N	2.66	0.48
1:B:351:PHE:HE1	1:B:369:LEU:O	1.96	0.48
1:A:373:ARG:NH1	1:A:373:ARG:HG3	2.28	0.48
2:F:360:PRO:HD3	2:F:368:TYR:CE2	2.48	0.48
2:F:88:PRO:HD2	2:F:89:GLU:OE2	2.14	0.48
1:B:211:SER:O	1:B:215:GLN:HG3	2.13	0.48
2:F:82:ILE:HD13	2:F:98:ILE:HG22	1.95	0.48
1:B:430:GLN:HB3	1:B:430:GLN:HE21	1.50	0.48
1:B:209:LYS:NZ	2:E:356:ARG:NH1	2.62	0.48
2:E:360:PRO:HD3	2:E:368:TYR:CD1	2.49	0.48
2:E:134:VAL:HG13	2:E:141:ASP:OD2	2.13	0.48
2:F:221:GLN:HA	2:F:221:GLN:HE21	1.78	0.48
2:E:374:VAL:O	2:E:377:ILE:HG22	2.14	0.48
1:A:417:LEU:HD23	1:A:417:LEU:H	1.77	0.48
4:H:41:GLN:HG2	4:H:57:VAL:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:125:LEU:HD11	3:G:151:SER:HB2	1.96	0.48
1:B:49:ALA:O	1:B:50:GLU:HB2	2.12	0.48
1:B:311:LYS:HD2	1:B:312:MET:O	2.13	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
1:C:488:LYS:HG2	1:C:489:ILE:N	2.28	0.48
3:G:39:LYS:N	3:G:40:PRO:HD2	2.28	0.48
1:B:240:ALA:N	1:B:241:PRO:CD	2.77	0.48
1:C:338:ILE:O	1:C:339:PRO:C	2.51	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
1:A:453:LEU:HD13	1:A:461:ILE:HG23	1.96	0.48
1:B:179:ALA:O	1:B:182:THR:HB	2.14	0.48
3:G:117:HIS:C	3:G:117:HIS:ND1	2.67	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: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
5:I:37:THR:HG22	5:I:38:SER:H	1.79	0.48
3:G:160:ILE:HG22	3:G:176:LYS:HB2	1.95	0.48
2:F:467:VAL:O	2:F:470:ALA:HB3	2.14	0.48
2:D:32:ILE:O	2:D:33:LEU:HB2	2.14	0.48
3:G:156:ASP:O	3:G:181:LEU:HB2	2.14	0.47
1:A:444:VAL:CG1	1:A:469:LEU:HD13	2.44	0.47
2:E:54:GLY:O	2:E:55:GLU:HB2	2.13	0.47
1:A:300:TYR:O	1:A:304:ARG:HG2	2.13	0.47
1:C:59:LEU:HD23	1:C:82:ILE:CD1	2.44	0.47
1:B:423:ARG:HE	1:B:458:PRO:CD	2.26	0.47
2:F:462:PRO:HG2	2:F:465:GLU:HG3	1.96	0.47
2:E:438:ILE:O	2:E:442:GLN:HB2	2.15	0.47
1:A:376:SER:O	1:A:378:ALA:N	2.48	0.47
1:A:211:SER:HA	2:D:126:MET:HE3	1.96	0.47
1:B:427:LEU:HD11	1:B:448:GLY:HA3	1.95	0.47
1:A:485:THR:HG22	1:A:486:ASP:N	2.29	0.47
2:F:205:VAL:HG23	2:F:215:VAL:HG21	1.96	0.47
1:C:292:GLU:O	1:C:293:ALA:CB	2.63	0.47
2:E:259:PHE:CE2	2:E:263:GLN:HG2	2.50	0.47
1:A:100:GLY:HA2	1:A:256:TYR:CD1	2.49	0.47
2:F:346:PRO:HG3	2:F:418:PHE:HZ	1.79	0.47
2:F:93:ARG:NH2	2:F:106:GLY:O	2.48	0.47
1:A:68:PRO:HD3	2:E:15:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:61:ILE:O	2:E:61:ILE:HG13	2.14	0.47
2:E:388:ILE:HG23	2:E:393:MET:CG	2.43	0.47
1:C:187:LYS:HE3	1:C:224:ASP:HB3	1.97	0.47
1:A:209:LYS:HE3	1:A:211:SER:CB	2.44	0.47
1:A:127:ARG:HE	1:A:131:LEU:CD1	2.27	0.47
1:B:171:ARG:HH11	1:B:171:ARG:HG3	1.79	0.47
1:C:44:LEU:HB3	1:C:47:VAL:HG22	1.95	0.47
2:E:242:TYR:C	2:E:244:ARG:H	2.18	0.47
1:C:313:ASN:OD1	1:C:315:ALA:HB3	2.14	0.47
4:H:57:VAL:HG13	5:I:11:TYR:CZ	2.50	0.47
2:F:357:ILE:HD12	2:F:362:ILE:HG21	1.95	0.47
5:I:35:MET:C	5:I:37:THR:N	2.68	0.47
2:D:200:MET:HE3	2:D:215:VAL:HG21	1.96	0.47
1:B:389:THR:HA	1:B:392:LEU:HG	1.96	0.47
1:A:166:LEU:HD13	1:A:342:VAL:HG12	1.95	0.47
4:H:47:ILE:H	4:H:47:ILE:HD12	1.79	0.47
1:A:85:GLY:O	1:A:86:ASP:C	2.53	0.47
4:H:62:LEU:CD1	4:H:144:ALA:HB2	2.34	0.47
2:F:409:LYS:HD3	2:F:457:PHE:HE2	1.78	0.47
1:C:91:THR:HG22	1:C:93:ALA:HB3	1.97	0.47
1:B:218:LYS:NZ	2:E:129:GLU:OE2	2.48	0.47
2:F:96:ASN:HD22	2:F:100:GLU:CB	2.27	0.47
3:G:179:PHE:HB3	3:G:184:ILE:HG21	1.96	0.47
2:E:204:GLY:C	2:E:206:ILE:N	2.68	0.47
3:G:144:ILE:HG21	3:G:213:ILE:HD13	1.97	0.47
3:G:207:TYR:CZ	4:H:80:GLY:HA2	2.50	0.47
1:B:400:VAL:HB	1:B:418:LEU:CD2	2.45	0.47
1:A:188:ARG:HE	1:A:437:ALA:HB2	1.79	0.47
2:E:116:ILE:HA	2:E:238:THR:OG1	2.14	0.47
2:D:154:LEU:HD13	2:D:165:LEU:HD23	1.96	0.47
1:C:441:GLN:O	1:C:445:ILE:HG12	2.14	0.47
2:F:310:ILE:HD13	2:F:325:THR:HG21	1.97	0.47
1:C:180:ILE:HG22	1:C:184:ILE:HD12	1.97	0.46
1:B:443:ALA:O	1:B:446:TYR:HB3	2.14	0.46
1:B:209:LYS:NZ	2:E:356:ARG:HH12	2.13	0.46
2:D:368:TYR:CE1	2:D:372:ARG:HG3	2.50	0.46
2:F:319:ASP:O	2:F:322:PRO:HD2	2.14	0.46
2:E:63:MET:CE	2:E:228:ALA:HA	2.45	0.46
3:G:179:PHE:O	3:G:181:LEU:N	2.48	0.46
2:F:200:MET:CG	2:F:206:ILE:HG12	2.46	0.46
1:A:293:ALA:HB2	3:G:265:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:VAL:HB	1:A:116:ASP:HB3	1.97	0.46
2:D:129:GLU:HA	2:D:129:GLU:OE1	2.15	0.46
1:A:78:ASN:OD1	1:A:80:LYS:HB3	2.15	0.46
1:C:30:ARG:HE	1:C:87:ILE:CD1	2.18	0.46
2:D:412:ARG:O	2:D:415:SER:OG	2.33	0.46
2:D:397:SER:O	2:D:400:ASP:N	2.45	0.46
2:E:431:LEU:O	2:E:431:LEU:HD12	2.15	0.46
2:E:343:GLY:O	2:E:345:TYR:HD1	1.99	0.46
2:F:339:ILE:CG2	2:F:344:ILE:HB	2.46	0.46
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.98	0.46
1:C:445:ILE:HG22	1:C:449:VAL:CG2	2.45	0.46
1:C:156:LEU:HD11	1:C:428:LEU:CD1	2.45	0.46
1:A:51:GLU:OE2	1:A:90:ARG:HB3	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
2:F:151:LYS:HD3	2:F:328:HIS:O	2.15	0.46
1:B:496:LYS:O	1:B:500:ILE:HG13	2.15	0.46
4:H:35:GLN:HB3	4:H:66:HIS:CD2	2.50	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:70:GLY:O	4:H:71:THR:C	2.53	0.46
3:G:51:LEU:HD13	4:H:55:LEU:HD21	1.97	0.46
2:D:469:LYS:O	2:D:473:LEU:HG	2.15	0.46
2:F:36:LEU:N	2:F:36:LEU:HD23	2.30	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:A:240:ALA:HB3	1:A:241:PRO:HD3	1.97	0.46
2:E:63:MET:HE3	2:E:228:ALA:HA	1.96	0.46
2:D:289:MET:SD	2:D:324:THR:HG22	2.56	0.46
1:B:469:LEU:HG	1:B:473:ILE:HD11	1.97	0.46
2:F:455:GLN:CD	2:F:455:GLN:H	2.18	0.46
2:E:67:GLU:H	2:E:67:GLU:HG3	1.16	0.46
2:D:432:VAL:HG13	2:D:433:PRO:HD2	1.97	0.46
3:G:178:ILE:C	3:G:180:SER:N	2.69	0.46
1:B:437:ALA:O	1:B:438:ILE:C	2.54	0.46
2:E:112:GLN:NE2	2:E:242:TYR:HE2	2.14	0.46
2:D:237:LEU:HD21	2:D:295:ARG:HB2	1.97	0.46
2:E:82:ILE:HB	2:E:116:ILE:CD1	2.45	0.46
1:C:45:ARG:HA	1:C:45:ARG:HD3	1.29	0.46
1:A:36:ASP:O	1:A:284:LEU:HD13	2.16	0.46
2:E:405:SER:OG	2:E:406:ARG:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:MET:HE2	1:A:76:PHE:HZ	1.81	0.46
2:F:243:PHE:O	2:F:249:GLN:HB2	2.16	0.46
2:F:390:ILE:CD1	3:G:242:MET:HE3	2.46	0.46
2:F:96:ASN:HB2	2:F:100:GLU:N	2.31	0.46
1:A:213:VAL:O	1:A:216:LEU:HB3	2.16	0.46
2:F:50:ALA:O	2:F:51:GLN:HB3	2.16	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:340:ALA:O	2:E:343:GLY:N	2.42	0.45
1:C:102:GLU:HG2	1:C:122:GLY:C	2.36	0.45
1:A:245:LEU:C	1:A:247:PRO:HD2	2.36	0.45
2:E:41:ARG:O	2:E:42:GLU:C	2.53	0.45
2:E:120:ALA:HB1	2:E:121:PRO:HD2	1.98	0.45
4:H:99:THR:O	4:H:102:MET:HG2	2.15	0.45
3:G:115:ILE:C	3:G:117:HIS:N	2.68	0.45
2:E:204:GLY:O	2:E:205:VAL:C	2.54	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
1:A:166:LEU:HD13	1:A:342:VAL:CG1	2.47	0.45
1:A:40:ARG:HH11	1:A:40:ARG:CG	2.27	0.45
2:F:345:TYR:HA	2:F:346:PRO:C	2.36	0.45
2:F:394:ASP:HB3	3:G:79:GLY:C	2.36	0.45
2:F:252:LEU:HA	2:F:252:LEU:HD23	1.81	0.45
2:E:443:GLN:HA	2:E:446:ALA:HB3	1.99	0.45
2:E:33:LEU:HD13	2:E:117:HIS:CG	2.50	0.45
1:B:353:GLU:HG3	1:B:366:ASN:HB2	1.98	0.45
2:D:35:ALA:HB1	2:D:46:VAL:CG1	2.47	0.45
3:G:259:THR:O	3:G:263:ILE:HG12	2.17	0.45
1:C:158:PRO:HB3	1:C:379:GLN:HG3	1.99	0.45
1:C:432:GLN:O	1:C:433:TYR:HB2	2.16	0.45
1:A:140:ILE:CG2	1:A:313:ASN:HA	2.47	0.45
1:B:358:TYR:C	1:B:360:GLY:N	2.69	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
2:D:345:TYR:HA	2:D:346:PRO:C	2.37	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:F:136:GLY:HA3	2:F:431:LEU:HD11	1.99	0.45
1:A:283:LEU:HD11	1:A:293:ALA:HB1	1.99	0.45
1:A:179:ALA:O	1:A:182:THR:HB	2.17	0.45
1:A:59:LEU:HD11	1:A:81:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:390:ILE:HD11	3:G:242:MET:SD	2.56	0.45
1:B:381:ARG:HG2	1:B:488:LYS:HG3	1.97	0.45
1:A:339:PRO:O	1:A:343:ILE:HG13	2.16	0.45
1:A:151:LYS:HE2	1:A:427:LEU:O	2.17	0.45
1:B:210:ARG:O	1:B:211:SER:C	2.54	0.45
1:A:142:VAL:HG22	1:A:161:ARG:O	2.16	0.45
2:D:452:LEU:HD12	2:D:457:PHE:CZ	2.52	0.45
2:F:346:PRO:HG3	2:F:418:PHE:CZ	2.52	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:319:ASP:O	2:D:320:PRO:C	2.55	0.45
1:C:474:SER:OG	1:C:475:GLN:N	2.49	0.45
2:E:397:SER:C	2:E:399:GLU:H	2.20	0.45
2:D:95:MET:HG2	2:D:99:GLY:HA2	1.99	0.45
1:B:76:PHE:HB3	1:B:242:LEU:HD21	1.99	0.45
3:G:13:ILE:HD13	3:G:242:MET:SD	2.57	0.45
1:A:97:VAL:HG11	1:A:249:SER:HB2	1.99	0.45
1:C:67:GLU:HB3	1:C:68:PRO:HD2	1.98	0.45
1:A:385:GLN:OE1	1:A:488:LYS:HB2	2.17	0.45
2:D:440:GLY:O	2:D:444:ILE:HG13	2.16	0.45
1:C:251:CYS:O	1:C:255:GLU:HG3	2.16	0.44
1:B:383:MET:O	1:B:384:LYS:C	2.52	0.44
4:H:55:LEU:O	4:H:56:GLN:HG3	2.17	0.44
2:F:29:LEU:HD11	2:F:58:VAL:HG13	1.98	0.44
1:C:390:MET:HE2	1:C:428:LEU:HD11	1.99	0.44
1:A:412:ALA:HA	1:A:415:GLN:HB3	1.98	0.44
2:D:298:THR:HG23	2:D:303:SER:HA	1.98	0.44
3:G:105:ILE:HG22	3:G:106:ILE:N	2.32	0.44
1:C:476:HIS:N	1:C:476:HIS:ND1	2.64	0.44
4:H:34:ARG:HH22	4:H:70:GLY:CA	2.24	0.44
2:E:321:ALA:N	2:E:322:PRO:HD2	2.32	0.44
2:D:366:GLU:O	2:D:370:VAL:HG23	2.17	0.44
3:G:228:ARG:O	3:G:232:MET:HG2	2.17	0.44
2:F:257:ASN:OD1	2:F:259:PHE:HB3	2.18	0.44
1:B:141:SER:HB2	1:B:143:ARG:NH1	2.31	0.44
1:A:392:LEU:O	1:A:396:GLN:HG3	2.18	0.44
2:E:281:TYR:CZ	2:E:321:ALA:HB2	2.52	0.44
4:H:33:VAL:HG11	4:H:65:VAL:HG13	1.99	0.44
1:C:436:MET:HE1	1:C:469:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:VAL:CG1	1:B:418:LEU:HD11	2.47	0.44
1:A:463:LYS:HD3	1:A:508:PHE:CZ	2.52	0.44
1:B:300:TYR:HA	1:B:303:SER:OG	2.17	0.44
2:D:103:ASP:O	2:D:104:GLU:HB2	2.18	0.44
2:F:469:LYS:O	2:F:473:LEU:HG	2.16	0.44
1:C:219:ARG:HD3	1:C:433:TYR:HE1	1.80	0.44
1:B:140:ILE:HG13	1:B:143:ARG:NH1	2.32	0.44
3:G:180:SER:O	3:G:181:LEU:C	2.56	0.44
1:A:379:GLN:HB2	1:A:384:LYS:HE3	2.00	0.44
2:F:188:GLU:H	2:F:221:GLN:NE2	2.15	0.44
2:D:170:ILE:O	2:D:174:ALA:HB3	2.17	0.44
3:G:117:HIS:CE1	3:G:118:ARG:NE	2.86	0.44
1:A:460:LYS:HD2	1:A:460:LYS:N	2.32	0.44
2:E:402:LEU:O	2:E:406:ARG:HG3	2.16	0.44
1:A:413:ALA:O	1:A:416:GLN:HB3	2.17	0.44
2:F:348:VAL:O	2:F:350:PRO:HD3	2.17	0.44
1:C:132:LYS:NZ	2:D:64:ASP:OD1	2.49	0.44
1:C:209:LYS:HE3	1:C:211:SER:OG	2.18	0.44
1:A:180:ILE:O	1:A:181:ASP:C	2.56	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:B:32:LEU:HD21	1:B:42:HIS:HB2	2.00	0.44
2:E:114:ALA:HB3	2:E:238:THR:CG2	2.47	0.44
1:A:74:VAL:HG13	1:A:241:PRO:HG3	2.00	0.44
1:B:389:THR:HA	1:B:392:LEU:CG	2.48	0.44
3:G:206:GLU:O	5:I:12:ILE:HD11	2.17	0.44
2:F:105:ARG:CZ	2:F:208:LEU:HD23	2.47	0.44
1:B:107:VAL:HG12	1:B:115:ILE:HD11	2.00	0.44
2:D:189:ARG:O	2:D:192:GLU:HB2	2.18	0.44
1:C:311:LYS:HE3	1:C:318:GLY:O	2.18	0.44
1:C:169:GLY:O	1:C:175:LYS:HE2	2.18	0.44
4:H:38:VAL:HA	4:H:39:PRO:HD3	1.83	0.44
3:G:113:ARG:O	3:G:117:HIS:HB2	2.18	0.44
2:F:357:ILE:O	2:F:359:ASP:N	2.48	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
1:A:244:TYR:HE1	1:A:301:LEU:HD11	1.82	0.44
2:E:316:ASP:OD2	3:G:255:GLN:NE2	2.39	0.44
1:C:208:GLN:HE21	1:C:208:GLN:HB2	1.37	0.44
1:A:420:ARG:HA	1:A:420:ARG:HD3	1.78	0.44
2:F:359:ASP:OD1	2:F:360:PRO:HD2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:MET:CG	1:A:95:VAL:HG22	2.48	0.43
2:F:31:PRO:O	2:F:34:ASN:HB2	2.18	0.43
1:B:294:TYR:CE2	1:B:338:ILE:HD13	2.53	0.43
1:C:335:SER:O	2:D:314:ALA:HA	2.18	0.43
1:C:90:ARG:HB3	1:C:90:ARG:HE	1.61	0.43
2:D:400:ASP:O	2:D:404:VAL:HG23	2.18	0.43
1:B:212:THR:O	1:B:216:LEU:HB2	2.18	0.43
1:A:471:HIS:ND1	1:A:475:GLN:HG3	2.33	0.43
1:B:423:ARG:HE	1:B:458:PRO:CG	2.31	0.43
2:E:136:GLY:HA2	2:E:432:VAL:O	2.18	0.43
1:A:133:ALA:HB1	1:A:134:PRO:HD2	1.99	0.43
1:B:423:ARG:O	1:B:426:GLU:N	2.51	0.43
1:B:269:ASP:HA	1:B:270:ASP:HA	1.78	0.43
2:E:35:ALA:HB2	2:E:82:ILE:HG13	1.99	0.43
2:E:376:LYS:O	2:E:379:GLN:HB2	2.18	0.43
1:C:32:LEU:HD21	1:C:42:HIS:HB2	2.00	0.43
2:E:166:ILE:O	2:E:170:ILE:HG13	2.18	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
1:B:400:VAL:HG12	1:B:418:LEU:HD11	2.00	0.43
4:H:41:GLN:CG	4:H:57:VAL:HG12	2.48	0.43
2:F:385:GLN:HA	2:F:388:ILE:HG12	2.01	0.43
4:H:112:LEU:HD21	4:H:135:ILE:HG23	1.99	0.43
2:D:275:ILE:HG23	3:G:269:ALA:CA	2.46	0.43
4:H:105:LEU:CD2	4:H:109:LYS:HE3	2.41	0.43
4:H:35:GLN:HG2	4:H:36:VAL:N	2.34	0.43
1:B:389:THR:HG22	1:B:392:LEU:HD12	2.00	0.43
1:A:62:MET:HE2	1:A:76:PHE:CZ	2.54	0.43
1:B:289:PRO:HG2	3:G:263:ILE:HD12	1.99	0.43
1:B:213:VAL:O	1:B:217:VAL:HG13	2.18	0.43
2:F:141:ASP:HB3	2:F:434:LEU:HD13	2.01	0.43
1:C:144:GLU:H	1:C:144:GLU:HG3	1.65	0.43
1:C:185:ASN:HB2	1:C:435:PRO:HB3	2.00	0.43
2:E:393:MET:HE3	2:E:396:LEU:HD12	1.99	0.43
1:C:51:GLU:HG2	1:C:52:MET:N	2.33	0.43
1:A:397:TYR:CD1	1:A:421:GLY:HA3	2.54	0.43
1:A:251:CYS:O	1:A:255:GLU:HG3	2.18	0.43
1:C:49:ALA:O	1:C:50:GLU:HB2	2.19	0.43
3:G:86:ALA:HA	3:G:89:MET:CE	2.49	0.43
2:D:274:ARG:HH11	2:D:274:ARG:HD2	1.50	0.43
2:D:108:ILE:HG22	2:D:110:THR:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:5:ARG:C	5:I:7:ALA:N	2.72	0.43
3:G:6:ILE:HG21	3:G:250:PHE:HB2	2.00	0.43
2:F:407:ALA:O	2:F:411:GLN:HB2	2.18	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:F:89:GLU:HG2	2:F:110:THR:CG2	2.44	0.43
1:A:45:ARG:HA	1:A:45:ARG:HD3	1.67	0.43
2:E:158:ALA:C	2:E:160:VAL:N	2.72	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
2:E:161:GLY:O	2:E:162:LYS:C	2.57	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
4:H:79:SER:O	4:H:94:ALA:HA	2.18	0.43
1:A:383:MET:O	1:A:386:VAL:HG23	2.19	0.43
2:F:144:ALA:N	2:F:145:PRO:CD	2.82	0.43
1:C:83:LYS:HE3	1:C:83:LYS:HB2	1.83	0.43
5:I:35:MET:O	5:I:37:THR:N	2.52	0.43
1:C:224:ASP:OD1	1:C:227:LYS:HE3	2.19	0.43
2:E:461:GLY:HA3	2:E:462:PRO:HD3	1.73	0.43
1:C:49:ALA:N	1:C:66:LEU:HD11	2.34	0.43
2:D:462:PRO:HD2	2:D:465:GLU:HG3	2.00	0.43
1:C:147:GLN:OE1	1:C:438:ILE:HD13	2.19	0.43
2:E:182:VAL:HG21	2:E:240:ALA:HB2	2.01	0.43
1:A:291:ARG:N	3:G:262:LEU:CD2	2.82	0.42
3:G:239:ALA:O	3:G:243:ILE:HG12	2.18	0.42
2:E:310:ILE:HD11	2:E:329:LEU:HD11	2.00	0.42
1:C:485:THR:O	1:C:486:ASP:C	2.57	0.42
3:G:192:ILE:HG22	4:H:53:PRO:HG2	2.00	0.42
2:D:145:PRO:HB2	2:D:357:ILE:HD11	2.01	0.42
2:E:441:PHE:O	2:E:445:LEU:HG	2.19	0.42
2:F:357:ILE:HD13	2:F:357:ILE:HA	1.80	0.42
1:C:107:VAL:O	1:C:115:ILE:HG12	2.18	0.42
1:A:99:VAL:HG23	1:A:253:MET:HA	2.01	0.42
2:D:410:ILE:HG23	2:D:441:PHE:CE1	2.54	0.42
4:H:131:ILE:HG23	4:H:134:ARG:HH21	1.84	0.42
3:G:203:ASN:HB3	4:H:57:VAL:HG21	2.01	0.42
2:F:452:LEU:HD22	2:F:470:ALA:CB	2.49	0.42
1:C:139:ARG:HB3	1:C:311:LYS:O	2.19	0.42
1:A:340:THR:O	1:A:344:SER:HB3	2.19	0.42
2:D:412:ARG:HG3	2:D:412:ARG:NH1	2.33	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:F:122:GLU:OE1	2:F:122:GLU:HA	2.19	0.42
1:B:385:GLN:NE2	1:B:489:ILE:HB	2.34	0.42
1:A:96:ASP:HA	1:A:128:ARG:HA	2.01	0.42
2:F:400:ASP:O	2:F:404:VAL:HG23	2.19	0.42
1:B:433:TYR:C	1:B:435:PRO:HD3	2.40	0.42
1:A:338:ILE:N	1:A:339:PRO:CD	2.83	0.42
2:F:438:ILE:H	2:F:438:ILE:HG12	1.73	0.42
2:F:95:MET:HG3	2:F:99:GLY:HA2	2.00	0.42
3:G:58:LYS:O	3:G:59:THR:OG1	2.31	0.42
1:A:184:ILE:HD12	1:A:223:ALA:CB	2.50	0.42
3:G:180:SER:O	3:G:182:ASP:N	2.52	0.42
2:E:425:THR:C	2:E:427:HIS:N	2.72	0.42
5:I:5:ARG:O	5:I:6:GLN:CB	2.68	0.42
2:E:296:ILE:HD13	2:E:306:SER:HB2	2.02	0.42
1:A:485:THR:C	1:A:487:GLY:H	2.23	0.42
1:C:137:ILE:HA	1:C:137:ILE:HD13	1.88	0.42
3:G:86:ALA:O	3:G:116:LEU:HD13	2.18	0.42
1:C:423:ARG:CD	1:C:461:ILE:HD11	2.49	0.42
1:B:485:THR:O	1:B:486:ASP:C	2.58	0.42
2:E:32:ILE:O	2:E:33:LEU:CB	2.68	0.42
2:F:47:LEU:HD23	2:F:62:ALA:HA	2.01	0.42
2:D:266:SER:CB	2:D:282:GLN:NE2	2.82	0.42
2:D:397:SER:O	2:D:398:GLU:C	2.58	0.42
2:E:95:MET:HA	2:E:100:GLU:O	2.20	0.42
2:E:412:ARG:NH1	2:E:454:GLU:OE1	2.53	0.42
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.48	0.42
2:F:251:VAL:HG12	2:F:252:LEU:N	2.35	0.42
2:E:282:GLN:HA	2:E:283:PRO:HD3	1.89	0.42
3:G:203:ASN:HB2	4:H:57:VAL:HG21	2.02	0.42
1:B:165:GLU:O	1:B:325:PRO:HD2	2.19	0.42
2:F:423:VAL:O	2:F:423:VAL:HG12	2.20	0.42
2:D:38:VAL:HG22	2:D:75:VAL:HG22	2.02	0.42
2:E:12:ARG:NH2	2:E:24:GLN:OE1	2.50	0.42
1:C:442:VAL:HG11	1:C:489:ILE:HD11	2.01	0.42
1:C:151:LYS:HE2	1:C:436:MET:SD	2.60	0.42
1:B:361:ILE:HD13	1:B:429:LYS:HE2	2.02	0.42
2:D:38:VAL:HG11	2:D:69:LEU:CD2	2.49	0.42
4:H:54:THR:O	4:H:55:LEU:HD23	2.20	0.42
2:E:105:ARG:NE	2:E:208:LEU:HD23	2.33	0.42
2:D:200:MET:CE	2:D:215:VAL:HG21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:475:GLU:OE1	2:D:475:GLU:HA	2.20	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
1:C:245:LEU:O	1:C:246:ALA:C	2.56	0.42
2:D:279:VAL:HG12	2:D:279:VAL:O	2.20	0.42
3:G:56:ASP:C	3:G:57:ILE:HG12	2.41	0.42
1:B:379:GLN:HB3	1:B:384:LYS:CE	2.46	0.42
2:D:471:ASP:O	2:D:472:LYS:C	2.57	0.42
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
2:E:396:LEU:CB	2:E:401:LYS:HG2	2.50	0.41
2:D:63:MET:CE	2:D:228:ALA:HA	2.50	0.41
1:C:467:ALA:O	1:C:470:SER:HB2	2.20	0.41
1:A:353:GLU:CD	1:A:366:ASN:HD22	2.23	0.41
1:C:340:THR:O	1:C:341:ASN:C	2.59	0.41
1:A:56:SER:O	1:A:58:GLY:N	2.53	0.41
3:G:87:LYS:HA	3:G:90:LYS:HE2	2.02	0.41
2:D:412:ARG:C	2:D:414:LEU:N	2.73	0.41
1:C:403:PHE:CZ	2:D:408:ARG:HD2	2.55	0.41
1:B:381:ARG:HA	1:B:384:LYS:HB2	2.01	0.41
1:A:139:ARG:C	1:A:140:ILE:HG22	2.40	0.41
2:E:360:PRO:HD3	2:E:368:TYR:CG	2.56	0.41
2:D:201:ILE:CD1	2:D:208:LEU:HD11	2.50	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:382:ALA:HB1	1:B:442:VAL:HG11	2.02	0.41
4:H:64:VAL:CG1	4:H:72:THR:HG21	2.50	0.41
2:F:167:MET:HB2	2:F:420:VAL:HG11	2.02	0.41
2:D:35:ALA:HB1	2:D:46:VAL:HG13	2.02	0.41
3:G:106:ILE:HG12	3:G:126:VAL:HG23	2.01	0.41
1:A:103:LEU:O	1:A:106:ARG:HB2	2.20	0.41
1:C:211:SER:HB3	2:F:126:MET:HE3	2.02	0.41
1:A:403:PHE:O	1:A:404:ALA:C	2.59	0.41
1:A:294:TYR:HB2	1:A:337:TYR:CE2	2.54	0.41
1:A:292:GLU:HB2	1:A:294:TYR:HD2	1.86	0.41
1:B:151:LYS:NZ	1:B:427:LEU:O	2.47	0.41
1:B:304:ARG:HD3	1:B:304:ARG:HH11	1.64	0.41
2:E:189:ARG:HB2	2:E:192:GLU:HG3	2.02	0.41
2:E:388:ILE:HD12	2:E:396:LEU:HD11	2.01	0.41
1:B:44:LEU:HB3	1:B:47:VAL:CG2	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:196:LEU:O	2:F:200:MET:HB2	2.19	0.41
1:B:423:ARG:HH21	1:B:458:PRO:HD3	1.86	0.41
1:B:366:ASN:ND2	1:B:369:LEU:HG	2.36	0.41
2:E:282:GLN:NE2	2:E:282:GLN:H	2.19	0.41
4:H:119:LEU:HD21	4:H:132:GLN:HE21	1.86	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
1:C:151:LYS:HG3	1:C:430:GLN:OE1	2.21	0.41
2:D:63:MET:CE	2:D:97:VAL:HG11	2.51	0.41
2:D:52:HIS:CD2	2:D:58:VAL:HG12	2.56	0.41
2:F:442:GLN:O	2:F:445:LEU:HB2	2.20	0.41
1:A:408:SER:O	1:A:409:ASP:HB2	2.20	0.41
3:G:120:HIS:HB3	3:G:123:GLN:HB2	2.03	0.41
2:E:167:MET:SD	2:E:200:MET:HA	2.61	0.41
1:A:206:ILE:O	1:A:273:LYS:HD2	2.20	0.41
1:A:492:GLU:C	1:A:494:ASP:N	2.74	0.41
1:B:78:ASN:ND2	1:B:80:LYS:HE2	2.35	0.41
2:E:82:ILE:CG2	2:E:116:ILE:HD13	2.51	0.41
2:D:360:PRO:HD3	2:D:368:TYR:CD2	2.56	0.41
2:D:13:ILE:HD12	2:D:73:GLN:HB3	2.03	0.41
2:F:471:ASP:O	2:F:474:ALA:N	2.53	0.41
2:F:282:GLN:HG2	2:F:282:GLN:H	1.07	0.41
1:B:206:ILE:HA	1:B:234:ALA:O	2.21	0.41
1:A:129:VAL:HG12	1:A:249:SER:HA	2.03	0.41
1:C:78:ASN:HD21	1:C:80:LYS:HD3	1.85	0.41
2:F:63:MET:HE1	2:F:97:VAL:HG11	2.03	0.41
2:D:112:GLN:NE2	2:D:242:TYR:CE1	2.88	0.41
1:A:498:LYS:O	1:A:502:THR:HG23	2.21	0.41
1:A:32:LEU:HD21	1:A:42:HIS:HB2	2.02	0.41
1:C:19:ALA:O	1:C:21:THR:HG23	2.21	0.41
1:A:105:GLY:HA2	1:A:226:MET:O	2.21	0.41
3:G:180:SER:O	3:G:205:GLN:NE2	2.50	0.41
2:D:398:GLU:HA	2:D:401:LYS:CG	2.51	0.41
2:D:393:MET:HE1	2:D:404:VAL:HG11	2.02	0.41
2:E:97:VAL:HG13	2:E:232:VAL:HG12	2.02	0.41
4:H:34:ARG:NH2	4:H:70:GLY:HA2	2.28	0.41
1:C:465:GLU:O	1:C:465:GLU:HG2	2.21	0.41
1:C:374:VAL:CG1	1:C:378:ALA:HB2	2.51	0.41
2:E:122:GLU:HB2	2:E:125:GLU:HG3	2.01	0.41
2:D:63:MET:HE1	2:D:231:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:SER:CA	2:D:126:MET:HE3	2.51	0.41
1:A:294:TYR:CE2	1:A:338:ILE:HD13	2.56	0.41
1:B:107:VAL:O	1:B:115:ILE:HG12	2.20	0.41
1:A:485:THR:C	1:A:487:GLY:N	2.73	0.41
3:G:85:VAL:HG12	3:G:173:THR:HG23	2.03	0.41
2:F:434:LEU:O	2:F:438:ILE:HG12	2.21	0.41
1:A:184:ILE:HD12	1:A:223:ALA:HB3	2.03	0.41
1:C:129:VAL:HG21	1:C:245:LEU:HD11	2.02	0.41
2:E:189:ARG:O	2:E:190:THR:C	2.58	0.41
1:B:201:CYS:O	1:B:229:THR:HA	2.21	0.41
2:F:228:ALA:O	2:F:232:VAL:HG22	2.21	0.41
2:E:256:ASP:HA	2:E:257:ASN:HA	1.65	0.41
2:E:165:LEU:HD22	2:E:335:LEU:HD21	2.02	0.41
2:E:227:GLY:O	2:E:231:ARG:HG2	2.21	0.41
2:E:231:ARG:O	2:E:232:VAL:C	2.60	0.41
2:E:397:SER:O	2:E:399:GLU:N	2.54	0.41
3:G:51:LEU:HD22	3:G:204:TYR:OH	2.21	0.41
2:D:86:VAL:HG11	2:D:114:ALA:HB3	2.02	0.41
1:C:423:ARG:HD2	1:C:461:ILE:HD11	2.03	0.41
1:B:423:ARG:NE	1:B:458:PRO:HD3	2.36	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
1:A:74:VAL:CG1	1:A:241:PRO:HG3	2.51	0.41
2:D:368:TYR:O	2:D:372:ARG:HG2	2.21	0.41
1:A:247:PRO:HG2	1:A:274:GLN:NE2	2.35	0.41
2:E:452:LEU:HA	2:E:453:PRO:HD3	1.85	0.41
1:B:30:ARG:HA	1:B:86:ASP:O	2.21	0.41
1:B:336:ALA:HB3	1:B:339:PRO:HD2	2.02	0.41
2:D:27:GLU:H	2:D:27:GLU:HG3	1.77	0.41
2:D:433:PRO:HG2	2:D:436:GLU:CG	2.44	0.40
2:E:434:LEU:O	2:E:437:THR:HB	2.21	0.40
2:E:393:MET:O	2:E:393:MET:HE2	2.21	0.40
2:E:105:ARG:NH1	2:E:208:LEU:HD23	2.36	0.40
1:A:440:GLU:HG2	1:A:473:ILE:HD11	2.03	0.40
1:B:99:VAL:HG13	1:B:256:TYR:HB2	2.02	0.40
1:A:147:GLN:OE1	1:A:438:ILE:HD13	2.21	0.40
3:G:12:SER:O	3:G:16:ILE:HD12	2.20	0.40
2:D:94:ILE:HG22	2:D:102:ILE:HD11	2.01	0.40
3:G:2:THR:C	3:G:4:LYS:N	2.75	0.40
3:G:73:SER:O	3:G:111:LYS:HB2	2.21	0.40
1:B:45:ARG:HD3	1:B:45:ARG:HH11	1.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:78:SER:HB3	5:I:22:VAL:HG21	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
1:A:479:LEU:O	1:A:482:LYS:HB2	2.22	0.40
1:C:465:GLU:O	1:C:469:LEU:HB2	2.21	0.40
2:E:77:ASP:C	2:E:79:GLY:H	2.24	0.40
1:A:267:ILE:HA	1:A:324:LEU:O	2.20	0.40
3:G:2:THR:HG22	3:G:4:LYS:H	1.86	0.40
2:D:281:TYR:HB3	2:D:285:LEU:HD12	2.03	0.40
1:A:69:ASP:O	1:A:70:ASN:HB3	2.21	0.40
3:G:113:ARG:HG3	3:G:127:THR:HG21	2.03	0.40
2:E:139:VAL:HG21	2:E:348:VAL:HB	2.02	0.40
1:B:452:TYR:CD2	1:B:501:VAL:HG21	2.56	0.40
3:G:39:LYS:CB	3:G:40:PRO:CD	2.99	0.40
1:B:439:GLU:HA	1:B:442:VAL:CG2	2.52	0.40
2:E:200:MET:CB	2:E:206:ILE:HD12	2.52	0.40
2:E:422:GLU:C	2:E:424:PHE:N	2.74	0.40
5:I:20:LYS:HA	5:I:23:ARG:NH1	2.36	0.40
1:C:240:ALA:N	1:C:241:PRO:CD	2.84	0.40
2:E:35:ALA:HB1	2:E:46:VAL:CG1	2.52	0.40
4:H:82:VAL:HB	4:H:92:LEU:CD1	2.52	0.40
2:D:203:SER:OG	2:D:205:VAL:HG23	2.21	0.40
1:B:376:SER:O	1:B:384:LYS:HE2	2.22	0.40
2:F:30:PRO:HA	2:F:31:PRO:HD3	1.98	0.40
2:E:329:LEU:O	2:E:356:ARG:CZ	2.70	0.40
4:H:62:LEU:HD23	4:H:75:TYR:O	2.22	0.40
2:E:434:LEU:CD1	2:E:438:ILE:HD11	2.52	0.40
1:B:388:GLY:O	1:B:392:LEU:HG	2.22	0.40
1:B:362:ARG:HA	1:B:364:ALA:N	2.37	0.40
4:H:95:GLU:O	4:H:96:GLU:HG2	2.22	0.40
2:F:38:VAL:HG11	2:F:69:LEU:CD2	2.50	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%)	14	58
1	B	475/553 (86%)	426 (90%)	42 (9%)	7 (2%)	13	58
1	C	490/553 (89%)	444 (91%)	38 (8%)	8 (2%)	12	57
2	D	465/528 (88%)	419 (90%)	43 (9%)	3 (1%)	30	74
2	E	464/528 (88%)	407 (88%)	47 (10%)	10 (2%)	8	50
2	F	464/528 (88%)	433 (93%)	29 (6%)	2 (0%)	39	80
3	G	257/298 (86%)	223 (87%)	26 (10%)	8 (3%)	5	43
4	H	129/168 (77%)	118 (92%)	8 (6%)	3 (2%)	8	49
5	I	45/51 (88%)	36 (80%)	4 (9%)	5 (11%)	0	11
All	All	3274/3760 (87%)	2949 (90%)	272 (8%)	53 (2%)	12	57

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

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Mol	Chain	Res	Type
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
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%)	351 (89%)	42 (11%)	8	38
1	B	388/444 (87%)	341 (88%)	47 (12%)	6	32
1	C	397/444 (89%)	369 (93%)	28 (7%)	18	57
2	D	377/417 (90%)	346 (92%)	31 (8%)	14	51
2	E	376/417 (90%)	343 (91%)	33 (9%)	12	47
2	F	376/417 (90%)	354 (94%)	22 (6%)	24	63
3	G	225/251 (90%)	210 (93%)	15 (7%)	20	59
4	H	104/128 (81%)	100 (96%)	4 (4%)	40	74
5	I	38/42 (90%)	35 (92%)	3 (8%)	15	53
All	All	2674/3004 (89%)	2449 (92%)	225 (8%)	14	50

All (225) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	40	ARG
1	A	45	ARG
1	A	47	VAL
1	A	48	GLN
1	A	50	GLU
1	A	56	SER
1	A	80	LYS
1	A	94	ILE
1	A	99	VAL
1	A	101	GLU
1	A	102	GLU
1	A	121	ILE
1	A	140	ILE
1	A	143	ARG
1	A	151	LYS
1	A	164	ARG
1	A	173	THR
1	A	188	ARG
1	A	193	THR
1	A	195	GLU
1	A	211	SER

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Mol	Chain	Res	Type
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	417	LEU
1	A	420	ARG
1	A	436	MET
1	A	444	VAL
1	A	457	GLU
1	A	472	VAL
1	A	474	SER
1	A	479	LEU
1	A	497	LEU
1	A	499	GLU
1	B	38	ILE
1	B	47	VAL
1	B	52	MET
1	B	79	ASP
1	B	80	LYS
1	B	123	SER
1	B	141	SER
1	B	143	ARG
1	B	145	PRO
1	B	164	ARG
1	B	173	THR
1	B	186	GLN
1	B	188	ARG
1	B	189	PHE
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

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Mol	Chain	Res	Type
1	B	256	TYR
1	B	270	ASP
1	B	298	VAL
1	B	299	PHE
1	B	335	SER
1	B	349	GLN
1	B	351	PHE
1	B	371	VAL
1	B	374	VAL
1	B	376	SER
1	B	380	THR
1	B	381	ARG
1	B	399	GLU
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	474	SER
1	B	479	LEU
1	B	482	LYS
1	B	484	ARG
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	87	ILE
1	C	101	GLU
1	C	164	ARG
1	C	189	PHE
1	C	195	GLU
1	C	208	GLN
1	C	227	LYS
1	C	270	ASP
1	C	282	SER
1	C	298	VAL
1	C	334	VAL
1	C	349	GLN

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Mol	Chain	Res	Type
1	C	399	GLU
1	C	400	VAL
1	C	406	PHE
1	C	440	GLU
1	C	444	VAL
1	C	474	SER
1	C	477	GLN
1	C	479	LEU
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	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	266	SER
2	D	282	GLN
2	D	306	SER
2	D	322	PRO
2	D	336	SER
2	D	361	ASN
2	D	365	SER
2	D	388	ILE
2	D	397	SER
2	D	400	ASP
2	D	401	LYS
2	D	405	SER
2	D	423	VAL
2	D	431	LEU
2	D	452	LEU
2	D	475	GLU

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Mol	Chain	Res	Type
2	E	9	THR
2	E	67	GLU
2	E	95	MET
2	E	127	SER
2	E	128	VAL
2	E	132	ILE
2	E	133	LEU
2	E	139	VAL
2	E	148	LYS
2	E	155	PHE
2	E	164	VAL
2	E	194	ASN
2	E	213	SER
2	E	215	VAL
2	E	223	ASN
2	E	225	PRO
2	E	257	ASN
2	E	282	GLN
2	E	293	GLN
2	E	297	THR
2	E	306	SER
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	412	ARG
2	E	431	LEU
2	E	438	ILE
2	E	452	LEU
2	F	10	THR
2	F	27	GLU
2	F	42	GLU
2	F	67	GLU
2	F	95	MET
2	F	112	GLN
2	F	127	SER
2	F	139	VAL
2	F	166	ILE

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Mol	Chain	Res	Type
2	F	191	ARG
2	F	200	MET
2	F	210	ASP
2	F	223	ASN
2	F	232	VAL
2	F	261	PHE
2	F	292	MET
2	F	386	ASP
2	F	387	ILE
2	F	397	SER
2	F	405	SER
2	F	428	LEU
2	F	455	GLN
3	G	35	GLU
3	G	67	LEU
3	G	110	ASP
3	G	113	ARG
3	G	118	ARG
3	G	125	LEU
3	G	126	VAL
3	G	130	GLU
3	G	180	SER
3	G	184	ILE
3	G	190	MET
3	G	205	GLN
3	G	212	ILE
3	G	213	ILE
3	G	262	LEU
4	H	54	THR
4	H	57	VAL
4	H	91	GLN
4	H	112	LEU
5	I	37	THR
5	I	41	THR
5	I	42	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	GLN
1	A	349	GLN
1	A	396	GLN

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Mol	Chain	Res	Type
1	A	432	GLN
1	B	48	GLN
1	B	65	ASN
1	B	349	GLN
1	B	432	GLN
1	C	208	GLN
1	C	260	ASN
1	C	349	GLN
1	C	432	GLN
2	D	130	GLN
2	D	194	ASN
2	D	221	GLN
2	D	223	ASN
2	D	282	GLN
2	D	328	HIS
2	D	442	GLN
2	E	39	GLN
2	E	130	GLN
2	E	194	ASN
2	E	223	ASN
2	E	246	GLN
2	E	367	HIS
2	F	39	GLN
2	F	96	ASN
2	F	221	GLN
2	F	223	ASN
2	F	282	GLN
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
4	H	132	GLN
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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%)	-0.12	2 (0%) 93 90	70, 70, 70, 70	0
1	B	479/553 (86%)	-0.09	1 (0%) 95 94	70, 70, 70, 70	0
1	C	492/553 (88%)	-0.20	0 100 100	70, 70, 70, 70	0
2	D	467/528 (88%)	-0.12	1 (0%) 95 94	70, 70, 70, 70	0
2	E	466/528 (88%)	0.08	4 (0%) 85 80	70, 70, 70, 70	0
2	F	466/528 (88%)	-0.13	0 100 100	70, 70, 70, 70	0
3	G	263/298 (88%)	0.26	4 (1%) 76 68	36, 68, 116, 133	0
4	H	131/168 (77%)	0.61	10 (7%) 17 14	67, 97, 131, 136	0
5	I	47/51 (92%)	0.11	0 100 100	58, 91, 127, 129	0
All	All	3298/3760 (87%)	-0.04	22 (0%) 89 84	36, 70, 90, 136	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	510	ALA	3.6
1	B	510	ALA	3.5
2	E	457	PHE	3.4
4	H	97	ALA	3.0
4	H	79	SER	2.8
3	G	101	LYS	2.6
4	H	122	ALA	2.6
4	H	86	ALA	2.5
1	A	408	SER	2.4
4	H	15	GLN	2.4
3	G	61	GLU	2.3
4	H	105	LEU	2.3
4	H	85	ASN	2.3
2	E	179	GLY	2.2
3	G	189	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	456	ALA	2.1
2	E	448	GLU	2.1
2	D	180	TYR	2.1
4	H	16	MET	2.1
3	G	1	ALA	2.1
4	H	144	ALA	2.1
4	H	84	VAL	2.1

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 carbohydrates 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.