



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:11 PM UTC

PDB ID : 2W6G / pdb_00002w6g
Title : Low resolution structures of bovine mitochondrial F1-ATPase during controlled dehydration: Hydration State 3.
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 : 6.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

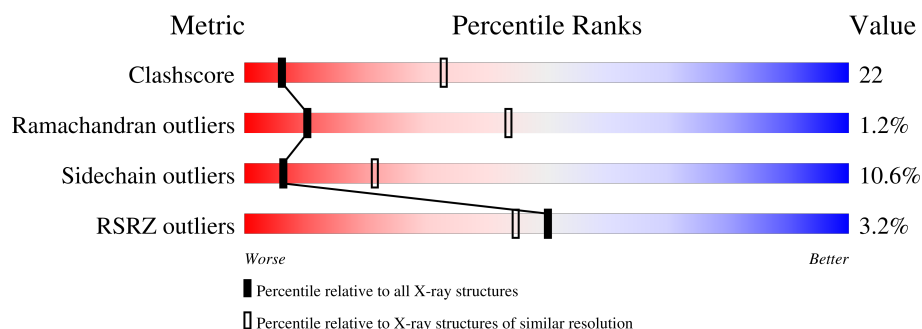
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.00 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	1210 (8.00-4.00)
Ramachandran outliers	187476	1034 (8.00-4.00)
Sidechain outliers	187428	1000 (8.00-4.00)
RSRZ outliers	180081	1136 (8.00-4.00)

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	3% 41% 36% 10% 12%
1	B	553	2% 41% 36% 8% 13%
1	C	553	3% 44% 35% 8% 11%
2	D	528	3% 51% 29% 7% 12%
2	E	528	2% 38% 38% 11% 12%
2	F	528	4% 49% 32% 6% 12%
3	G	298	2% 33% 13% 53%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22795 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			

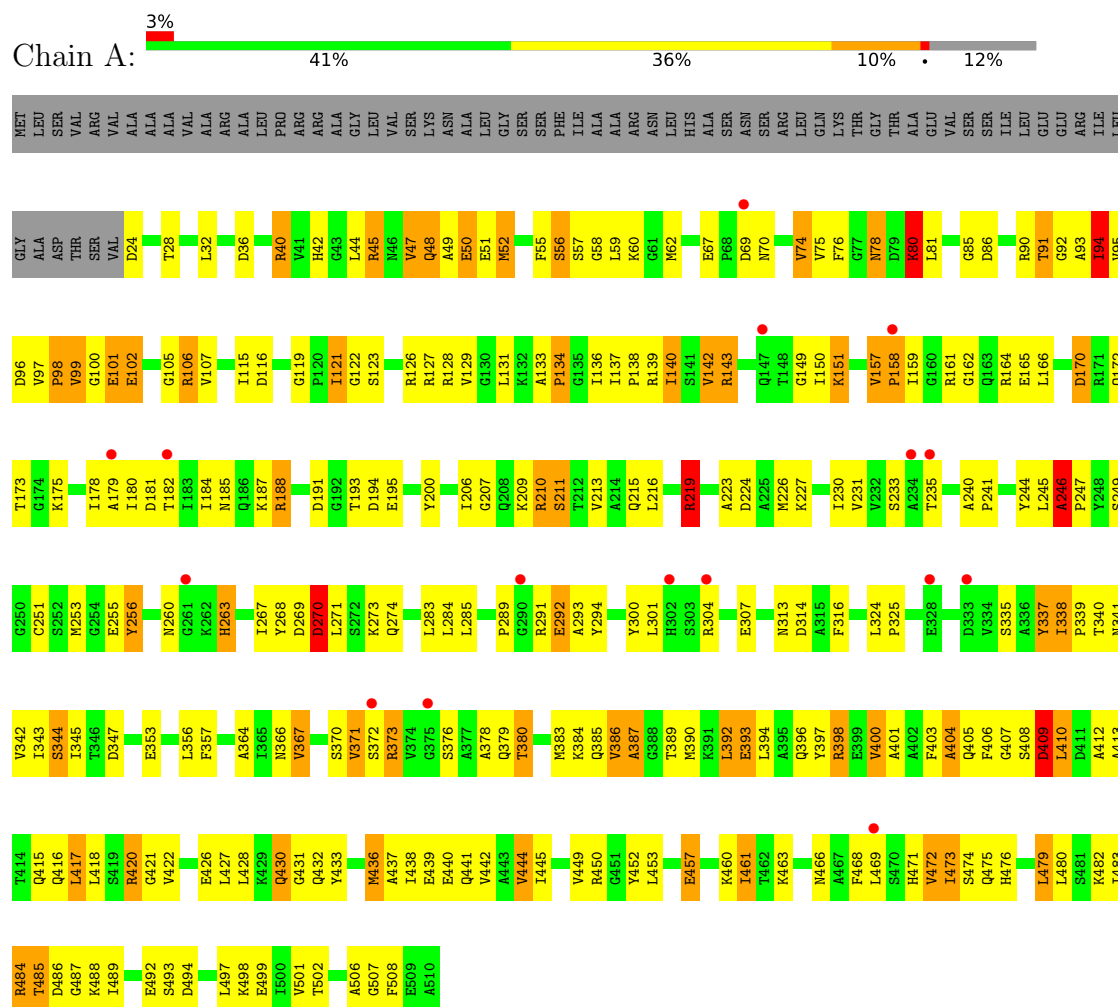
- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	140	Total	C	N	O	S	0	0	0
			1077	671	195	205	6			

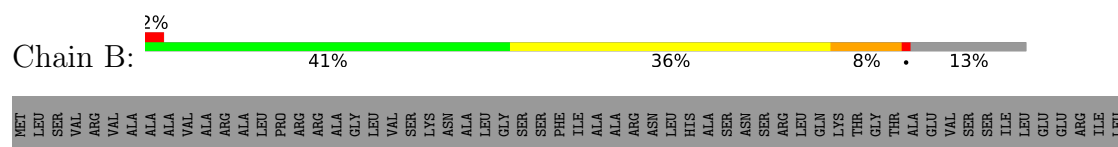
3 Residue-property plots

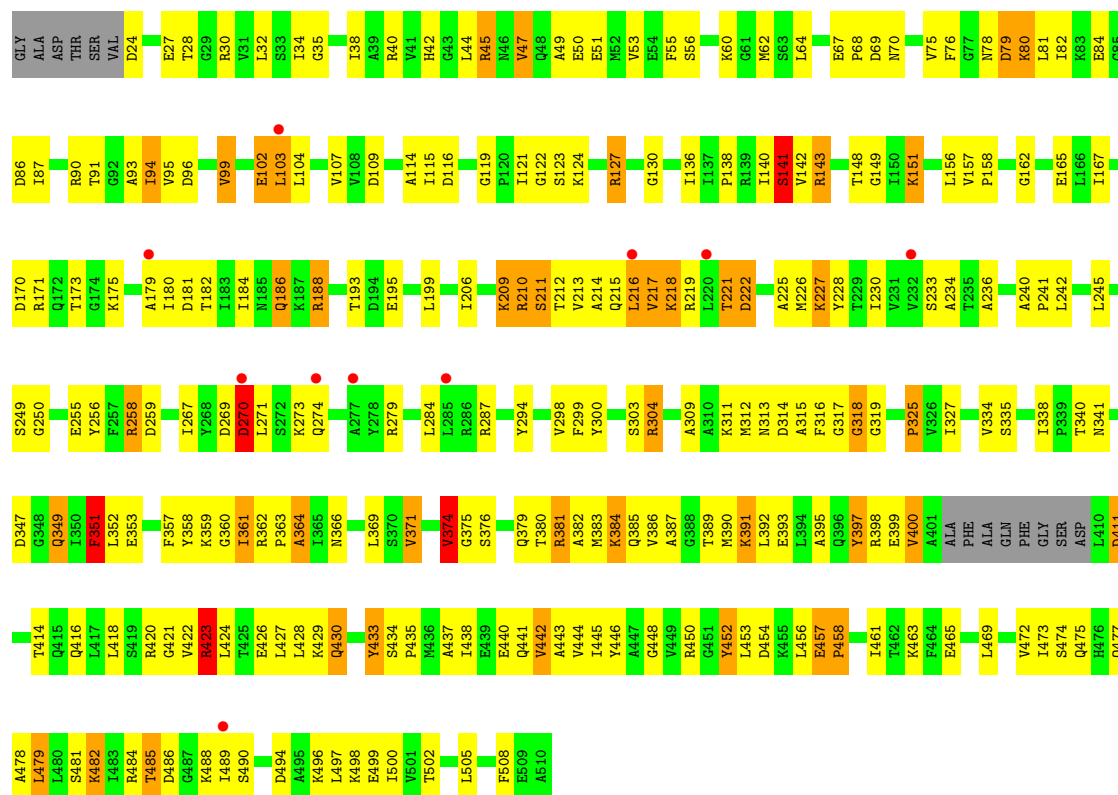
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

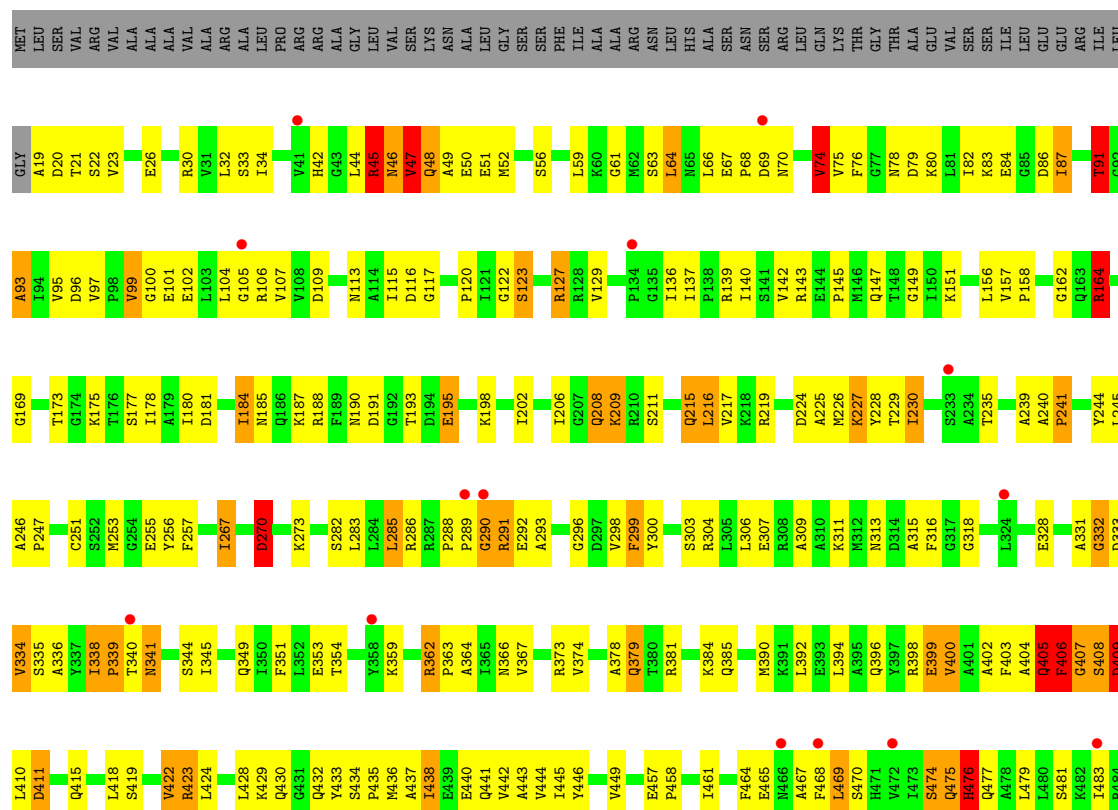
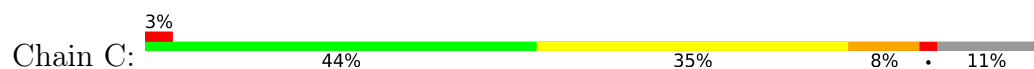


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL



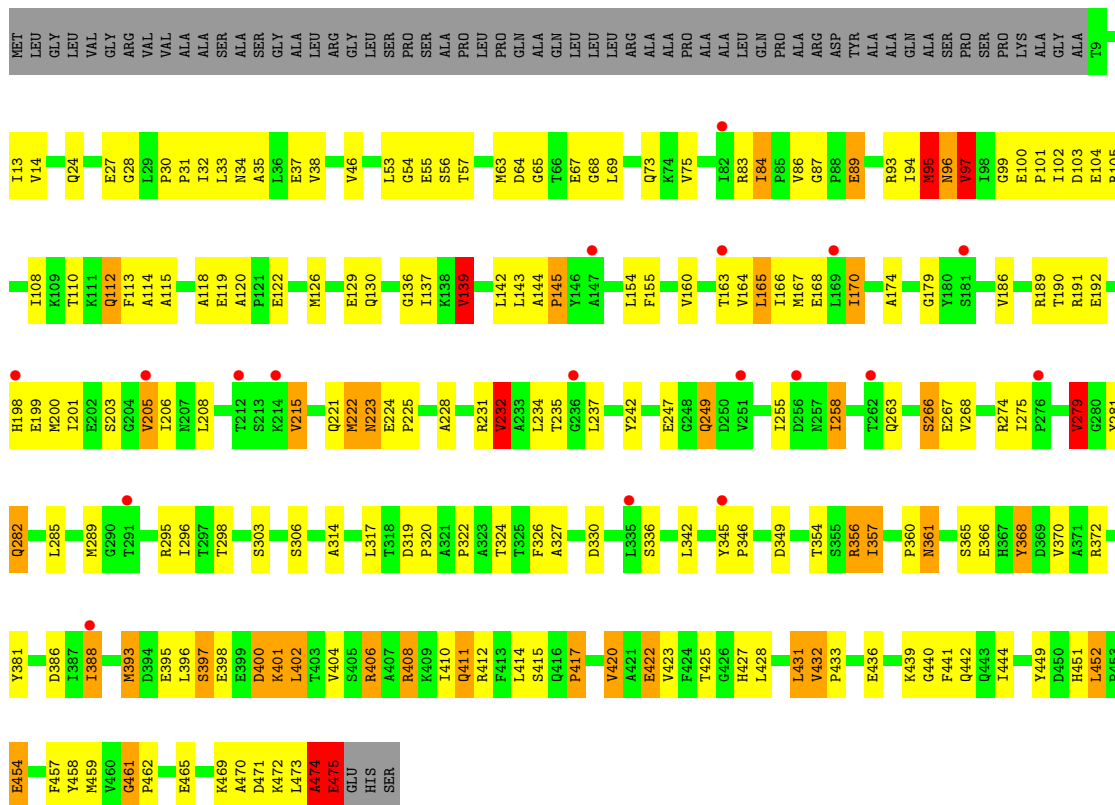


- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL

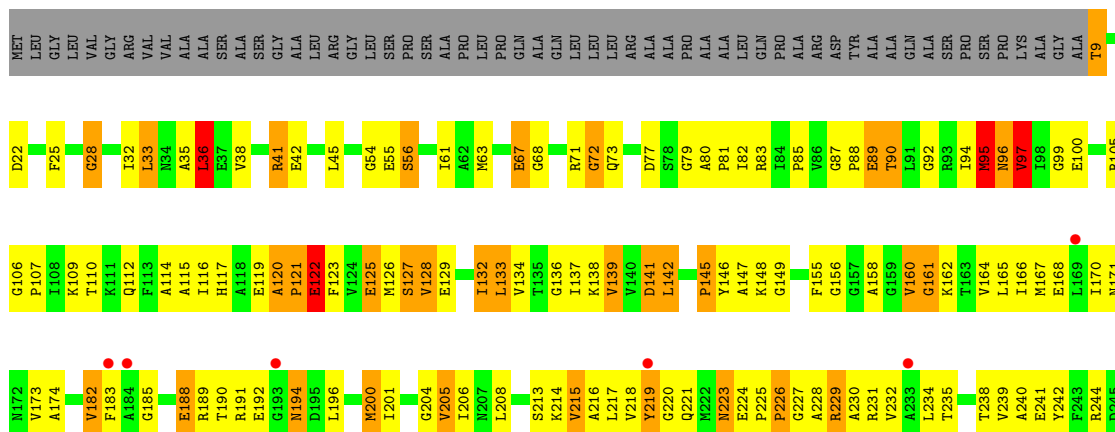


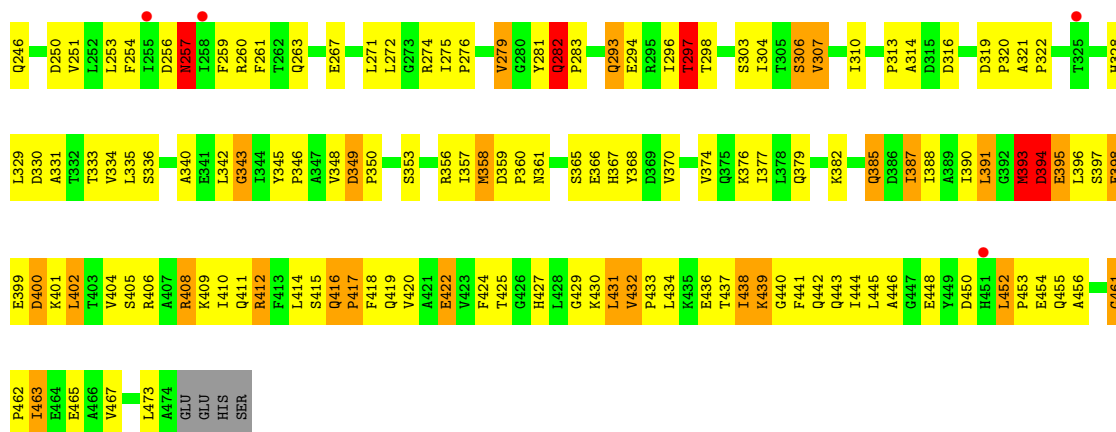


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

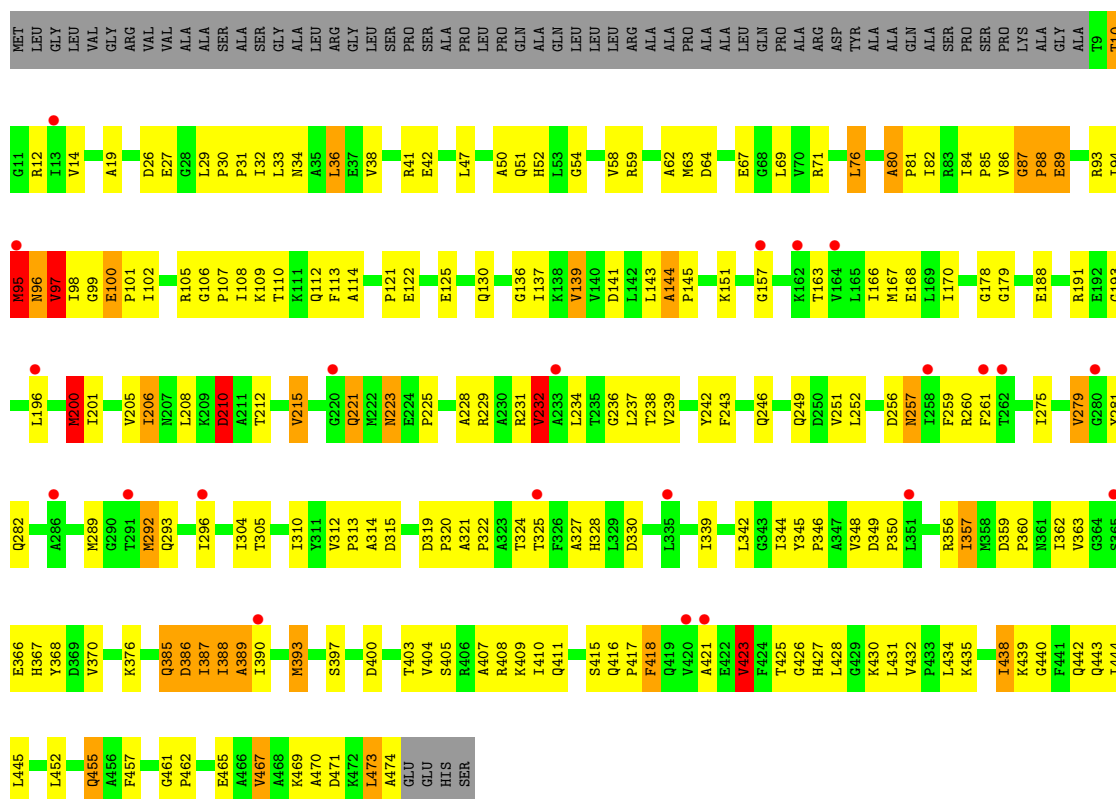


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

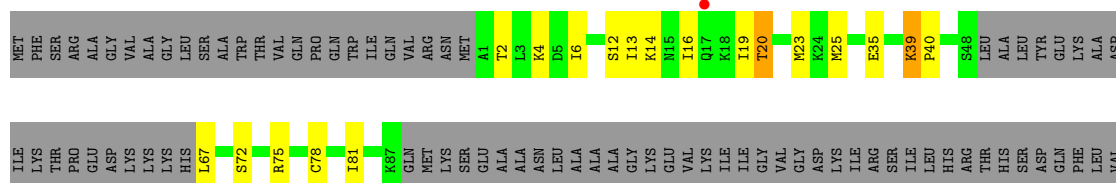
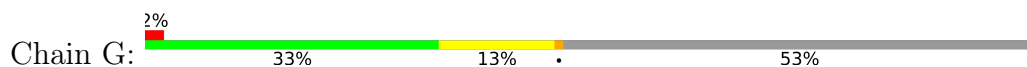


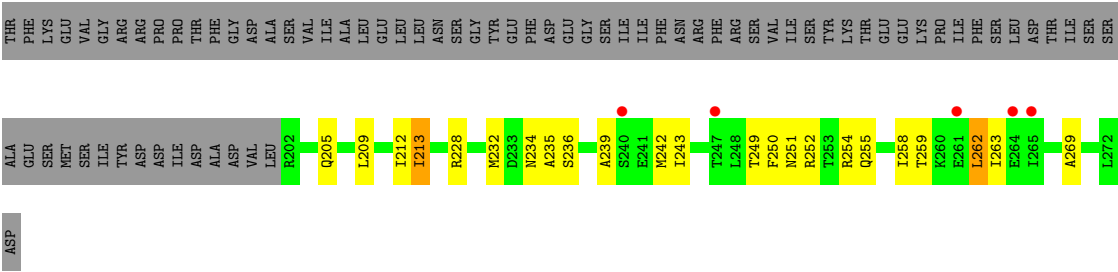


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.35Å 132.93Å 275.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.53 – 6.00 101.53 – 6.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (101.53-6.00) 65.8 (101.53-6.00)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 6.18Å)	Xtriage
Refinement program	REFMAC 5.5.0038	Depositor
R, R_{free}	0.330 , (Not available) 0.329 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	156.4	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	22795	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.56% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.76	0/3766	1.74	68/5080 (1.3%)
1	B	0.77	0/3704	1.76	70/4995 (1.4%)
1	C	0.80	1/3799 (0.0%)	1.80	73/5126 (1.4%)
2	D	0.81	1/3596 (0.0%)	1.78	69/4879 (1.4%)
2	E	0.78	0/3587	1.78	86/4867 (1.8%)
2	F	0.80	1/3587 (0.0%)	1.79	93/4867 (1.9%)
3	G	0.41	0/1083	0.93	2/1448 (0.1%)
All	All	0.77	3/23122 (0.0%)	1.74	461/31262 (1.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	96	ASN	CA-CB	5.51	1.62	1.53
2	D	96	ASN	CA-CB	5.26	1.61	1.53
1	C	290	GLY	N-CA	5.04	1.49	1.44

All (461) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	408	ARG	CD-NE-CZ	22.73	156.22	124.40
2	F	282	GLN	CB-CG-CD	15.17	138.39	112.60
2	E	408	ARG	CD-NE-CZ	13.40	143.16	124.40
1	B	351	PHE	CA-CB-CG	11.08	124.88	113.80
1	A	270	ASP	CA-CB-CG	10.88	123.48	112.60
2	F	139	VAL	CB-CA-C	-10.76	98.11	111.88
1	B	270	ASP	CA-CB-CG	10.44	123.04	112.60
1	B	375	GLY	N-CA-C	9.70	125.34	114.67
1	B	40	ARG	CD-NE-CZ	9.31	137.44	124.40
2	F	97	VAL	CB-CA-C	-9.10	99.85	112.14
2	D	139	VAL	CB-CA-C	-8.68	100.59	111.70
2	D	96	ASN	CA-CB-CG	-8.66	103.94	112.60
2	D	95	MET	CA-C-N	8.61	138.29	122.02
2	D	95	MET	C-N-CA	8.61	138.29	122.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	503	ASN	CA-CB-CG	-8.60	104.00	112.60
2	E	307	VAL	N-CA-CB	8.51	122.05	111.41
1	C	113	ASN	CA-CB-CG	-8.35	104.25	112.60
2	F	96	ASN	CB-CA-C	-8.30	93.22	110.40
1	A	269	ASP	CA-C-N	8.17	136.40	121.70
1	A	269	ASP	C-N-CA	8.17	136.40	121.70
1	C	74	VAL	N-CA-CB	-8.02	101.97	110.72
2	F	427	HIS	CA-CB-CG	8.02	121.82	113.80
2	F	95	MET	CA-C-N	7.96	138.50	121.45
2	F	95	MET	C-N-CA	7.96	138.50	121.45
2	D	349	ASP	CA-C-N	7.87	127.59	119.56
2	D	349	ASP	C-N-CA	7.87	127.59	119.56
1	C	476	HIS	N-CA-C	7.87	127.56	110.80
1	A	123	SER	N-CA-C	7.83	121.23	109.25
2	D	474	ALA	CA-C-N	7.81	135.76	121.70
2	D	474	ALA	C-N-CA	7.81	135.76	121.70
1	B	309	ALA	N-CA-C	-7.79	99.52	110.50
1	C	409	ASP	CA-CB-CG	7.64	120.24	112.60
2	E	349	ASP	CA-C-O	7.63	124.25	119.29
1	B	270	ASP	CB-CA-C	-7.60	95.66	110.10
2	E	95	MET	CA-C-O	7.54	129.94	121.11
2	F	221	GLN	N-CA-C	7.47	120.66	110.35
1	B	475	GLN	N-CA-C	7.47	119.50	111.36
2	F	95	MET	CA-CB-CG	7.46	129.02	114.10
1	A	91	THR	N-CA-C	-7.40	104.78	113.88
1	A	270	ASP	CB-CA-C	-7.36	96.12	110.10
2	E	276	PRO	CA-C-O	-7.33	112.69	122.08
2	E	395	GLU	N-CA-C	-7.25	104.56	113.19
1	C	501	VAL	N-CA-CB	7.24	118.51	110.62
2	D	417	PRO	N-CA-CB	7.24	106.97	102.92
1	A	170	ASP	CA-CB-CG	7.21	119.81	112.60
1	A	392	LEU	N-CA-C	7.19	119.20	111.36
1	B	53	VAL	CA-C-O	-7.17	114.36	121.67
1	C	429	LYS	CA-C-O	-7.16	113.56	121.87
2	D	393	MET	N-CA-C	7.16	122.19	113.38
1	B	219	ARG	NE-CZ-NH2	7.12	125.60	119.20
2	D	97	VAL	CB-CA-C	-7.10	102.42	112.22
2	F	232	VAL	CB-CA-C	-7.10	101.68	112.05
2	E	129	GLU	N-CA-C	7.08	120.21	109.23
1	A	210	ARG	CA-C-O	-7.07	112.11	120.10
2	D	249	GLN	N-CA-C	7.04	119.62	110.53
2	F	256	ASP	CA-CB-CG	7.04	119.64	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	431	GLY	N-CA-C	-7.03	101.53	112.85
1	A	260	ASN	CA-CB-CG	-7.03	105.57	112.60
2	E	343	GLY	N-CA-C	-7.01	106.74	115.08
2	F	59	ARG	NE-CZ-NH1	-6.99	114.51	121.50
1	B	349	GLN	CA-CB-CG	6.96	128.03	114.10
2	E	160	VAL	N-CA-C	-6.96	98.56	108.58
2	F	179	GLY	N-CA-C	-6.93	103.66	111.63
1	A	149	GLY	N-CA-C	-6.93	105.50	115.27
2	E	95	MET	CA-CB-CG	6.91	127.92	114.10
2	D	406	ARG	NE-CZ-NH1	-6.89	114.61	121.50
1	A	476	HIS	N-CA-C	6.89	121.61	112.25
2	F	312	VAL	CA-C-N	6.87	127.25	119.83
2	F	312	VAL	C-N-CA	6.87	127.25	119.83
1	C	476	HIS	CA-CB-CG	-6.84	106.95	113.80
2	E	261	PHE	CA-C-N	6.83	129.32	120.44
2	E	261	PHE	C-N-CA	6.83	129.32	120.44
2	E	306	SER	N-CA-C	6.78	119.99	109.07
2	E	22	ASP	CA-CB-CG	6.73	119.33	112.60
2	D	96	ASN	CB-CA-C	-6.72	97.00	111.78
1	A	314	ASP	CA-CB-CG	-6.69	105.91	112.60
1	C	149	GLY	N-CA-C	-6.68	105.38	115.00
2	E	342	LEU	N-CA-C	-6.67	105.12	113.20
2	F	385	GLN	N-CA-C	6.66	120.27	111.75
2	F	349	ASP	CA-C-N	6.65	126.28	119.56
2	F	349	ASP	C-N-CA	6.65	126.28	119.56
2	E	156	GLY	N-CA-C	-6.64	104.44	112.48
1	C	164	ARG	CD-NE-CZ	-6.62	115.13	124.40
1	C	47	VAL	CB-CA-C	-6.61	104.04	111.45
2	D	400	ASP	CA-CB-CG	6.61	119.21	112.60
1	A	285	LEU	CA-C-O	6.59	127.25	119.28
2	D	101	PRO	N-CA-CB	6.59	109.08	103.35
1	C	328	GLU	CB-CG-CD	-6.58	101.42	112.60
1	C	235	THR	N-CA-C	6.57	119.00	110.53
2	E	394	ASP	CA-CB-CG	-6.57	106.03	112.60
1	C	215	GLN	OE1-CD-NE2	6.56	129.16	122.60
2	E	87	GLY	CA-C-N	6.56	126.33	119.05
2	E	87	GLY	C-N-CA	6.56	126.33	119.05
1	B	258	ARG	CD-NE-CZ	6.56	133.58	124.40
1	B	209	LYS	CA-C-O	-6.55	113.53	120.80
1	A	80	LYS	N-CA-C	-6.53	104.34	112.90
2	E	41	ARG	CD-NE-CZ	6.52	133.53	124.40
2	F	313	PRO	N-CA-CB	6.49	109.11	103.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	GLY	CA-C-N	6.49	126.51	119.89
1	B	119	GLY	C-N-CA	6.49	126.51	119.89
2	E	141	ASP	CA-CB-CG	6.46	119.06	112.60
2	E	432	VAL	CA-C-N	6.45	126.98	120.14
2	E	432	VAL	C-N-CA	6.45	126.98	120.14
2	F	143	LEU	N-CA-C	6.45	121.35	112.90
1	B	279	ARG	CD-NE-CZ	6.45	133.43	124.40
2	D	113	PHE	CA-CB-CG	-6.45	107.36	113.80
2	F	225	PRO	CA-C-N	6.45	127.90	119.84
2	F	225	PRO	C-N-CA	6.45	127.90	119.84
1	A	230	ILE	CA-C-N	-6.42	114.56	123.10
1	A	230	ILE	C-N-CA	-6.42	114.56	123.10
2	F	193	GLY	N-CA-C	-6.42	105.06	112.50
1	A	172	GLN	N-CA-CB	-6.41	102.45	111.62
2	D	84	ILE	N-CA-C	6.37	114.91	107.84
2	E	394	ASP	N-CA-C	6.36	123.61	114.39
2	D	420	VAL	N-CA-CB	-6.36	104.06	112.26
2	E	125	GLU	N-CA-C	-6.35	105.84	113.97
2	F	59	ARG	NE-CZ-NH2	6.34	124.90	119.20
1	B	299	PHE	N-CA-C	-6.33	104.46	111.36
1	A	78	ASN	CA-CB-CG	6.31	118.91	112.60
2	D	144	ALA	CA-C-N	6.31	126.33	119.90
2	D	144	ALA	C-N-CA	6.31	126.33	119.90
2	F	64	ASP	CA-C-O	-6.30	114.71	121.45
2	D	221	GLN	N-CA-C	6.30	118.16	110.41
2	F	275	ILE	N-CA-C	-6.28	102.80	108.95
1	A	231	VAL	CA-C-N	-6.28	115.02	122.93
1	A	231	VAL	C-N-CA	-6.28	115.02	122.93
2	F	403	THR	N-CA-C	-6.28	104.36	111.14
1	A	371	VAL	CB-CA-C	-6.27	99.20	110.48
1	A	337	TYR	CA-C-N	6.25	124.17	120.24
1	A	337	TYR	C-N-CA	6.25	124.17	120.24
2	E	225	PRO	N-CA-CB	6.24	109.13	103.08
1	A	157	VAL	CA-C-N	6.23	126.60	119.93
1	A	157	VAL	C-N-CA	6.23	126.60	119.93
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
1	B	93	ALA	N-CA-C	6.20	118.51	108.41
1	C	291	ARG	NE-CZ-NH2	-6.17	113.65	119.20
2	E	106	GLY	CA-C-N	6.17	126.11	119.76
2	E	106	GLY	C-N-CA	6.17	126.11	119.76
1	B	142	VAL	N-CA-CB	6.16	118.38	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	GLU	CB-CG-CD	6.15	123.06	112.60
1	C	288	PRO	N-CA-CB	6.15	109.05	103.08
1	C	164	ARG	NE-CZ-NH1	-6.15	115.35	121.50
1	A	158	PRO	N-CA-CB	6.14	108.72	103.19
2	D	422	GLU	N-CA-C	-6.14	104.69	111.82
2	F	26	ASP	CA-CB-CG	-6.13	106.47	112.60
2	E	94	ILE	N-CA-CB	6.13	119.59	111.25
2	E	145	PRO	N-CA-CB	6.13	108.71	103.19
1	C	70	ASN	CA-C-O	-6.12	114.89	121.38
1	B	210	ARG	N-CA-CB	6.12	118.88	110.01
1	C	405	GLN	CA-C-N	6.08	133.16	121.54
1	C	405	GLN	C-N-CA	6.08	133.16	121.54
1	B	287	ARG	CB-CA-C	6.08	118.20	109.26
1	A	162	GLY	N-CA-C	-6.07	106.73	114.37
2	D	120	ALA	CA-C-N	6.06	126.08	119.90
2	D	120	ALA	C-N-CA	6.06	126.08	119.90
2	F	261	PHE	CA-C-O	6.06	126.97	120.55
1	C	157	VAL	CA-C-N	6.05	126.07	119.90
1	C	157	VAL	C-N-CA	6.05	126.07	119.90
1	B	374	VAL	N-CA-C	6.05	120.02	113.43
2	F	80	ALA	CA-C-N	6.05	126.24	120.31
2	F	80	ALA	C-N-CA	6.05	126.24	120.31
2	E	422	GLU	N-CA-C	-6.04	105.94	113.55
2	F	206	ILE	N-CA-CB	6.03	119.06	111.46
2	E	90	THR	N-CA-C	-6.03	106.05	113.41
1	A	94	ILE	CB-CA-C	6.02	119.81	111.38
1	C	45	ARG	N-CA-C	6.01	118.62	111.71
2	F	229	ARG	NE-CZ-NH1	-6.00	115.50	121.50
1	B	423	ARG	CD-NE-CZ	6.00	132.80	124.40
2	F	144	ALA	CA-C-N	6.00	126.02	119.90
2	F	144	ALA	C-N-CA	6.00	126.02	119.90
2	F	342	LEU	N-CA-C	-5.99	105.93	113.18
1	C	162	GLY	N-CA-C	-5.99	107.14	114.92
1	C	406	PHE	CA-CB-CG	5.99	119.79	113.80
2	F	432	VAL	CB-CA-C	-5.99	104.19	110.53
1	C	400	VAL	N-CA-CB	5.98	117.94	110.47
1	C	507	GLY	N-CA-C	-5.97	105.57	112.73
2	E	461	GLY	CA-C-N	5.96	125.87	119.85
2	E	461	GLY	C-N-CA	5.96	125.87	119.85
1	C	345	ILE	N-CA-C	-5.96	106.92	111.62
1	C	341	ASN	CA-C-O	-5.95	114.53	120.90
2	F	461	GLY	CA-C-N	5.95	126.28	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	461	GLY	C-N-CA	5.95	126.28	119.92
2	D	139	VAL	N-CA-CB	5.95	116.86	110.62
1	A	67	GLU	CA-C-N	5.94	125.42	119.24
1	A	67	GLU	C-N-CA	5.94	125.42	119.24
2	D	402	LEU	N-CA-C	-5.93	105.13	112.90
1	A	75	VAL	N-CA-C	5.92	116.70	109.30
1	B	167	ILE	N-CA-CB	5.92	118.14	111.21
2	F	96	ASN	N-CA-CB	-5.92	101.98	110.44
1	C	46	ASN	CA-CB-CG	5.91	118.51	112.60
1	B	371	VAL	CB-CA-C	-5.91	99.85	110.48
1	B	91	THR	N-CA-C	-5.90	105.42	114.16
1	C	422	VAL	CB-CA-C	-5.90	104.18	112.14
1	C	336	ALA	O-C-N	-5.88	116.06	123.12
2	F	388	ILE	CB-CA-C	-5.88	104.33	112.04
1	B	162	GLY	N-CA-C	-5.88	106.87	115.63
1	A	106	ARG	CD-NE-CZ	5.88	132.63	124.40
2	F	221	GLN	CA-C-N	5.88	130.09	120.63
2	F	221	GLN	C-N-CA	5.88	130.09	120.63
1	B	109	ASP	CA-CB-CG	5.88	118.47	112.60
1	B	45	ARG	CB-CG-CD	-5.87	97.80	111.30
1	C	69	ASP	CA-CB-CG	-5.87	106.73	112.60
2	D	247	GLU	N-CA-C	-5.87	106.76	114.04
1	C	91	THR	N-CA-C	-5.86	107.12	114.56
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
2	D	143	LEU	N-CA-C	5.85	120.55	113.41
2	F	370	VAL	N-CA-C	-5.85	105.03	110.53
2	F	426	GLY	N-CA-C	-5.85	107.17	115.30
1	B	351	PHE	N-CA-CB	5.83	119.92	110.42
1	C	93	ALA	N-CA-C	5.82	118.44	109.07
1	B	136	ILE	CA-C-N	5.81	124.98	120.33
1	B	136	ILE	C-N-CA	5.81	124.98	120.33
1	C	379	GLN	N-CA-C	5.81	118.94	109.59
2	E	229	ARG	N-CA-C	-5.81	106.04	113.01
1	C	109	ASP	CA-CB-CG	5.80	118.41	112.60
1	C	241	PRO	N-CA-CB	5.80	109.66	103.39
2	F	236	GLY	N-CA-C	-5.80	105.77	112.73
2	D	225	PRO	N-CA-CB	5.80	106.23	103.22
2	F	210	ASP	CB-CA-C	-5.79	100.41	111.48
1	A	370	SER	CA-C-O	-5.79	114.98	121.81
2	E	349	ASP	CA-C-N	5.78	125.88	119.87
2	E	349	ASP	C-N-CA	5.78	125.88	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	ARG	NE-CZ-NH2	5.78	124.40	119.20
2	D	454	GLU	CA-CB-CG	5.78	125.65	114.10
1	B	79	ASP	CA-CB-CG	5.76	118.36	112.60
1	C	341	ASN	O-C-N	5.76	128.08	122.09
1	A	98	PRO	N-CA-CB	5.74	108.79	103.39
2	E	97	VAL	CB-CA-C	-5.73	102.82	112.16
2	F	229	ARG	NE-CZ-NH2	5.73	124.35	119.20
1	C	230	ILE	CA-C-N	-5.72	115.22	123.11
1	C	230	ILE	C-N-CA	-5.72	115.22	123.11
2	D	96	ASN	N-CA-CB	-5.71	101.76	110.49
2	D	225	PRO	CA-C-N	5.70	126.97	119.84
2	D	225	PRO	C-N-CA	5.70	126.97	119.84
2	F	157	GLY	CA-C-O	-5.70	115.51	122.75
2	F	389	ALA	N-CA-C	5.70	118.27	111.71
1	B	304	ARG	NE-CZ-NH1	-5.69	115.81	121.50
1	C	303	SER	CA-C-N	5.69	129.36	120.82
1	C	303	SER	C-N-CA	5.69	129.36	120.82
2	E	36	LEU	CA-C-O	-5.69	114.73	121.16
1	B	433	TYR	CA-C-N	-5.69	116.27	122.59
1	B	433	TYR	C-N-CA	-5.69	116.27	122.59
1	C	100	GLY	N-CA-C	5.69	117.83	112.08
2	D	356	ARG	CD-NE-CZ	-5.67	116.45	124.40
1	C	120	PRO	N-CA-CB	5.67	108.72	103.39
1	B	245	LEU	N-CA-C	5.66	117.13	111.07
2	D	368	TYR	N-CA-C	5.66	117.45	111.28
1	A	194	ASP	CA-CB-CG	5.65	118.25	112.60
1	A	335	SER	CB-CA-C	-5.65	99.84	110.01
2	D	145	PRO	CA-C-O	-5.65	114.97	121.36
2	F	84	ILE	N-CA-C	5.64	113.82	109.19
1	C	381	ARG	CD-NE-CZ	5.63	132.28	124.40
1	A	200	TYR	CA-CB-CG	-5.62	103.78	113.90
2	F	473	LEU	N-CA-C	-5.62	105.92	112.89
2	D	145	PRO	N-CA-CB	5.62	108.19	103.25
1	B	103	LEU	N-CA-C	-5.62	106.56	113.41
2	D	163	THR	N-CA-C	5.60	117.39	111.28
1	C	362	ARG	NE-CZ-NH2	5.60	124.24	119.20
1	B	127	ARG	CD-NE-CZ	5.59	132.23	124.40
1	A	92	GLY	N-CA-C	-5.59	108.32	115.42
2	D	215	VAL	CA-C-O	-5.58	113.80	120.78
2	E	133	LEU	CA-C-O	-5.58	114.39	120.36
2	F	113	PHE	CA-CB-CG	-5.58	108.22	113.80
2	E	239	VAL	N-CA-CB	-5.58	104.76	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	304	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	A	164	ARG	CA-C-O	-5.58	113.55	120.57
2	E	219	TYR	N-CA-C	5.56	118.47	109.40
2	F	96	ASN	N-CA-C	5.56	117.70	110.53
2	F	88	PRO	N-CA-CB	5.55	108.84	103.51
1	A	420	ARG	NE-CZ-NH1	-5.55	115.95	121.50
2	E	96	ASN	CA-CB-CG	5.54	118.14	112.60
1	B	141	SER	CA-C-O	-5.54	114.92	120.96
1	B	151	LYS	N-CA-C	5.54	117.76	111.11
2	E	216	ALA	CA-C-N	-5.53	115.38	123.00
2	E	216	ALA	C-N-CA	-5.53	115.38	123.00
2	E	120	ALA	CA-C-N	5.52	126.74	119.84
2	E	120	ALA	C-N-CA	5.52	126.74	119.84
2	F	95	MET	O-C-N	-5.52	116.49	123.17
2	D	164	VAL	N-CA-C	-5.51	105.13	110.42
2	E	336	SER	N-CA-C	5.51	117.89	108.90
1	A	367	VAL	CB-CA-C	5.51	119.58	112.14
1	C	423	ARG	CD-NE-CZ	5.50	132.10	124.40
2	E	95	MET	CA-C-N	5.50	132.04	121.54
2	E	95	MET	C-N-CA	5.50	132.04	121.54
2	E	272	LEU	N-CA-C	-5.50	106.89	113.21
1	A	233	SER	N-CA-CB	-5.50	102.14	110.77
2	E	260	ARG	NE-CZ-NH1	-5.50	116.00	121.50
2	D	30	PRO	N-CA-CB	5.49	108.41	103.08
2	F	282	GLN	OE1-CD-NE2	-5.49	117.11	122.60
1	A	235	THR	N-CA-C	5.49	118.55	110.59
1	C	74	VAL	CB-CA-C	5.49	117.71	110.91
1	A	271	LEU	CA-C-O	5.47	125.67	119.27
2	F	408	ARG	NE-CZ-NH2	5.47	124.12	119.20
2	F	215	VAL	N-CA-C	5.46	115.98	108.12
2	D	232	VAL	N-CA-CB	5.46	120.23	111.23
1	A	466	ASN	OD1-CG-ND2	5.45	128.05	122.60
2	D	179	GLY	CA-C-O	-5.45	116.27	121.83
1	C	366	ASN	CA-C-O	5.45	126.59	120.92
2	D	198	HIS	CA-CB-CG	-5.45	108.35	113.80
1	A	172	GLN	N-CA-C	5.43	118.69	111.30
2	E	127	SER	N-CA-C	-5.43	101.68	110.32
2	E	196	LEU	N-CA-C	-5.43	105.01	111.69
2	E	282	GLN	CA-C-N	5.42	125.07	119.05
2	E	282	GLN	C-N-CA	5.42	125.07	119.05
2	E	257	ASN	CA-CB-CG	5.42	118.02	112.60
1	A	93	ALA	CA-C-N	-5.42	114.81	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	ALA	C-N-CA	-5.42	114.81	122.34
1	C	106	ARG	CA-CB-CG	-5.42	103.27	114.10
1	A	263	HIS	CA-CB-CG	-5.40	108.40	113.80
1	A	74	VAL	N-CA-CB	-5.39	105.51	111.66
1	A	398	ARG	NE-CZ-NH1	-5.39	116.11	121.50
2	E	331	ALA	CA-C-O	5.38	128.21	120.51
2	F	121	PRO	N-CA-CB	5.38	107.99	103.25
1	C	285	LEU	N-CA-C	-5.37	106.50	113.16
2	D	155	PHE	CA-CB-CG	5.37	119.17	113.80
2	F	12	ARG	CD-NE-CZ	-5.36	116.89	124.40
1	B	478	ALA	N-CA-C	5.35	117.11	111.28
3	G	39	LYS	CA-C-N	5.35	124.54	118.97
3	G	39	LYS	C-N-CA	5.35	124.54	118.97
1	C	123	SER	N-CA-C	5.35	117.98	109.96
2	E	83	ARG	CD-NE-CZ	-5.35	116.91	124.40
2	E	297	THR	CB-CA-C	-5.35	101.19	111.78
2	E	96	ASN	N-CA-CB	-5.34	101.46	110.49
1	C	299	PHE	N-CA-C	-5.34	105.15	110.97
2	D	222	MET	CB-CA-C	-5.34	98.52	110.21
1	B	40	ARG	NE-CZ-NH1	5.34	126.84	121.50
1	C	309	ALA	N-CA-C	-5.34	101.95	109.96
2	F	330	ASP	CA-CB-CG	-5.34	107.26	112.60
2	E	200	MET	N-CA-C	-5.34	105.12	111.69
2	F	225	PRO	N-CA-C	-5.34	104.19	110.70
1	A	52	MET	CA-C-N	-5.33	115.24	122.92
1	A	52	MET	C-N-CA	-5.33	115.24	122.92
2	E	83	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	B	259	ASP	CA-CB-CG	-5.33	107.27	112.60
2	D	268	VAL	CA-C-O	5.33	123.59	118.90
2	E	393	MET	N-CA-C	5.32	122.13	110.80
2	E	398	GLU	N-CA-C	-5.32	105.42	112.34
1	C	48	GLN	CA-C-O	-5.31	115.16	121.16
2	E	358	MET	N-CA-CB	5.31	117.00	110.53
2	F	76	LEU	N-CA-C	5.31	117.17	108.52
1	C	411	ASP	CA-CB-CG	5.30	117.90	112.60
1	B	148	THR	N-CA-C	-5.30	106.95	113.41
2	F	366	GLU	N-CA-C	-5.30	105.40	111.07
1	C	304	ARG	NE-CZ-NH2	5.29	123.96	119.20
2	D	160	VAL	N-CA-CB	5.29	118.03	112.21
2	D	411	GLN	CA-C-O	5.29	126.34	120.63
2	F	41	ARG	CG-CD-NE	5.29	123.64	112.00
2	D	322	PRO	N-CA-C	-5.29	105.91	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	423	VAL	CB-CA-C	-5.29	101.69	111.79
2	D	119	GLU	CA-C-O	-5.29	115.80	121.56
1	A	372	SER	N-CA-CB	5.28	120.09	110.95
2	E	400	ASP	CA-CB-CG	-5.28	107.32	112.60
1	C	75	VAL	N-CA-C	5.28	115.70	107.99
2	F	393	MET	N-CA-C	5.28	119.77	113.23
1	A	134	PRO	N-CA-C	-5.28	102.91	111.14
2	E	417	PRO	CB-CA-C	-5.27	104.94	111.11
1	C	33	SER	CA-C-O	-5.26	115.60	121.23
2	E	122	GLU	CA-CB-CG	5.25	124.61	114.10
1	B	318	GLY	N-CA-C	-5.25	108.59	115.47
2	F	387	ILE	CB-CA-C	-5.25	105.14	112.02
1	C	296	GLY	N-CA-C	-5.25	108.89	114.67
1	C	405	GLN	CA-C-O	5.25	128.02	120.51
2	F	87	GLY	CA-C-N	5.25	124.86	119.56
2	F	87	GLY	C-N-CA	5.25	124.86	119.56
2	F	416	GLN	CA-C-N	5.24	126.06	120.13
2	F	416	GLN	C-N-CA	5.24	126.06	120.13
1	C	127	ARG	NE-CZ-NH1	-5.22	116.28	121.50
2	D	432	VAL	CA-C-N	5.22	125.12	119.85
2	D	432	VAL	C-N-CA	5.22	125.12	119.85
2	D	327	ALA	CA-C-O	-5.21	113.18	119.49
2	E	251	VAL	CB-CA-C	-5.21	105.85	111.59
1	B	116	ASP	N-CA-C	-5.21	106.70	113.16
1	B	287	ARG	CA-C-N	5.21	125.75	120.38
1	B	287	ARG	C-N-CA	5.21	125.75	120.38
2	E	137	ILE	CA-C-O	5.21	126.79	120.74
1	B	130	GLY	O-C-N	-5.20	115.94	122.70
2	E	439	LYS	O-C-N	5.20	127.42	122.07
2	F	257	ASN	OD1-CG-ND2	5.20	127.80	122.60
1	B	219	ARG	NE-CZ-NH1	-5.19	116.31	121.50
1	C	336	ALA	N-CA-C	5.18	117.61	110.35
1	C	336	ALA	CA-C-O	5.18	126.66	121.07
2	F	19	ALA	CA-C-N	-5.18	116.07	123.11
2	F	19	ALA	C-N-CA	-5.18	116.07	123.11
2	F	101	PRO	N-CA-CB	5.18	107.86	103.35
2	F	178	GLY	CA-C-N	-5.18	114.33	122.92
2	F	178	GLY	C-N-CA	-5.18	114.33	122.92
1	B	279	ARG	NE-CZ-NH1	5.17	126.67	121.50
1	B	309	ALA	CA-C-O	-5.17	115.93	121.56
1	B	397	TYR	N-CA-C	-5.17	107.52	113.88
2	E	72	GLY	N-CA-C	-5.17	108.54	114.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	136	ILE	CA-C-N	5.16	124.46	120.33
1	C	136	ILE	C-N-CA	5.16	124.46	120.33
2	D	165	LEU	N-CA-CB	5.16	117.70	110.12
2	E	107	PRO	N-CA-CB	5.15	107.89	103.31
2	E	171	ASN	OD1-CG-ND2	5.14	127.74	122.60
2	D	357	ILE	N-CA-CB	5.14	119.70	112.15
2	F	200	MET	N-CA-CB	-5.14	102.56	110.16
1	B	149	GLY	N-CA-C	-5.13	108.53	115.21
2	D	118	ALA	CA-C-O	-5.13	115.74	121.23
2	E	250	ASP	CA-CB-CG	-5.13	107.47	112.60
2	D	170	ILE	N-CA-C	-5.12	105.55	110.72
2	E	330	ASP	CA-CB-CG	-5.12	107.48	112.60
2	F	388	ILE	N-CA-CB	5.12	116.87	110.47
2	D	224	GLU	CA-C-N	5.12	123.34	119.66
2	D	224	GLU	C-N-CA	5.12	123.34	119.66
2	F	200	MET	CA-C-O	5.12	125.84	120.42
2	E	125	GLU	CA-C-O	5.11	124.44	118.97
2	D	454	GLU	CB-CA-C	-5.11	102.80	110.92
2	D	475	GLU	N-CA-CB	5.11	119.18	110.50
2	F	281	TYR	CA-C-N	5.10	127.74	120.49
2	F	281	TYR	C-N-CA	5.10	127.74	120.49
2	D	361	ASN	CA-CB-CG	-5.09	107.51	112.60
2	F	59	ARG	CD-NE-CZ	-5.09	117.27	124.40
1	B	230	ILE	CA-C-O	-5.09	115.96	121.92
2	F	330	ASP	N-CA-C	-5.09	107.20	113.41
1	A	219	ARG	CD-NE-CZ	5.08	131.52	124.40
1	A	338	ILE	N-CA-CB	5.08	113.70	110.50
1	A	387	ALA	CA-C-N	5.08	125.58	119.94
1	A	387	ALA	C-N-CA	5.08	125.58	119.94
1	B	457	GLU	N-CA-C	5.08	116.30	109.24
1	B	391	LYS	N-CA-C	-5.08	105.93	111.82
1	C	145	PRO	N-CA-CB	5.08	108.16	103.39
2	E	173	VAL	N-CA-C	-5.08	105.47	111.00
1	A	400	VAL	N-CA-C	5.07	119.50	112.35
1	B	141	SER	CB-CA-C	-5.07	102.23	109.84
1	B	94	ILE	N-CA-C	-5.07	102.53	109.37
1	C	483	ILE	N-CA-C	-5.06	105.56	110.42
2	D	354	THR	CA-C-O	-5.06	115.68	121.40
2	F	293	GLN	CA-C-O	-5.06	115.19	120.55
1	A	101	GLU	N-CA-C	5.06	118.91	112.34
2	D	461	GLY	CA-C-N	5.06	124.96	119.85
2	D	461	GLY	C-N-CA	5.06	124.96	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	170	ILE	N-CA-C	-5.05	105.46	110.62
2	F	418	PHE	CA-CB-CG	5.05	118.85	113.80
1	A	178	ILE	CB-CA-C	-5.05	105.42	111.88
1	B	222	ASP	CA-C-N	-5.05	114.21	122.54
1	B	222	ASP	C-N-CA	-5.05	114.21	122.54
1	B	325	PRO	CA-C-N	-5.05	116.59	123.10
1	B	325	PRO	C-N-CA	-5.05	116.59	123.10
2	F	100	GLU	CA-C-O	-5.05	115.95	120.19
2	E	226	PRO	CA-C-N	5.04	125.68	120.03
2	E	226	PRO	C-N-CA	5.04	125.68	120.03
1	A	246	ALA	CA-C-N	5.04	124.83	119.28
1	A	246	ALA	C-N-CA	5.04	124.83	119.28
2	F	417	PRO	CB-CA-C	-5.04	105.21	111.11
1	B	274	GLN	N-CA-C	-5.04	105.87	111.36
1	C	438	ILE	N-CA-C	5.03	115.64	110.36
1	B	167	ILE	N-CA-C	-5.03	100.65	107.99
1	B	349	GLN	N-CA-CB	5.03	120.44	111.69
2	D	97	VAL	O-C-N	5.03	127.01	121.83
1	B	374	VAL	CB-CA-C	-5.02	104.56	110.84
2	F	107	PRO	N-CA-CB	5.02	108.00	103.33
1	C	270	ASP	CA-CB-CG	5.02	117.62	112.60
1	C	209	LYS	N-CA-CB	-5.01	102.70	110.57
1	C	415	GLN	N-CA-C	-5.01	105.92	112.23
2	E	56	SER	CA-C-N	-5.01	115.43	122.94
2	E	56	SER	C-N-CA	-5.01	115.43	122.94
2	F	85	PRO	N-CA-CB	5.01	107.63	103.17
2	E	415	SER	CA-C-O	-5.00	116.03	121.89

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3715	0	3813	197	0
1	B	3656	0	3764	165	58

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3748	0	3843	180	56
2	D	3539	0	3593	167	0
2	E	3530	0	3587	234	0
2	F	3530	0	3587	131	2
3	G	1077	0	1139	70	0
All	All	22795	0	23326	1034	58

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 (1034) 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:F:390:ILE:CD1	3:G:242:MET:HE1	1.54	1.37
2:F:390:ILE:HD11	3:G:242:MET:CE	1.54	1.36
2:F:390:ILE:CD1	3:G:242:MET:CE	2.07	1.29
2:E:390:ILE:HG13	3:G:25:MET:SD	1.75	1.25
1:C:127:ARG:HH12	1:C:255:GLU:HB2	1.00	1.13
2:E:390:ILE:HG21	3:G:25:MET:HB3	1.30	1.06
1:C:215:GLN:HG3	2:F:356:ARG:HH22	0.95	1.05
1:A:291:ARG:CA	3:G:262:LEU:HD22	1.86	1.04
1:A:291:ARG:HA	3:G:262:LEU:HD22	1.04	1.01
1:A:291:ARG:HA	3:G:262:LEU:CD2	1.90	1.01
1:C:344:SER:O	2:D:222:MET:HE1	1.59	1.00
1:B:214:ALA:HA	2:E:123:PHE:CZ	1.96	0.99
1:C:215:GLN:HG3	2:F:356:ARG:NH2	1.77	0.98
2:E:223:ASN:HD22	2:E:223:ASN:H	1.00	0.98
3:G:19:ILE:HG22	3:G:23:MET:HE2	1.49	0.95
2:E:314:ALA:CB	3:G:254:ARG:CZ	2.44	0.95
1:C:404:ALA:C	1:C:406:PHE:H	1.64	0.94
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.48	0.93
2:F:223:ASN:HD22	2:F:223:ASN:H	1.07	0.93
2:F:390:ILE:HD11	3:G:242:MET:HE1	0.92	0.92
1:B:214:ALA:HB2	2:E:123:PHE:CE1	2.05	0.91
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.52	0.91
1:C:127:ARG:NH1	1:C:255:GLU:HB2	1.84	0.90
1:A:215:GLN:HG3	2:D:356:ARG:NH1	1.88	0.88
2:D:395:GLU:OE2	3:G:75:ARG:NE	2.05	0.88
1:C:30:ARG:HE	1:C:87:ILE:HD11	1.37	0.88
2:E:89:GLU:HG2	2:E:110:THR:HG22	1.55	0.87
2:E:390:ILE:CG1	3:G:25:MET:SD	2.63	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:84:ILE:HD12	2:D:95:MET:HE1	1.57	0.87
2:E:314:ALA:HB3	3:G:254:ARG:NH2	1.90	0.86
2:E:223:ASN:H	2:E:223:ASN:ND2	1.72	0.85
2:F:390:ILE:CD1	3:G:242:MET:HE3	2.06	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	0.84
2:F:390:ILE:HD11	3:G:242:MET:SD	2.18	0.83
1:B:456:LEU:HD12	1:B:457:GLU:H	1.42	0.83
2:E:132:ILE:HD12	2:E:145:PRO:HB3	1.61	0.82
1:A:406:PHE:CD1	3:G:19:ILE:HD13	2.15	0.81
2:E:314:ALA:HB2	3:G:254:ARG:CZ	2.11	0.81
1:A:291:ARG:N	3:G:262:LEU:HD21	1.96	0.80
1:A:347:ASP:OD1	2:E:191:ARG:NH1	2.14	0.80
1:B:214:ALA:CA	2:E:123:PHE:CE1	2.65	0.79
1:B:141:SER:O	1:B:143:ARG:HD2	1.83	0.79
2:E:370:VAL:HG21	2:E:438:ILE:HG22	1.65	0.79
2:D:139:VAL:HG13	2:D:414:LEU:HD22	1.65	0.79
2:F:390:ILE:HD13	3:G:242:MET:HE1	1.60	0.79
2:D:136:GLY:HA3	2:D:431:LEU:HD13	1.66	0.78
1:B:186:GLN:HG3	1:B:199:LEU:HB3	1.65	0.78
2:D:404:VAL:O	2:D:408:ARG:HG3	1.84	0.78
1:A:291:ARG:CA	3:G:262:LEU:CD2	2.55	0.77
1:A:392:LEU:HG	1:A:396:GLN:HE21	1.50	0.76
1:B:379:GLN:HB3	1:B:384:LYS:HE2	1.68	0.76
1:C:52:MET:HE3	1:C:95:VAL:HG22	1.68	0.76
2:D:282:GLN:H	2:D:282:GLN:HE21	1.30	0.76
2:E:394:ASP:C	2:E:396:LEU:H	1.93	0.75
2:D:53:LEU:HD12	2:D:57:THR:HG22	1.66	0.75
2:F:130:GLN:HB3	2:F:357:ILE:HD11	1.67	0.75
2:D:433:PRO:HG2	2:D:436:GLU:HG2	1.70	0.74
2:E:89:GLU:HG3	2:E:109:LYS:O	1.87	0.74
2:E:345:TYR:HA	2:E:346:PRO:C	2.13	0.74
2:F:223:ASN:H	2:F:223:ASN:ND2	1.85	0.74
1:B:214:ALA:CB	2:E:123:PHE:CE1	2.71	0.74
2:D:223:ASN:H	2:D:223:ASN:HD22	1.35	0.73
2:E:390:ILE:HG22	2:E:391:LEU:HD23	1.70	0.73
2:E:139:VAL:HG13	2:E:414:LEU:HD22	1.71	0.73
2:E:96:ASN:HB3	2:E:100:GLU:H	1.52	0.73
2:E:38:VAL:HG21	2:E:45:LEU:HD23	1.71	0.72
1:C:34:ILE:HD11	1:C:79:ASP:HB2	1.72	0.72
2:E:314:ALA:CB	3:G:254:ARG:NH2	2.50	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:183:PHE:HB3	2:E:217:LEU:HD22	1.72	0.72
1:B:209:LYS:HG2	2:E:294:GLU:OE2	1.89	0.71
2:F:89:GLU:HG3	2:F:109:LYS:O	1.89	0.71
2:D:275:ILE:HG23	3:G:269:ALA:HB2	1.73	0.71
1:B:180:ILE:HD11	1:B:216:LEU:HD21	1.71	0.71
2:D:96:ASN:HB2	2:D:100:GLU:H	1.56	0.71
2:E:433:PRO:HD2	2:E:436:GLU:HB2	1.73	0.70
2:E:388:ILE:HG23	2:E:393:MET:HG3	1.73	0.70
1:A:407:GLY:HA2	1:A:410:LEU:HD21	1.74	0.70
2:D:200:MET:HE3	2:D:215:VAL:HG21	1.74	0.69
1:B:214:ALA:CA	2:E:123:PHE:CZ	2.74	0.69
1:A:215:GLN:HG3	2:D:356:ARG:HH12	1.57	0.69
2:F:390:ILE:HD13	3:G:242:MET:CE	2.14	0.69
1:C:211:SER:O	1:C:215:GLN:HG2	1.91	0.69
2:E:105:ARG:CZ	2:E:208:LEU:HD23	2.23	0.69
1:B:452:TYR:OH	1:B:498:LYS:HG3	1.92	0.69
1:A:97:VAL:HA	1:A:126:ARG:HH21	1.56	0.68
1:A:479:LEU:HA	1:A:482:LYS:HE3	1.73	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
2:F:223:ASN:HD22	2:F:223:ASN:N	1.85	0.68
1:A:97:VAL:HB	1:A:98:PRO:HD2	1.76	0.68
1:A:44:LEU:O	1:A:47:VAL:HG22	1.94	0.68
1:C:385:GLN:OE1	1:C:488:LYS:HG2	1.93	0.68
1:A:134:PRO:O	1:A:139:ARG:NH2	2.27	0.67
1:A:383:MET:HE2	1:A:438:ILE:HD11	1.77	0.67
1:A:376:SER:C	1:A:378:ALA:H	2.02	0.67
1:A:440:GLU:O	1:A:444:VAL:HG13	1.94	0.67
1:B:156:LEU:HD22	1:B:391:LYS:HD2	1.77	0.67
2:E:223:ASN:HD22	2:E:223:ASN:N	1.84	0.67
2:F:89:GLU:HG2	2:F:110:THR:HG22	1.75	0.67
2:F:252:LEU:HD23	2:F:305:THR:HB	1.75	0.67
2:E:313:PRO:HD2	2:E:322:PRO:HG3	1.75	0.67
1:B:44:LEU:HB3	1:B:47:VAL:HG22	1.76	0.66
1:C:59:LEU:HD23	1:C:82:ILE:HD11	1.77	0.66
2:E:390:ILE:CG2	3:G:25:MET:HB3	2.18	0.66
3:G:14:LYS:HG3	3:G:243:ILE:HD12	1.76	0.66
2:F:80:ALA:HB1	2:F:81:PRO:CD	2.25	0.66
2:F:409:LYS:HD3	2:F:457:PHE:CE2	2.30	0.66
1:C:418:LEU:O	1:C:422:VAL:HG23	1.94	0.66
2:E:359:ASP:OD2	2:E:361:ASN:HB2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:THR:HG22	1:C:354:THR:HG22	1.77	0.65
2:D:167:MET:HB3	2:D:420:VAL:HG11	1.78	0.65
2:D:200:MET:HB3	2:D:206:ILE:HG13	1.79	0.65
2:F:314:ALA:O	2:F:315:ASP:HB2	1.95	0.65
1:B:362:ARG:HA	1:B:363:PRO:C	2.22	0.65
1:C:44:LEU:O	1:C:47:VAL:HG22	1.96	0.65
1:B:188:ARG:HH21	1:B:437:ALA:HB2	1.62	0.65
1:C:99:VAL:HG22	1:C:253:MET:HA	1.78	0.65
2:E:314:ALA:HB1	3:G:254:ARG:NE	2.12	0.65
1:A:471:HIS:CE1	1:A:475:GLN:HG3	2.32	0.65
1:B:214:ALA:N	2:E:123:PHE:HE1	1.94	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	0.64
2:E:314:ALA:CB	3:G:254:ARG:NE	2.60	0.64
2:F:344:ILE:HG23	2:F:415:SER:HB3	1.78	0.64
2:F:136:GLY:HA3	2:F:431:LEU:CD1	2.26	0.64
1:C:188:ARG:HH21	1:C:437:ALA:HB2	1.62	0.64
1:C:488:LYS:HG2	1:C:489:ILE:H	1.63	0.64
2:D:54:GLY:O	2:D:55:GLU:HB2	1.96	0.64
2:E:136:GLY:HA3	2:E:431:LEU:HD13	1.77	0.64
1:C:419:SER:O	1:C:423:ARG:HG2	1.98	0.64
2:E:346:PRO:HG3	2:E:418:PHE:CZ	2.33	0.64
1:B:437:ALA:O	1:B:440:GLU:N	2.30	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
1:B:214:ALA:HA	2:E:123:PHE:HZ	1.59	0.64
1:C:202:ILE:HG12	1:C:230:ILE:HD12	1.80	0.64
2:F:200:MET:HG3	2:F:205:VAL:HG23	1.80	0.64
2:D:223:ASN:H	2:D:223:ASN:ND2	1.93	0.64
1:A:291:ARG:HH21	3:G:258:ILE:CD1	2.10	0.63
1:B:214:ALA:HA	2:E:123:PHE:CE1	2.32	0.63
2:E:443:GLN:HG2	2:E:448:GLU:OE2	1.98	0.63
2:F:200:MET:HG3	2:F:205:VAL:CG2	2.27	0.63
1:C:52:MET:HE2	1:C:76:PHE:HE2	1.62	0.63
2:E:139:VAL:CG1	2:E:414:LEU:HD22	2.28	0.63
2:E:400:ASP:O	2:E:404:VAL:HG23	1.98	0.63
3:G:39:LYS:HB3	3:G:40:PRO:HD3	1.80	0.63
1:A:344:SER:O	2:E:189:ARG:NH2	2.32	0.63
1:A:376:SER:C	1:A:378:ALA:N	2.55	0.63
2:F:94:ILE:HG22	2:F:102:ILE:HD11	1.80	0.63
2:E:425:THR:O	2:E:427:HIS:ND1	2.21	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ARG:N	3:G:262:LEU:CD2	2.59	0.63
2:E:298:THR:HG23	2:E:303:SER:HB3	1.81	0.63
2:F:363:VAL:HG23	2:F:367:HIS:HB3	1.81	0.63
1:C:436:MET:HE3	1:C:469:LEU:HD21	1.79	0.63
2:E:204:GLY:O	2:E:206:ILE:N	2.32	0.62
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.64	0.62
1:B:67:GLU:O	2:F:71:ARG:NH1	2.31	0.62
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.34	0.62
1:C:52:MET:O	1:C:91:THR:HB	1.99	0.62
2:E:138:LYS:HE2	2:E:432:VAL:HG21	1.81	0.62
1:B:390:MET:HE1	1:B:428:LEU:HD21	1.80	0.62
1:C:151:LYS:HE3	1:C:430:GLN:HG3	1.82	0.62
1:A:341:ASN:O	1:A:345:ILE:HG13	1.99	0.62
2:E:158:ALA:C	2:E:160:VAL:H	2.08	0.62
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.34	0.62
1:A:394:LEU:HD11	1:A:428:LEU:HD11	1.82	0.62
1:B:389:THR:HA	1:B:392:LEU:CD1	2.29	0.62
2:E:422:GLU:HG2	2:E:427:HIS:O	1.99	0.61
2:F:63:MET:HE1	2:F:97:VAL:HG11	1.82	0.61
1:B:102:GLU:HG3	1:B:122:GLY:O	2.00	0.61
1:C:99:VAL:HG13	1:C:256:TYR:HB2	1.82	0.61
2:D:396:LEU:HD22	2:D:400:ASP:CB	2.30	0.61
1:A:283:LEU:HD21	1:A:289:PRO:HB3	1.83	0.61
2:E:224:GLU:O	2:E:229:ARG:NH1	2.32	0.61
1:A:209:LYS:HZ1	2:D:330:ASP:CG	2.08	0.61
2:E:397:SER:C	2:E:399:GLU:N	2.58	0.61
1:C:292:GLU:O	1:C:293:ALA:HB3	2.00	0.61
1:A:291:ARG:HH21	3:G:258:ILE:HD13	1.66	0.61
1:B:389:THR:HA	1:B:392:LEU:HD12	1.82	0.60
1:C:408:SER:O	1:C:409:ASP:C	2.44	0.60
1:C:373:ARG:CZ	2:D:189:ARG:NH2	2.64	0.60
2:E:201:ILE:HD13	2:E:208:LEU:HD11	1.82	0.60
1:B:184:ILE:HG22	1:B:435:PRO:HG2	1.81	0.60
1:A:52:MET:O	1:A:91:THR:HG23	2.02	0.60
1:B:422:VAL:O	1:B:426:GLU:HG2	2.00	0.60
1:A:166:LEU:HA	1:A:325:PRO:HD2	1.83	0.60
1:A:270:ASP:OD1	1:A:273:LYS:HG3	2.01	0.60
1:B:218:LYS:HG2	2:E:128:VAL:HG11	1.84	0.60
1:A:457:GLU:CB	1:A:460:LYS:HD3	2.31	0.60
1:B:51:GLU:HA	1:B:94:ILE:HA	1.83	0.60
2:D:89:GLU:HG2	2:D:110:THR:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:93:ARG:HG3	2:D:93:ARG:HH11	1.66	0.60
2:E:32:ILE:O	2:E:33:LEU:HB2	2.02	0.60
2:E:419:GLN:HG3	2:E:429:GLY:HA3	1.84	0.60
1:A:439:GLU:HG2	1:A:484:ARG:HB2	1.83	0.60
1:A:121:ILE:HD13	1:A:121:ILE:H	1.66	0.60
2:E:397:SER:H	2:E:400:ASP:HB2	1.66	0.60
1:A:40:ARG:HH11	1:A:40:ARG:HG3	1.66	0.59
1:B:438:ILE:O	1:B:442:VAL:HG22	2.02	0.59
1:B:479:LEU:HD11	1:B:497:LEU:HD13	1.83	0.59
2:D:393:MET:HE3	2:D:404:VAL:HG21	1.84	0.59
2:E:149:GLY:HA2	2:E:304:ILE:O	2.02	0.59
1:B:499:GLU:O	1:B:502:THR:HB	2.03	0.59
2:D:63:MET:HE3	2:D:228:ALA:HA	1.83	0.59
2:D:473:LEU:C	2:D:475:GLU:H	2.08	0.59
1:C:405:GLN:C	1:C:406:PHE:HD1	2.11	0.59
1:C:433:TYR:C	1:C:435:PRO:HD3	2.26	0.59
2:F:96:ASN:HD22	2:F:100:GLU:HB2	1.68	0.59
1:A:157:VAL:N	1:A:158:PRO:CD	2.65	0.59
1:B:214:ALA:N	2:E:123:PHE:CE1	2.70	0.59
1:C:102:GLU:OE2	1:C:123:SER:HA	2.03	0.59
2:D:263:GLN:O	2:D:267:GLU:HG3	2.03	0.59
1:B:400:VAL:HB	1:B:418:LEU:HD21	1.85	0.59
2:E:408:ARG:O	2:E:412:ARG:HG3	2.02	0.59
1:B:170:ASP:O	1:B:175:LYS:HE2	2.03	0.59
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.37	0.59
1:B:452:TYR:O	1:B:453:LEU:HD23	2.03	0.59
2:F:105:ARG:NH1	2:F:208:LEU:HD23	2.18	0.59
1:A:432:GLN:HB3	1:A:433:TYR:CD2	2.37	0.59
1:B:391:LYS:O	1:B:395:ALA:N	2.36	0.59
1:C:140:ILE:HD11	1:C:143:ARG:NH2	2.18	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:313:ASN:OD1	1:C:316:PHE:HD1	1.85	0.59
1:C:344:SER:O	2:D:222:MET:CE	2.44	0.59
2:D:186:VAL:HG13	2:D:232:VAL:HG23	1.85	0.59
2:F:122:GLU:HB2	2:F:125:GLU:HG3	1.84	0.59
1:C:407:GLY:HA2	1:C:410:LEU:HD11	1.84	0.58
1:C:374:VAL:HG11	1:C:378:ALA:HB2	1.85	0.58
1:B:358:TYR:C	1:B:360:GLY:H	2.11	0.58
1:C:464:PHE:CE1	1:C:505:LEU:HD23	2.39	0.58
2:E:122:GLU:N	2:E:125:GLU:OE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:200:MET:HB3	2:E:205:VAL:HG23	1.84	0.58
2:F:29:LEU:HD12	2:F:30:PRO:HD2	1.85	0.58
1:B:352:LEU:HA	1:B:364:ALA:O	2.04	0.58
2:E:95:MET:CG	2:E:99:GLY:HA2	2.34	0.58
2:E:226:PRO:HB3	2:E:267:GLU:HB2	1.84	0.58
1:B:411:ASP:HB3	1:B:414:THR:OG1	2.03	0.58
1:C:396:GLN:HG3	2:D:458:TYR:CE2	2.38	0.58
1:C:406:PHE:O	1:C:408:SER:N	2.36	0.58
2:E:85:PRO:HD2	2:E:95:MET:HE2	1.86	0.58
2:D:431:LEU:C	2:D:431:LEU:HD12	2.29	0.58
1:A:472:VAL:HG23	1:A:480:LEU:HD11	1.85	0.58
2:E:138:LYS:O	2:E:142:LEU:HB3	2.04	0.58
1:C:396:GLN:NE2	2:D:342:LEU:O	2.35	0.57
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.85	0.57
2:E:433:PRO:HG2	2:E:436:GLU:HG2	1.86	0.57
1:A:48:GLN:HB3	2:E:68:GLY:HA2	1.87	0.57
1:B:393:GLU:OE1	1:B:424:LEU:HD11	2.05	0.57
1:C:184:ILE:HG22	1:C:435:PRO:HG2	1.87	0.57
1:C:404:ALA:O	1:C:406:PHE:N	2.37	0.57
1:A:291:ARG:NH2	3:G:258:ILE:HD13	2.19	0.57
2:F:440:GLY:O	2:F:444:ILE:HG13	2.04	0.57
1:B:51:GLU:OE2	1:B:90:ARG:HB3	2.05	0.57
1:B:180:ILE:O	1:B:181:ASP:C	2.47	0.57
1:C:78:ASN:ND2	1:C:80:LYS:HD3	2.19	0.57
2:D:473:LEU:C	2:D:475:GLU:N	2.62	0.57
2:E:77:ASP:OD1	2:E:79:GLY:N	2.34	0.57
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.85	0.57
1:A:406:PHE:CG	3:G:19:ILE:HG21	2.40	0.57
1:C:107:VAL:HG12	1:C:115:ILE:HD11	1.86	0.57
2:E:105:ARG:NH2	2:E:208:LEU:HA	2.20	0.57
1:B:357:PHE:CE1	1:B:362:ARG:HD3	2.40	0.57
2:E:246:GLN:HA	2:E:246:GLN:NE2	2.19	0.57
2:F:14:VAL:O	2:F:71:ARG:HG2	2.05	0.57
1:A:219:ARG:HH11	1:A:219:ARG:HB2	1.69	0.56
2:D:282:GLN:H	2:D:282:GLN:NE2	2.01	0.56
1:A:107:VAL:HG12	1:A:115:ILE:HD11	1.87	0.56
2:E:155:PHE:CE1	2:E:310:ILE:HD12	2.40	0.56
1:A:185:ASN:O	1:A:188:ARG:HG3	2.05	0.56
1:B:214:ALA:HB2	2:E:123:PHE:CD1	2.41	0.56
1:C:52:MET:HE2	1:C:76:PHE:CE2	2.41	0.56
1:C:156:LEU:HD13	1:C:367:VAL:HG22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:126:MET:HE1	2:E:297:THR:HG21	1.86	0.56
2:F:32:ILE:O	2:F:33:LEU:HB2	2.05	0.56
3:G:209:LEU:O	3:G:213:ILE:HG22	2.05	0.56
1:A:209:LYS:NZ	2:D:330:ASP:OD1	2.31	0.56
1:A:450:ARG:NH2	1:A:494:ASP:OD2	2.38	0.56
2:E:267:GLU:O	2:E:271:LEU:HG	2.05	0.56
1:B:62:MET:HE3	1:B:64:LEU:HD13	1.87	0.56
1:A:209:LYS:HE3	1:A:211:SER:HB2	1.88	0.56
1:B:423:ARG:HE	1:B:458:PRO:HG3	1.71	0.56
2:D:471:ASP:O	2:D:474:ALA:N	2.39	0.56
2:F:98:ILE:HG13	2:F:100:GLU:HG3	1.88	0.56
1:B:351:PHE:CE1	1:B:369:LEU:HB3	2.41	0.56
1:C:173:THR:CG2	1:C:354:THR:HG22	2.35	0.56
1:A:224:ASP:CG	1:A:227:LYS:HE3	2.31	0.56
1:B:80:LYS:HG3	1:B:81:LEU:HD23	1.88	0.56
1:B:347:ASP:HB3	1:B:374:VAL:HG22	1.88	0.56
2:D:366:GLU:HG3	2:D:442:GLN:HE22	1.71	0.56
2:E:174:ALA:CB	2:E:214:LYS:HD3	2.35	0.56
1:C:219:ARG:HD3	1:C:433:TYR:CE1	2.41	0.55
2:D:84:ILE:CD1	2:D:95:MET:HE1	2.34	0.55
2:F:324:THR:O	2:F:324:THR:HG22	2.05	0.55
1:C:187:LYS:HE2	1:C:191:ASP:OD2	2.05	0.55
2:E:138:LYS:HG3	2:E:416:GLN:OE1	2.06	0.55
2:E:244:ARG:HG3	2:E:303:SER:N	2.22	0.55
2:E:92:GLY:N	2:E:215:VAL:O	2.29	0.55
1:A:99:VAL:CG2	1:A:253:MET:HA	2.36	0.55
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.89	0.55
2:D:255:ILE:HG21	2:D:258:ILE:HD13	1.87	0.55
2:E:396:LEU:HB3	2:E:401:LYS:HG2	1.88	0.55
2:D:395:GLU:CD	3:G:75:ARG:HH21	2.13	0.55
1:A:457:GLU:HB3	1:A:460:LYS:HD3	1.89	0.55
1:A:479:LEU:HD21	1:A:493:SER:HB3	1.89	0.55
1:C:403:PHE:CD2	2:D:408:ARG:CZ	2.89	0.55
1:C:394:LEU:HD22	1:C:398:ARG:HH21	1.71	0.55
2:D:87:GLY:HA2	2:D:242:TYR:CE2	2.42	0.55
1:A:207:GLY:HA3	1:A:273:LYS:HD3	1.90	0.54
2:D:451:HIS:CD2	2:D:452:LEU:HD23	2.42	0.54
2:D:473:LEU:O	2:D:475:GLU:N	2.40	0.54
1:B:423:ARG:HE	1:B:458:PRO:HD3	1.72	0.54
1:B:114:ALA:HB2	1:B:121:ILE:HD11	1.89	0.54
1:B:441:GLN:O	1:B:445:ILE:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:GLU:HG2	2:D:342:LEU:HD22	1.90	0.54
2:E:201:ILE:CD1	2:E:208:LEU:HD11	2.37	0.54
2:E:397:SER:O	2:E:401:LYS:HG3	2.07	0.54
1:A:159:ILE:HD12	1:A:165:GLU:HG2	1.88	0.54
1:A:373:ARG:HG3	1:A:373:ARG:HH11	1.72	0.54
1:B:479:LEU:HA	1:B:482:LYS:HE3	1.89	0.54
1:C:442:VAL:CG1	1:C:489:ILE:HD11	2.37	0.54
2:F:63:MET:CE	2:F:97:VAL:HG11	2.37	0.54
1:B:446:TYR:CD2	1:B:497:LEU:HD23	2.43	0.54
1:C:52:MET:HG3	1:C:61:GLY:O	2.07	0.54
2:D:142:LEU:HD22	2:D:441:PHE:CD2	2.42	0.54
1:C:102:GLU:HG2	1:C:122:GLY:O	2.06	0.54
2:D:388:ILE:HD12	2:D:393:MET:SD	2.48	0.54
2:E:263:GLN:O	2:E:267:GLU:HG3	2.07	0.54
2:D:122:GLU:OE1	2:D:122:GLU:HA	2.07	0.54
2:F:10:THR:HG23	2:F:76:LEU:HD12	1.88	0.54
2:F:439:LYS:HE3	2:F:443:GLN:HE22	1.73	0.54
2:F:390:ILE:CD1	3:G:242:MET:SD	2.86	0.54
2:D:83:ARG:HA	2:D:114:ALA:O	2.07	0.54
1:A:170:ASP:O	1:A:175:LYS:HE2	2.08	0.54
1:A:463:LYS:HD3	1:A:508:PHE:HZ	1.73	0.54
1:A:468:PHE:CE1	1:A:501:VAL:HG12	2.43	0.54
1:B:270:ASP:OD1	1:B:273:LYS:HG3	2.08	0.54
1:A:161:ARG:HH11	1:A:263:HIS:CG	2.26	0.53
1:A:245:LEU:O	1:A:246:ALA:C	2.52	0.53
1:B:44:LEU:O	1:B:47:VAL:HG22	2.09	0.53
1:B:456:LEU:HD12	1:B:457:GLU:N	2.20	0.53
1:A:100:GLY:HA2	1:A:256:TYR:CE1	2.42	0.53
2:D:396:LEU:HD22	2:D:400:ASP:HB3	1.89	0.53
3:G:249:THR:HA	3:G:252:ARG:NH1	2.24	0.53
1:C:239:ALA:HB1	1:C:241:PRO:HD2	1.90	0.53
2:D:356:ARG:O	2:D:356:ARG:HG2	2.09	0.53
2:F:292:MET:CE	2:F:296:ILE:HD11	2.38	0.53
3:G:39:LYS:HB3	3:G:40:PRO:CD	2.38	0.53
1:A:150:ILE:HA	1:A:430:GLN:OE1	2.08	0.53
1:A:179:ALA:HB1	1:A:267:ILE:HG12	1.91	0.53
1:A:452:TYR:OH	1:A:498:LYS:HG3	2.08	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	1.74	0.53
1:A:406:PHE:HB2	3:G:19:ILE:HG23	1.90	0.53
1:C:390:MET:HE3	1:C:424:LEU:HD22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:167:MET:CB	2:D:420:VAL:HG11	2.38	0.53
2:D:412:ARG:HH11	2:D:412:ARG:HG3	1.73	0.53
1:B:482:LYS:O	1:B:486:ASP:N	2.38	0.53
1:C:404:ALA:C	1:C:406:PHE:N	2.44	0.53
1:A:291:ARG:HG3	3:G:258:ILE:CG2	2.39	0.53
1:C:91:THR:HG22	1:C:93:ALA:H	1.72	0.53
2:D:31:PRO:HD2	2:D:34:ASN:ND2	2.24	0.53
2:D:136:GLY:CA	2:D:431:LEU:HD13	2.37	0.53
2:E:220:GLY:HA3	2:E:232:VAL:HG21	1.91	0.53
2:E:9:THR:HG21	2:E:28:GLY:O	2.09	0.52
2:E:218:VAL:HG11	2:E:235:THR:CG2	2.38	0.52
1:B:140:ILE:HG23	1:B:311:LYS:HG3	1.92	0.52
1:B:180:ILE:CD1	1:B:216:LEU:HD21	2.39	0.52
1:B:383:MET:O	1:B:384:LYS:C	2.52	0.52
1:B:423:ARG:HD2	1:B:461:ILE:HD11	1.92	0.52
2:D:84:ILE:HD13	2:D:235:THR:HG23	1.92	0.52
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.75	0.52
2:D:412:ARG:HD2	2:D:454:GLU:HB3	1.90	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:D:422:GLU:HG2	2:D:427:HIS:O	2.09	0.52
2:F:210:ASP:HB2	2:F:212:THR:HG23	1.91	0.52
1:C:64:LEU:HD23	1:C:74:VAL:HG21	1.92	0.52
1:C:443:ALA:O	1:C:446:TYR:HB3	2.10	0.52
2:D:366:GLU:CG	2:D:442:GLN:HE22	2.23	0.52
2:E:97:VAL:HG13	2:E:232:VAL:CG1	2.39	0.52
1:B:386:VAL:HG22	1:B:442:VAL:HG12	1.91	0.52
1:C:140:ILE:HD11	1:C:143:ARG:HH22	1.74	0.52
1:C:267:ILE:N	1:C:267:ILE:HD12	2.25	0.52
1:C:270:ASP:OD1	1:C:273:LYS:HG3	2.09	0.52
2:D:96:ASN:CB	2:D:100:GLU:H	2.22	0.52
2:E:81:PRO:HG2	2:E:115:ALA:HB1	1.91	0.52
2:E:334:VAL:HG23	2:E:353:SER:HA	1.92	0.52
3:G:23:MET:SD	3:G:232:MET:HE2	2.50	0.52
1:B:157:VAL:N	1:B:158:PRO:CD	2.73	0.52
1:C:338:ILE:O	1:C:339:PRO:C	2.51	0.52
2:E:25:PHE:O	2:E:56:SER:HB3	2.10	0.52
1:A:436:MET:HG3	1:A:441:GLN:HG2	1.91	0.52
1:A:457:GLU:HB2	1:A:460:LYS:HD3	1.92	0.52
1:C:190:ASN:HA	1:C:198:LYS:HG2	1.91	0.52
1:C:335:SER:O	2:D:314:ALA:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:242:TYR:C	2:E:244:ARG:H	2.18	0.52
2:E:279:VAL:HG12	2:E:279:VAL:O	2.10	0.52
1:B:69:ASP:O	1:B:70:ASN:HB3	2.09	0.51
2:E:254:PHE:CD1	2:E:307:VAL:HB	2.45	0.51
1:C:45:ARG:NH2	1:C:68:PRO:O	2.44	0.51
1:C:156:LEU:HD11	1:C:428:LEU:HD13	1.91	0.51
2:E:377:ILE:HG21	2:E:410:ILE:CD1	2.40	0.51
1:A:187:LYS:HE2	1:A:191:ASP:OD2	2.11	0.51
1:B:489:ILE:HG22	1:B:494:ASP:HB2	1.93	0.51
2:D:381:TYR:HE2	2:D:411:GLN:HE22	1.56	0.51
1:A:140:ILE:HG21	1:A:313:ASN:HA	1.92	0.51
1:A:85:GLY:O	1:A:86:ASP:C	2.53	0.51
2:E:444:ILE:HD11	2:E:463:ILE:HD11	1.93	0.51
1:C:436:MET:CE	1:C:469:LEU:HD21	2.41	0.51
2:E:293:GLN:HG3	2:E:328:HIS:CG	2.45	0.51
2:E:443:GLN:O	2:E:446:ALA:HB3	2.10	0.51
2:F:257:ASN:HB3	2:F:260:ARG:HG2	1.92	0.51
2:F:360:PRO:HD3	2:F:368:TYR:CD2	2.46	0.51
1:B:157:VAL:N	1:B:158:PRO:HD3	2.25	0.51
1:C:399:GLU:CG	2:D:342:LEU:HD22	2.41	0.51
2:E:377:ILE:HG21	2:E:410:ILE:HD12	1.92	0.51
1:A:245:LEU:C	1:A:247:PRO:HD2	2.36	0.51
1:C:23:VAL:HG12	1:C:23:VAL:O	2.11	0.51
2:D:275:ILE:HG23	3:G:269:ALA:CB	2.40	0.51
2:E:204:GLY:O	2:E:205:VAL:C	2.54	0.51
2:E:41:ARG:O	2:E:42:GLU:C	2.53	0.50
1:A:406:PHE:CB	3:G:19:ILE:HG23	2.41	0.50
2:E:204:GLY:C	2:E:206:ILE:N	2.68	0.50
2:E:218:VAL:HG11	2:E:235:THR:HG22	1.91	0.50
2:E:382:LYS:O	2:E:385:GLN:HB2	2.11	0.50
2:F:421:ALA:O	2:F:425:THR:HG23	2.11	0.50
1:A:140:ILE:HD11	1:A:143:ARG:NE	2.26	0.50
1:C:34:ILE:HD11	1:C:79:ASP:CB	2.41	0.50
1:C:105:GLY:HA2	1:C:226:MET:HE3	1.93	0.50
1:C:244:TYR:O	1:C:247:PRO:HD2	2.11	0.50
2:D:406:ARG:O	2:D:410:ILE:HG13	2.11	0.50
2:E:241:GLU:HA	2:E:304:ILE:HD11	1.94	0.50
2:E:275:ILE:O	2:E:283:PRO:HG3	2.12	0.50
1:B:151:LYS:NZ	1:B:429:LYS:O	2.45	0.50
2:F:386:ASP:O	2:F:389:ALA:HB3	2.12	0.50
1:A:45:ARG:HA	2:E:71:ARG:NH2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:VAL:CG2	1:B:442:VAL:HG12	2.41	0.50
1:C:331:ALA:O	1:C:333:ASP:N	2.44	0.50
2:E:142:LEU:HD21	2:E:374:VAL:HG21	1.93	0.50
2:F:234:LEU:O	2:F:237:LEU:HB3	2.10	0.50
1:B:210:ARG:O	1:B:211:SER:C	2.54	0.50
1:B:390:MET:CE	1:B:428:LEU:HD21	2.42	0.50
2:D:168:GLU:HG3	2:D:168:GLU:O	2.11	0.50
2:E:221:GLN:N	2:E:224:GLU:OE1	2.44	0.50
2:F:242:TYR:CD1	2:F:246:GLN:HG3	2.46	0.50
2:F:345:TYR:HA	2:F:346:PRO:C	2.36	0.50
1:B:27:GLU:O	1:B:90:ARG:HG3	2.12	0.50
1:C:102:GLU:HG2	1:C:122:GLY:C	2.36	0.50
1:C:164:ARG:HD2	1:C:306:LEU:O	2.11	0.50
1:C:406:PHE:N	1:C:406:PHE:CD1	2.79	0.50
1:B:284:LEU:HD21	2:E:274:ARG:HD3	1.94	0.50
1:C:434:SER:N	1:C:435:PRO:HD3	2.27	0.50
1:C:359:LYS:O	2:F:376:LYS:HE2	2.11	0.50
2:E:155:PHE:HE1	2:E:310:ILE:HD12	1.77	0.50
2:F:86:VAL:HG11	2:F:114:ALA:HB3	1.93	0.50
2:F:455:GLN:H	2:F:455:GLN:CD	2.18	0.50
1:B:358:TYR:C	1:B:360:GLY:N	2.69	0.49
1:C:96:ASP:O	1:C:97:VAL:HG13	2.12	0.49
1:C:225:ALA:HA	1:C:228:TYR:CE1	2.47	0.49
2:F:80:ALA:HB1	2:F:81:PRO:HD2	1.94	0.49
1:C:403:PHE:CZ	2:D:408:ARG:HD2	2.48	0.49
2:D:14:VAL:HG11	2:D:24:GLN:HB2	1.95	0.49
2:D:154:LEU:HD22	2:D:165:LEU:HD23	1.92	0.49
1:A:313:ASN:O	1:A:316:PHE:N	2.37	0.49
1:B:96:ASP:HB2	1:B:127:ARG:O	2.12	0.49
1:B:463:LYS:HE2	1:B:508:PHE:CZ	2.48	0.49
1:C:30:ARG:HA	1:C:86:ASP:O	2.12	0.49
2:D:96:ASN:HB2	2:D:100:GLU:N	2.27	0.49
2:F:96:ASN:ND2	2:F:100:GLU:HB2	2.26	0.49
1:A:137:ILE:N	1:A:138:PRO:CD	2.75	0.49
1:C:307:GLU:HG3	2:D:223:ASN:HB3	1.95	0.49
2:E:397:SER:C	2:E:399:GLU:H	2.20	0.49
1:A:294:TYR:HB2	1:A:337:TYR:HE2	1.76	0.49
1:C:392:LEU:HD11	2:D:425:THR:HA	1.95	0.49
2:D:345:TYR:HA	2:D:346:PRO:C	2.37	0.49
2:E:463:ILE:O	2:E:467:VAL:HG23	2.12	0.49
1:A:136:ILE:HG13	2:E:194:ASN:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ALA:N	1:A:241:PRO:HD2	2.27	0.49
2:D:83:ARG:HA	2:D:115:ALA:HA	1.95	0.49
2:D:93:ARG:HG3	2:D:93:ARG:NH1	2.27	0.49
2:F:409:LYS:HD3	2:F:457:PHE:HE2	1.78	0.49
1:C:402:ALA:O	1:C:405:GLN:HG3	2.12	0.49
1:B:107:VAL:HG12	1:B:115:ILE:CG1	2.42	0.49
1:B:437:ALA:O	1:B:438:ILE:C	2.54	0.49
1:C:362:ARG:HG3	1:C:362:ARG:NH1	2.27	0.49
1:C:396:GLN:HG3	2:D:458:TYR:CZ	2.48	0.49
2:D:136:GLY:HA2	2:D:432:VAL:O	2.12	0.49
1:A:94:ILE:HG12	1:A:95:VAL:N	2.27	0.49
1:B:99:VAL:HG21	1:B:127:ARG:HB3	1.94	0.49
2:D:360:PRO:HD3	2:D:368:TYR:CE2	2.48	0.49
2:E:227:GLY:O	2:E:230:ALA:HB3	2.13	0.49
1:B:24:ASP:O	1:B:28:THR:HB	2.12	0.48
1:B:423:ARG:HE	1:B:458:PRO:CD	2.26	0.48
2:E:462:PRO:HD2	2:E:465:GLU:HG3	1.94	0.48
3:G:39:LYS:N	3:G:40:PRO:HD2	2.28	0.48
1:A:373:ARG:HG3	1:A:373:ARG:NH1	2.28	0.48
1:B:211:SER:O	1:B:215:GLN:HG3	2.13	0.48
1:B:311:LYS:HD2	1:B:312:MET:O	2.13	0.48
2:D:397:SER:O	2:D:400:ASP:N	2.45	0.48
2:F:163:THR:O	2:F:167:MET:HG2	2.12	0.48
2:F:221:GLN:HE21	2:F:221:GLN:HA	1.78	0.48
2:F:321:ALA:HB3	2:F:322:PRO:HD3	1.95	0.48
1:A:209:LYS:NZ	2:D:330:ASP:CG	2.70	0.48
2:E:393:MET:HE3	2:E:396:LEU:HD12	1.95	0.48
2:F:339:ILE:HG22	2:F:344:ILE:HB	1.95	0.48
2:F:82:ILE:HD13	2:F:98:ILE:HG22	1.96	0.48
1:A:300:TYR:O	1:A:304:ARG:HG2	2.13	0.48
1:A:380:THR:O	1:A:384:LYS:HG3	2.12	0.48
1:A:444:VAL:CG1	1:A:469:LEU:HD13	2.44	0.48
1:C:48:GLN:HB3	2:D:68:GLY:HA2	1.95	0.48
2:E:134:VAL:HG13	2:E:141:ASP:OD2	2.13	0.48
2:F:168:GLU:OE1	2:F:418:PHE:HB3	2.12	0.48
1:B:351:PHE:HE1	1:B:369:LEU:O	1.96	0.48
2:D:319:ASP:O	2:D:320:PRO:C	2.55	0.48
1:A:389:THR:O	1:A:393:GLU:HG2	2.13	0.48
1:B:218:LYS:HB2	2:E:128:VAL:HG12	1.95	0.48
2:E:360:PRO:HD3	2:E:368:TYR:CD1	2.49	0.48
2:F:360:PRO:HD3	2:F:368:TYR:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ALA:O	1:B:50:GLU:HB2	2.13	0.48
1:B:225:ALA:HA	1:B:228:TYR:CE2	2.49	0.48
1:B:427:LEU:HD11	1:B:448:GLY:HA3	1.95	0.48
1:C:403:PHE:CD2	2:D:408:ARG:NH1	2.82	0.48
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.41	0.48
2:F:357:ILE:HD12	2:F:362:ILE:HG21	1.95	0.48
2:F:467:VAL:O	2:F:470:ALA:HB3	2.14	0.48
1:A:49:ALA:O	1:A:50:GLU:HB2	2.13	0.48
1:A:406:PHE:CB	3:G:19:ILE:CG2	2.92	0.48
1:A:485:THR:HG22	1:A:486:ASP:N	2.29	0.48
1:B:171:ARG:HG3	1:B:171:ARG:HH11	1.79	0.48
1:B:300:TYR:O	1:B:304:ARG:HG2	2.13	0.48
2:E:416:GLN:HG3	2:E:417:PRO:HD2	1.96	0.48
2:E:444:ILE:HD11	2:E:463:ILE:CD1	2.43	0.48
2:F:390:ILE:HD12	3:G:242:MET:CE	2.27	0.48
1:A:100:GLY:HA2	1:A:256:TYR:CD1	2.49	0.48
1:A:417:LEU:HD23	1:A:417:LEU:H	1.77	0.48
1:B:240:ALA:N	1:B:241:PRO:CD	2.77	0.48
1:C:245:LEU:O	1:C:246:ALA:C	2.56	0.48
1:C:313:ASN:OD1	1:C:315:ALA:HB3	2.14	0.48
2:E:253:LEU:O	2:E:306:SER:HA	2.14	0.48
2:D:425:THR:HB	2:D:459:MET:HE2	1.96	0.47
2:F:88:PRO:HD2	2:F:89:GLU:OE2	2.14	0.47
1:C:180:ILE:HG22	1:C:184:ILE:HD12	1.97	0.47
2:E:161:GLY:O	2:E:162:LYS:C	2.57	0.47
2:E:404:VAL:O	2:E:408:ARG:HG3	2.13	0.47
1:A:180:ILE:O	1:A:181:ASP:C	2.57	0.47
1:B:151:LYS:NZ	1:B:427:LEU:O	2.47	0.47
1:C:292:GLU:O	1:C:293:ALA:CB	2.63	0.47
2:E:116:ILE:HA	2:E:238:THR:OG1	2.15	0.47
2:E:158:ALA:C	2:E:160:VAL:N	2.72	0.47
1:A:453:LEU:HD13	1:A:461:ILE:HG23	1.96	0.47
1:C:334:VAL:HG13	1:C:351:PHE:CE1	2.48	0.47
1:C:445:ILE:HG22	1:C:449:VAL:CG2	2.44	0.47
2:D:32:ILE:O	2:D:33:LEU:HB2	2.14	0.47
2:E:374:VAL:O	2:E:377:ILE:HG22	2.14	0.47
2:F:36:LEU:N	2:F:36:LEU:HD23	2.29	0.47
1:A:166:LEU:HD13	1:A:342:VAL:HG12	1.95	0.47
1:A:376:SER:O	1:A:378:ALA:N	2.48	0.47
1:B:389:THR:HA	1:B:392:LEU:HG	1.97	0.47
2:E:61:ILE:HG13	2:E:61:ILE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:96:ASN:HD22	2:F:100:GLU:CB	2.27	0.47
1:C:481:SER:O	1:C:485:THR:HB	2.14	0.47
2:E:259:PHE:CE2	2:E:263:GLN:HG2	2.50	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	2.34	0.47
1:A:240:ALA:HB3	1:A:241:PRO:HD3	1.97	0.47
1:A:406:PHE:CE1	3:G:19:ILE:HD13	2.50	0.47
1:B:443:ALA:O	1:B:446:TYR:HB3	2.14	0.47
1:C:187:LYS:HE3	1:C:224:ASP:HB3	1.96	0.47
1:C:488:LYS:HG2	1:C:489:ILE:N	2.28	0.47
2:D:393:MET:HE1	2:D:404:VAL:HG11	1.96	0.47
2:E:54:GLY:O	2:E:55:GLU:HB2	2.13	0.47
1:C:164:ARG:HD2	1:C:164:ARG:HH11	1.41	0.47
2:D:417:PRO:HA	2:D:459:MET:HE1	1.96	0.47
2:F:93:ARG:NH2	2:F:106:GLY:O	2.48	0.47
1:A:52:MET:HE1	1:A:60:LYS:HD3	1.97	0.47
1:A:188:ARG:HE	1:A:437:ALA:HB2	1.80	0.47
1:A:209:LYS:HE3	1:A:211:SER:CB	2.45	0.47
1:A:485:THR:C	1:A:487:GLY:N	2.73	0.47
1:B:400:VAL:HB	1:B:418:LEU:CD2	2.45	0.47
2:F:63:MET:HE1	2:F:231:ARG:HB2	1.95	0.47
1:A:51:GLU:OE2	1:A:90:ARG:HB3	2.16	0.47
1:B:179:ALA:O	1:B:182:THR:HB	2.14	0.47
1:B:209:LYS:CG	2:E:294:GLU:OE2	2.59	0.47
1:B:481:SER:O	1:B:485:THR:HB	2.14	0.47
1:C:44:LEU:HB3	1:C:47:VAL:HG22	1.95	0.47
2:E:438:ILE:O	2:E:442:GLN:HB2	2.15	0.47
2:F:205:VAL:HG23	2:F:215:VAL:HG21	1.97	0.47
1:B:485:THR:O	1:B:486:ASP:C	2.58	0.46
1:B:496:LYS:O	1:B:500:ILE:HG13	2.15	0.46
2:D:84:ILE:N	2:D:114:ALA:O	2.42	0.46
2:D:129:GLU:OE1	2:D:129:GLU:HA	2.14	0.46
2:D:154:LEU:HD13	2:D:165:LEU:HD23	1.96	0.46
2:D:469:LYS:O	2:D:473:LEU:HG	2.15	0.46
2:E:319:ASP:HA	3:G:255:GLN:OE1	2.15	0.46
2:E:431:LEU:HD12	2:E:431:LEU:O	2.15	0.46
1:A:313:ASN:OD1	1:A:316:PHE:HD2	1.98	0.46
1:C:156:LEU:HD11	1:C:428:LEU:CD1	2.46	0.46
1:A:107:VAL:HB	1:A:116:ASP:HB3	1.97	0.46
1:A:353:GLU:CD	1:A:366:ASN:HD22	2.24	0.46
1:C:91:THR:HG22	1:C:93:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:THR:O	1:C:486:ASP:C	2.57	0.46
2:E:112:GLN:NE2	2:E:242:TYR:HE2	2.14	0.46
2:F:200:MET:CG	2:F:206:ILE:HG12	2.46	0.46
2:F:462:PRO:HG2	2:F:465:GLU:HG3	1.96	0.46
3:G:78:CYS:O	3:G:81:ILE:HD13	2.15	0.46
1:B:45:ARG:HH11	1:B:45:ARG:HD3	1.53	0.46
2:E:82:ILE:HB	2:E:116:ILE:CD1	2.45	0.46
2:F:346:PRO:HG3	2:F:418:PHE:HZ	1.80	0.46
1:A:127:ARG:HE	1:A:131:LEU:CD1	2.27	0.46
1:B:433:TYR:C	1:B:435:PRO:HD3	2.40	0.46
2:F:89:GLU:HG2	2:F:110:THR:CG2	2.44	0.46
2:F:151:LYS:HD3	2:F:328:HIS:O	2.15	0.46
1:A:403:PHE:O	1:A:404:ALA:C	2.58	0.46
2:E:33:LEU:HD13	2:E:117:HIS:CG	2.50	0.46
2:F:339:ILE:CG2	2:F:344:ILE:HB	2.46	0.46
1:A:36:ASP:O	1:A:284:LEU:HD13	2.16	0.46
2:D:368:TYR:CE1	2:D:372:ARG:HG3	2.50	0.46
2:E:77:ASP:C	2:E:79:GLY:H	2.23	0.46
2:E:256:ASP:HA	2:E:257:ASN:HA	1.64	0.46
2:F:310:ILE:HD13	2:F:325:THR:HG21	1.98	0.46
1:A:139:ARG:C	1:A:140:ILE:HG22	2.41	0.46
2:E:343:GLY:O	2:E:345:TYR:HD1	1.99	0.46
1:A:78:ASN:OD1	1:A:80:LYS:HB3	2.15	0.46
1:A:485:THR:C	1:A:487:GLY:H	2.23	0.46
1:B:84:GLU:CD	2:E:56:SER:H	2.23	0.46
1:C:392:LEU:CD1	2:D:425:THR:HA	2.45	0.46
2:E:120:ALA:HB1	2:E:121:PRO:HD2	1.98	0.46
2:E:223:ASN:ND2	2:E:223:ASN:N	2.46	0.46
1:C:441:GLN:O	1:C:445:ILE:HG12	2.15	0.46
2:D:130:GLN:HE22	2:D:356:ARG:HD3	1.81	0.46
2:D:289:MET:SD	2:D:324:THR:HG22	2.56	0.46
2:E:95:MET:HE2	2:E:99:GLY:CA	2.45	0.46
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.98	0.46
2:F:319:ASP:O	2:F:322:PRO:HD2	2.14	0.46
1:B:34:ILE:HD12	1:B:35:GLY:H	1.81	0.45
1:B:465:GLU:O	1:B:469:LEU:HB2	2.17	0.45
2:D:471:ASP:O	2:D:472:LYS:C	2.58	0.45
2:F:289:MET:HE3	2:F:289:MET:HB2	1.73	0.45
1:A:40:ARG:HH11	1:A:40:ARG:CG	2.27	0.45
1:A:300:TYR:HE1	2:E:223:ASN:O	1.99	0.45
1:A:339:PRO:O	1:A:343:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ASP:HA	1:B:270:ASP:HA	1.77	0.45
1:C:251:CYS:O	1:C:255:GLU:HG3	2.16	0.45
2:F:96:ASN:HB2	2:F:100:GLU:N	2.31	0.45
1:A:412:ALA:HA	1:A:415:GLN:HB3	1.98	0.45
1:C:180:ILE:CD1	1:C:216:LEU:HD21	2.34	0.45
1:C:432:GLN:O	1:C:433:TYR:HB2	2.16	0.45
2:E:146:TYR:O	2:E:357:ILE:HD11	2.16	0.45
2:E:443:GLN:HA	2:E:446:ALA:HB3	1.99	0.45
2:F:136:GLY:HA3	2:F:431:LEU:HD11	1.99	0.45
1:B:141:SER:HB2	1:B:143:ARG:NH1	2.31	0.45
1:B:271:LEU:HD12	1:B:325:PRO:HB2	1.98	0.45
2:D:432:VAL:HG13	2:D:433:PRO:HD2	1.97	0.45
2:E:316:ASP:CG	3:G:251:ASN:HB3	2.42	0.45
2:E:405:SER:OG	2:E:406:ARG:N	2.49	0.45
2:F:469:LYS:O	2:F:473:LEU:HG	2.16	0.45
1:A:166:LEU:HD13	1:A:342:VAL:CG1	2.47	0.45
1:C:26:GLU:HB3	1:C:46:ASN:ND2	2.32	0.45
1:C:83:LYS:HB3	2:F:52:HIS:CE1	2.52	0.45
2:D:201:ILE:HD13	2:D:208:LEU:HD11	1.98	0.45
2:E:63:MET:CE	2:E:228:ALA:HA	2.46	0.45
2:E:388:ILE:HG23	2:E:393:MET:CG	2.43	0.45
1:A:151:LYS:HE2	1:A:427:LEU:O	2.17	0.45
1:A:398:ARG:HH11	1:A:398:ARG:HD2	1.53	0.45
1:A:492:GLU:C	1:A:494:ASP:N	2.73	0.45
2:D:440:GLY:O	2:D:444:ILE:HG13	2.16	0.45
2:E:281:TYR:CZ	2:E:321:ALA:HB2	2.52	0.45
1:B:353:GLU:HG3	1:B:366:ASN:HB2	1.98	0.45
2:D:366:GLU:O	2:D:370:VAL:HG23	2.17	0.45
2:D:386:ASP:HB3	3:G:12:SER:CB	2.46	0.45
2:D:417:PRO:HB3	2:D:459:MET:HE3	1.99	0.45
2:E:85:PRO:HD2	2:E:95:MET:CE	2.47	0.45
2:F:252:LEU:HD23	2:F:252:LEU:HA	1.81	0.45
1:A:179:ALA:O	1:A:182:THR:HB	2.17	0.45
1:B:27:GLU:OE1	1:B:90:ARG:HD3	2.16	0.45
1:C:84:GLU:OE1	2:F:54:GLY:HA2	2.17	0.45
1:C:158:PRO:HB3	1:C:379:GLN:HG3	1.99	0.45
1:C:476:HIS:ND1	1:C:476:HIS:N	2.64	0.45
2:D:237:LEU:HD21	2:D:295:ARG:HB2	1.97	0.45
2:D:452:LEU:HD12	2:D:457:PHE:CZ	2.52	0.45
2:E:147:ALA:HB2	2:E:357:ILE:HD13	1.99	0.45
2:F:81:PRO:O	2:F:82:ILE:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:VAL:HG22	1:A:161:ARG:O	2.16	0.45
1:A:213:VAL:O	1:A:216:LEU:HB3	2.16	0.45
1:A:283:LEU:HD11	1:A:293:ALA:HB1	1.99	0.45
1:C:67:GLU:HB3	1:C:68:PRO:HD2	1.98	0.45
2:E:77:ASP:CG	2:E:79:GLY:H	2.23	0.45
2:E:409:LYS:NZ	2:E:450:ASP:HA	2.30	0.45
2:F:346:PRO:HG3	2:F:418:PHE:CZ	2.52	0.45
3:G:13:ILE:HD13	3:G:242:MET:SD	2.57	0.45
1:A:59:LEU:HD11	1:A:81:LEU:HD12	1.99	0.45
1:A:471:HIS:ND1	1:A:475:GLN:HG3	2.32	0.45
1:B:140:ILE:HG13	1:B:143:ARG:NH1	2.32	0.45
1:B:469:LEU:HG	1:B:473:ILE:HD11	1.98	0.45
1:C:311:LYS:HE3	1:C:318:GLY:O	2.17	0.45
2:E:461:GLY:HA3	2:E:462:PRO:HD3	1.73	0.45
2:F:50:ALA:O	2:F:51:GLN:HB3	2.16	0.45
2:F:243:PHE:O	2:F:249:GLN:HB2	2.16	0.45
1:B:76:PHE:HB3	1:B:242:LEU:HD21	1.99	0.44
2:D:231:ARG:O	2:D:234:LEU:N	2.50	0.44
2:D:231:ARG:O	2:D:232:VAL:C	2.60	0.44
2:E:189:ARG:O	2:E:190:THR:C	2.58	0.44
2:F:348:VAL:O	2:F:350:PRO:HD3	2.17	0.44
1:A:97:VAL:HG11	1:A:249:SER:HB2	1.99	0.44
1:A:244:TYR:HE1	1:A:301:LEU:HD11	1.83	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:E:402:LEU:O	2:E:406:ARG:HG3	2.17	0.44
2:F:221:GLN:HA	2:F:221:GLN:NE2	2.31	0.44
1:A:379:GLN:HB2	1:A:384:LYS:HE3	2.00	0.44
1:B:32:LEU:HD21	1:B:42:HIS:HB2	1.99	0.44
1:C:403:PHE:CG	2:D:408:ARG:NH2	2.85	0.44
2:D:63:MET:HE1	2:D:231:ARG:HB2	1.99	0.44
2:D:95:MET:HG2	2:D:99:GLY:HA2	1.99	0.44
2:D:170:ILE:O	2:D:174:ALA:HB3	2.17	0.44
2:F:29:LEU:HD11	2:F:58:VAL:HG13	1.98	0.44
3:G:259:THR:O	3:G:263:ILE:HG12	2.17	0.44
1:A:385:GLN:OE1	1:A:488:LYS:HB2	2.17	0.44
1:B:80:LYS:HA	2:E:32:ILE:HB	1.98	0.44
1:B:423:ARG:HE	1:B:458:PRO:CG	2.30	0.44
1:C:177:SER:O	1:C:178:ILE:C	2.60	0.44
2:D:35:ALA:HB1	2:D:46:VAL:CG1	2.47	0.44
2:E:114:ALA:HB3	2:E:238:THR:CG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:105:ARG:CZ	2:F:208:LEU:HD23	2.46	0.44
3:G:228:ARG:O	3:G:232:MET:HG2	2.17	0.44
1:A:24:ASP:OD1	1:A:24:ASP:C	2.60	0.44
1:C:219:ARG:HD3	1:C:433:TYR:HE1	1.81	0.44
1:C:474:SER:OG	1:C:475:GLN:N	2.49	0.44
2:D:298:THR:HG23	2:D:303:SER:HA	1.98	0.44
2:E:321:ALA:N	2:E:322:PRO:HD2	2.32	0.44
2:F:359:ASP:OD1	2:F:360:PRO:HD2	2.17	0.44
1:A:74:VAL:HG13	1:A:241:PRO:HG3	1.99	0.44
1:C:45:ARG:HH11	1:C:45:ARG:HD2	1.67	0.44
2:D:400:ASP:O	2:D:404:VAL:HG23	2.18	0.44
2:E:422:GLU:C	2:E:424:PHE:N	2.74	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:B:212:THR:O	1:B:216:LEU:HB2	2.17	0.44
1:B:249:SER:O	1:B:250:GLY:C	2.61	0.44
1:C:209:LYS:HE3	1:C:211:SER:OG	2.18	0.44
2:D:274:ARG:HH11	2:D:274:ARG:HD2	1.50	0.44
2:F:319:ASP:O	2:F:320:PRO:C	2.60	0.44
1:A:211:SER:N	2:D:126:MET:HE2	2.33	0.44
1:B:381:ARG:HG2	1:B:488:LYS:HG3	1.98	0.44
1:B:400:VAL:HG12	1:B:418:LEU:HD11	2.00	0.44
1:C:169:GLY:O	1:C:175:LYS:HE2	2.18	0.44
2:D:93:ARG:NH1	2:D:108:ILE:HG12	2.33	0.44
1:A:55:PHE:O	1:A:56:SER:C	2.61	0.44
1:A:97:VAL:N	1:A:127:ARG:O	2.41	0.44
1:A:251:CYS:O	1:A:255:GLU:HG3	2.18	0.44
1:A:392:LEU:O	1:A:396:GLN:HG3	2.18	0.44
1:B:107:VAL:HG12	1:B:115:ILE:HD11	2.00	0.44
1:C:59:LEU:HD23	1:C:82:ILE:CD1	2.45	0.44
2:F:407:ALA:O	2:F:411:GLN:HB2	2.18	0.44
1:A:460:LYS:N	1:A:460:LYS:HD2	2.32	0.43
1:C:489:ILE:HG22	1:C:494:ASP:HB2	1.99	0.43
2:D:412:ARG:O	2:D:415:SER:OG	2.33	0.43
3:G:6:ILE:HG21	3:G:250:PHE:HB2	2.00	0.43
1:A:140:ILE:CG2	1:A:313:ASN:HA	2.47	0.43
1:A:291:ARG:HH21	3:G:258:ILE:HD11	1.80	0.43
1:A:133:ALA:HB1	1:A:134:PRO:HD2	1.99	0.43
2:D:38:VAL:HG11	2:D:69:LEU:CD2	2.48	0.43
2:D:461:GLY:HA3	2:D:462:PRO:HD3	1.74	0.43
2:E:136:GLY:HA2	2:E:432:VAL:O	2.18	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: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:137:ILE:HD13	1:C:137:ILE:HA	1.88	0.43
1:C:353:GLU:O	1:C:364:ALA:HB1	2.18	0.43
2:D:189:ARG:O	2:D:192:GLU:HB2	2.19	0.43
2:D:425:THR:HG21	2:D:459:MET:HE1	1.99	0.43
1:B:213:VAL:O	1:B:217:VAL:HG13	2.18	0.43
1:B:389:THR:HG22	1:B:392:LEU:HD12	2.00	0.43
1:C:32:LEU:HD21	1:C:42:HIS:HB2	2.01	0.43
1:C:404:ALA:HB1	1:C:410:LEU:HD11	1.99	0.43
2:D:108:ILE:HG22	2:D:110:THR:HG23	2.00	0.43
2:D:470:ALA:O	2:D:474:ALA:N	2.51	0.43
2:E:439:LYS:O	2:E:440:GLY:C	2.61	0.43
2:F:385:GLN:HA	2:F:388:ILE:HG12	2.01	0.43
2:F:439:LYS:HG2	2:F:443:GLN:NE2	2.33	0.43
1:A:397:TYR:CD1	1:A:421:GLY:HA3	2.54	0.43
1:A:482:LYS:O	1:A:483:ILE:C	2.61	0.43
1:B:94:ILE:O	1:B:95:VAL:C	2.61	0.43
1:C:187:LYS:O	1:C:188:ARG:C	2.61	0.43
1:C:193:THR:O	1:C:195:GLU:OE1	2.36	0.43
1:C:390:MET:HE1	1:C:428:LEU:HD21	1.99	0.43
2:D:103:ASP:O	2:D:104:GLU:HB2	2.17	0.43
2:D:397:SER:O	2:D:398:GLU:C	2.58	0.43
2:E:72:GLY:O	2:E:73:GLN:C	2.60	0.43
2:E:376:LYS:O	2:E:379:GLN:HB2	2.18	0.43
2:F:141:ASP:HB3	2:F:434:LEU:HD13	2.01	0.43
2:F:257:ASN:OD1	2:F:259:PHE:HB3	2.17	0.43
1:B:450:ARG:HD3	1:B:450:ARG:HA	1.87	0.43
1:A:136:ILE:O	2:E:194:ASN:OD1	2.35	0.43
1:B:381:ARG:HA	1:B:384:LYS:HB2	2.01	0.43
1:B:434:SER:N	1:B:435:PRO:CD	2.81	0.43
1:C:116:ASP:O	1:C:117:GLY:C	2.60	0.43
2:E:310:ILE:HD11	2:E:329:LEU:HD11	2.00	0.43
2:F:95:MET:HG3	2:F:99:GLY:HA2	2.01	0.43
2:F:452:LEU:HD22	2:F:470:ALA:CB	2.49	0.43
1:B:385:GLN:NE2	1:B:489:ILE:HB	2.34	0.43
1:C:139:ARG:HB3	1:C:311:LYS:O	2.19	0.43
2:D:412:ARG:C	2:D:414:LEU:N	2.73	0.43
2:D:462:PRO:HD2	2:D:465:GLU:HG3	2.00	0.43
2:E:35:ALA:HB2	2:E:82:ILE:HG13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:182:VAL:HG21	2:E:240:ALA:HB2	2.01	0.43
2:F:31:PRO:O	2:F:34:ASN:HB2	2.18	0.43
1:B:255:GLU:HG2	1:B:258:ARG:CZ	2.49	0.43
2:E:242:TYR:C	2:E:242:TYR:CD1	2.96	0.43
2:E:433:PRO:HG2	2:E:436:GLU:CG	2.48	0.43
1:C:180:ILE:O	1:C:181:ASP:C	2.62	0.42
1:C:185:ASN:HB2	1:C:435:PRO:HB3	2.00	0.42
2:D:386:ASP:CB	3:G:12:SER:HB3	2.49	0.42
2:D:412:ARG:HG3	2:D:412:ARG:NH1	2.33	0.42
2:E:296:ILE:HD13	2:E:306:SER:HB2	2.02	0.42
2:E:441:PHE:O	2:E:445:LEU:HG	2.19	0.42
2:F:144:ALA:N	2:F:145:PRO:CD	2.82	0.42
1:A:463:LYS:HD3	1:A:508:PHE:CZ	2.53	0.42
1:C:285:LEU:C	1:C:286:ARG:HG2	2.44	0.42
2:E:95:MET:HE2	2:E:99:GLY:HA2	2.01	0.42
2:E:231:ARG:O	2:E:232:VAL:C	2.60	0.42
2:E:349:ASP:HA	2:E:350:PRO:HD2	1.87	0.42
3:G:239:ALA:O	3:G:243:ILE:HG12	2.18	0.42
1:A:45:ARG:HA	2:E:71:ARG:HH21	1.84	0.42
1:C:49:ALA:O	1:C:50:GLU:HB2	2.19	0.42
1:C:51:GLU:HG2	1:C:52:MET:N	2.33	0.42
1:C:442:VAL:HG11	1:C:489:ILE:HD11	2.01	0.42
2:D:410:ILE:HG23	2:D:441:PHE:CE1	2.54	0.42
3:G:2:THR:C	3:G:4:LYS:N	2.75	0.42
1:A:136:ILE:CG1	2:E:194:ASN:HB2	2.49	0.42
1:A:184:ILE:HD12	1:A:223:ALA:CB	2.50	0.42
1:A:291:ARG:HG3	3:G:258:ILE:HG23	2.00	0.42
1:A:340:THR:O	1:A:344:SER:HB3	2.19	0.42
1:B:389:THR:HA	1:B:392:LEU:CG	2.49	0.42
1:C:84:GLU:CD	2:F:54:GLY:HA2	2.45	0.42
1:C:107:VAL:O	1:C:115:ILE:HG12	2.18	0.42
2:D:38:VAL:HG22	2:D:75:VAL:HG22	2.02	0.42
2:D:145:PRO:HB2	2:D:357:ILE:HD11	2.01	0.42
2:D:396:LEU:HD22	2:D:400:ASP:HB2	2.01	0.42
2:E:105:ARG:NE	2:E:208:LEU:HD23	2.33	0.42
2:F:122:GLU:OE1	2:F:122:GLU:HA	2.19	0.42
2:F:196:LEU:O	2:F:200:MET:HB2	2.19	0.42
1:A:96:ASP:HA	1:A:128:ARG:HA	2.02	0.42
1:A:136:ILE:HG21	1:A:136:ILE:HD13	1.83	0.42
1:A:347:ASP:C	1:A:373:ARG:HH11	2.28	0.42
1:C:44:LEU:HD23	1:C:44:LEU:HA	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:ALA:N	1:C:66:LEU:HD11	2.34	0.42
1:C:224:ASP:OD1	1:C:227:LYS:HE3	2.20	0.42
1:C:423:ARG:CD	1:C:461:ILE:HD11	2.49	0.42
2:D:84:ILE:HB	2:D:95:MET:HE3	2.02	0.42
2:D:266:SER:CB	2:D:282:GLN:NE2	2.82	0.42
2:E:166:ILE:O	2:E:170:ILE:HG13	2.18	0.42
1:A:338:ILE:N	1:A:339:PRO:CD	2.83	0.42
1:B:165:GLU:O	1:B:325:PRO:HD2	2.19	0.42
1:B:438:ILE:HD12	1:B:438:ILE:HA	1.87	0.42
2:E:396:LEU:CB	2:E:401:LYS:HG2	2.50	0.42
2:E:397:SER:O	2:E:398:GLU:C	2.62	0.42
2:F:251:VAL:HG12	2:F:252:LEU:N	2.35	0.42
1:A:407:GLY:CA	1:A:410:LEU:HD21	2.48	0.42
2:D:395:GLU:CD	3:G:75:ARG:NH2	2.77	0.42
2:E:32:ILE:O	2:E:33:LEU:CB	2.68	0.42
2:E:231:ARG:O	2:E:234:LEU:N	2.50	0.42
1:A:136:ILE:HD11	2:E:219:TYR:HE2	1.85	0.42
1:B:420:ARG:O	1:B:423:ARG:N	2.50	0.42
1:C:147:GLN:OE1	1:C:438:ILE:HD13	2.19	0.42
1:C:340:THR:O	1:C:341:ASN:C	2.59	0.42
2:D:396:LEU:HD23	2:D:396:LEU:HA	1.87	0.42
2:F:47:LEU:HD23	2:F:62:ALA:HA	2.01	0.42
2:F:80:ALA:CB	2:F:81:PRO:CD	2.94	0.42
1:B:361:ILE:HD13	1:B:429:LYS:HE2	2.02	0.42
1:C:30:ARG:HE	1:C:87:ILE:CD1	2.18	0.42
1:C:384:LYS:HB2	1:C:384:LYS:HE3	1.94	0.42
2:D:449:TYR:C	2:D:451:HIS:H	2.28	0.42
2:E:97:VAL:HG13	2:E:232:VAL:HG12	2.01	0.42
2:F:423:VAL:O	2:F:423:VAL:HG12	2.20	0.42
1:A:247:PRO:HG2	1:A:274:GLN:NE2	2.35	0.42
1:B:103:LEU:O	1:B:104:LEU:C	2.63	0.42
1:B:382:ALA:HB1	1:B:442:VAL:HG11	2.02	0.42
1:C:457:GLU:O	1:C:458:PRO:C	2.62	0.42
2:D:95:MET:HE2	2:D:235:THR:CG2	2.49	0.42
2:D:190:THR:O	2:D:191:ARG:C	2.60	0.42
1:A:78:ASN:ND2	1:A:80:LYS:HD2	2.34	0.41
1:C:331:ALA:O	1:C:332:GLY:C	2.63	0.41
1:C:390:MET:HE2	1:C:428:LEU:HD11	2.02	0.41
2:D:112:GLN:NE2	2:D:242:TYR:HE1	2.18	0.41
2:E:67:GLU:H	2:E:67:GLU:HG3	1.16	0.41
2:E:320:PRO:HD3	3:G:255:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:410:ILE:O	2:E:411:GLN:C	2.63	0.41
1:A:56:SER:O	1:A:58:GLY:N	2.53	0.41
1:A:99:VAL:HG23	1:A:253:MET:HA	2.01	0.41
1:A:383:MET:O	1:A:386:VAL:HG23	2.19	0.41
2:D:94:ILE:HG22	2:D:102:ILE:HD11	2.01	0.41
2:D:279:VAL:HG12	2:D:279:VAL:O	2.20	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
1:A:356:LEU:O	1:A:357:PHE:C	2.63	0.41
1:B:55:PHE:O	1:B:56:SER:C	2.61	0.41
1:B:75:VAL:HG21	1:B:82:ILE:HD12	2.02	0.41
2:E:82:ILE:CG2	2:E:116:ILE:HD13	2.51	0.41
2:E:340:ALA:O	2:E:343:GLY:N	2.42	0.41
2:E:434:LEU:O	2:E:437:THR:HB	2.20	0.41
2:F:38:VAL:HG11	2:F:69:LEU:CD2	2.50	0.41
2:F:400:ASP:O	2:F:404:VAL:HG23	2.19	0.41
1:A:105:GLY:HA2	1:A:226:MET:O	2.21	0.41
1:B:78:ASN:ND2	1:B:80:LYS:HE2	2.36	0.41
2:D:35:ALA:HB1	2:D:46:VAL:HG13	2.02	0.41
2:D:401:LYS:H	2:D:401:LYS:HG2	1.72	0.41
2:E:189:ARG:HB2	2:E:192:GLU:HG3	2.02	0.41
2:E:397:SER:O	2:E:399:GLU:N	2.54	0.41
2:F:471:ASP:O	2:F:474:ALA:N	2.53	0.41
1:A:383:MET:HG3	1:A:387:ALA:HB2	2.02	0.41
1:B:44:LEU:HB3	1:B:47:VAL:CG2	2.47	0.41
1:C:151:LYS:HE2	1:C:436:MET:SD	2.60	0.41
2:D:86:VAL:HG11	2:D:114:ALA:HB3	2.02	0.41
2:E:95:MET:HA	2:E:100:GLU:O	2.20	0.41
2:E:183:PHE:HB3	2:E:217:LEU:CD2	2.47	0.41
2:E:185:GLY:HA3	2:E:188:GLU:HG3	2.02	0.41
2:F:434:LEU:O	2:F:438:ILE:HG12	2.21	0.41
3:G:39:LYS:CB	3:G:40:PRO:CD	2.99	0.41
1:A:32:LEU:HD21	1:A:42:HIS:HB2	2.02	0.41
1:A:74:VAL:CG1	1:A:241:PRO:HG3	2.51	0.41
1:A:90:ARG:HB3	1:A:90:ARG:HE	1.73	0.41
1:A:267:ILE:HA	1:A:324:LEU:O	2.20	0.41
1:A:408:SER:O	1:A:409:ASP:HB2	2.20	0.41
1:A:461:ILE:H	1:A:461:ILE:HG12	1.60	0.41
1:B:30:ARG:HA	1:B:86:ASP:O	2.21	0.41
1:B:221:THR:HG22	1:B:222:ASP:N	2.36	0.41
1:B:366:ASN:ND2	1:B:369:LEU:HG	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:VAL:HG21	1:C:245:LEU:HD11	2.02	0.41
1:C:373:ARG:NH2	2:D:189:ARG:NH2	2.68	0.41
2:D:112:GLN:NE2	2:D:242:TYR:CE1	2.88	0.41
2:D:203:SER:OG	2:D:205:VAL:HG23	2.20	0.41
2:D:360:PRO:HD3	2:D:368:TYR:CD2	2.56	0.41
2:E:227:GLY:O	2:E:231:ARG:HG2	2.21	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:430:LYS:HA	2:F:430:LYS:HD3	1.93	0.41
2:F:442:GLN:O	2:F:445:LEU:HB2	2.21	0.41
2:F:445:LEU:HD23	2:F:445:LEU:HA	1.92	0.41
1:B:107:VAL:O	1:B:115:ILE:HG12	2.20	0.41
1:B:218:LYS:CG	2:E:128:VAL:HG11	2.48	0.41
1:C:78:ASN:HD21	1:C:80:LYS:HD3	1.85	0.41
1:C:465:GLU:O	1:C:469:LEU:HB2	2.21	0.41
2:D:201:ILE:CD1	2:D:208:LEU:HD11	2.50	0.41
2:D:398:GLU:HA	2:D:401:LYS:CG	2.51	0.41
2:D:402:LEU:O	2:D:406:ARG:HG3	2.21	0.41
2:E:35:ALA:C	2:E:36:LEU:HD23	2.46	0.41
2:E:139:VAL:HG21	2:E:348:VAL:HB	2.02	0.41
3:G:12:SER:O	3:G:16:ILE:HD12	2.20	0.41
1:B:423:ARG:NE	1:B:458:PRO:HD3	2.36	0.41
1:B:430:GLN:HE21	1:B:430:GLN:HB3	1.50	0.41
1:C:290:GLY:O	1:C:291:ARG:C	2.61	0.41
2:D:13:ILE:HD12	2:D:73:GLN:HB3	2.03	0.41
2:E:387:ILE:HG22	2:E:388:ILE:HD13	2.02	0.41
1:A:506:ALA:O	1:A:507:GLY:C	2.63	0.41
1:B:210:ARG:C	1:B:212:THR:N	2.79	0.41
1:B:383:MET:O	1:B:387:ALA:N	2.53	0.41
1:B:423:ARG:HH21	1:B:458:PRO:HD3	1.86	0.41
1:C:468:PHE:CZ	1:C:501:VAL:HG12	2.56	0.41
1:C:485:THR:C	1:C:487:GLY:N	2.76	0.41
2:D:63:MET:CE	2:D:97:VAL:HG11	2.51	0.41
2:D:95:MET:HE3	2:D:99:GLY:HA2	2.02	0.41
2:E:122:GLU:HB2	2:E:125:GLU:HG3	2.01	0.41
2:E:167:MET:SD	2:E:200:MET:HA	2.61	0.41
2:E:319:ASP:HA	3:G:255:GLN:CD	2.46	0.41
2:E:360:PRO:HD3	2:E:368:TYR:CG	2.56	0.41
2:E:452:LEU:HA	2:E:453:PRO:HD3	1.85	0.41
2:F:95:MET:HE3	2:F:108:ILE:HD13	2.02	0.41
3:G:2:THR:HG22	3:G:4:LYS:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ARG:HH11	1:A:210:ARG:HD2	1.69	0.41
1:A:307:GLU:OE1	2:E:190:THR:HB	2.21	0.41
1:A:422:VAL:O	1:A:426:GLU:HG2	2.21	0.41
1:C:104:LEU:HD21	1:C:257:PHE:CZ	2.56	0.41
1:C:240:ALA:N	1:C:241:PRO:CD	2.84	0.41
1:C:362:ARG:HG3	1:C:362:ARG:HH11	1.86	0.41
1:C:374:VAL:CG1	1:C:378:ALA:HB2	2.51	0.41
2:E:409:LYS:HZ2	2:E:450:ASP:HA	1.85	0.41
1:A:129:VAL:HG12	1:A:249:SER:HA	2.03	0.40
1:A:206:ILE:O	1:A:273:LYS:HD2	2.21	0.40
1:A:400:VAL:O	1:A:401:ALA:C	2.64	0.40
1:B:99:VAL:HG13	1:B:256:TYR:HB2	2.02	0.40
1:C:142:VAL:C	1:C:143:ARG:HG3	2.46	0.40
1:C:423:ARG:HD2	1:C:461:ILE:HD11	2.03	0.40
1:C:467:ALA:O	1:C:470:SER:HB2	2.20	0.40
2:D:105:ARG:NH1	2:D:208:LEU:HD23	2.36	0.40
2:D:433:PRO:HG2	2:D:436:GLU:CG	2.45	0.40
2:D:449:TYR:C	2:D:451:HIS:N	2.78	0.40
2:E:168:GLU:OE1	2:E:420:VAL:HG23	2.22	0.40
2:E:412:ARG:NH1	2:E:454:GLU:OE1	2.53	0.40
2:E:416:GLN:NE2	2:E:430:LYS:O	2.54	0.40
2:E:454:GLU:C	2:E:456:ALA:H	2.29	0.40
2:F:200:MET:HE2	2:F:205:VAL:CG2	2.51	0.40
2:F:357:ILE:HD13	2:F:357:ILE:HA	1.80	0.40
1:A:69:ASP:O	1:A:70:ASN:HB3	2.21	0.40
1:A:292:GLU:HB2	1:A:294:TYR:HD2	1.86	0.40
1:A:294:TYR:HB2	1:A:337:TYR:CE2	2.54	0.40
1:A:390:MET:HE1	1:A:428:LEU:HD21	2.02	0.40
1:A:441:GLN:O	1:A:445:ILE:HG12	2.21	0.40
1:B:138:PRO:HB2	1:B:312:MET:HE1	2.03	0.40
1:B:206:ILE:HA	1:B:234:ALA:O	2.21	0.40
1:C:392:LEU:HD11	2:D:425:THR:HG22	2.03	0.40
2:D:281:TYR:HB3	2:D:285:LEU:HD12	2.03	0.40
2:E:33:LEU:HD23	2:E:33:LEU:HA	1.92	0.40
2:E:319:ASP:O	2:E:322:PRO:HD2	2.22	0.40
2:E:359:ASP:HA	2:E:360:PRO:HD2	1.87	0.40
2:E:425:THR:C	2:E:427:HIS:H	2.28	0.40
2:F:304:ILE:HD13	2:F:304:ILE:HG21	1.92	0.40
1:A:485:THR:O	1:A:487:GLY:N	2.55	0.40
1:A:498:LYS:O	1:A:502:THR:HG23	2.21	0.40
1:B:423:ARG:O	1:B:426:GLU:N	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:GLY:N	1:C:229:THR:O	2.41	0.40
1:C:299:PHE:O	1:C:300:TYR:C	2.62	0.40
2:E:165:LEU:HD22	2:E:335:LEU:HD21	2.02	0.40
1:A:102:GLU:HG3	1:A:122:GLY:C	2.46	0.40
1:A:268:TYR:HB2	1:A:325:PRO:HA	2.03	0.40
1:A:383:MET:HE2	1:A:438:ILE:CD1	2.48	0.40
1:A:440:GLU:HG2	1:A:473:ILE:HD11	2.03	0.40
1:A:479:LEU:O	1:A:482:LYS:HB2	2.22	0.40
1:B:340:THR:O	1:B:341:ASN:C	2.63	0.40
1:B:488:LYS:HG2	1:B:489:ILE:N	2.37	0.40
1:C:19:ALA:O	1:C:21:THR:HG23	2.21	0.40
1:C:45:ARG:HD3	1:C:45:ARG:HA	1.29	0.40
1:C:151:LYS:HG3	1:C:430:GLN:OE1	2.21	0.40
2:E:454:GLU:C	2:E:456:ALA:N	2.80	0.40
2:F:228:ALA:O	2:F:232:VAL:HG22	2.21	0.40
2:F:238:THR:O	2:F:239:VAL:C	2.64	0.40
1:A:62:MET:HE2	1:A:76:PHE:CZ	2.57	0.40
1:A:106:ARG:NH2	1:A:119:GLY:O	2.46	0.40
1:B:226:MET:O	1:B:227:LYS:C	2.65	0.40
1:C:206:ILE:C	1:C:208:GLN:H	2.29	0.40
2:D:64:ASP:CG	2:D:65:GLY:H	2.28	0.40
2:E:329:LEU:O	2:E:356:ARG:CZ	2.69	0.40

All (58) 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:314:ASP:O	1:C:22:SER:C[4_455]	0.42	1.78
1:B:314:ASP:CA	1:C:22:SER:N[4_455]	0.82	1.38
1:B:318:GLY:C	1:C:20:ASP:OD2[4_455]	0.87	1.33
1:B:314:ASP:O	1:C:23:VAL:N[4_455]	0.93	1.27
1:B:314:ASP:OD1	1:C:20:ASP:O[4_455]	0.94	1.26
1:B:314:ASP:CA	1:C:21:THR:C[4_455]	1.04	1.16
1:B:314:ASP:N	1:C:22:SER:N[4_455]	1.12	1.08
1:B:313:ASN:O	1:C:22:SER:CB[4_455]	1.15	1.05
1:B:318:GLY:O	1:C:20:ASP:OD2[4_455]	1.15	1.05
1:B:314:ASP:C	1:C:22:SER:CA[4_455]	1.20	1.00
1:B:318:GLY:CA	1:C:20:ASP:CG[4_455]	1.22	0.98
1:B:124:LYS:NZ	2:F:31:PRO:CB[4_455]	1.27	0.93
1:B:314:ASP:C	1:C:22:SER:C[4_455]	1.29	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ASP:N	1:C:21:THR:C[4_455]	1.30	0.90
1:B:318:GLY:CA	1:C:20:ASP:OD1[4_455]	1.38	0.82
1:B:318:GLY:CA	1:C:20:ASP:OD2[4_455]	1.39	0.81
1:B:314:ASP:CB	1:C:21:THR:C[4_455]	1.44	0.76
1:B:314:ASP:CG	1:C:21:THR:CA[4_455]	1.48	0.72
1:B:314:ASP:CB	1:C:21:THR:CA[4_455]	1.48	0.72
1:B:314:ASP:OD1	1:C:20:ASP:C[4_455]	1.51	0.69
1:B:314:ASP:C	1:C:22:SER:N[4_455]	1.53	0.67
1:B:314:ASP:O	1:C:22:SER:O[4_455]	1.53	0.67
1:B:124:LYS:NZ	2:F:31:PRO:CG[4_455]	1.55	0.65
1:B:318:GLY:N	1:C:22:SER:OG[4_455]	1.57	0.63
1:B:313:ASN:O	1:C:22:SER:OG[4_455]	1.62	0.58
1:B:315:ALA:C	1:C:22:SER:O[4_455]	1.66	0.54
1:B:313:ASN:C	1:C:22:SER:N[4_455]	1.68	0.52
1:B:314:ASP:O	1:C:22:SER:CA[4_455]	1.71	0.49
1:B:315:ALA:N	1:C:22:SER:CA[4_455]	1.73	0.47
1:B:315:ALA:N	1:C:21:THR:O[4_455]	1.75	0.45
1:B:313:ASN:O	1:C:22:SER:CA[4_455]	1.79	0.41
1:B:317:GLY:CA	1:C:23:VAL:CG2[4_455]	1.81	0.39
1:B:314:ASP:C	1:C:23:VAL:N[4_455]	1.84	0.36
1:B:314:ASP:N	1:C:21:THR:CA[4_455]	1.85	0.35
1:B:316:PHE:N	1:C:22:SER:CB[4_455]	1.85	0.35
1:B:314:ASP:N	1:C:21:THR:N[4_455]	1.88	0.32
1:B:314:ASP:CG	1:C:20:ASP:O[4_455]	1.90	0.30
1:B:317:GLY:N	1:C:22:SER:OG[4_455]	1.91	0.29
1:B:314:ASP:C	1:C:21:THR:C[4_455]	1.93	0.27
1:B:311:LYS:NZ	1:C:20:ASP:CB[4_455]	1.96	0.24
1:B:318:GLY:C	1:C:20:ASP:CG[4_455]	1.96	0.24
1:B:313:ASN:O	1:C:22:SER:N[4_455]	1.97	0.23
1:B:314:ASP:CA	1:C:22:SER:CA[4_455]	1.99	0.21
1:B:314:ASP:CB	1:C:21:THR:O[4_455]	2.01	0.19
1:B:314:ASP:CA	1:C:21:THR:CA[4_455]	2.01	0.19
1:B:314:ASP:OD1	1:C:21:THR:N[4_455]	2.02	0.18
1:B:314:ASP:CA	1:C:21:THR:O[4_455]	2.04	0.16
1:B:315:ALA:CA	1:C:22:SER:O[4_455]	2.05	0.15
1:B:316:PHE:N	1:C:22:SER:CA[4_455]	2.06	0.14
1:B:318:GLY:N	1:C:20:ASP:OD1[4_455]	2.06	0.14
1:B:314:ASP:C	1:C:21:THR:O[4_455]	2.08	0.12
1:B:316:PHE:N	1:C:22:SER:O[4_455]	2.09	0.11
1:B:315:ALA:N	1:C:22:SER:C[4_455]	2.11	0.09
1:B:319:GLY:N	1:C:20:ASP:OD2[4_455]	2.12	0.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ASP:O	1:C:23:VAL:CA[4_455]	2.13	0.07
1:B:314:ASP:OD1	1:C:21:THR:CA[4_455]	2.15	0.05
1:B:318:GLY:O	1:C:20:ASP:CG[4_455]	2.17	0.03
1:B:314:ASP:OD2	1:C:21:THR:CA[4_455]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/553 (88%)	443 (91%)	35 (7%)	7 (1%)	9	40
1	B	475/553 (86%)	427 (90%)	41 (9%)	7 (2%)	8	39
1	C	490/553 (89%)	444 (91%)	38 (8%)	8 (2%)	7	37
2	D	465/528 (88%)	419 (90%)	43 (9%)	3 (1%)	21	59
2	E	464/528 (88%)	407 (88%)	48 (10%)	9 (2%)	6	32
2	F	464/528 (88%)	432 (93%)	30 (6%)	2 (0%)	30	67
3	G	134/298 (45%)	130 (97%)	3 (2%)	1 (1%)	18	56
All	All	2977/3541 (84%)	2702 (91%)	238 (8%)	37 (1%)	10	44

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	407	GLY
2	E	393	MET
1	A	57	SER
1	A	405	GLN
1	A	409	ASP
1	B	364	ALA
1	C	332	GLY
1	C	408	SER
1	C	411	ASP

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Mol	Chain	Res	Type
1	C	476	HIS
2	D	28	GLY
2	E	161	GLY
2	E	205	VAL
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
1	B	411	ASP
1	C	405	GLN
1	C	475	GLN
2	D	474	ALA
2	E	122	GLU
2	F	327	ALA
1	A	484	ARG
1	B	359	LYS
2	E	33	LEU
1	B	458	PRO
1	C	409	ASP
2	E	28	GLY
2	E	279	VAL
1	B	68	PRO
2	F	279	VAL
2	D	279	VAL
1	A	246	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/444 (88%)	343 (87%)	50 (13%)	4	16
1	B	388/444 (87%)	334 (86%)	54 (14%)	3	14
1	C	397/444 (89%)	359 (90%)	38 (10%)	8	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	377/417 (90%)	344 (91%)	33 (9%)	9	28
2	E	376/417 (90%)	335 (89%)	41 (11%)	6	21
2	F	376/417 (90%)	343 (91%)	33 (9%)	9	28
3	G	116/251 (46%)	109 (94%)	7 (6%)	17	39
All	All	2423/2834 (86%)	2167 (89%)	256 (11%)	6	21

All (256) 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	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

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Mol	Chain	Res	Type
1	A	410	LEU
1	A	417	LEU
1	A	420	ARG
1	A	430	GLN
1	A	436	MET
1	A	442	VAL
1	A	444	VAL
1	A	449	VAL
1	A	457	GLU
1	A	461	ILE
1	A	472	VAL
1	A	473	ILE
1	A	474	SER
1	A	479	LEU
1	A	485	THR
1	A	489	ILE
1	A	497	LEU
1	A	499	GLU
1	B	38	ILE
1	B	47	VAL
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	195	GLU
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

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Mol	Chain	Res	Type
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	384	LYS
1	B	398	ARG
1	B	399	GLU
1	B	400	VAL
1	B	416	GLN
1	B	423	ARG
1	B	430	GLN
1	B	442	VAL
1	B	444	VAL
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

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Mol	Chain	Res	Type
1	C	195	GLU
1	C	208	GLN
1	C	216	LEU
1	C	217	VAL
1	C	227	LYS
1	C	267	ILE
1	C	270	ASP
1	C	282	SER
1	C	298	VAL
1	C	334	VAL
1	C	338	ILE
1	C	339	PRO
1	C	349	GLN
1	C	399	GLU
1	C	400	VAL
1	C	406	PHE
1	C	440	GLU
1	C	444	VAL
1	C	469	LEU
1	C	474	SER
1	C	477	GLN
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

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Mol	Chain	Res	Type
2	D	258	ILE
2	D	266	SER
2	D	279	VAL
2	D	282	GLN
2	D	306	SER
2	D	336	SER
2	D	361	ASN
2	D	365	SER
2	D	388	ILE
2	D	397	SER
2	D	401	LYS
2	D	423	VAL
2	D	428	LEU
2	D	431	LEU
2	D	439	LYS
2	D	452	LEU
2	D	475	GLU
2	E	9	THR
2	E	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

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Mol	Chain	Res	Type
2	E	333	THR
2	E	358	MET
2	E	365	SER
2	E	385	GLN
2	E	387	ILE
2	E	391	LEU
2	E	393	MET
2	E	394	ASP
2	E	395	GLU
2	E	402	LEU
2	E	412	ARG
2	E	431	LEU
2	E	438	ILE
2	E	452	LEU
2	E	463	ILE
2	E	473	LEU
2	F	10	THR
2	F	27	GLU
2	F	36	LEU
2	F	42	GLU
2	F	67	GLU
2	F	89	GLU
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

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Mol	Chain	Res	Type
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	67	LEU
3	G	205	GLN
3	G	212	ILE
3	G	213	ILE
3	G	262	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	GLN
1	A	396	GLN
1	A	476	HIS
1	B	42	HIS
1	B	172	GLN
1	B	330	GLN
1	B	415	GLN
1	B	466	ASN
1	C	208	GLN
1	C	260	ASN
1	C	416	GLN
1	C	432	GLN
1	C	475	GLN
2	D	24	GLN
2	D	130	GLN
2	D	171	ASN
2	D	221	GLN
2	D	223	ASN
2	D	282	GLN
2	D	328	HIS
2	D	442	GLN
2	E	39	GLN
2	E	51	GLN
2	E	194	ASN

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Mol	Chain	Res	Type
2	E	223	ASN
2	E	246	GLN
2	E	282	GLN
2	E	367	HIS
2	E	442	GLN
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	225	GLN
3	G	234	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	487/553 (88%)	0.09	16 (3%) 49 44	20, 20, 20, 20	0
1	B	479/553 (86%)	0.09	10 (2%) 63 54	20, 20, 20, 20	0
1	C	492/553 (88%)	0.14	14 (2%) 55 47	20, 20, 20, 20	0
2	D	467/528 (88%)	0.13	18 (3%) 43 41	20, 20, 20, 20	0
2	E	466/528 (88%)	0.13	10 (2%) 63 54	20, 20, 20, 20	0
2	F	466/528 (88%)	0.20	22 (4%) 36 36	20, 20, 20, 20	0
3	G	140/298 (46%)	0.25	6 (4%) 40 39	36, 59, 81, 89	0
All	All	2997/3541 (84%)	0.13	96 (3%) 50 45	20, 20, 20, 89	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	220	GLY	10.5
1	A	234	ALA	7.5
2	F	335	LEU	5.4
1	B	274	GLN	4.9
1	B	489	ILE	4.6
1	B	179	ALA	4.5
1	B	270	ASP	4.5
3	G	265	ILE	4.5
2	E	233	ALA	4.0
2	F	261	PHE	3.9
1	C	468	PHE	3.9
2	F	420	VAL	3.8
1	C	289	PRO	3.7
1	C	472	VAL	3.7
1	C	483	ILE	3.7
2	D	256	ASP	3.7
2	D	236	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	105	GLY	3.6
3	G	247	THR	3.6
2	F	421	ALA	3.5
2	F	296	ILE	3.4
2	D	345	TYR	3.3
2	D	291	THR	3.3
2	D	82	ILE	3.3
2	F	291	THR	3.3
1	B	216	LEU	3.2
1	B	220	LEU	3.2
1	C	233	SER	3.2
2	F	162	LYS	3.1
2	F	233	ALA	3.0
3	G	17	GLN	3.0
3	G	261	GLU	3.0
2	E	325	THR	2.9
2	F	157	GLY	2.9
2	E	183	PHE	2.9
2	F	196	LEU	2.9
2	E	258	ILE	2.9
2	D	163	THR	2.8
2	F	164	VAL	2.8
2	D	214	LYS	2.8
2	D	212	THR	2.7
2	E	219	TYR	2.7
1	A	304	ARG	2.7
1	A	182	THR	2.6
1	A	290	GLY	2.6
1	A	302	HIS	2.6
2	D	335	LEU	2.6
2	D	169	LEU	2.6
2	F	13	ILE	2.5
2	E	451	HIS	2.5
2	E	255	ILE	2.5
2	D	181	SER	2.5
2	F	286	ALA	2.5
2	E	184	ALA	2.5
1	C	69	ASP	2.5
1	B	103	LEU	2.4
1	A	235	THR	2.4
1	C	358	TYR	2.4
1	C	466	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	179	ALA	2.4
1	A	375	GLY	2.4
1	B	277	ALA	2.4
2	F	280	GLY	2.3
1	C	290	GLY	2.3
1	B	285	LEU	2.3
1	C	41	VAL	2.3
1	A	469	LEU	2.3
2	D	147	ALA	2.3
1	C	324	LEU	2.2
2	E	169	LEU	2.2
1	A	372	SER	2.2
2	D	205	VAL	2.2
3	G	264	GLU	2.2
1	A	158	PRO	2.2
1	A	69	ASP	2.2
1	A	147	GLN	2.2
1	C	340	THR	2.2
2	F	365	SER	2.2
2	D	262	THR	2.1
2	F	325	THR	2.1
2	D	251	VAL	2.1
1	A	333	ASP	2.1
1	A	261	GLY	2.1
1	B	232	VAL	2.1
2	D	198	HIS	2.1
2	E	193	GLY	2.1
2	F	351	LEU	2.1
2	F	258	ILE	2.1
1	A	328	GLU	2.1
1	C	134	PRO	2.1
2	D	276	PRO	2.1
2	D	388	ILE	2.0
2	F	262	THR	2.0
2	F	95	MET	2.0
2	F	390	ILE	2.0
3	G	240	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [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.