



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:30 am GMT

PDB ID : 2W6I
Title : LOW RESOLUTION STRUCTURES OF BOVINE MITOCHONDRIAL F1-ATPASE DURING CONTROLLED DEHYDRATION: HYDRATION STATE 4B.
Authors : Sanchez-Weatherby, J.; Felisaz, F.; Gobbo, A.; Huet, J.; Ravelli, R.B.G.; Bowler, M.W.; Cipriani, F.
Deposited on : 2008-12-18
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

<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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

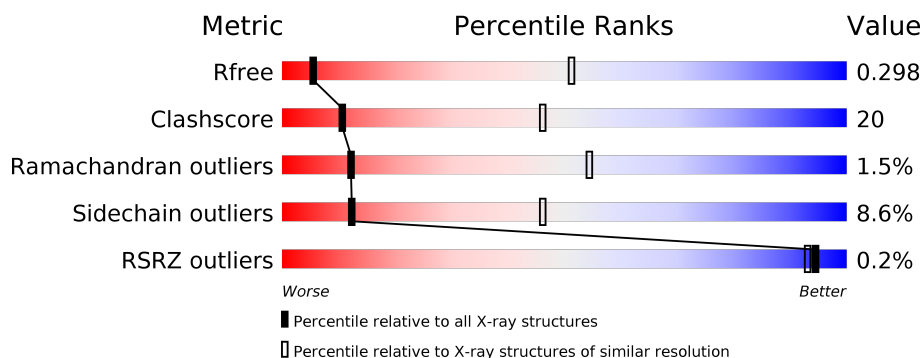
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1088 (4.40-3.60)
Clashscore	112137	1187 (4.40-3.60)
Ramachandran outliers	110173	1139 (4.40-3.60)
Sidechain outliers	110143	1126 (4.40-3.60)
RSRZ outliers	101464	1099 (4.40-3.60)

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	
1	B	553	
1	C	553	
2	D	528	
2	E	528	
2	F	528	

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Mol	Chain	Length	Quality of chain
3	G	298	<div><div></div><div>54%30%5%12%</div></div>
4	H	168	<div><div></div><div>9%9%82%</div></div>
5	I	51	<div><div></div><div>33%20%45%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24216 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL.

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

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

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

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

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

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

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

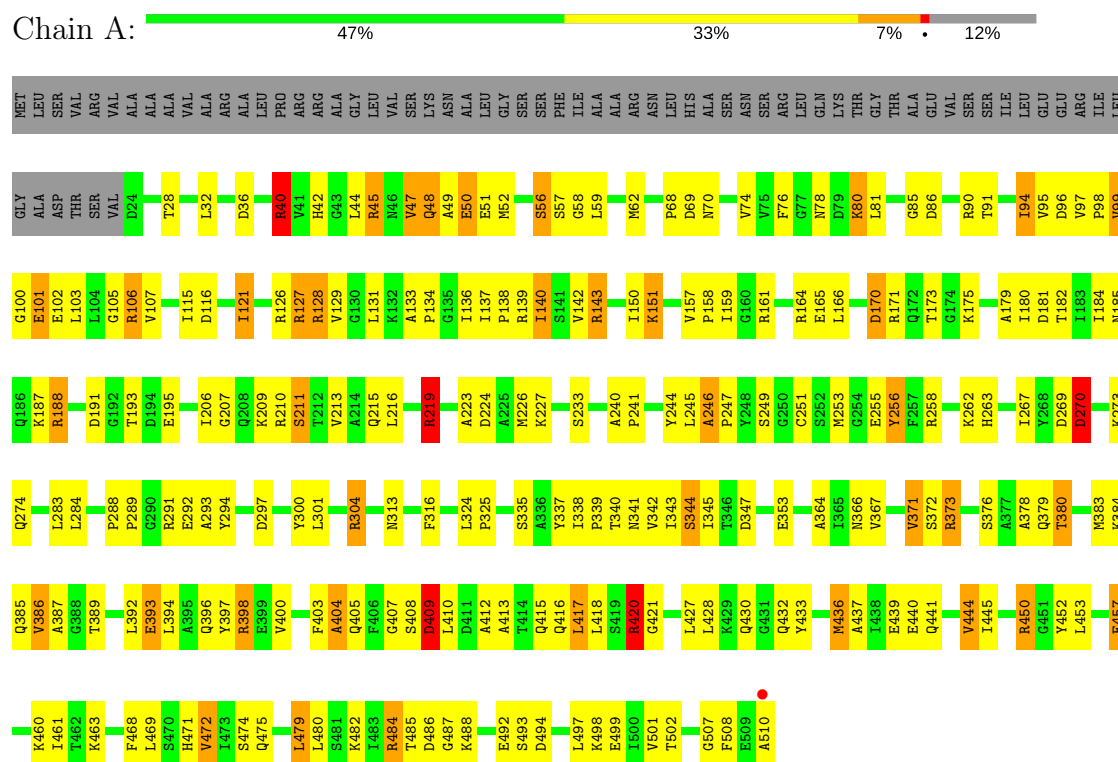
- Molecule 5 is a protein called ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL.

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

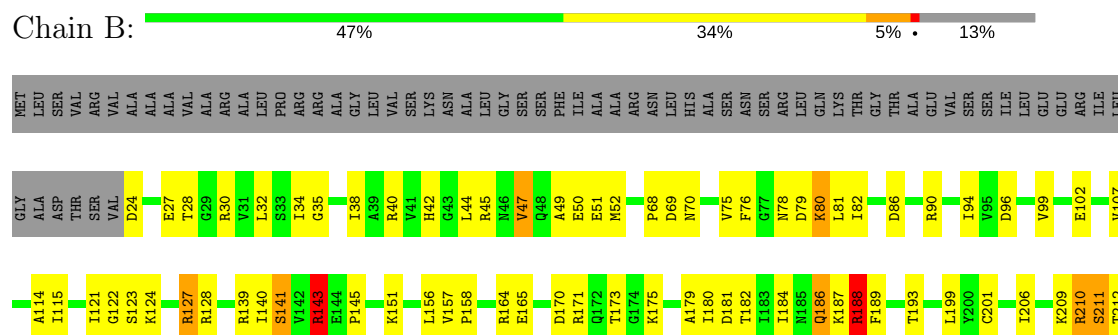
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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

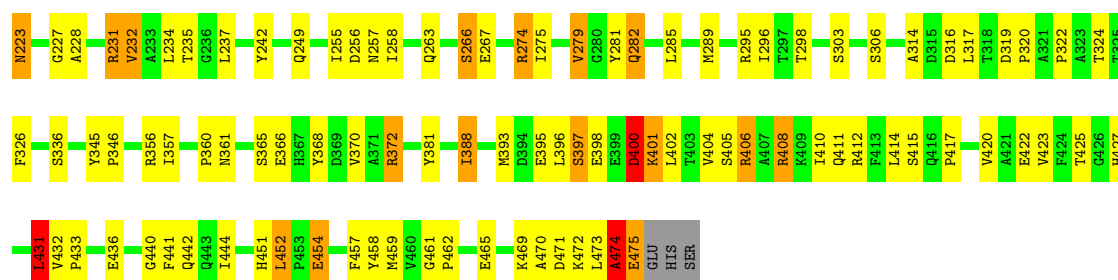




MET	LEU	VAL	ARG	ALA	VAL	VAL	ARG	ALA	GLY	VAL	LEU	GLN	LYS	THR	GLY	THR	ALA	GLU	VAL	SER	SER	ILE	LEU	GLU	ARG	ILE	LEU	ILE																																																																																																																																																																																																																																																																																										
	GLY	ALA	VAL	ARG	ALA	VAL	ARG	ALA	GLY	VAL	LEU	GLN	LYS	THR	GLY	THR	ALA	GLU	VAL	SER	SER	ILE	LEU	GLU	ARG	ILE	LEU	ILE																																																																																																																																																																																																																																																																																										
	A19	D20	T21	S22	V23	E26	R30	V41	L32	S33	I34	G122	S123	D224	A225	M226	R127	R128	V129	R139	I140	R143	A239	A240	P241	Q147	S56	L59	K60	G61	M62	S63	L64	N65	L66	E67	P68	V74	N78	D79	K80	L81	I82	K83	D86	I87	T91	G92	A93	I94	V95	D96	ARG	V97	D98																																																																																																																																																																																																																																																															
	Q100	E101	E102	L103	L104	G105	R106	V107	I115	D116	G117	G122	S123	D224	A225	M226	R127	R128	V129	R139	I140	R143	A239	A240	P241	Q147	S56	L59	K60	G61	M62	S63	L64	N65	L66	E67	P68	V74	N78	D79	K80	L81	I82	K83	D86	I87	T91	G92	A93	I94	V95	D96	ARG	V97	D98																																																																																																																																																																																																																																																															
	K198	I202	Q208	K209	R210	S211	Q215	L216	V217	K218	R219	G122	S123	D224	A225	M226	R127	R128	V129	R139	I140	R143	A239	A240	P241	Q147	S56	L59	K60	G61	M62	S63	L64	N65	L66	E67	P68	V74	N78	D79	K80	L81	I82	K83	D86	I87	T91	G92	A93	I94	V95	D96	ARG	V97	D98																																																																																																																																																																																																																																																															
	K311	K312	K313	K314	K315	K316	K317	K318	K319	K320	K321	K322	K323	K324	K325	K326	K327	K328	K329	K330	K331	K332	K333	K334	K335	K336	K337	K338	K339	K340	K341	K342	K343	K344	K345	K346	K347	K348	K349	K350	K351	K352	K353	K354	K355	K356	K357	K358	K359	K360	K361	K362	K363	K364	K365	K366	K367	K368	K369	K370	K371	K372	K373	K374	K375	K376	K377	K378	K379	K380	K381	K382	K383	K384	K385	K386	K387	K388	K389	K390	K391	K392	K393	K394	K395	K396	K397	K398	K399	K400	K401	K402	K403	K404	K405	K406	K407	K408	K409	K410	K411	K412	K413	K414	K415	K416	K417	K418	K419	K420	K421	K422	K423	K424	K425	K426	K427	K428	K429	K430	K431	K432	K433	K434	K435	K436	K437	K438	K439	K440	K441	K442	K443	K444	K445	K446	K447	K448	K449	K450	K451	K452	K453	K454	K455	K456	K457	K458	K459	K460	K461	K462	K463	K464	K465	K466	K467	K468	K469	K470	K471	K472	K473	K474	K475	K476	K477	K478	K479	K480	K481	K482	K483	K484	K485	K486	K487	K488	K489	K490	K491	K492	K493	K494	K495	K496	K497	K498	K499	K500	K501	K502	K503	K504	K505	K506	K507	K508	K509	K510	K511	K512	K513	K514	K515	K516	K517	K518	K519	K520	K521	K522	K523	K524	K525	K526	K527	K528	K529	K530	K531	K532	K533	K534	K535	K536	K537	K538	K539	K540	K541	K542	K543	K544	K545	K546	K547	K548	K549	K550	K551	K552	K553	K554	K555	K556	K557	K558	K559	K560	K561	K562	K563	K564	K565	K566	K567	K568	K569	K570	K571	K572	K573	K574	K575	K576	K577	K578	K579	K580	K581	K582	K583	K584	K585	K586	K587	K588	K589	K590	K591	K592	K593	K594	K595	K596	K597	K598	K599	K600	K601	K602	K603	K604	K605	K606	K607	K608	K609	K610	K611	K612	K613	K614	K615	K616	K617	K618	K619	K620

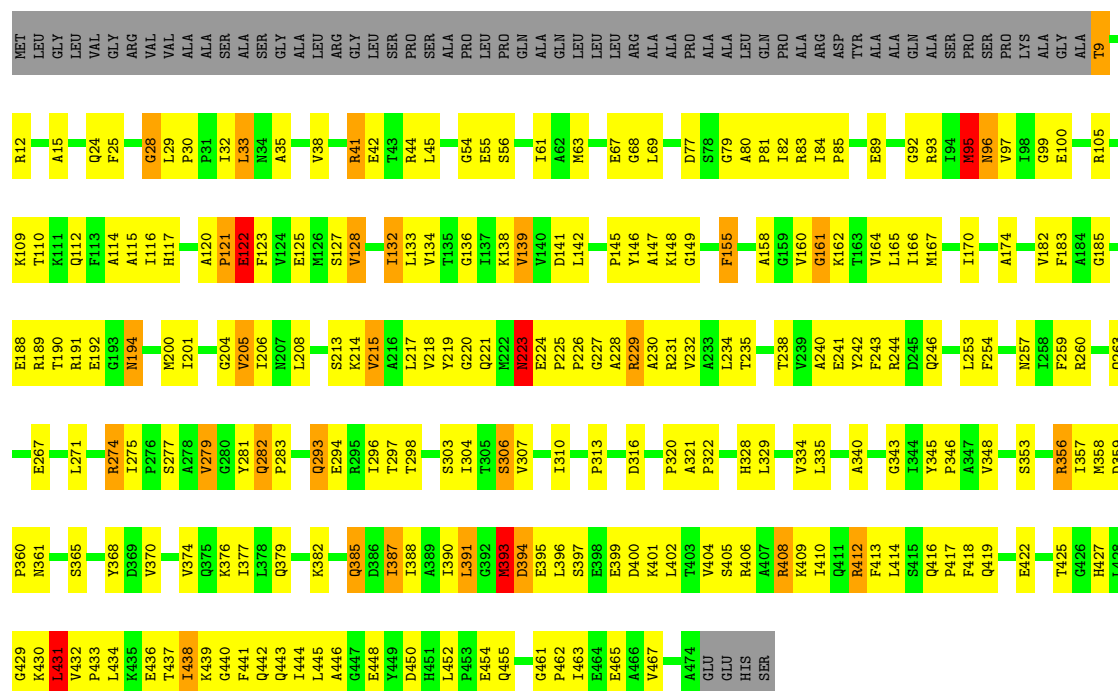
- Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

E104	I108	K109	T110	K111	Q112	F113	A114	A115	E122	E125	M126	E129	Q130	G136	I137	K138	V139	L142	P145	L154	L165	I166	M167	E168	L169	I170	A174	V186	R189	T190	R191	E192	E199	M200	I201	E202	S203	G204	V205	I206	M207	L208	V215	T220									
R12	I13	I14	Q24	E27	G28	P31	I32	L33	N34	A35	L36	E37	V38	R44	L45	V46	H52	L53	G54	E55	S56	T57	V58	R59	M63	E67	G68	L69	Q73	K74	V75	R83	I84	P85	V86	G87	P88	E89	R93	I94	N95	N96	V97	G98	L99	E100	P101	I102	N103				
MET	GLY	GLY	LEU	VAL	GLY	ARG	VAL	VAL	ALA	SER	ALA	ALA	LEU	ARG	GLY	LEU	SER	PRO	SER	ALA	PRO	LEU	GLN	ALA	GLN	LEU	LEU	ARG	ALA	ALA	PRO	ALA	ALA	LEU	GLN	PRO	ALA	ARG	ASP	TYR	ALA	ALA	GLN	ALA	SER	PRO	SER	PRO	LYS	ALA	GLY	ALA	T9



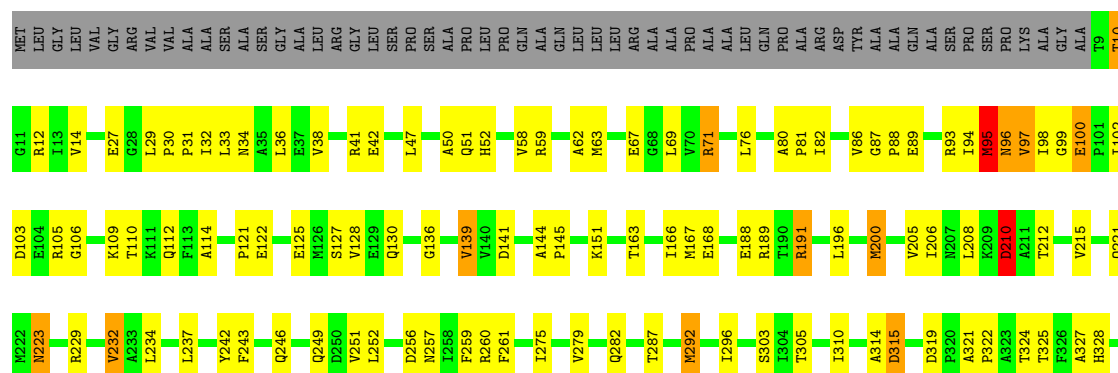
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

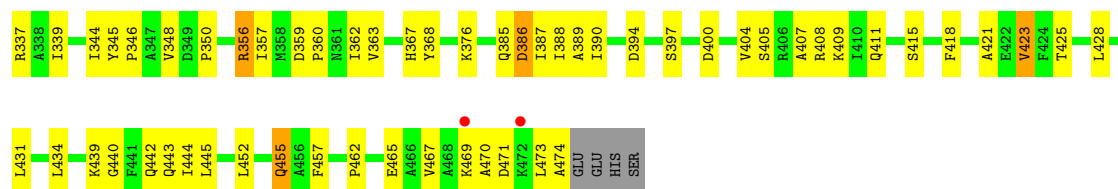
Chain E: 44% 38% 5% 12%



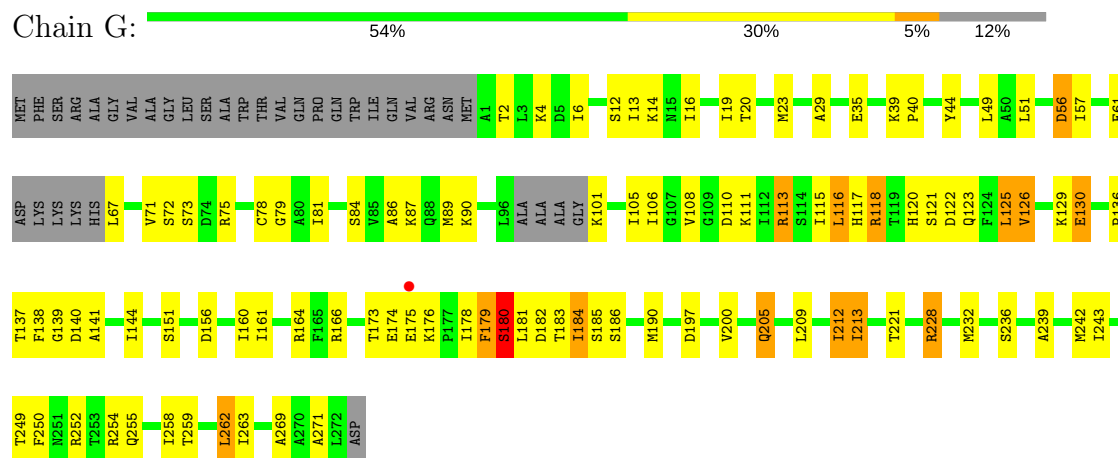
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain F: 57% 28% 12%

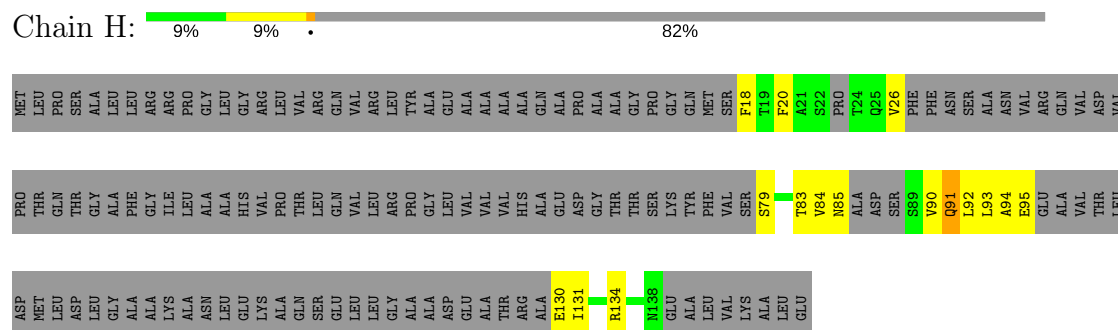




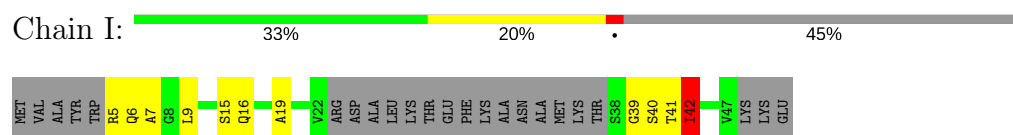
- Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL



- Molecule 4: F1-ATPASE DELTA SUBUNIT



- Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.92Å 131.33Å 267.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 4.00 100.87 – 4.00	Depositor EDS
% Data completeness (in resolution range)	92.8 (30.00-4.00) 92.7 (100.87-4.00)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 4.01Å)	Xtriage
Refinement program	REFMAC 5.5.0038	Depositor
R, R_{free}	0.299 , 0.300 0.303 , 0.298	Depositor DCC
R_{free} test set	1557 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	92.8	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 9.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	24216	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.60	0/3766	1.31	26/5080 (0.5%)
1	B	0.61	0/3704	1.36	30/4995 (0.6%)
1	C	0.62	0/3799	1.38	25/5126 (0.5%)
2	D	0.62	0/3596	1.36	22/4879 (0.5%)
2	E	0.60	0/3587	1.32	17/4867 (0.3%)
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	0.31	0/232	0.61	0/308
5	I	0.34	0/212	0.75	0/281
All	All	0.59	0/24557	1.30	151/33188 (0.5%)

There are no bond length outliers.

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	408	ARG	CD-NE-CZ	23.38	156.33	123.60
2	E	408	ARG	CD-NE-CZ	13.90	143.07	123.60
1	C	291	ARG	NE-CZ-NH2	-13.42	113.59	120.30
1	B	40	ARG	NE-CZ-NH1	13.11	126.85	120.30
1	B	279	ARG	NE-CZ-NH1	12.83	126.71	120.30
2	F	356	ARG	NE-CZ-NH1	11.71	126.15	120.30
2	D	406	ARG	NE-CZ-NH1	-11.61	114.50	120.30
2	F	59	ARG	NE-CZ-NH1	-11.33	114.64	120.30
2	D	408	ARG	NE-CZ-NH1	11.06	125.83	120.30
2	F	282	GLN	CB-CG-CD	10.34	138.48	111.60
1	B	219	ARG	NE-CZ-NH2	10.23	125.42	120.30
1	C	164	ARG	NE-CZ-NH1	-10.04	115.28	120.30
1	B	40	ARG	CD-NE-CZ	9.82	137.35	123.60
1	C	258	ARG	NE-CZ-NH1	9.80	125.20	120.30
2	F	229	ARG	NE-CZ-NH1	-9.54	115.53	120.30
2	F	356	ARG	NE-CZ-NH2	-9.54	115.53	120.30
2	D	44	ARG	NE-CZ-NH2	-9.27	115.66	120.30
1	B	304	ARG	NE-CZ-NH1	-9.15	115.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	59	ARG	NE-CZ-NH2	9.12	124.86	120.30
2	F	95	MET	CA-CB-CG	9.10	128.77	113.30
1	A	420	ARG	NE-CZ-NH1	-8.94	115.83	120.30
1	C	161	ARG	NE-CZ-NH1	8.89	124.74	120.30
2	E	95	MET	CA-CB-CG	8.59	127.90	113.30
2	E	260	ARG	NE-CZ-NH1	-8.59	116.01	120.30
1	A	398	ARG	NE-CZ-NH1	-8.57	116.02	120.30
2	F	96	ASN	CB-CA-C	-8.57	93.27	110.40
1	C	450	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	A	450	ARG	NE-CZ-NH2	-8.49	116.06	120.30
2	E	83	ARG	NE-CZ-NH1	-8.46	116.07	120.30
1	A	373	ARG	NE-CZ-NH2	8.37	124.48	120.30
2	F	229	ARG	NE-CZ-NH2	8.15	124.38	120.30
1	B	304	ARG	NE-CZ-NH2	8.12	124.36	120.30
1	C	127	ARG	NE-CZ-NH1	-8.10	116.25	120.30
2	D	125	GLU	OE1-CD-OE2	-7.95	113.77	123.30
1	C	362	ARG	NE-CZ-NH2	7.92	124.26	120.30
2	E	229	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	C	450	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	B	219	ARG	NE-CZ-NH1	-7.57	116.52	120.30
1	B	279	ARG	NE-CZ-NH2	-7.48	116.56	120.30
2	F	408	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	C	304	ARG	NE-CZ-NH2	7.41	124.01	120.30
1	B	270	ASP	CB-CA-C	-7.37	95.66	110.40
1	A	450	ARG	NE-CZ-NH1	7.28	123.94	120.30
2	E	356	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	B	258	ARG	CD-NE-CZ	7.24	133.73	123.60
1	C	161	ARG	NE-CZ-NH2	-7.18	116.71	120.30
2	D	93	ARG	NE-CZ-NH1	-7.18	116.71	120.30
1	C	45	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	A	270	ASP	CB-CA-C	-7.14	96.11	110.40
2	E	41	ARG	CD-NE-CZ	7.12	133.56	123.60
2	E	356	ARG	NE-CZ-NH1	7.10	123.85	120.30
2	F	139	VAL	CB-CA-C	-7.02	98.07	111.40
1	B	279	ARG	CD-NE-CZ	6.92	133.29	123.60
2	F	95	MET	C-N-CA	6.77	138.62	121.70
2	D	96	ASN	CB-CA-C	-6.73	96.94	110.40
2	D	95	MET	C-N-CA	6.67	138.37	121.70
1	A	127	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	B	349	GLN	CA-CB-CG	6.62	127.96	113.40
1	C	308	ARG	NE-CZ-NH1	-6.61	117.00	120.30
2	D	231	ARG	NE-CZ-NH1	6.49	123.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	423	ARG	CD-NE-CZ	6.48	132.68	123.60
1	A	372	SER	N-CA-CB	6.46	120.19	110.50
2	F	256	ASP	CB-CG-OD1	6.46	124.11	118.30
1	A	106	ARG	CD-NE-CZ	6.45	132.63	123.60
1	A	371	VAL	CB-CA-C	-6.45	99.15	111.40
2	D	274	ARG	NE-CZ-NH1	-6.44	117.08	120.30
1	A	170	ASP	CB-CG-OD1	6.42	124.08	118.30
2	D	59	ARG	NE-CZ-NH1	-6.42	117.09	120.30
2	F	189	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	B	270	ASP	CB-CG-OD1	6.39	124.05	118.30
2	D	191	ARG	NE-CZ-NH1	-6.39	117.11	120.30
2	E	431	LEU	CA-CB-CG	6.38	129.97	115.30
2	E	44	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	C	291	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	A	171	ARG	NE-CZ-NH2	6.36	123.48	120.30
1	C	308	ARG	NE-CZ-NH2	6.33	123.47	120.30
1	A	398	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	A	210	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	C	381	ARG	CD-NE-CZ	6.19	132.26	123.60
1	C	476	HIS	N-CA-C	6.18	127.69	111.00
2	E	274	ARG	NE-CZ-NH2	-6.18	117.21	120.30
2	D	372	ARG	NE-CZ-NH2	6.16	123.38	120.30
1	B	127	ARG	CD-NE-CZ	6.16	132.22	123.60
1	B	371	VAL	CB-CA-C	-6.12	99.76	111.40
1	B	128	ARG	NE-CZ-NH1	6.11	123.35	120.30
2	F	97	VAL	CB-CA-C	-6.11	99.80	111.40
1	C	423	ARG	CD-NE-CZ	6.08	132.10	123.60
2	F	12	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	B	300	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	C	164	ARG	CD-NE-CZ	-5.95	115.27	123.60
1	B	398	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	A	40	ARG	NE-CZ-NH2	5.93	123.27	120.30
2	D	222	MET	CB-CA-C	-5.89	98.61	110.40
1	A	269	ASP	C-N-CA	5.82	136.24	121.70
1	B	337	TYR	CB-CG-CD1	5.75	124.45	121.00
1	A	219	ARG	CD-NE-CZ	5.71	131.59	123.60
1	A	297	ASP	CB-CG-OD2	-5.70	113.17	118.30
2	F	41	ARG	CG-CD-NE	5.69	123.75	111.80
2	F	103	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	A	297	ASP	CB-CG-OD1	5.66	123.39	118.30
1	B	139	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	210	ARG	NE-CZ-NH1	-5.64	117.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	474	ALA	C-N-CA	5.61	135.73	121.70
2	D	139	VAL	CB-CA-C	-5.61	100.74	111.40
2	D	454	GLU	CA-CB-CG	5.60	125.72	113.40
2	D	431	LEU	CA-CB-CG	5.59	128.16	115.30
3	G	254	ARG	NE-CZ-NH2	-5.57	117.51	120.30
2	D	372	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	A	233	SER	N-CA-CB	-5.51	102.23	110.50
1	B	40	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	C	170	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	349	GLN	N-CA-CB	5.50	120.50	110.60
1	B	423	ARG	NE-CZ-NH1	5.49	123.04	120.30
2	F	191	ARG	NE-CZ-NH2	-5.47	117.57	120.30
2	F	191	ARG	CD-NE-CZ	5.46	131.25	123.60
3	G	254	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	304	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	A	335	SER	CB-CA-C	-5.42	99.80	110.10
1	B	222	ASP	CB-CG-OD2	-5.40	113.44	118.30
2	F	71	ARG	NE-CZ-NH2	5.38	122.99	120.30
2	E	408	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	C	349	GLN	CB-CA-C	-5.36	99.69	110.40
1	C	241	PRO	N-CA-CB	5.34	109.71	103.30
2	E	93	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	C	171	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	B	45	ARG	CB-CG-CD	-5.25	97.95	111.60
1	B	188	ARG	CG-CD-NE	5.24	122.80	111.80
1	C	336	ALA	N-CA-CB	-5.23	102.78	110.10
2	F	100	GLU	OE1-CD-OE2	5.23	129.57	123.30
1	B	143	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	C	127	ARG	NH1-CZ-NH2	5.22	125.14	119.40
2	D	12	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	258	ARG	CD-NE-CZ	5.19	130.86	123.60
2	E	260	ARG	NE-CZ-NH2	5.17	122.89	120.30
2	F	423	VAL	CB-CA-C	-5.17	101.58	111.40
3	G	228	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	351	PHE	N-CA-CB	5.14	119.84	110.60
2	E	122	GLU	CA-CB-CG	5.13	124.69	113.40
2	F	232	VAL	CB-CA-C	-5.11	101.69	111.40
2	D	316	ASP	CB-CG-OD2	-5.09	113.72	118.30
2	F	337	ARG	CD-NE-CZ	5.09	130.72	123.60
1	A	40	ARG	CG-CD-NE	5.08	122.48	111.80
1	A	128	ARG	NE-CZ-NH1	-5.08	117.76	120.30
2	E	223	ASN	CB-CA-C	-5.08	100.25	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	303	SER	N-CA-CB	-5.08	102.89	110.50
1	A	270	ASP	CB-CG-OD1	5.07	122.86	118.30
2	E	96	ASN	N-CA-CB	-5.07	101.47	110.60
2	D	400	ASP	CB-CG-OD1	5.07	122.86	118.30
2	F	210	ASP	CB-CA-C	-5.04	100.32	110.40
2	F	315	ASP	CB-CG-OD1	5.01	122.81	118.30
1	C	161	ARG	CD-NE-CZ	5.01	130.61	123.60

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	165	3
1	B	3656	0	3764	149	52
1	C	3748	0	3843	152	53
2	D	3539	0	3593	146	0
2	E	3530	0	3587	198	0
2	F	3530	0	3586	123	2
3	G	2051	0	2115	114	0
4	H	235	0	230	18	0
5	I	212	0	232	13	0
All	All	24216	0	24763	1003	55

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (1003) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:ARG:HH12	1:C:255:GLU:HB2	1.00	1.16
1:A:291:ARG:HA	3:G:262:LEU:HD22	1.25	1.11
1:C:215:GLN:HG3	2:F:356:ARG:HH22	1.11	1.07
3:G:90:LYS:HB3	3:G:116:LEU:HD11	1.38	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:GLN:HG3	2:D:356:ARG:NH1	1.73	1.03
1:C:404:ALA:C	1:C:406:PHE:H	1.64	1.00
2:E:223:ASN:H	2:E:223:ASN:HD22	1.00	0.96
4:H:85:ASN:HD21	4:H:91:GLN:HE22	1.13	0.96
2:F:223:ASN:HD22	2:F:223:ASN:H	1.08	0.95
1:A:215:GLN:HG3	2:D:356:ARG:HH12	1.30	0.94
1:C:127:ARG:NH1	1:C:255:GLU:HB2	1.84	0.93
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.48	0.91
4:H:79:SER:OG	5:I:15:SER:HA	1.72	0.90
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.52	0.89
2:F:394:ASP:CG	3:G:79:GLY:HA2	1.93	0.88
1:C:30:ARG:HE	1:C:87:ILE:HD11	1.37	0.88
4:H:130:GLU:HG2	5:I:9:LEU:HD21	1.56	0.87
2:E:89:GLU:HG2	2:E:110:THR:HG22	1.56	0.87
3:G:20:THR:HG22	3:G:236:SER:HB3	1.57	0.86
2:E:223:ASN:H	2:E:223:ASN:ND2	1.72	0.86
1:C:215:GLN:HG3	2:F:356:ARG:NH2	1.91	0.86
1:B:456:LEU:HD12	1:B:457:GLU:H	1.42	0.84
2:D:275:ILE:HG23	3:G:269:ALA:HB2	1.60	0.84
2:E:132:ILE:HD12	2:E:145:PRO:HB3	1.61	0.83
1:A:400:VAL:HG12	1:A:418:LEU:HD21	1.60	0.82
3:G:137:THR:HG21	5:I:39:GLY:H	1.46	0.80
1:A:291:ARG:CA	3:G:262:LEU:HD22	2.08	0.80
3:G:178:ILE:HG22	3:G:180:SER:HB2	1.64	0.79
3:G:161:ILE:HG12	3:G:175:GLU:HG2	1.63	0.79
3:G:89:MET:HB3	3:G:116:LEU:HD22	1.63	0.78
2:D:136:GLY:HA3	2:D:431:LEU:HD13	1.66	0.78
1:B:141:SER:O	1:B:143:ARG:HD2	1.83	0.78
2:D:139:VAL:HG13	2:D:414:LEU:HD22	1.65	0.77
2:E:370:VAL:HG21	2:E:438:ILE:HG22	1.65	0.77
1:A:392:LEU:HG	1:A:396:GLN:HE21	1.50	0.77
2:F:130:GLN:HB3	2:F:357:ILE:HD11	1.67	0.77
1:B:186:GLN:HG3	1:B:199:LEU:HB3	1.65	0.76
2:D:282:GLN:H	2:D:282:GLN:HE21	1.30	0.76
2:D:53:LEU:HD12	2:D:57:THR:HG22	1.66	0.76
2:D:404:VAL:O	2:D:408:ARG:HG3	1.84	0.76
3:G:117:HIS:ND1	3:G:118:ARG:N	2.34	0.76
2:D:223:ASN:H	2:D:223:ASN:HD22	1.34	0.75
2:E:391:LEU:HD22	3:G:29:ALA:HB2	1.68	0.75
2:D:395:GLU:OE2	3:G:75:ARG:NE	2.19	0.74
2:F:223:ASN:H	2:F:223:ASN:ND2	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:390:ILE:HG22	2:E:391:LEU:HD23	1.70	0.74
2:E:89:GLU:HG3	2:E:109:LYS:O	1.87	0.74
1:B:379:GLN:HB3	1:B:384:LYS:HE2	1.68	0.73
2:F:89:GLU:HG3	2:F:109:LYS:O	1.89	0.73
1:B:180:ILE:HD11	1:B:216:LEU:HD21	1.72	0.72
2:D:433:PRO:HG2	2:D:436:GLU:HG2	1.69	0.72
2:E:96:ASN:HB3	2:E:100:GLU:H	1.52	0.72
1:A:291:ARG:HA	3:G:262:LEU:CD2	2.13	0.72
2:E:38:VAL:HG21	2:E:45:LEU:HD23	1.71	0.72
2:E:139:VAL:HG13	2:E:414:LEU:HD22	1.71	0.72
3:G:121:SER:C	3:G:123:GLN:H	1.91	0.72
3:G:57:ILE:CG2	3:G:184:ILE:HD12	2.19	0.71
4:H:84:VAL:HG12	4:H:90:VAL:HG22	1.72	0.71
1:C:34:ILE:HD11	1:C:79:ASP:HB2	1.71	0.71
2:E:388:ILE:HG23	2:E:393:MET:HG3	1.73	0.71
1:C:404:ALA:C	1:C:406:PHE:N	2.44	0.71
1:B:452:TYR:OH	1:B:498:LYS:HG3	1.92	0.70
2:D:96:ASN:HB2	2:D:100:GLU:H	1.56	0.70
1:A:407:GLY:HA2	1:A:410:LEU:HD21	1.73	0.70
1:A:479:LEU:HA	1:A:482:LYS:HE3	1.73	0.70
2:E:183:PHE:HB3	2:E:217:LEU:HD22	1.73	0.70
4:H:85:ASN:HD21	4:H:91:GLN:NE2	1.87	0.70
2:D:393:MET:HE3	2:D:404:VAL:HG21	1.73	0.70
1:A:97:VAL:HA	1:A:126:ARG:HH21	1.56	0.69
1:C:211:SER:O	1:C:215:GLN:HG2	1.91	0.69
2:D:84:ILE:HB	2:D:95:MET:HE3	1.73	0.69
2:E:394:ASP:C	2:E:396:LEU:H	1.93	0.69
2:E:433:PRO:HD2	2:E:436:GLU:HB2	1.74	0.69
2:F:252:LEU:HD23	2:F:305:THR:HB	1.75	0.69
2:E:105:ARG:CZ	2:E:208:LEU:HD23	2.23	0.69
1:C:385:GLN:OE1	1:C:488:LYS:HG2	1.93	0.68
2:E:321:ALA:HB3	2:E:322:PRO:HD3	1.75	0.68
2:F:89:GLU:HG2	2:F:110:THR:HG22	1.75	0.68
2:E:345:TYR:HA	2:E:346:PRO:C	2.13	0.68
3:G:14:LYS:HG3	3:G:243:ILE:HD12	1.76	0.68
2:E:313:PRO:HD2	2:E:322:PRO:HG3	1.76	0.68
2:F:314:ALA:O	2:F:315:ASP:HB2	1.95	0.67
1:A:440:GLU:O	1:A:444:VAL:HG13	1.94	0.67
1:B:156:LEU:HD22	1:B:391:LYS:HD2	1.77	0.67
1:A:97:VAL:HB	1:A:98:PRO:HD2	1.76	0.67
2:E:136:GLY:HA3	2:E:431:LEU:HD13	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:130:GLU:CG	5:I:9:LEU:HD21	2.23	0.67
1:A:44:LEU:O	1:A:47:VAL:HG22	1.94	0.67
1:A:134:PRO:O	1:A:139:ARG:NH2	2.27	0.66
1:C:59:LEU:HD23	1:C:82:ILE:HD11	1.77	0.66
1:B:289:PRO:HG2	3:G:263:ILE:HD12	1.78	0.66
1:C:99:VAL:HG22	1:C:253:MET:HA	1.78	0.66
2:D:223:ASN: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:C:418:LEU:O	1:C:422:VAL:HG23	1.94	0.66
2:D:223:ASN:N	2:D:223:ASN:HD22	1.89	0.66
3:G:137:THR:HG22	3:G:139:GLY:H	1.60	0.66
1:A:136:ILE:HD11	2:E:219:TYR:HE2	1.60	0.66
1:A:376:SER:HB3	1:A:384:LYS:HE2	1.78	0.66
1:B:44:LEU:HB3	1:B:47:VAL:HG22	1.76	0.66
2:F:136:GLY:HA3	2:F:431:LEU:CD1	2.26	0.66
2:F:80:ALA:HB1	2:F:81:PRO:CD	2.26	0.66
1:C:173:THR:HG22	1:C:354:THR:HG22	1.77	0.65
2:D:167:MET:HB3	2:D:420:VAL:HG11	1.79	0.65
2:F:344:ILE:HG23	2:F:415:SER:HB3	1.78	0.65
1:B:188:ARG:HH21	1:B:437:ALA:HB2	1.62	0.65
1:C:44:LEU:O	1:C:47:VAL:HG22	1.96	0.64
2:F:200:MET:HG3	2:F:205:VAL:CG2	2.27	0.64
3:G:115:ILE:C	3:G:117:HIS:H	2.01	0.64
2:E:359:ASP:OD2	2:E:361:ASN:HB2	1.97	0.64
1:C:188:ARG:HH21	1:C:437:ALA:HB2	1.62	0.64
1:B:389:THR:HA	1:B:392:LEU:CD1	2.28	0.64
2:F:94:ILE:HG22	2:F:102:ILE:HD11	1.80	0.64
1:C:419:SER:O	1:C:423:ARG:HG2	1.98	0.63
2:E:139:VAL:CG1	2:E:414:LEU:HD22	2.28	0.63
2:E:443:GLN:HG2	2:E:448:GLU:OE2	1.98	0.63
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.63	0.63
1:A:471:HIS:CE1	1:A:475:GLN:HG3	2.33	0.63
1:C:202:ILE:HG12	1:C:230:ILE:HD12	1.80	0.63
1:C:488:LYS:HG2	1:C:489:ILE:H	1.63	0.63
2:E:346:PRO:HG3	2:E:418:PHE:CZ	2.33	0.63
1:B:437:ALA:O	1:B:440:GLU:N	2.30	0.63
2:D:54:GLY:O	2:D:55:GLU:HB2	1.96	0.63
1:B:184:ILE:HG22	1:B:435:PRO:HG2	1.81	0.63
2:E:138:LYS:HE2	2:E:432:VAL:HG21	1.80	0.63
2:E:400:ASP:O	2:E:404:VAL:HG23	1.98	0.63
2:E:425:THR:O	2:E:427:HIS:ND1	2.20	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:200:MET:HB3	2:D:206:ILE:HG13	1.79	0.63
2:E:298:THR:HG23	2:E:303:SER:HB3	1.81	0.63
2:F:136:GLY:HA3	2:F:431:LEU:HD12	1.80	0.63
3:G:61:GLU:OE1	3:G:101:LYS:HG2	1.99	0.63
3:G:141:ALA:HB1	3:G:213:ILE:HG23	1.81	0.63
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.34	0.62
1:C:52:MET:O	1:C:91:THR:HB	1.98	0.62
4:H:79:SER:OG	5:I:15:SER:CA	2.46	0.62
1:A:394:LEU:HD11	1:A:428:LEU:HD11	1.82	0.62
2:E:204:GLY:O	2:E:206:ILE:N	2.32	0.62
3:G:39:LYS:HB3	3:G:40:PRO:HD3	1.80	0.62
1:A:341:ASN:O	1:A:345:ILE:HG13	1.99	0.62
2:F:390:ILE:HD11	3:G:242:MET:CE	2.30	0.62
2:F:200:MET:HG3	2:F:205:VAL:HG23	1.80	0.62
1:B:102:GLU:HG3	1:B:122:GLY:O	2.00	0.62
1:B:389:THR:HA	1:B:392:LEU:HD12	1.81	0.61
2:E:422:GLU:HG2	2:E:427:HIS:O	1.99	0.61
1:B:422:VAL:O	1:B:426:GLU:HG2	2.00	0.61
2:E:394:ASP:C	2:E:396:LEU:N	2.54	0.61
2:F:363:VAL:HG23	2:F:367:HIS:HB3	1.81	0.61
1:C:151:LYS:HE3	1:C:430:GLN:HG3	1.82	0.61
1:C:292:GLU:O	1:C:293:ALA:HB3	2.00	0.61
2:D:396:LEU:HD22	2:D:400:ASP:CB	2.30	0.61
1:B:214:ALA:HA	2:E:123:PHE:CZ	2.35	0.61
2:E:391:LEU:CD2	3:G:29:ALA:HB2	2.28	0.61
2:E:201:ILE:HD13	2:E:208:LEU:HD11	1.81	0.61
1:A:121:ILE:H	1:A:121:ILE:HD13	1.66	0.61
1:C:362:ARG:HA	1:C:363:PRO:C	2.21	0.61
2:E:397:SER:H	2:E:400:ASP:HB2	1.66	0.61
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.34	0.61
1:A:376:SER:C	1:A:378:ALA:H	2.03	0.61
1:A:439:GLU:HG2	1:A:484:ARG:HB2	1.83	0.61
1:A:52:MET:O	1:A:91:THR:HG23	2.01	0.60
1:C:99:VAL:HG13	1:C:256:TYR:HB2	1.83	0.60
2:E:149:GLY:HA2	2:E:304:ILE:O	2.01	0.60
1:A:270:ASP:OD1	1:A:273:LYS:HG3	2.00	0.60
1:A:283:LEU:HD21	1:A:289:PRO:HB3	1.82	0.60
1:A:40:ARG:HH11	1:A:40:ARG:HG3	1.66	0.60
1:B:51:GLU:HA	1:B:94:ILE:HA	1.83	0.60
1:A:457:GLU:CB	1:A:460:LYS:HD3	2.32	0.60
1:C:313:ASN:OD1	1:C:316:PHE:HD1	1.85	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:122:GLU:HB2	2:F:125:GLU:HG3	1.84	0.60
1:A:376:SER:C	1:A:378:ALA:N	2.55	0.60
1:C:403:PHE:CZ	2:D:408:ARG:HD2	2.37	0.60
2:D:93:ARG:HH11	2:D:93:ARG:HG3	1.66	0.60
1:A:166:LEU:HA	1:A:325:PRO:HD2	1.83	0.60
1:A:432:GLN:HB3	1:A:433:TYR:CD2	2.37	0.60
2:E:224:GLU:O	2:E:229:ARG:NH1	2.32	0.60
1:B:362:ARG:HA	1:B:363:PRO:C	2.21	0.59
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.37	0.59
1:C:210:ARG:NH1	2:F:121:PRO:O	2.35	0.59
1:B:411:ASP:HB3	1:B:414:THR:OG1	2.02	0.59
1:B:499:GLU:O	1:B:502:THR:HB	2.02	0.59
2:D:89:GLU:HG2	2:D:110:THR:HG22	1.83	0.59
2:E:419:GLN:HG3	2:E:429:GLY:HA3	1.84	0.59
1:A:157:VAL:N	1:A:158:PRO:CD	2.65	0.59
1:B:438:ILE:O	1:B:442:VAL:HG22	2.02	0.59
2:E:32:ILE:O	2:E:33:LEU:HB2	2.02	0.59
2:D:317:LEU:HD22	2:D:326:PHE:HZ	1.67	0.59
1:B:452:TYR:O	1:B:453:LEU:HD23	2.03	0.59
1:B:479:LEU:HD11	1:B:497:LEU:HD13	1.83	0.59
1:C:102:GLU:OE2	1:C:123:SER:HA	2.03	0.59
3:G:178:ILE:C	3:G:180:SER:H	2.04	0.59
3:G:156:ASP:HA	3:G:181:LEU:HD13	1.85	0.59
1:B:170:ASP:O	1:B:175:LYS:HE2	2.03	0.59
1:C:140:ILE:HD11	1:C:143:ARG:NH2	2.17	0.59
2:E:200:MET:HB3	2:E:205:VAL:HG23	1.84	0.59
2:E:408:ARG:O	2:E:412:ARG:HG3	2.03	0.59
2:F:105:ARG:NH1	2:F:208:LEU:HD23	2.18	0.59
1:C:407:GLY:HA2	1:C:410:LEU:HD11	1.84	0.59
2:D:263:GLN:O	2:D:267:GLU:HG3	2.03	0.59
1:B:391:LYS:O	1:B:395:ALA:N	2.36	0.58
1:C:335:SER:O	2:D:314:ALA:HA	2.02	0.58
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.85	0.58
1:A:472:VAL:HG23	1:A:480:LEU:HD11	1.85	0.58
2:E:122:GLU:N	2:E:125:GLU:OE2	2.37	0.58
2:E:226:PRO:HB3	2:E:267:GLU:HB2	1.84	0.58
2:F:29:LEU:HD12	2:F:30:PRO:HD2	1.85	0.58
3:G:57:ILE:CG2	3:G:184:ILE:CD1	2.81	0.58
1:B:283:LEU:CD1	2:E:277:SER:HB3	2.32	0.58
2:D:186:VAL:HG13	2:D:232:VAL:HG23	1.85	0.58
3:G:87:LYS:O	3:G:90:LYS:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:246:GLN:NE2	2:E:246:GLN:HA	2.18	0.58
1:C:406:PHE:O	1:C:408:SER:N	2.36	0.58
5:I:5:ARG:C	5:I:7:ALA:H	2.06	0.58
1:B:434:SER:N	1:B:435:PRO:HD3	2.18	0.58
1:A:219:ARG:HH11	1:A:219:ARG:HB2	1.69	0.58
1:C:404:ALA:O	1:C:406:PHE:N	2.37	0.58
1:C:396:GLN:HG3	2:D:458:TYR:CE2	2.38	0.58
2:E:267:GLU:O	2:E:271:LEU:HG	2.04	0.58
4:H:95:GLU:OE2	5:I:16:GLN:HA	2.04	0.58
1:C:374:VAL:HG11	1:C:378:ALA:HB2	1.85	0.57
1:B:214:ALA:HB2	2:E:123:PHE:CE1	2.38	0.57
2:E:158:ALA:C	2:E:160:VAL:H	2.08	0.57
2:E:223:ASN:ND2	2:E:223:ASN:N	2.46	0.57
2:E:95:MET:CG	2:E:99:GLY:HA2	2.34	0.57
2:F:96:ASN:HD22	2:F:100:GLU:HB2	1.68	0.57
2:F:440:GLY:O	2:F:444:ILE:HG13	2.04	0.57
2:F:14:VAL:O	2:F:71:ARG:HG2	2.05	0.57
3:G:57:ILE:HG23	3:G:184:ILE:CD1	2.35	0.57
3:G:19:ILE:HG22	3:G:23:MET:HE2	1.86	0.57
1:B:51:GLU:OE2	1:B:90:ARG:HB3	2.05	0.57
2:E:433:PRO:HG2	2:E:436:GLU:HG2	1.86	0.57
1:C:464:PHE:CE1	1:C:505:LEU:HD23	2.38	0.57
1:B:400:VAL:HB	1:B:418:LEU:HD21	1.85	0.57
1:C:107:VAL:HG12	1:C:115:ILE:HD11	1.86	0.57
2:E:138:LYS:O	2:E:142:LEU:HB3	2.04	0.57
1:A:136:ILE:HD11	2:E:219:TYR:CE2	2.39	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	1.86	0.57
1:B:352:LEU:HA	1:B:364:ALA:O	2.04	0.57
2:E:92:GLY:N	2:E:215:VAL:O	2.29	0.57
1:A:107:VAL:HG12	1:A:115:ILE:HD11	1.87	0.57
2:F:324:THR:O	2:F:324:THR:HG22	2.05	0.57
3:G:180:SER:O	3:G:205:GLN:HG3	2.04	0.57
3:G:209:LEU:O	3:G:213:ILE:HG22	2.05	0.57
2:F:223:ASN:N	2:F:223:ASN:HD22	1.85	0.56
3:G:164:ARG:NH2	3:G:166:ARG:HD3	2.20	0.56
3:G:184:ILE:C	3:G:186:SER:H	2.08	0.56
1:C:78:ASN:ND2	1:C:80:LYS:HD3	2.19	0.56
2:F:394:ASP:CB	3:G:79:GLY:HA2	2.34	0.56
1:A:347:ASP:OD1	2:E:191:ARG:NH1	2.38	0.56
1:A:159:ILE:HD12	1:A:165:GLU:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:PHE:CE1	1:B:362:ARG:HD3	2.40	0.56
1:B:283:LEU:HD12	2:E:277:SER:HB3	1.87	0.56
1:C:173:THR:CG2	1:C:354:THR:HG22	2.35	0.56
1:C:102:GLU:HG2	1:C:122:GLY:O	2.06	0.56
1:C:156:LEU:HD13	1:C:367:VAL:HG22	1.86	0.56
1:C:408:SER:O	1:C:409:ASP:C	2.44	0.56
2:D:275:ILE:HG23	3:G:269:ALA:CB	2.33	0.56
2:E:105:ARG:NH2	2:E:208:LEU:HA	2.20	0.56
2:E:174:ALA:CB	2:E:214:LYS:HD3	2.35	0.56
1:A:450:ARG:NH2	1:A:494:ASP:OD2	2.38	0.56
2:D:473:LEU:C	2:D:475:GLU:H	2.08	0.56
2:E:155:PHE:CE1	2:E:310:ILE:HD12	2.40	0.56
3:G:71:VAL:HG13	3:G:108:VAL:HG22	1.88	0.56
2:E:397:SER:C	2:E:399:GLU:N	2.57	0.56
1:C:219:ARG:HD3	1:C:433:TYR:CE1	2.41	0.56
1:C:433:TYR:C	1:C:435:PRO:HD3	2.26	0.56
1:A:185:ASN:O	1:A:188:ARG:HG3	2.05	0.56
1:C:187:LYS:HE2	1:C:191:ASP:OD2	2.05	0.56
2:D:425:THR:HG21	2:D:459:MET:HE1	1.88	0.56
1:B:423:ARG:HE	1:B:458:PRO:HD3	1.71	0.56
2:E:396:LEU:HB3	2:E:401:LYS:HG2	1.88	0.56
1:B:393:GLU:OE1	1:B:424:LEU:HD11	2.05	0.55
2:E:138:LYS:HG3	2:E:416:GLN:OE1	2.06	0.55
2:F:98:ILE:HG13	2:F:100:GLU:HG3	1.88	0.55
3:G:121:SER:C	3:G:123:GLN:N	2.60	0.55
1:A:291:ARG:N	3:G:262:LEU:HD21	2.21	0.55
1:B:351:PHE:CE1	1:B:369:LEU:HB3	2.41	0.55
1:C:442:VAL:CG1	1:C:489:ILE:HD11	2.37	0.55
1:B:80:LYS:HG3	1:B:81:LEU:HD23	1.88	0.55
1:A:99:VAL:CG2	1:A:253:MET:HA	2.36	0.55
2:D:87:GLY:HA2	2:D:242:TYR:CE2	2.42	0.55
2:D:451:HIS:CD2	2:D:452:LEU:HD23	2.42	0.55
2:D:471:ASP:O	2:D:474:ALA:N	2.39	0.55
3:G:164:ARG:HD3	3:G:174:GLU:OE2	2.06	0.55
1:C:184:ILE:HG22	1:C:435:PRO:HG2	1.87	0.55
1:C:394:LEU:HD22	1:C:398:ARG:HH21	1.71	0.55
2:E:244:ARG:HG3	2:E:303:SER:N	2.22	0.55
1:A:479:LEU:HD21	1:A:493:SER:HB3	1.89	0.55
2:D:255:ILE:HG21	2:D:258:ILE:HD13	1.87	0.55
2:D:366:GLU:HG3	2:D:442:GLN:HE22	1.71	0.55
2:E:263:GLN:O	2:E:267:GLU:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:32:ILE:O	2:F:33:LEU:HB2	2.06	0.55
3:G:117:HIS:O	3:G:120:HIS:N	2.35	0.55
2:F:63:MET:CE	2:F:97:VAL:HG11	2.36	0.55
1:A:100:GLY:HA2	1:A:256:TYR:CE1	2.42	0.55
2:F:10:THR:HG23	2:F:76:LEU:HD12	1.88	0.55
1:A:209:LYS:HE3	1:A:211:SER:HB2	1.88	0.54
1:C:91:THR:HG22	1:C:93:ALA:H	1.72	0.54
2:D:473:LEU:O	2:D:475:GLU:N	2.40	0.54
3:G:57:ILE:HG22	3:G:184:ILE:HD12	1.87	0.54
1:B:423:ARG:HE	1:B:458:PRO:HG3	1.71	0.54
2:D:142:LEU:HD22	2:D:441:PHE:CD2	2.42	0.54
2:E:174:ALA:HB2	2:E:214:LYS:HD3	1.89	0.54
3:G:144:ILE:HD13	3:G:213:ILE:HD11	1.90	0.54
3:G:160:ILE:CG2	3:G:176:LYS:HB2	2.37	0.54
1:B:347:ASP:HB3	1:B:374:VAL:HG22	1.88	0.54
2:D:83:ARG:HA	2:D:114:ALA:O	2.07	0.54
1:A:452:TYR:OH	1:A:498:LYS:HG3	2.08	0.54
2:D:122:GLU:HA	2:D:122:GLU:OE1	2.07	0.54
2:E:218:VAL:HG11	2:E:235:THR:CG2	2.38	0.54
3:G:117:HIS:CE1	3:G:121:SER:HB2	2.42	0.54
3:G:181:LEU:HB3	3:G:184:ILE:HG22	1.89	0.54
3:G:181:LEU:HG	3:G:183:THR:HB	1.89	0.54
3:G:39:LYS:HB3	3:G:40:PRO:CD	2.38	0.54
1:A:373:ARG:HG3	1:A:373:ARG:HH11	1.72	0.54
2:D:282:GLN:H	2:D:282:GLN:NE2	2.01	0.54
2:E:63:MET:HE3	2:E:228:ALA:HA	1.90	0.54
1:A:161:ARG:HH11	1:A:263:HIS:CG	2.26	0.54
1:C:239:ALA:HB1	1:C:241:PRO:HD2	1.90	0.54
1:C:405:GLN:C	1:C:406:PHE:HD1	2.11	0.54
1:C:52:MET:HG3	1:C:61:GLY:O	2.07	0.54
1:C:218:LYS:HD2	2:F:128:VAL:HG21	1.88	0.54
1:B:218:LYS:HB2	2:E:128:VAL:HG12	1.89	0.54
1:B:446:TYR:CD2	1:B:497:LEU:HD23	2.43	0.54
1:A:468:PHE:CE1	1:A:501:VAL:HG12	2.43	0.54
1:B:479:LEU:HA	1:B:482:LYS:HE3	1.89	0.54
2:D:167:MET:CB	2:D:420:VAL:HG11	2.38	0.54
2:F:439:LYS:HE3	2:F:443:GLN:HE22	1.73	0.54
1:A:463:LYS:HD3	1:A:508:PHE:HZ	1.73	0.53
1:B:270:ASP:OD1	1:B:273:LYS:HG3	2.07	0.53
1:B:358:TYR:C	1:B:360:GLY:H	2.12	0.53
1:C:190:ASN:HA	1:C:198:LYS:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ILE:HA	1:A:430:GLN:OE1	2.08	0.53
1:B:44:LEU:O	1:B:47:VAL:HG22	2.09	0.53
1:B:69:ASP:O	1:B:70:ASN:HB3	2.09	0.53
2:D:396:LEU:HD22	2:D:400:ASP:HB3	1.89	0.53
2:E:220:GLY:HA3	2:E:232:VAL:HG21	1.91	0.53
1:B:482:LYS:O	1:B:486:ASP:N	2.37	0.53
2:D:381:TYR:HE2	2:D:411:GLN:HE22	1.56	0.53
2:D:431:LEU:C	2:D:431:LEU:HD12	2.29	0.53
1:A:207:GLY:HA3	1:A:273:LYS:HD3	1.89	0.53
1:A:436:MET:HG3	1:A:441:GLN:HG2	1.90	0.53
2:D:388:ILE:HD12	2:D:393:MET:SD	2.48	0.53
2:D:412:ARG:HG3	2:D:412:ARG:HH11	1.73	0.53
1:A:48:GLN:HB3	2:E:68:GLY:O	2.07	0.53
2:F:292:MET:CE	2:F:296:ILE:HD11	2.38	0.53
3:G:249:THR:HA	3:G:252:ARG:NH1	2.24	0.53
1:A:170:ASP:O	1:A:175:LYS:HE2	2.08	0.53
1:C:140:ILE:HD11	1:C:143:ARG:HH22	1.74	0.53
2:D:136:GLY:CA	2:D:431:LEU:HD13	2.37	0.53
2:D:473:LEU:C	2:D:475:GLU:N	2.62	0.53
2:D:84:ILE:HD12	2:D:95:MET:HE1	1.90	0.53
2:E:81:PRO:HG2	2:E:115:ALA:HB1	1.91	0.53
1:B:441:GLN:O	1:B:445:ILE:HG12	2.08	0.53
2:D:422:GLU:HG2	2:D:427:HIS:O	2.09	0.53
1:A:457:GLU:HB3	1:A:460:LYS:HD3	1.89	0.53
1:C:48:GLN:HB3	2:D:68:GLY:HA2	1.90	0.53
2:E:397:SER:O	2:E:401:LYS:HG3	2.07	0.53
2:E:97:VAL:HG13	2:E:232:VAL:CG1	2.39	0.53
3:G:117:HIS:ND1	3:G:118:ARG:HA	2.22	0.53
1:A:291:ARG:HG3	3:G:258:ILE:CG2	2.38	0.53
1:B:114:ALA:HB2	1:B:121:ILE:HD11	1.90	0.53
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.89	0.53
2:D:31:PRO:HD2	2:D:34:ASN:ND2	2.24	0.53
2:D:417:PRO:HB3	2:D:459:MET:HE3	1.91	0.53
2:D:96:ASN:CB	2:D:100:GLU:H	2.22	0.53
2:E:9:THR:HG21	2:E:28:GLY:O	2.09	0.53
1:B:386:VAL:HG22	1:B:442:VAL:HG12	1.91	0.53
1:C:180:ILE:CD1	1:C:216:LEU:HD21	2.34	0.53
3:G:86:ALA:HA	3:G:89:MET:HE2	1.90	0.53
2:E:201:ILE:CD1	2:E:208:LEU:HD11	2.37	0.53
1:A:140:ILE:HG21	1:A:313:ASN:HA	1.92	0.52
2:E:279:VAL:O	2:E:279:VAL:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:19:ILE:HG22	3:G:23:MET:CE	2.40	0.52
1:C:64:LEU:HD23	1:C:74:VAL:HG21	1.91	0.52
2:F:96:ASN:HB2	2:F:100:GLU:H	1.73	0.52
2:E:391:LEU:HD22	3:G:29:ALA:CB	2.36	0.52
3:G:137:THR:HG22	3:G:138:PHE:N	2.24	0.52
1:C:270:ASP:OD1	1:C:273:LYS:HG3	2.09	0.52
1:A:179:ALA:HB1	1:A:267:ILE:HG12	1.91	0.52
1:C:156:LEU:HD11	1:C:428:LEU:HD13	1.91	0.52
2:D:412:ARG:HD2	2:D:454:GLU:HB3	1.90	0.52
2:E:316:ASP:OD2	3:G:255:GLN:NE2	2.30	0.52
1:C:267:ILE:N	1:C:267:ILE:HD12	2.25	0.52
2:D:366:GLU:CG	2:D:442:GLN:HE22	2.23	0.52
3:G:140:ASP:HB3	5:I:42:ILE:HG13	1.92	0.52
3:G:181:LEU:O	3:G:184:ILE:HG22	2.08	0.52
1:B:423:ARG:HD2	1:B:461:ILE:HD11	1.92	0.52
2:D:356:ARG:HG2	2:D:356:ARG:O	2.09	0.52
2:E:377:ILE:HG21	2:E:410:ILE:HD12	1.92	0.52
1:A:136:ILE:O	2:E:194:ASN:HB2	2.10	0.52
4:H:83:THR:HB	4:H:91:GLN:HE21	1.75	0.52
2:E:25:PHE:O	2:E:56:SER:HB3	2.10	0.52
2:E:80:ALA:HB1	2:E:81:PRO:HD2	1.91	0.52
2:F:210:ASP:HB2	2:F:212:THR:HG23	1.91	0.52
1:A:140:ILE:HD11	1:A:143:ARG:NE	2.25	0.51
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.75	0.51
2:E:254:PHE:CD1	2:E:307:VAL:HB	2.45	0.51
2:E:377:ILE:HG21	2:E:410:ILE:CD1	2.40	0.51
3:G:117:HIS:ND1	3:G:118:ARG:CA	2.74	0.51
1:B:157:VAL:N	1:B:158:PRO:CD	2.73	0.51
1:B:386:VAL:CG2	1:B:442:VAL:HG12	2.41	0.51
2:E:218:VAL:HG11	2:E:235:THR:HG22	1.92	0.51
1:C:215:GLN:HE22	2:F:128:VAL:HA	1.75	0.51
2:F:234:LEU:O	2:F:237:LEU:HB3	2.11	0.51
2:F:360:PRO:HD3	2:F:368:TYR:CD2	2.45	0.51
1:A:224:ASP:CG	1:A:227:LYS:HE3	2.31	0.51
1:B:180:ILE:O	1:B:181:ASP:C	2.47	0.51
1:C:436:MET:CE	1:C:469:LEU:HD21	2.40	0.51
1:C:45:ARG:NH2	1:C:68:PRO:O	2.44	0.51
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.40	0.51
2:E:382:LYS:O	2:E:385:GLN:HB2	2.11	0.51
1:B:140:ILE:HG23	1:B:311:LYS:HG3	1.92	0.51
2:D:154:LEU:HD22	2:D:165:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:444:ILE:HD11	2:E:463:ILE:HD11	1.93	0.51
5:I:5:ARG:O	5:I:6:GLN:HB3	2.10	0.51
1:B:157:VAL:N	1:B:158:PRO:HD3	2.26	0.51
1:C:406:PHE:N	1:C:406:PHE:CD1	2.79	0.51
2:E:293:GLN:HG3	2:E:328:HIS:CG	2.46	0.51
2:E:142:LEU:HD21	2:E:374:VAL:HG21	1.93	0.51
1:C:443:ALA:O	1:C:446:TYR:HB3	2.10	0.51
1:B:180:ILE:CD1	1:B:216:LEU:HD21	2.39	0.51
1:C:164:ARG:HD2	1:C:306:LEU:O	2.11	0.51
3:G:23:MET:SD	3:G:232:MET:HE2	2.50	0.51
1:B:456:LEU:HD12	1:B:457:GLU:N	2.20	0.51
1:B:489:ILE:HG22	1:B:494:ASP:HB2	1.93	0.51
2:F:421:ALA:O	2:F:425:THR:HG23	2.11	0.51
1:A:457:GLU:HB2	1:A:460:LYS:HD3	1.92	0.51
1:C:244:TYR:O	1:C:247:PRO:HD2	2.11	0.51
2:E:443:GLN:O	2:E:446:ALA:HB3	2.10	0.51
1:A:137:ILE:N	1:A:138:PRO:CD	2.74	0.50
1:C:23:VAL:O	1:C:23:VAL:HG12	2.11	0.50
2:D:84:ILE:HD13	2:D:235:THR:HG23	1.92	0.50
2:E:82:ILE:HB	2:E:116:ILE:HD13	1.92	0.50
2:F:96:ASN:ND2	2:F:100:GLU:HB2	2.26	0.50
2:F:242:TYR:CD1	2:F:246:GLN:HG3	2.46	0.50
2:F:390:ILE:HD11	3:G:242:MET:SD	2.51	0.50
1:A:187:LYS:HE2	1:A:191:ASP:OD2	2.11	0.50
1:A:240:ALA:N	1:A:241:PRO:HD2	2.27	0.50
1:C:331:ALA:O	1:C:333:ASP:N	2.44	0.50
2:D:93:ARG:NH1	2:D:93:ARG:HG3	2.27	0.50
2:E:241:GLU:HA	2:E:304:ILE:HD11	1.93	0.50
2:E:334:VAL:HG23	2:E:353:SER:HA	1.92	0.50
3:G:49:LEU:HD21	3:G:212:ILE:CD1	2.41	0.50
2:D:406:ARG:O	2:D:410:ILE:HG13	2.11	0.50
2:E:155:PHE:HE1	2:E:310:ILE:HD12	1.77	0.50
2:F:386:ASP:O	2:F:389:ALA:HB3	2.11	0.50
4:H:79:SER:CB	5:I:15:SER:HA	2.41	0.50
1:A:291:ARG:CA	3:G:262:LEU:CD2	2.81	0.50
1:B:390:MET:CE	1:B:428:LEU:HD21	2.42	0.50
2:E:462:PRO:HD2	2:E:465:GLU:HG3	1.94	0.50
2:E:463:ILE:O	2:E:467:VAL:HG23	2.12	0.50
2:F:257:ASN:HB3	2:F:260:ARG:HG2	1.93	0.50
1:A:380:THR:O	1:A:384:LYS:HG3	2.12	0.50
2:D:136:GLY:HA2	2:D:432:VAL:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:221:GLN:N	2:E:224:GLU:OE1	2.44	0.50
1:C:359:LYS:O	2:F:376:LYS:HE2	2.12	0.50
1:A:94:ILE:HG12	1:A:95:VAL:N	2.27	0.50
1:C:52:MET:HE3	1:C:95:VAL:HG13	1.93	0.50
1:C:30:ARG:HE	1:C:87:ILE:CD1	2.18	0.50
1:C:402:ALA:O	1:C:405:GLN:HG3	2.12	0.50
1:B:49:ALA:O	1:B:50:GLU:HB2	2.12	0.49
1:B:107:VAL:HG12	1:B:115:ILE:CG1	2.43	0.49
1:B:423:ARG:HE	1:B:458:PRO:CD	2.25	0.49
2:E:275:ILE:O	2:E:283:PRO:HG3	2.12	0.49
2:F:168:GLU:OE1	2:F:418:PHE:HB3	2.12	0.49
4:H:18:PHE:CZ	4:H:20:PHE:HB2	2.46	0.49
4:H:130:GLU:HG3	5:I:9:LEU:HD11	1.93	0.49
1:A:294:TYR:HB2	1:A:337:TYR:HE2	1.76	0.49
1:A:417:LEU:HD23	1:A:417:LEU:H	1.77	0.49
1:B:27:GLU:O	1:B:90:ARG:HG3	2.12	0.49
2:E:54:GLY:O	2:E:55:GLU:HB2	2.13	0.49
2:F:339:ILE:HG22	2:F:344:ILE:HB	1.94	0.49
3:G:197:ASP:O	3:G:200:VAL:HG12	2.13	0.49
1:B:151:LYS:NZ	1:B:429:LYS:O	2.45	0.49
2:F:360:PRO:HD3	2:F:368:TYR:CE2	2.48	0.49
1:B:96:ASP:HB2	1:B:127:ARG:O	2.13	0.49
2:E:84:ILE:HB	2:E:95:MET:HE1	1.94	0.49
2:F:394:ASP:HB3	3:G:79:GLY:O	2.12	0.49
1:C:225:ALA:HA	1:C:228:TYR:CE1	2.47	0.49
1:C:96:ASP:O	1:C:97:VAL:HG13	2.12	0.49
2:D:84:ILE:N	2:D:114:ALA:O	2.42	0.49
2:E:444:ILE:HD11	2:E:463:ILE:CD1	2.43	0.49
1:A:300:TYR:O	1:A:304:ARG:HG2	2.13	0.49
1:C:30:ARG:HA	1:C:86:ASP:O	2.13	0.49
1:C:83:LYS:HB3	2:F:52:HIS:CE1	2.48	0.49
2:F:163:THR:O	2:F:167:MET:HG2	2.12	0.49
2:F:80:ALA:HB1	2:F:81:PRO:HD2	1.95	0.49
1:B:211:SER:O	1:B:215:GLN:HG3	2.13	0.49
1:B:24:ASP:O	1:B:28:THR:HB	2.12	0.49
1:B:463:LYS:HE2	1:B:508:PHE:CZ	2.48	0.49
3:G:179:PHE:C	3:G:181:LEU:N	2.66	0.49
1:B:427:LEU:HD11	1:B:448:GLY:HA3	1.95	0.48
1:C:362:ARG:HG3	1:C:362:ARG:NH1	2.27	0.48
1:C:436:MET:HE1	1:C:469:LEU:HD21	1.94	0.48
2:D:83:ARG:HA	2:D:115:ALA:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:86:VAL:HG11	2:F:114:ALA:HB3	1.94	0.48
3:G:71:VAL:HG13	3:G:108:VAL:CG2	2.43	0.48
2:F:82:ILE:HD13	2:F:98:ILE:HG22	1.95	0.48
3:G:156:ASP:O	3:G:181:LEU:HB2	2.13	0.48
1:B:99:VAL:HG21	1:B:127:ARG:HB3	1.94	0.48
1:B:300:TYR:O	1:B:304:ARG:HG2	2.13	0.48
2:D:168:GLU:O	2:D:168:GLU:HG3	2.11	0.48
2:D:360:PRO:HD3	2:D:368:TYR:CE2	2.48	0.48
2:E:134:VAL:HG13	2:E:141:ASP:OD2	2.13	0.48
2:E:227:GLY:O	2:E:230:ALA:HB3	2.13	0.48
3:G:160:ILE:HG22	3:G:176:LYS:HB2	1.96	0.48
1:C:164:ARG:HD2	1:C:164:ARG:HH11	1.41	0.48
2:D:63:MET:HE3	2:D:228:ALA:HA	1.94	0.48
2:F:357:ILE:HD12	2:F:362:ILE:HG21	1.95	0.48
3:G:39:LYS:N	3:G:40:PRO:HD2	2.28	0.48
1:C:434:SER:N	1:C:435:PRO:HD3	2.27	0.48
1:C:488:LYS:HG2	1:C:489:ILE:N	2.28	0.48
2:E:223:ASN:HD22	2:E:223:ASN:N	1.84	0.48
3:G:136:PRO:HD3	3:G:221:THR:HG21	1.95	0.48
1:A:127:ARG:HE	1:A:131:LEU:CD1	2.27	0.48
1:C:334:VAL:HG13	1:C:351:PHE:CE1	2.48	0.48
1:C:403:PHE:CD2	2:D:408:ARG:CZ	2.97	0.48
2:E:374:VAL:O	2:E:377:ILE:HG22	2.14	0.48
2:E:404:VAL:O	2:E:408:ARG:HG3	2.14	0.48
2:F:321:ALA:HB3	2:F:322:PRO:HD3	1.94	0.48
1:A:373:ARG:NH1	1:A:373:ARG:HG3	2.28	0.48
1:A:40:ARG:HH11	1:A:40:ARG:CG	2.27	0.48
2:E:416:GLN:HG3	2:E:417:PRO:HD2	1.96	0.48
2:F:221:GLN:HA	2:F:221:GLN:HE21	1.78	0.48
1:A:453:LEU:HD13	1:A:461:ILE:HG23	1.96	0.48
1:C:44:LEU:HB3	1:C:47:VAL:HG22	1.95	0.48
3:G:129:LYS:HG2	3:G:130:GLU:OE1	2.14	0.48
1:A:389:THR:O	1:A:393:GLU:HG2	2.13	0.48
1:B:481:SER:O	1:B:485:THR:HB	2.14	0.48
2:F:319:ASP:O	2:F:322:PRO:HD2	2.14	0.48
3:G:179:PHE:HB3	3:G:184:ILE:HG21	1.96	0.48
1:C:481:SER:O	1:C:485:THR:HB	2.14	0.47
2:D:32:ILE:O	2:D:33:LEU:HB2	2.14	0.47
3:G:89:MET:CB	3:G:116:LEU:HD22	2.38	0.47
1:A:100:GLY:HA2	1:A:256:TYR:CD1	2.49	0.47
1:C:313:ASN:OD1	1:C:315:ALA:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:GLN:O	1:C:445:ILE:HG12	2.14	0.47
2:D:14:VAL:HG11	2:D:24:GLN:HB2	1.95	0.47
2:E:253:LEU:O	2:E:306:SER:HA	2.14	0.47
3:G:117:HIS:C	3:G:117:HIS:ND1	2.67	0.47
1:A:136:ILE:CD1	2:E:219:TYR:CE2	2.97	0.47
1:A:209:LYS:HE3	1:A:211:SER:CB	2.44	0.47
1:B:225:ALA:HA	1:B:228:TYR:CE2	2.49	0.47
1:C:180:ILE:HG22	1:C:184:ILE:HD12	1.97	0.47
2:E:360:PRO:HD3	2:E:368:TYR:CD1	2.49	0.47
2:E:388:ILE:HG23	2:E:393:MET:CG	2.43	0.47
1:A:444:VAL:CG1	1:A:469:LEU:HD13	2.44	0.47
1:A:49:ALA:O	1:A:50:GLU:HB2	2.13	0.47
1:B:443:ALA:O	1:B:446:TYR:HB3	2.14	0.47
2:E:116:ILE:HA	2:E:238:THR:OG1	2.14	0.47
2:F:93:ARG:NH2	2:F:106:GLY:O	2.48	0.47
1:A:291:ARG:HG3	3:G:258:ILE:HG23	1.96	0.47
1:B:179:ALA:O	1:B:182:THR:HB	2.14	0.47
1:B:311:LYS:HD2	1:B:312:MET:O	2.13	0.47
2:D:129:GLU:HA	2:D:129:GLU:OE1	2.15	0.47
2:F:88:PRO:HD2	2:F:89:GLU:OE2	2.14	0.47
3:G:144:ILE:HG21	3:G:213:ILE:HD13	1.97	0.47
1:A:245:LEU:O	1:A:246:ALA:C	2.51	0.47
1:B:351:PHE:HE1	1:B:369:LEU:O	1.97	0.47
1:B:383:MET:O	1:B:384:LYS:C	2.52	0.47
2:E:82:ILE:HB	2:E:116:ILE:CD1	2.45	0.47
2:F:467:VAL:O	2:F:470:ALA:HB3	2.14	0.47
1:A:188:ARG:HE	1:A:437:ALA:HB2	1.79	0.47
1:B:171:ARG:HH11	1:B:171:ARG:HG3	1.79	0.47
2:D:368:TYR:CE1	2:D:372:ARG:HG3	2.50	0.47
2:F:462:PRO:HG2	2:F:465:GLU:HG3	1.96	0.47
3:G:115:ILE:C	3:G:117:HIS:N	2.68	0.47
3:G:125:LEU:HD11	3:G:151:SER:HB2	1.96	0.47
1:C:445:ILE:HG22	1:C:449:VAL:CG2	2.44	0.47
1:C:59:LEU:HD23	1:C:82:ILE:CD1	2.44	0.47
2:E:33:LEU:HD13	2:E:117:HIS:CG	2.50	0.47
2:F:346:PRO:HG3	2:F:418:PHE:HZ	1.79	0.47
2:F:36:LEU:N	2:F:36:LEU:HD23	2.30	0.47
1:A:291:ARG:N	3:G:262:LEU:CD2	2.78	0.47
1:A:107:VAL:HB	1:A:116:ASP:HB3	1.97	0.47
1:A:166:LEU:HD13	1:A:342:VAL:HG12	1.95	0.47
1:C:219:ARG:HD3	1:C:433:TYR:HE1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:204:GLY:C	2:E:206:ILE:N	2.68	0.47
2:E:41:ARG:O	2:E:42:GLU:C	2.53	0.47
2:E:431:LEU:O	2:E:431:LEU:HD12	2.15	0.47
2:F:409:LYS:HD3	2:F:457:PHE:HE2	1.78	0.47
3:G:78:CYS:O	3:G:81:ILE:HD13	2.15	0.47
1:A:78:ASN:OD1	1:A:80:LYS:HB3	2.15	0.47
1:B:240:ALA:N	1:B:241:PRO:CD	2.77	0.47
2:E:393:MET:HE3	2:E:396:LEU:HD12	1.97	0.47
2:F:151:LYS:HD3	2:F:328:HIS:O	2.15	0.47
1:A:245:LEU:C	1:A:247:PRO:HD2	2.36	0.46
1:B:400:VAL:HB	1:B:418:LEU:CD2	2.45	0.46
1:C:102:GLU:HG2	1:C:122:GLY:C	2.36	0.46
1:C:34:ILE:HD11	1:C:79:ASP:CB	2.41	0.46
2:D:469:LYS:O	2:D:473:LEU:HG	2.15	0.46
1:B:271:LEU:HD12	1:B:325:PRO:HB2	1.98	0.46
2:E:259:PHE:CE2	2:E:263:GLN:HG2	2.50	0.46
2:E:438:ILE:O	2:E:442:GLN:HB2	2.15	0.46
2:F:200:MET:CG	2:F:206:ILE:HG12	2.46	0.46
3:G:179:PHE:O	3:G:181:LEU:N	2.48	0.46
1:B:389:THR:HA	1:B:392:LEU:HG	1.96	0.46
1:C:403:PHE:CG	2:D:408:ARG:CZ	2.99	0.46
2:E:409:LYS:NZ	2:E:450:ASP:HA	2.30	0.46
2:E:61:ILE:O	2:E:61:ILE:HG13	2.14	0.46
2:F:205:VAL:HG23	2:F:215:VAL:HG21	1.96	0.46
2:F:455:GLN:CD	2:F:455:GLN:H	2.18	0.46
1:A:313:ASN:OD1	1:A:316:PHE:HD2	1.98	0.46
1:A:376:SER:O	1:A:378:ALA:N	2.48	0.46
1:B:353:GLU:HG3	1:B:366:ASN:HB2	1.98	0.46
2:D:201:ILE:HD13	2:D:208:LEU:HD11	1.98	0.46
2:F:89:GLU:HG2	2:F:110:THR:CG2	2.44	0.46
1:A:240:ALA:HB3	1:A:241:PRO:HD3	1.97	0.46
1:C:187:LYS:HE3	1:C:224:ASP:HB3	1.97	0.46
2:D:96:ASN:HB2	2:D:100:GLU:N	2.27	0.46
2:D:289:MET:SD	2:D:324:THR:HG22	2.56	0.46
2:E:120:ALA:HB1	2:E:121:PRO:HD2	1.98	0.46
2:E:204:GLY:O	2:E:205:VAL:C	2.54	0.46
2:F:345:TYR:HA	2:F:346:PRO:C	2.36	0.46
1:A:339:PRO:O	1:A:343:ILE:HG13	2.16	0.46
1:A:62:MET:HE2	1:A:76:PHE:HZ	1.81	0.46
2:E:146:TYR:O	2:E:357:ILE:HD11	2.16	0.46
1:A:36:ASP:O	1:A:284:LEU:HD13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:GLU:OE1	1:B:90:ARG:HD3	2.16	0.46
1:C:156:LEU:HD11	1:C:428:LEU:CD1	2.46	0.46
1:C:26:GLU:HB3	1:C:46:ASN:ND2	2.31	0.46
2:D:154:LEU:HD13	2:D:165:LEU:HD23	1.96	0.46
2:F:469:LYS:O	2:F:473:LEU:HG	2.16	0.46
1:B:381:ARG:HG2	1:B:488:LYS:HG3	1.98	0.46
2:D:298:THR:HG23	2:D:303:SER:HA	1.98	0.46
1:B:284:LEU:CD2	2:E:274:ARG:HD3	2.46	0.46
2:E:85:PRO:HD2	2:E:95:MET:CE	2.46	0.46
2:F:29:LEU:HD11	2:F:58:VAL:HG13	1.98	0.46
2:F:339:ILE:CG2	2:F:344:ILE:HB	2.46	0.46
1:A:213:VAL:O	1:A:216:LEU:HB3	2.16	0.46
1:B:358:TYR:C	1:B:360:GLY:N	2.69	0.46
1:C:251:CYS:O	1:C:255:GLU:HG3	2.16	0.46
1:C:338:ILE:O	1:C:339:PRO:C	2.51	0.46
1:C:45:ARG:HA	1:C:45:ARG:HD3	1.29	0.46
1:C:91:THR:HG22	1:C:93:ALA:HB3	1.97	0.46
2:D:200:MET:HE3	2:D:215:VAL:HG21	1.98	0.46
2:D:432:VAL:HG13	2:D:433:PRO:HD2	1.97	0.46
2:D:440:GLY:O	2:D:444:ILE:HG13	2.16	0.46
2:D:461:GLY:HA3	2:D:462:PRO:HD3	1.74	0.46
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.97	0.46
1:B:210:ARG:O	1:B:211:SER:C	2.54	0.45
1:B:469:LEU:HG	1:B:473:ILE:HD11	1.97	0.45
1:C:292:GLU:O	1:C:293:ALA:CB	2.63	0.45
2:E:63:MET:CE	2:E:228:ALA:HA	2.45	0.45
2:F:243:PHE:O	2:F:249:GLN:HB2	2.16	0.45
2:F:390:ILE:CD1	3:G:242:MET:CE	2.94	0.45
2:F:96:ASN:HD22	2:F:100:GLU:CB	2.27	0.45
1:A:142:VAL:HG22	1:A:161:ARG:O	2.16	0.45
1:A:485:THR:HG22	1:A:486:ASP:N	2.29	0.45
1:A:48:GLN:HA	2:E:69:LEU:O	2.16	0.45
1:B:141:SER:HB2	1:B:143:ARG:NH1	2.31	0.45
1:C:67:GLU:HB3	1:C:68:PRO:HD2	1.98	0.45
2:F:275:ILE:HD13	3:G:271:ALA:HB1	1.98	0.45
1:B:496:LYS:O	1:B:500:ILE:HG13	2.15	0.45
1:C:158:PRO:HB3	1:C:379:GLN:HG3	1.99	0.45
1:C:390:MET:HE2	1:C:428:LEU:HD11	1.98	0.45
2:D:274:ARG:HH11	2:D:274:ARG:HD2	1.49	0.45
2:D:237:LEU:HD21	2:D:295:ARG:HB2	1.97	0.45
2:E:147:ALA:HB2	2:E:357:ILE:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:405:SER:OG	2:E:406:ARG:N	2.49	0.45
2:F:221:GLN:HA	2:F:221:GLN:NE2	2.31	0.45
3:G:259:THR:O	3:G:263:ILE:HG12	2.17	0.45
1:C:476:HIS:N	1:C:476:HIS:ND1	2.64	0.45
2:E:112:GLN:NE2	2:E:242:TYR:HE2	2.14	0.45
2:F:96:ASN:HB2	2:F:100:GLU:N	2.31	0.45
1:A:313:ASN:O	1:A:316:PHE:N	2.37	0.45
1:B:465:GLU:O	1:B:469:LEU:HB2	2.16	0.45
1:C:432:GLN:O	1:C:433:TYR:HB2	2.16	0.45
1:C:474:SER:OG	1:C:475:GLN:N	2.49	0.45
2:E:321:ALA:N	2:E:322:PRO:HD2	2.32	0.45
2:E:343:GLY:O	2:E:345:TYR:HD1	1.99	0.45
2:E:402:LEU:O	2:E:406:ARG:HG3	2.16	0.45
3:G:178:ILE:C	3:G:180:SER:N	2.69	0.45
3:G:44:TYR:CD2	4:H:93:LEU:HD22	2.52	0.45
1:A:211:SER:HA	2:D:126:MET:HE3	1.99	0.45
1:A:59:LEU:HD11	1:A:81:LEU:HD12	1.99	0.45
1:A:51:GLU:OE2	1:A:90:ARG:HB3	2.16	0.45
1:B:140:ILE:HG13	1:B:143:ARG:NH1	2.32	0.45
1:B:269:ASP:HA	1:B:270:ASP:HA	1.78	0.45
1:B:400:VAL:CG1	1:B:418:LEU:HD11	2.47	0.45
2:D:452:LEU:HD12	2:D:457:PHE:CZ	2.52	0.45
1:A:133:ALA:HB1	1:A:134:PRO:HD2	1.99	0.45
1:A:179:ALA:O	1:A:182:THR:HB	2.17	0.45
1:A:74:VAL:HG13	1:A:241:PRO:HG3	1.99	0.45
1:B:300:TYR:HA	1:B:303:SER:OG	2.17	0.45
2:D:35:ALA:HB1	2:D:46:VAL:CG1	2.47	0.45
2:E:242:TYR:C	2:E:244:ARG:H	2.18	0.45
2:F:346:PRO:HG3	2:F:418:PHE:CZ	2.52	0.45
3:G:40:PRO:HB3	4:H:26:VAL:HG12	1.99	0.45
2:D:345:TYR:HA	2:D:346:PRO:C	2.37	0.45
2:F:105:ARG:CZ	2:F:208:LEU:HD23	2.47	0.45
2:F:348:VAL:O	2:F:350:PRO:HD3	2.17	0.45
1:A:413:ALA:O	1:A:416:GLN:HB3	2.17	0.45
2:D:170:ILE:O	2:D:174:ALA:HB3	2.17	0.45
2:D:130:GLN:HE22	2:D:356:ARG:HD3	1.81	0.45
2:F:310:ILE:HD13	2:F:325:THR:HG21	1.98	0.45
3:G:84:SER:HB3	3:G:173:THR:OG1	2.17	0.45
3:G:13:ILE:HD13	3:G:242:MET:SD	2.57	0.45
1:A:412:ALA:HA	1:A:415:GLN:HB3	1.98	0.44
1:A:463:LYS:HD3	1:A:508:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:HD13	1:A:342:VAL:CG1	2.47	0.44
1:A:244:TYR:HE1	1:A:301:LEU:HD11	1.83	0.44
1:A:461:ILE:HG12	1:A:461:ILE:H	1.60	0.44
1:B:76:PHE:HB3	1:B:242:LEU:HD21	1.98	0.44
2:D:400:ASP:O	2:D:404:VAL:HG23	2.18	0.44
1:A:140:ILE:CG2	1:A:313:ASN:HA	2.47	0.44
1:B:437:ALA:O	1:B:438:ILE:C	2.54	0.44
1:C:311:LYS:HE3	1:C:318:GLY:O	2.18	0.44
2:D:366:GLU:O	2:D:370:VAL:HG23	2.17	0.44
2:D:433:PRO:HG2	2:D:436:GLU:CG	2.44	0.44
2:F:359:ASP:OD1	2:F:360:PRO:HD2	2.18	0.44
1:A:471:HIS:ND1	1:A:475:GLN:HG3	2.33	0.44
2:E:282:GLN:HA	2:E:283:PRO:HD3	1.88	0.44
2:E:443:GLN:HA	2:E:446:ALA:HB3	1.99	0.44
2:F:257:ASN:OD1	2:F:259:PHE:HB3	2.18	0.44
3:G:86:ALA:O	3:G:116:LEU:HD13	2.18	0.44
1:A:392:LEU:O	1:A:396:GLN:HG3	2.18	0.44
1:B:34:ILE:HD12	1:B:35:GLY:H	1.81	0.44
2:D:108:ILE:HG22	2:D:110:THR:HG23	1.99	0.44
2:D:95:MET:HG2	2:D:99:GLY:HA2	1.99	0.44
2:E:114:ALA:HB3	2:E:238:THR:CG2	2.48	0.44
2:E:320:PRO:HD3	3:G:255:GLN:OE1	2.18	0.44
2:E:281:TYR:CZ	2:E:321:ALA:HB2	2.52	0.44
1:C:245:LEU:O	1:C:246:ALA:C	2.56	0.44
2:D:103:ASP:O	2:D:104:GLU:HB2	2.18	0.44
2:D:412:ARG:O	2:D:415:SER:OG	2.33	0.44
2:E:433:PRO:HG2	2:E:436:GLU:CG	2.48	0.44
2:E:89:GLU:HG2	2:E:110:THR:CG2	2.39	0.44
1:A:97:VAL:HG11	1:A:249:SER:HB2	1.99	0.44
1:A:379:GLN:HB2	1:A:384:LYS:HE3	2.00	0.44
1:A:460:LYS:HD2	1:A:460:LYS:N	2.32	0.44
2:E:136:GLY:HA2	2:E:432:VAL:O	2.18	0.44
3:G:239:ALA:O	3:G:243:ILE:HG12	2.18	0.44
1:A:398:ARG:HH11	1:A:398:ARG:HD2	1.53	0.44
1:B:212:THR:O	1:B:216:LEU:HB2	2.18	0.44
1:B:32:LEU:HD21	1:B:42:HIS:HB2	2.00	0.44
1:B:400:VAL:HG12	1:B:418:LEU:HD11	2.00	0.44
1:C:404:ALA:HB1	1:C:410:LEU:HD11	1.99	0.44
1:C:83:LYS:HB3	2:F:52:HIS:HE1	1.83	0.44
2:D:397:SER:O	2:D:400:ASP:N	2.45	0.44
2:E:166:ILE:O	2:E:170:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:188:GLU:H	2:F:221:GLN:NE2	2.15	0.44
2:F:407:ALA:O	2:F:411:GLN:HB2	2.18	0.44
1:B:213:VAL:O	1:B:217:VAL:HG13	2.18	0.44
1:C:209:LYS:HE3	1:C:211:SER:OG	2.18	0.44
2:D:470:ALA:O	2:D:474:ALA:N	2.50	0.44
2:F:136:GLY:HA3	2:F:431:LEU:HD11	1.99	0.44
2:F:63:MET:HE3	2:F:97:VAL:HG11	2.00	0.44
3:G:105:ILE:HG22	3:G:106:ILE:N	2.32	0.44
1:A:385:GLN:OE1	1:A:488:LYS:HB2	2.17	0.43
1:A:151:LYS:HE2	1:A:427:LEU:O	2.17	0.43
1:B:389:THR:HA	1:B:392:LEU:CG	2.48	0.43
1:C:193:THR:O	1:C:195:GLU:OE1	2.36	0.43
3:G:228:ARG:O	3:G:232:MET:HG2	2.17	0.43
1:A:251:CYS:O	1:A:255:GLU:HG3	2.18	0.43
2:D:412:ARG:HG3	2:D:412:ARG:NH1	2.33	0.43
2:E:310:ILE:HD11	2:E:329:LEU:HD11	2.00	0.43
2:E:425:THR:C	2:E:427:HIS:N	2.71	0.43
2:F:439:LYS:HG2	2:F:443:GLN:NE2	2.33	0.43
2:D:319:ASP:O	2:D:320:PRO:C	2.55	0.43
2:E:161:GLY:O	2:E:162:LYS:C	2.57	0.43
2:F:50:ALA:O	2:F:51:GLN:HB3	2.16	0.43
1:A:99:VAL:HG23	1:A:253:MET:HA	2.00	0.43
1:B:450:ARG:HA	1:B:450:ARG:HD3	1.87	0.43
1:C:485:THR:O	1:C:486:ASP:C	2.57	0.43
2:D:38:VAL:HG11	2:D:69:LEU:CD2	2.49	0.43
3:G:117:HIS:CE1	3:G:118:ARG:NE	2.86	0.43
3:G:180:SER:O	3:G:181:LEU:C	2.56	0.43
1:B:289:PRO:CG	3:G:263:ILE:HD12	2.47	0.43
1:A:45:ARG:HA	1:A:45:ARG:HD3	1.66	0.43
1:A:283:LEU:HD11	1:A:293:ALA:HB1	1.98	0.43
1:A:62:MET:HE2	1:A:76:PHE:CZ	2.54	0.43
1:C:49:ALA:N	1:C:66:LEU:HD11	2.34	0.43
2:D:93:ARG:NH1	2:D:108:ILE:HG12	2.33	0.43
2:E:105:ARG:NE	2:E:208:LEU:HD23	2.33	0.43
2:E:397:SER:C	2:E:399:GLU:H	2.20	0.43
2:F:144:ALA:N	2:F:145:PRO:CD	2.82	0.43
1:A:85:GLY:O	1:A:86:ASP:C	2.53	0.43
1:B:294:TYR:CE2	1:B:338:ILE:HD13	2.53	0.43
1:C:147:GLN:OE1	1:C:438:ILE:HD13	2.19	0.43
1:C:32:LEU:HD21	1:C:42:HIS:HB2	2.00	0.43
1:C:403:PHE:CD2	2:D:408:ARG:NH1	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:GLU:HG2	1:C:52:MET:N	2.33	0.43
2:E:461:GLY:HA3	2:E:462:PRO:HD3	1.73	0.43
2:F:122:GLU:OE1	2:F:122:GLU:HA	2.19	0.43
2:F:95:MET:HG3	2:F:99:GLY:HA2	2.00	0.43
1:A:397:TYR:CD1	1:A:421:GLY:HA3	2.53	0.43
1:A:52:MET:CG	1:A:95:VAL:HG22	2.48	0.43
1:B:107:VAL:HG12	1:B:115:ILE:HD11	2.00	0.43
1:C:353:GLU:O	1:C:364:ALA:HB1	2.19	0.43
1:C:423:ARG:CD	1:C:461:ILE:HD11	2.49	0.43
1:C:49:ALA:O	1:C:50:GLU:HB2	2.19	0.43
2:D:63:MET:HE1	2:D:227:GLY:O	2.19	0.43
2:D:231:ARG:O	2:D:234:LEU:N	2.50	0.43
2:F:141:ASP:HB3	2:F:434:LEU:HD13	2.01	0.43
2:F:196:LEU:O	2:F:200:MET:HB2	2.19	0.43
2:F:357:ILE:O	2:F:359:ASP:N	2.48	0.43
4:H:79:SER:O	4:H:94:ALA:HA	2.18	0.43
1:A:78:ASN:ND2	1:A:80:LYS:HD2	2.34	0.43
1:B:423:ARG:HE	1:B:458:PRO:CG	2.31	0.43
2:F:31:PRO:O	2:F:34:ASN:HB2	2.18	0.43
3:G:113:ARG:O	3:G:117:HIS:HB2	2.18	0.43
1:A:96:ASP:HA	1:A:128:ARG:HA	2.01	0.43
1:B:434:SER:N	1:B:435:PRO:CD	2.82	0.43
2:D:189:ARG:O	2:D:192:GLU:HB2	2.18	0.43
2:D:94:ILE:HG22	2:D:102:ILE:HD11	2.01	0.43
2:E:35:ALA:HB2	2:E:82:ILE:HG13	1.99	0.43
2:F:452:LEU:HD22	2:F:470:ALA:CB	2.49	0.43
3:G:106:ILE:HG12	3:G:126:VAL:HG23	2.01	0.43
1:C:107:VAL:O	1:C:115:ILE:HG12	2.18	0.42
1:C:269:ASP:HA	1:C:270:ASP:HA	1.79	0.42
2:E:376:LYS:O	2:E:379:GLN:HB2	2.19	0.42
1:C:344:SER:O	2:D:222:MET:CE	2.67	0.42
2:F:400:ASP:O	2:F:404:VAL:HG23	2.19	0.42
1:A:101:GLU:OE2	1:A:262:LYS:NZ	2.44	0.42
1:A:180:ILE:O	1:A:181:ASP:C	2.56	0.42
1:A:340:THR:O	1:A:344:SER:HB3	2.19	0.42
1:C:185:ASN:HB2	1:C:435:PRO:HB3	2.00	0.42
2:D:258:ILE:HA	2:D:258:ILE:HD12	1.94	0.42
2:E:189:ARG:HB2	2:E:192:GLU:HG3	2.01	0.42
2:E:387:ILE:HG22	2:E:388:ILE:HD13	2.01	0.42
3:G:86:ALA:HA	3:G:89:MET:CE	2.49	0.42
1:A:485:THR:C	1:A:487:GLY:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:GLU:O	1:B:325:PRO:HD2	2.19	0.42
2:D:266:SER:CB	2:D:282:GLN:NE2	2.82	0.42
2:D:35:ALA:HB1	2:D:46:VAL:HG13	2.02	0.42
2:E:158:ALA:C	2:E:160:VAL:N	2.72	0.42
1:B:284:LEU:HD21	2:E:274:ARG:HD3	2.00	0.42
3:G:180:SER:O	3:G:182:ASP:N	2.52	0.42
1:B:385:GLN:NE2	1:B:489:ILE:HB	2.34	0.42
2:E:441:PHE:O	2:E:445:LEU:HG	2.19	0.42
2:D:471:ASP:O	2:D:472:LYS:C	2.57	0.42
2:E:189:ARG:O	2:E:190:THR:C	2.58	0.42
2:F:385:GLN:HA	2:F:388:ILE:HG12	2.01	0.42
2:F:471:ASP:O	2:F:474:ALA:N	2.53	0.42
3:G:6:ILE:HG21	3:G:250:PHE:HB2	2.00	0.42
5:I:5:ARG:O	5:I:6:GLN:CB	2.68	0.42
1:A:383:MET:O	1:A:386:VAL:HG23	2.19	0.42
1:B:353:GLU:OE2	1:B:366:ASN:ND2	2.50	0.42
1:B:99:VAL:HG13	1:B:256:TYR:HB2	2.02	0.42
1:C:169:GLY:O	1:C:175:LYS:HE2	2.18	0.42
1:C:489:ILE:HG22	1:C:494:ASP:HB2	1.99	0.42
2:D:396:LEU:HD22	2:D:400:ASP:HB2	2.00	0.42
2:D:84:ILE:HD12	2:D:95:MET:CE	2.50	0.42
2:E:388:ILE:HD12	2:E:396:LEU:HD11	2.01	0.42
1:A:184:ILE:HD12	1:A:223:ALA:CB	2.49	0.42
1:B:255:GLU:HG2	1:B:258:ARG:CZ	2.50	0.42
2:D:279:VAL:HG12	2:D:279:VAL:O	2.20	0.42
2:E:412:ARG:NH1	2:E:454:GLU:OE1	2.53	0.42
2:E:97:VAL:HG13	2:E:232:VAL:HG12	2.02	0.42
2:F:47:LEU:HD23	2:F:62:ALA:HA	2.01	0.42
3:G:12:SER:O	3:G:16:ILE:HD12	2.20	0.42
2:F:390:ILE:CD1	3:G:242:MET:HE3	2.50	0.42
4:H:20:PHE:CD1	4:H:92:LEU:HD23	2.54	0.42
1:A:247:PRO:HG2	1:A:274:GLN:NE2	2.35	0.42
1:A:294:TYR:HB2	1:A:337:TYR:CE2	2.54	0.42
1:A:267:ILE:HA	1:A:324:LEU:O	2.20	0.42
1:B:381:ARG:HA	1:B:384:LYS:HB2	2.01	0.42
1:C:224:ASP:OD1	1:C:227:LYS:HE3	2.19	0.42
1:C:129:VAL:HG21	1:C:245:LEU:HD11	2.02	0.42
1:C:392:LEU:HD11	2:D:425:THR:HA	2.01	0.42
2:D:112:GLN:NE2	2:D:242:TYR:HE1	2.18	0.42
2:D:201:ILE:CD1	2:D:208:LEU:HD11	2.50	0.42
2:D: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:462:PRO:HD2	2:D:465:GLU:HG3	2.01	0.42
2:E:185:GLY:HA3	2:E:188:GLU:HG3	2.02	0.42
2:E:346:PRO:HG3	2:E:418:PHE:HZ	1.83	0.42
2:E:95:MET:HA	2:E:100:GLU:O	2.20	0.42
2:F:423:VAL:HG12	2:F:423:VAL:O	2.20	0.42
1:A:56:SER:O	1:A:58:GLY:N	2.53	0.42
1:B:420:ARG:O	1:B:423:ARG:N	2.50	0.42
1:C:78:ASN:HD21	1:C:80:LYS:HD3	1.85	0.42
2:D:112:GLN:NE2	2:D:242:TYR:CE1	2.88	0.42
2:D:410:ILE:HG23	2:D:441:PHE:CE1	2.54	0.42
2:D:475:GLU:HA	2:D:475:GLU:OE1	2.20	0.42
4:H:95:GLU:HB3	5:I:19:ALA:HB2	2.01	0.42
1:A:353:GLU:CD	1:A:366:ASN:HD22	2.23	0.41
1:A:68:PRO:HD3	2:E:15:ALA:HB2	2.02	0.41
1:B:433:TYR:C	1:B:435:PRO:HD3	2.40	0.41
1:B:78:ASN:ND2	1:B:80:LYS:HE2	2.35	0.41
1:C:105:GLY:N	1:C:229:THR:O	2.41	0.41
2:F:252:LEU:HA	2:F:252:LEU:HD23	1.81	0.41
2:F:357:ILE:HD13	2:F:357:ILE:HA	1.80	0.41
1:A:206:ILE:O	1:A:273:LYS:HD2	2.20	0.41
1:B:389:THR:HG22	1:B:392:LEU:HD12	2.00	0.41
1:B:485:THR:O	1:B:486:ASP:C	2.58	0.41
1:B:75:VAL:HG21	1:B:82:ILE:HD12	2.02	0.41
1:C:467:ALA:O	1:C:470:SER:HB2	2.20	0.41
2:D:145:PRO:HB2	2:D:357:ILE:HD11	2.01	0.41
2:E:340:ALA:O	2:E:343:GLY:N	2.42	0.41
2:E:396:LEU:CB	2:E:401:LYS:HG2	2.50	0.41
1:A:139:ARG:C	1:A:140:ILE:HG22	2.41	0.41
1:A:105:GLY:HA2	1:A:226:MET:O	2.21	0.41
1:A:338:ILE:N	1:A:339:PRO:CD	2.83	0.41
1:B:107:VAL:O	1:B:115:ILE:HG12	2.20	0.41
1:C:151:LYS:HE2	1:C:436:MET:SD	2.60	0.41
1:C:139:ARG:HB3	1:C:311:LYS:O	2.19	0.41
2:E:122:GLU:HB2	2:E:125:GLU:HG3	2.01	0.41
2:D:398:GLU:HA	2:D:401:LYS:CG	2.51	0.41
2:D:63:MET:CE	2:D:97:VAL:HG11	2.51	0.41
2:E:165:LEU:HD22	2:E:335:LEU:HD21	2.02	0.41
2:E:182:VAL:HG21	2:E:240:ALA:HB2	2.01	0.41
2:E:282:GLN:NE2	2:E:282:GLN:H	2.19	0.41
2:E:29:LEU:HA	2:E:30:PRO:HD2	1.92	0.41
2:E:139:VAL:HG21	2:E:348:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:434:LEU:O	2:E:437:THR:HB	2.21	0.41
2:F:81:PRO:O	2:F:82:ILE:C	2.58	0.41
4:H:131:ILE:HG23	4:H:134:ARG:HH21	1.84	0.41
1:A:288:PRO:HA	1:A:289:PRO:HD3	1.88	0.41
1:B:366:ASN:ND2	1:B:369:LEU:HG	2.35	0.41
1:B:461:ILE:HG12	1:B:461:ILE:H	1.75	0.41
2:E:12:ARG:NH2	2:E:24:GLN:OE1	2.50	0.41
1:B:361:ILE:HD13	1:B:429:LYS:HE2	2.02	0.41
2:D:86:VAL:HG11	2:D:114:ALA:HB3	2.02	0.41
2:D:52:HIS:CD2	2:D:58:VAL:HG12	2.56	0.41
2:E:32:ILE:O	2:E:33:LEU:CB	2.68	0.41
2:E:397:SER:O	2:E:399:GLU:N	2.54	0.41
2:F:38:VAL:HG11	2:F:69:LEU:CD2	2.50	0.41
1:A:441:GLN:O	1:A:445:ILE:HG12	2.21	0.41
1:B:382:ALA:HB1	1:B:442:VAL:HG11	2.02	0.41
1:C:104:LEU:HD21	1:C:257:PHE:CZ	2.56	0.41
2:D:281:TYR:HB3	2:D:285:LEU:HD12	2.03	0.41
2:D:281:TYR:CD2	2:D:320:PRO:HG2	2.56	0.41
2:E:387:ILE:HG22	2:E:388:ILE:N	2.36	0.41
2:F:445:LEU:HD23	2:F:445:LEU:HA	1.92	0.41
2:F:80:ALA:HB1	2:F:81:PRO:HD3	2.03	0.41
3:G:129:LYS:O	3:G:130:GLU:HB2	2.21	0.41
1:A:103:LEU:O	1:A:106:ARG:HB2	2.20	0.41
1:A:403:PHE:O	1:A:404:ALA:C	2.59	0.41
1:B:423:ARG:O	1:B:426:GLU:N	2.51	0.41
1:C:151:LYS:HG3	1:C:430:GLN:OE1	2.21	0.41
1:C:280:GLN:OE1	2:F:287:THR:HG23	2.20	0.41
2:D:402:LEU:O	2:D:406:ARG:HG3	2.21	0.41
2:E:77:ASP:C	2:E:79:GLY:H	2.24	0.41
2:F:251:VAL:HG12	2:F:252:LEU:N	2.35	0.41
1:A:408:SER:O	1:A:409:ASP:HB2	2.21	0.41
1:A:420:ARG:HA	1:A:420:ARG:HD3	1.78	0.41
1:A:498:LYS:O	1:A:502:THR:HG23	2.21	0.41
1:B:221:THR:HG22	1:B:222:ASP:N	2.36	0.41
1:B:44:LEU:HB3	1:B:47:VAL:CG2	2.47	0.41
1:B:423:ARG:NE	1:B:458:PRO:HD3	2.35	0.41
2:D:256:ASP:HA	2:D:257:ASN:HA	1.87	0.41
2:D:397:SER:O	2:D:398:GLU:C	2.58	0.41
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.48	0.41
2:E:167:MET:SD	2:E:200:MET:HA	2.61	0.41
2:E:296:ILE:HD13	2:E:306:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:184:ILE:C	3:G:186:SER:N	2.72	0.41
2:D:63:MET:CE	2:D:228:ALA:HA	2.50	0.41
2:E:360:PRO:HD3	2:E:368:TYR:CG	2.56	0.41
2:E:82:ILE:CG2	2:E:116:ILE:HD13	2.51	0.41
2:E:97:VAL:HG13	2:E:232:VAL:HG13	2.03	0.41
3:G:73:SER:O	3:G:111:LYS:HB2	2.21	0.41
3:G:120:HIS:HB3	3:G:123:GLN:HB2	2.03	0.41
1:A:32:LEU:HD21	1:A:42:HIS:HB2	2.03	0.41
1:A:151:LYS:NZ	1:A:427:LEU:O	2.53	0.41
1:A:485:THR:O	1:A:487:GLY:N	2.54	0.41
1:B:201:CYS:O	1:B:229:THR:HA	2.21	0.41
1:B:206:ILE:HA	1:B:234:ALA:O	2.21	0.41
1:B:452:TYR:CD2	1:B:501:VAL:HG21	2.56	0.41
2:D:97:VAL:HG11	2:D:231:ARG:HB2	2.03	0.41
2:D:38:VAL:HG22	2:D:75:VAL:HG22	2.02	0.41
2:E:430:LYS:HD3	2:E:430:LYS:HA	1.97	0.41
2:E:77:ASP:CG	2:E:79:GLY:H	2.24	0.41
1:A:74:VAL:CG1	1:A:241:PRO:HG3	2.51	0.40
1:A:492:GLU:C	1:A:494:ASP:N	2.73	0.40
1:C:44:LEU:HA	1:C:44:LEU:HD23	1.92	0.40
1:C:465:GLU:HG2	1:C:465:GLU:O	2.21	0.40
1:C:465:GLU:O	1:C:469:LEU:HB2	2.21	0.40
1:C:442:VAL:HG11	1:C:489:ILE:HD11	2.01	0.40
2:D:203:SER:OG	2:D:205:VAL:HG23	2.21	0.40
2:E:231:ARG:O	2:E:234:LEU:N	2.50	0.40
3:G:87:LYS:HA	3:G:90:LYS:HE2	2.02	0.40
1:A:129:VAL:HG12	1:A:249:SER:HA	2.03	0.40
1:B:187:LYS:HE3	1:B:227:LYS:NZ	2.37	0.40
1:B:297:ASP:N	1:B:297:ASP:OD1	2.52	0.40
1:C:116:ASP:O	1:C:117:GLY:C	2.60	0.40
2:D:412:ARG:C	2:D:414:LEU:N	2.73	0.40
2:E:227:GLY:O	2:E:231:ARG:HG2	2.21	0.40
2:E:439:LYS:O	2:E:442:GLN:HB3	2.22	0.40
3:G:56:ASP:C	3:G:57:ILE:HG12	2.41	0.40
1:A:292:GLU:HB2	1:A:294:TYR:HD2	1.86	0.40
1:A:383:MET:HG3	1:A:387:ALA:HB2	2.02	0.40
1:A:69:ASP:O	1:A:70:ASN:HB3	2.21	0.40
1:B:239:ALA:HB1	1:B:241:PRO:HD2	2.03	0.40
1:B:30:ARG:HA	1:B:86:ASP:O	2.21	0.40
1:B:336:ALA:HB3	1:B:339:PRO:HD2	2.02	0.40
1:B:382:ALA:O	1:B:385:GLN:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:ARG:HH21	1:B:458:PRO:HD3	1.86	0.40
1:C:30:ARG:HG2	1:C:87:ILE:HD12	2.04	0.40
1:C:342:VAL:HA	1:C:345:ILE:HD12	2.03	0.40
1:B:209:LYS:HG2	2:E:294:GLU:OE2	2.21	0.40
2:E:329:LEU:O	2:E:356:ARG:CZ	2.70	0.40
3:G:2:THR:HG22	3:G:4:LYS:H	1.86	0.40
1:C:469:LEU:HD12	1:C:469:LEU:HA	1.96	0.40
2:D:13:ILE:HD12	2:D:73:GLN:HB3	2.03	0.40
2:D:406:ARG:HH11	2:D:406:ARG:HD2	1.60	0.40
2:E:413:PHE:HE2	2:E:440:GLY:HA3	1.87	0.40
2:D:360:PRO:HD3	2:D:368:TYR:CD2	2.56	0.40
2:E:84:ILE:HD13	2:E:235:THR:HG23	2.03	0.40
2:F:94:ILE:CG2	2:F:102:ILE:HD11	2.50	0.40
2:F:442:GLN:O	2:F:445:LEU:HB2	2.20	0.40
3:G:115:ILE:O	3:G:117:HIS:N	2.54	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:GLY:O	1:C:20:ASP:OD2[4_555]	0.43	1.77
1:B:314:ASP:N	1:C:21:THR:C[4_555]	0.83	1.37
1:B:318:GLY:N	1:C:22:SER:OG[4_555]	0.92	1.28
1:B:313:ASN:O	1:C:22:SER:CA[4_555]	0.99	1.21
1:B:314:ASP:O	1:C:22:SER:O[4_555]	1.06	1.14
1:B:313:ASN:O	1:C:22:SER:CB[4_555]	1.08	1.12
1:B:124:LYS:NZ	2:F:31:PRO:CB[4_555]	1.10	1.10
1:B:311:LYS:NZ	1:C:20:ASP:CB[4_555]	1.14	1.06
1:B:314:ASP:O	1:C:22:SER:C[4_555]	1.18	1.02
1:B:314:ASP:CA	1:C:21:THR:C[4_555]	1.23	0.97
1:B:314:ASP:CA	1:C:21:THR:O[4_555]	1.26	0.94
1:B:314:ASP:N	1:C:21:THR:O[4_555]	1.28	0.92
1:B:318:GLY:CA	1:C:20:ASP:OD1[4_555]	1.29	0.91
1:B:314:ASP:N	1:C:22:SER:N[4_555]	1.30	0.90
1:B:317:GLY:CA	1:C:23:VAL:CG2[4_555]	1.31	0.89
1:B:318:GLY:O	1:C:20:ASP:CG[4_555]	1.31	0.89
1:B:318:GLY:C	1:C:20:ASP:OD2[4_555]	1.47	0.73
1:B:314:ASP:OD1	1:C:21:THR:CA[4_555]	1.49	0.71
1:B:313:ASN:C	1:C:22:SER:N[4_555]	1.50	0.70
1:B:143:ARG:CG	1:C:19:ALA:N[4_555]	1.52	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ASP:CB	1:C:21:THR:O[4_555]	1.53	0.67
1:B:314:ASP:CG	1:C:21:THR:CA[4_555]	1.59	0.61
1:B:313:ASN:C	1:C:22:SER:CA[4_555]	1.60	0.60
1:B:314:ASP:CA	1:C:22:SER:N[4_555]	1.60	0.60
1:B:314:ASP:C	1:C:22:SER:C[4_555]	1.69	0.51
1:B:311:LYS:NZ	1:C:20:ASP:CA[4_555]	1.76	0.44
1:A:510:ALA:CB	1:C:508:PHE:CD1[3_444]	1.83	0.37
1:B:314:ASP:O	1:C:23:VAL:N[4_555]	1.84	0.36
1:B:314:ASP:CB	1:C:21:THR:C[4_555]	1.84	0.36
1:B:311:LYS:NZ	1:C:20:ASP:CG[4_555]	1.84	0.36
1:B:318:GLY:C	1:C:20:ASP:CG[4_555]	1.85	0.35
1:B:318:GLY:CA	1:C:22:SER:OG[4_555]	1.88	0.32
1:B:317:GLY:C	1:C:23:VAL:CG2[4_555]	1.89	0.31
1:B:313:ASN:O	1:C:22:SER:N[4_555]	1.90	0.30
1:B:317:GLY:N	1:C:22:SER:O[4_555]	1.94	0.26
1:B:314:ASP:C	1:C:22:SER:O[4_555]	1.97	0.23
1:B:316:PHE:N	1:C:22:SER:O[4_555]	1.98	0.22
1:B:314:ASP:CA	1:C:22:SER:CA[4_555]	1.99	0.21
1:B:318:GLY:C	1:C:20:ASP:OD1[4_555]	2.00	0.20
1:B:314:ASP:N	1:C:22:SER:CA[4_555]	2.02	0.18
1:B:317:GLY:O	1:C:23:VAL:CG2[4_555]	2.04	0.16
1:B:313:ASN:C	1:C:21:THR:C[4_555]	2.04	0.16
1:B:317:GLY:C	1:C:22:SER:OG[4_555]	2.05	0.15
1:A:510:ALA:O	1:C:508:PHE:CE1[3_444]	2.05	0.15
1:B:314:ASP:C	1:C:22:SER:CA[4_555]	2.05	0.15
1:B:318:GLY:N	1:C:22:SER:CB[4_555]	2.06	0.14
1:B:318:GLY:CA	1:C:20:ASP:CG[4_555]	2.07	0.13
1:B:314:ASP:OD1	1:C:20:ASP:O[4_555]	2.09	0.11
1:B:314:ASP:CG	1:C:21:THR:C[4_555]	2.11	0.09
1:B:317:GLY:N	1:C:22:SER:C[4_555]	2.11	0.09
1:B:124:LYS:CE	2:F:31:PRO:CB[4_555]	2.13	0.07
1:B:314:ASP:C	1:C:21:THR:O[4_555]	2.14	0.06
1:B:314:ASP:N	1:C:21:THR:CA[4_555]	2.15	0.05
1:A:507:GLY:CA	1:C:504:PHE:O[3_444]	2.17	0.03
1:B:314:ASP:OD1	1:C:21:THR:C[4_555]	2.19	0.01

5.3 Torsion angles ⓘ

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%)	13	55
1	B	475/553 (86%)	427 (90%)	41 (9%)	7 (2%)	12	54
1	C	490/553 (89%)	444 (91%)	38 (8%)	8 (2%)	11	53
2	D	465/528 (88%)	419 (90%)	43 (9%)	3 (1%)	28	70
2	E	464/528 (88%)	407 (88%)	47 (10%)	10 (2%)	8	47
2	F	464/528 (88%)	433 (93%)	29 (6%)	2 (0%)	38	77
3	G	257/298 (86%)	223 (87%)	26 (10%)	8 (3%)	5	40
4	H	21/168 (12%)	21 (100%)	0	0	100	100
5	I	24/51 (47%)	20 (83%)	2 (8%)	2 (8%)	1	16
All	All	3145/3760 (84%)	2837 (90%)	261 (8%)	47 (2%)	12	54

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	407	GLY
2	E	393	MET
1	A	57	SER
1	A	405	GLN
1	A	409	ASP
1	B	364	ALA
1	C	332	GLY
1	C	408	SER
1	C	411	ASP
1	C	476	HIS
2	D	28	GLY
2	E	161	GLY
2	E	205	VAL
3	G	51	LEU
3	G	56	ASP
1	A	364	ALA

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/444 (88%)	351 (89%)	42 (11%)	8	36
1	B	388/444 (87%)	341 (88%)	47 (12%)	6	30
1	C	397/444 (89%)	369 (93%)	28 (7%)	17	53
2	D	377/417 (90%)	346 (92%)	31 (8%)	13	47
2	E	376/417 (90%)	343 (91%)	33 (9%)	12	44
2	F	376/417 (90%)	354 (94%)	22 (6%)	23	59
3	G	225/251 (90%)	210 (93%)	15 (7%)	19	55
4	H	27/128 (21%)	26 (96%)	1 (4%)	39	71
5	I	23/42 (55%)	21 (91%)	2 (9%)	12	45
All	All	2582/3004 (86%)	2361 (91%)	221 (9%)	12	46

All (221) 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
1	A	219	ARG

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Mol	Chain	Res	Type
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
1	B	256	TYR

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Mol	Chain	Res	Type
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
1	C	399	GLU

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Mol	Chain	Res	Type
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
2	E	9	THR

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Mol	Chain	Res	Type
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
2	F	191	ARG

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Mol	Chain	Res	Type
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	91	GLN
5	I	41	THR
5	I	42	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	GLN
1	A	349	GLN
1	A	396	GLN
1	A	432	GLN
1	B	48	GLN
1	B	65	ASN
1	B	349	GLN
1	B	432	GLN

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Mol	Chain	Res	Type
1	C	208	GLN
1	C	260	ASN
1	C	349	GLN
1	C	432	GLN
2	D	130	GLN
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	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
5	I	16	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates 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%)	-0.04	1 (0%) 94 93	20, 20, 20, 20	0
1	B	479/553 (86%)	-0.10	1 (0%) 94 93	20, 20, 20, 20	0
1	C	492/553 (88%)	-0.17	1 (0%) 94 93	20, 20, 20, 20	0
2	D	467/528 (88%)	-0.15	0 100 100	20, 20, 20, 20	0
2	E	466/528 (88%)	-0.12	0 100 100	20, 20, 20, 20	0
2	F	466/528 (88%)	-0.16	2 (0%) 92 88	20, 20, 20, 20	0
3	G	263/298 (88%)	0.31	1 (0%) 92 88	20, 20, 20, 20	0
4	H	31/168 (18%)	0.32	0 100 100	20, 20, 20, 20	0
5	I	28/51 (54%)	0.44	0 100 100	20, 20, 20, 20	0
All	All	3179/3760 (84%)	-0.08	6 (0%) 94 93	20, 20, 20, 20	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	510	ALA	3.6
1	C	19	ALA	3.1
3	G	175	GLU	2.4
2	F	469	LYS	2.4
1	B	448	GLY	2.4
2	F	472	LYS	2.3

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 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.