



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:52 AM UTC

PDB ID : 2W6E / pdb_00002w6e
Title : Low resolution structures of bovine mitochondrial F1-ATPase during controlled dehydration:hydration state 1.
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 : 6.50 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:

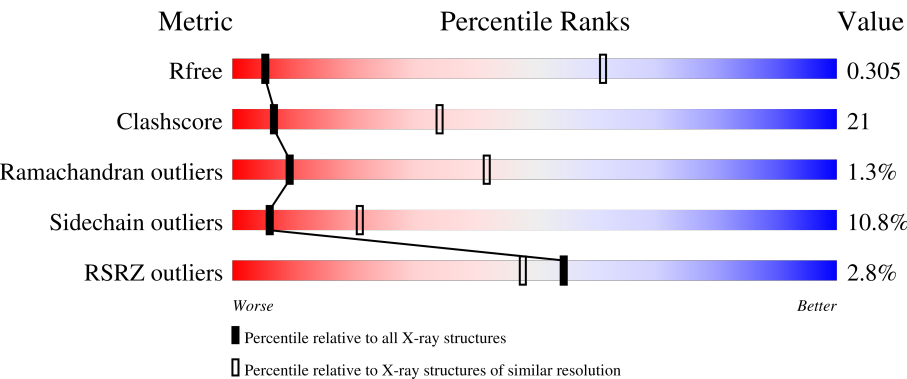
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 6.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1162 (9.00-4.00)
Clashscore	190562	1020 (8.98-4.02)
Ramachandran outliers	187476	1050 (9.00-4.00)
Sidechain outliers	187428	1014 (9.00-4.00)
RSRZ outliers	180081	1155 (9.00-4.00)

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% 42% 35% 10% • 12%
1	B	553	2% 42% 36% 8% • 13%
1	C	553	3% 46% 34% 7% • 11%
2	D	528	3% 50% 30% 7% • 12%

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Mol	Chain	Length	Quality of chain
2	E	528	% 38% 38% 10% • 12%
2	F	528	3% 49% 31% 6% • 12%
3	G	298	21% 15% • 59%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22690 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			

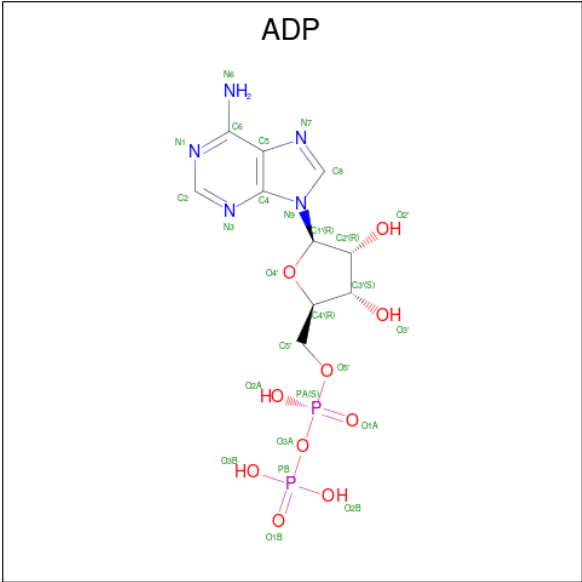
- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

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	122	Total	C	N	O	S	0	0	0
			945	591	171	176	7			

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

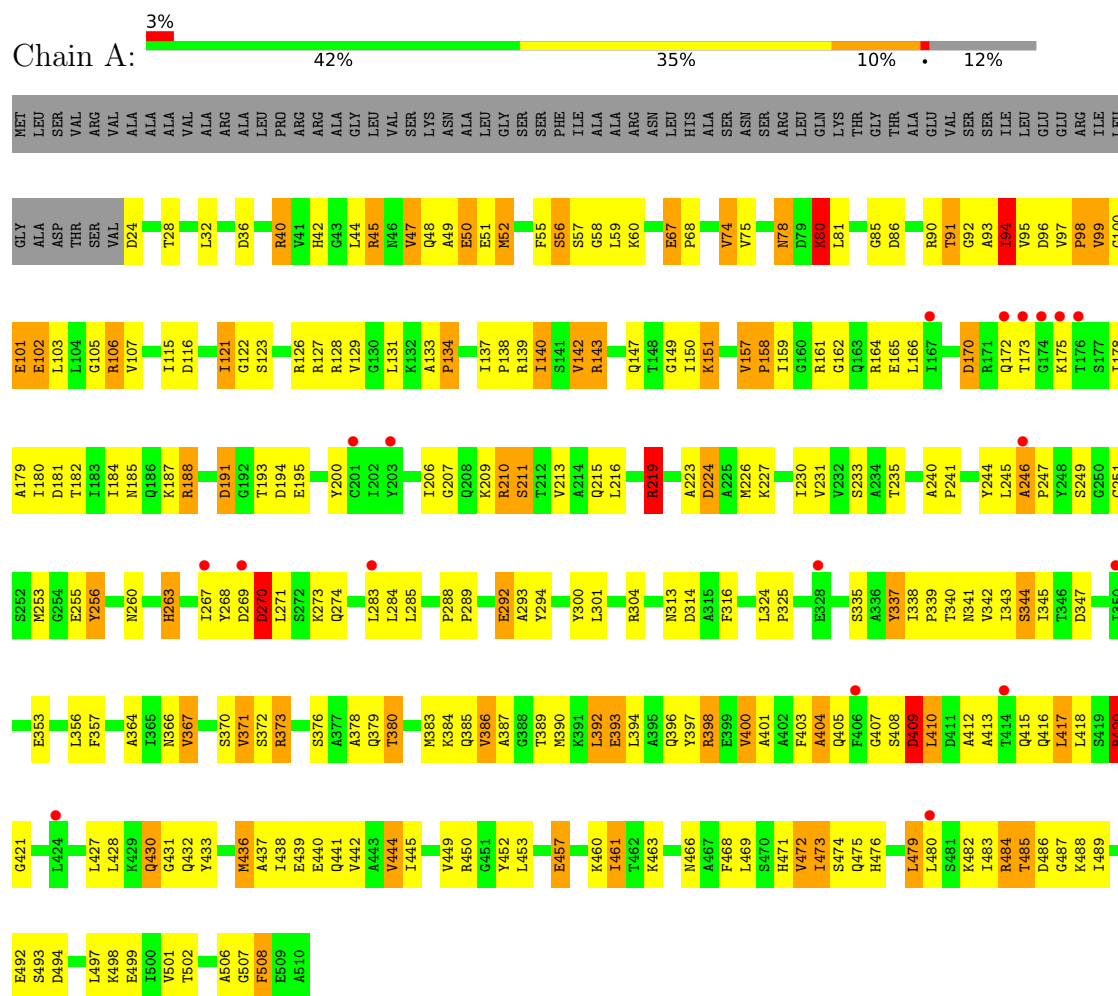


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

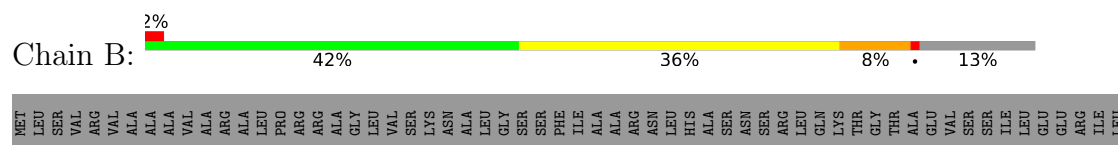
3 Residue-property plots

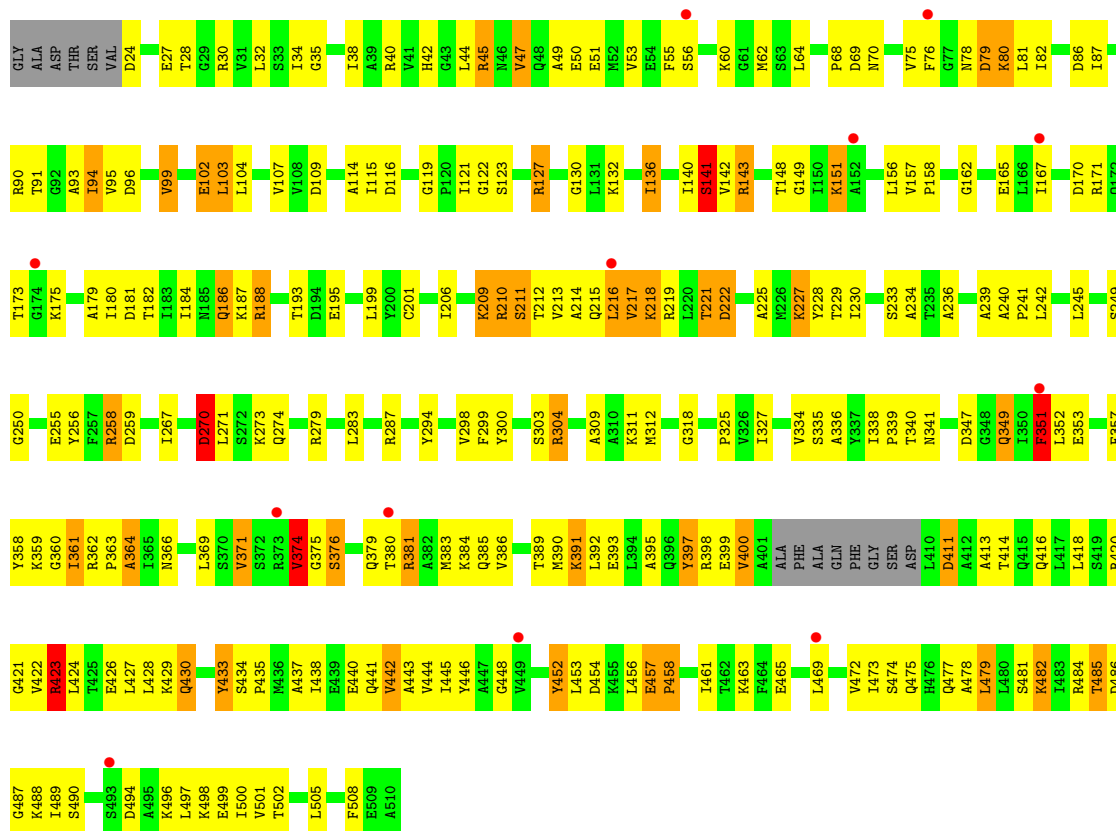
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

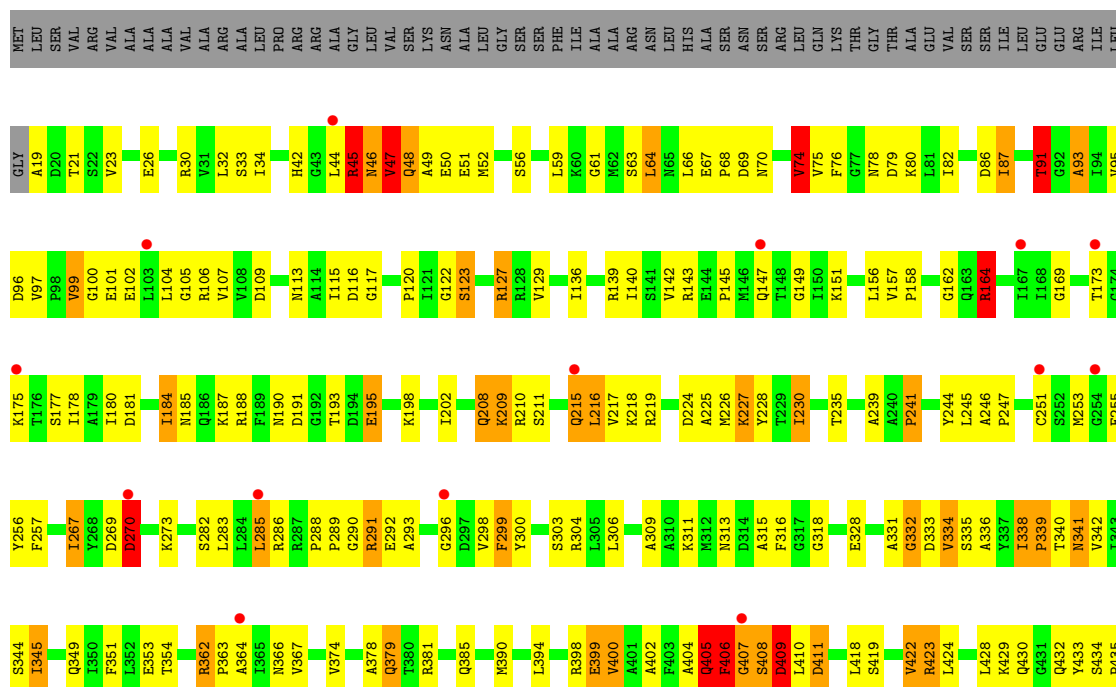


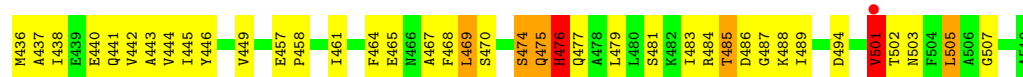
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL



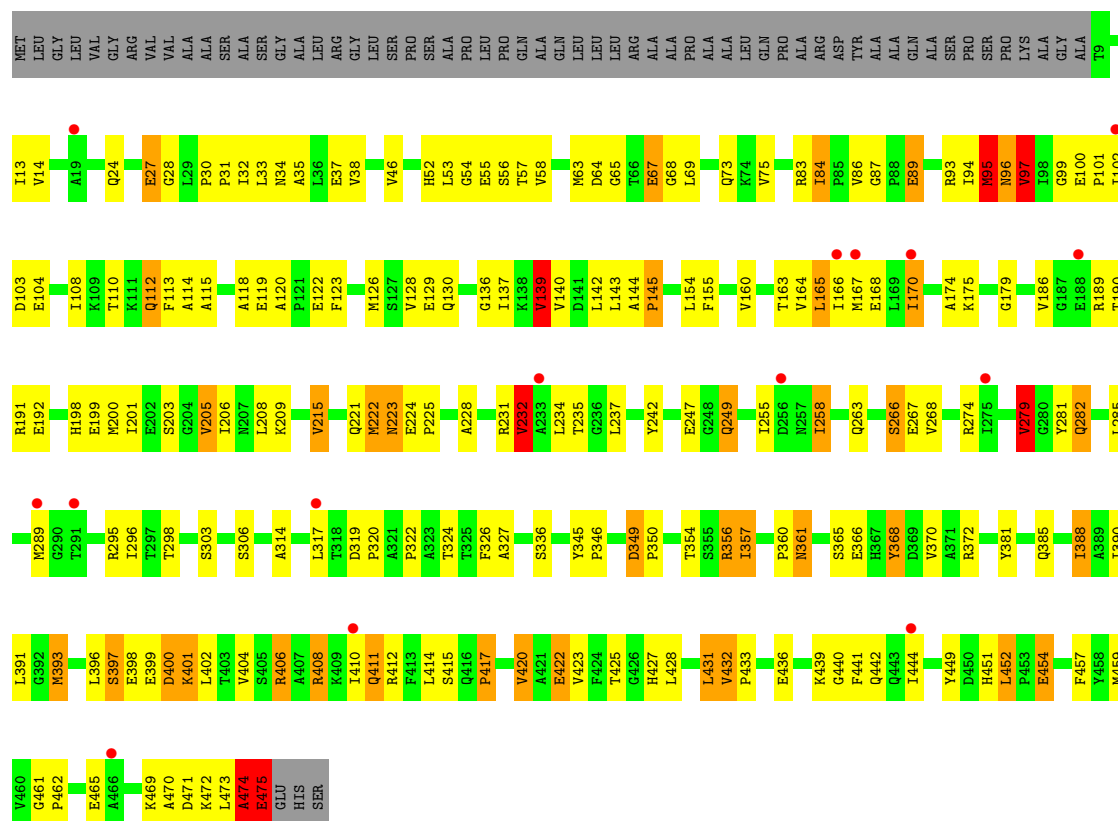


● Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL

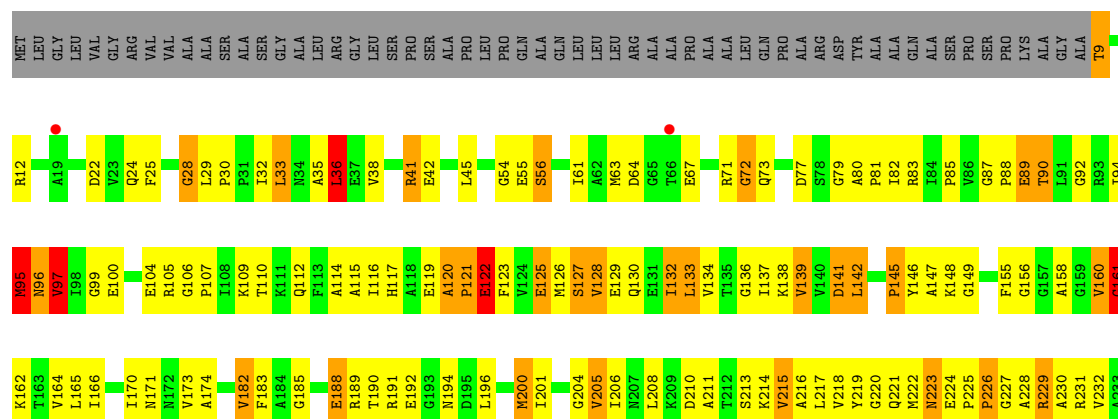


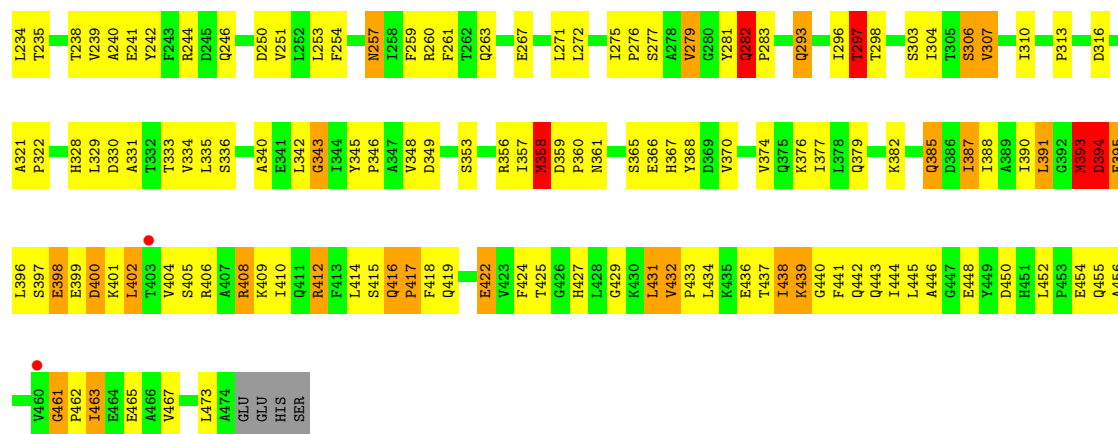


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

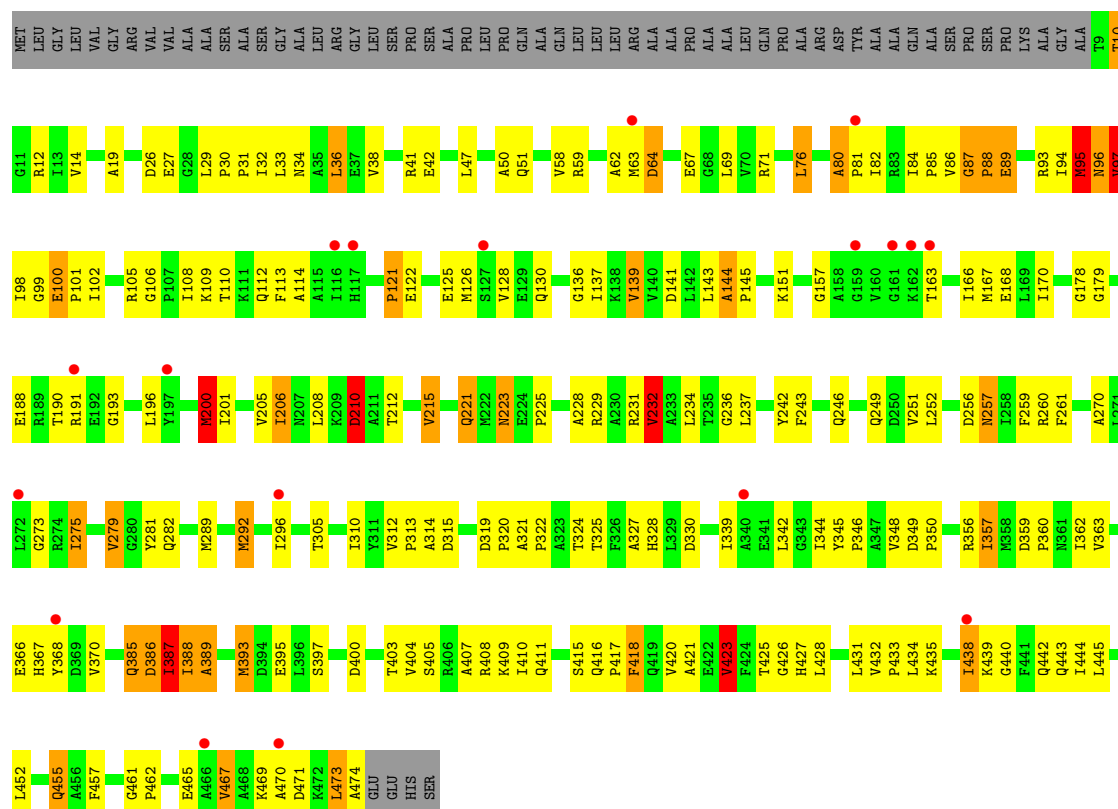


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

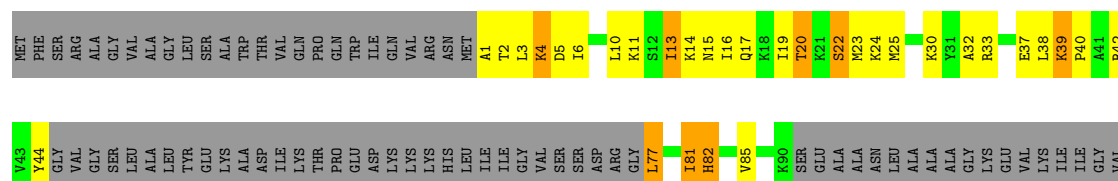




• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL



GLY	ILE	ILE	GLY
ASP	SER	SER	ASP
LYS	LYS	LYS	LYS
ILE	THR	THR	ILE
ARG	THR	THR	ARG
SER	GLU	GLU	SER
ILE	GLU	GLU	ILE
LEU	LYS	LYS	LEU
HIS	PRO	PRO	HIS
THR	ILE	ILE	THR
THR	PHE	PHE	THR
HIS	SER	SER	HIS
SER	LEU	LEU	SER
ASP	ASP	ASP	ASP
GLN	THR	THR	GLN
PHE	ILE	ILE	PHE
LEU	SER	SER	LEU
VAL	SER	SER	VAL
THR	ALA	ALA	THR
PHE	GLU	GLU	PHE
LYS	SER	SER	LYS
GLU	MET	MET	GLU
VAL	SER	SER	VAL
GLY	ILE	ILE	GLY
ARG	TYR	TYR	ARG
ARG	ASP	ASP	ARG
PRO	ASP	ASP	PRO
THR	ILE	ILE	THR
PHE	ALA	ALA	PHE
GLY	ASP	ASP	GLY
ASP	VAL	VAL	ASP
ALA	LEU	LEU	ALA
SER	ARG	ARG	SER
VAL	ASN	ASN	VAL
ILE	TYR	TYR	ILE
ALA	GLN	GLN	ALA
LEU	GLU	GLU	LEU
GLU	TYR	TYR	GLU
LEU	SER	SER	LEU
LEU	SER	SER	LEU
ASN	L209	L209	ASN
SER	A210	A210	SER
GLY	N211	N211	GLY
TYR	I212	I212	TYR
GLU	I213	I213	GLU
PHE	Y214	Y214	PHE
ASP	L217	L217	ASP
GLU	K218	K218	GLU
GLY	E219	E219	GLY
SER	S220	S220	SER
ILE	T221	T221	ILE
ILE	T222	T222	ILE
PHE	M232	M232	PHE
ASN	D233	D233	ASN
ARG	N234	N234	ARG
PHE	A235	A235	PHE
ARG	S236	S236	ARG
SER	K237	K237	SER
VAL			VAL

N238	N239	A239	S240	E241	M242	I243	D244	K245	L246	F250	R254	T258	T259	I263	A271	L272	ASP
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.49Å 141.15Å 285.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 6.50 30.00 – 6.50	Depositor EDS
% Data completeness (in resolution range)	86.9 (30.00-6.50) 85.8 (30.00-6.50)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 6.68Å)	Xtriage
Refinement program	REFMAC 5.5.0038	Depositor
R, R_{free}	0.290 , 0.285 0.303 , 0.305	Depositor DCC
R_{free} test set	378 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	176.4	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	22690	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 3.25% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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	66/5080 (1.3%)
1	B	0.77	0/3704	1.76	70/4995 (1.4%)
1	C	0.80	0/3799	1.80	72/5126 (1.4%)
2	D	0.81	1/3596 (0.0%)	1.78	67/4879 (1.4%)
2	E	0.78	0/3587	1.78	88/4867 (1.8%)
2	F	0.80	1/3587 (0.0%)	1.79	92/4867 (1.9%)
3	G	0.67	0/949	1.55	12/1266 (0.9%)
All	All	0.78	2/22988 (0.0%)	1.77	467/31080 (1.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	96	ASN	CA-CB	5.37	1.61	1.53
2	D	96	ASN	CA-CB	5.33	1.61	1.53

All (467) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	408	ARG	CD-NE-CZ	22.72	156.21	124.40
2	F	282	GLN	CB-CG-CD	15.19	138.42	112.60
2	E	408	ARG	CD-NE-CZ	13.46	143.24	124.40
1	B	351	PHE	CA-CB-CG	11.12	124.92	113.80
1	A	270	ASP	CA-CB-CG	10.90	123.50	112.60
2	F	139	VAL	CB-CA-C	-10.82	98.03	111.88
1	B	270	ASP	CA-CB-CG	10.48	123.08	112.60
1	B	375	GLY	N-CA-C	9.75	125.40	114.67
1	B	40	ARG	CD-NE-CZ	9.32	137.45	124.40
3	G	15	ASN	CA-CB-CG	-9.24	103.36	112.60
2	F	97	VAL	CB-CA-C	-9.15	99.79	112.14
2	D	96	ASN	CA-CB-CG	-8.73	103.86	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	139	VAL	CB-CA-C	-8.62	100.67	111.70
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
1	C	503	ASN	CA-CB-CG	-8.52	104.08	112.60
2	E	307	VAL	N-CA-CB	8.45	121.98	111.41
1	C	113	ASN	CA-CB-CG	-8.38	104.22	112.60
2	F	96	ASN	CB-CA-C	-8.27	93.28	110.40
1	A	269	ASP	CA-C-N	8.20	136.46	121.70
1	A	269	ASP	C-N-CA	8.20	136.46	121.70
2	F	427	HIS	CA-CB-CG	8.13	121.93	113.80
1	C	74	VAL	N-CA-CB	-8.10	101.89	110.72
2	F	95	MET	CA-C-N	8.02	138.61	121.45
2	F	95	MET	C-N-CA	8.02	138.61	121.45
2	D	349	ASP	CA-C-N	7.93	127.65	119.56
2	D	349	ASP	C-N-CA	7.93	127.65	119.56
1	C	476	HIS	N-CA-C	7.91	127.64	110.80
1	A	123	SER	N-CA-C	7.87	121.29	109.25
2	D	474	ALA	CA-C-N	7.82	135.78	121.70
2	D	474	ALA	C-N-CA	7.82	135.78	121.70
1	B	309	ALA	N-CA-C	-7.73	99.60	110.50
1	C	409	ASP	CA-CB-CG	7.65	120.25	112.60
1	B	270	ASP	CB-CA-C	-7.60	95.67	110.10
2	E	95	MET	CA-C-O	7.58	129.97	121.11
2	E	349	ASP	CA-C-O	7.53	124.18	119.29
2	F	221	GLN	N-CA-C	7.48	120.67	110.35
1	B	475	GLN	N-CA-C	7.48	119.51	111.36
2	F	95	MET	CA-CB-CG	7.47	129.04	114.10
1	A	91	THR	N-CA-C	-7.45	104.72	113.88
2	E	276	PRO	CA-C-O	-7.40	112.60	122.08
1	A	270	ASP	CB-CA-C	-7.33	96.18	110.10
1	A	170	ASP	CA-CB-CG	7.31	119.91	112.60
2	D	417	PRO	N-CA-CB	7.27	106.99	102.92
1	A	392	LEU	N-CA-C	7.25	119.26	111.36
1	B	53	VAL	CA-C-O	-7.18	114.35	121.67
1	C	501	VAL	N-CA-CB	7.17	118.44	110.62
2	E	395	GLU	N-CA-C	-7.17	104.66	113.19
1	C	429	LYS	CA-C-O	-7.15	113.57	121.87
2	E	129	GLU	N-CA-C	7.14	120.29	109.23
2	D	393	MET	N-CA-C	7.10	122.11	113.38
2	D	97	VAL	CB-CA-C	-7.08	102.45	112.22
2	D	249	GLN	N-CA-C	7.06	119.64	110.53
2	F	256	ASP	CA-CB-CG	7.06	119.66	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	ASN	CA-CB-CG	-7.05	105.55	112.60
2	E	343	GLY	N-CA-C	-7.04	106.71	115.08
1	A	210	ARG	CA-C-O	-7.02	112.16	120.10
2	F	232	VAL	CB-CA-C	-7.01	101.81	112.05
1	A	431	GLY	N-CA-C	-7.00	101.57	112.85
1	B	219	ARG	NE-CZ-NH2	6.96	125.47	119.20
2	E	160	VAL	N-CA-C	-6.95	98.57	108.58
1	B	349	GLN	CA-CB-CG	6.94	127.99	114.10
2	F	179	GLY	N-CA-C	-6.92	103.67	111.63
1	A	149	GLY	N-CA-C	-6.91	105.53	115.27
2	E	261	PHE	CA-C-N	6.87	129.38	120.44
2	E	261	PHE	C-N-CA	6.87	129.38	120.44
2	D	406	ARG	NE-CZ-NH1	-6.87	114.63	121.50
1	C	476	HIS	CA-CB-CG	-6.86	106.94	113.80
2	F	312	VAL	CA-C-N	6.86	127.24	119.83
2	F	312	VAL	C-N-CA	6.86	127.24	119.83
2	E	95	MET	CA-CB-CG	6.84	127.78	114.10
2	E	22	ASP	CA-CB-CG	6.84	119.44	112.60
1	A	314	ASP	CA-CB-CG	-6.83	105.77	112.60
2	F	59	ARG	NE-CZ-NH1	-6.83	114.67	121.50
1	A	476	HIS	N-CA-C	6.79	121.48	112.25
2	E	306	SER	N-CA-C	6.78	119.99	109.07
1	C	149	GLY	N-CA-C	-6.70	105.35	115.00
2	D	96	ASN	CB-CA-C	-6.70	97.04	111.78
2	F	349	ASP	CA-C-N	6.69	126.31	119.56
2	F	349	ASP	C-N-CA	6.69	126.31	119.56
1	A	285	LEU	CA-C-O	6.66	127.34	119.28
2	D	101	PRO	N-CA-CB	6.64	109.13	103.35
2	E	342	LEU	N-CA-C	-6.64	105.16	113.20
2	E	87	GLY	CA-C-N	6.63	126.41	119.05
2	E	87	GLY	C-N-CA	6.63	126.41	119.05
2	F	385	GLN	N-CA-C	6.61	120.21	111.75
1	C	47	VAL	CB-CA-C	-6.60	104.06	111.45
2	E	141	ASP	CA-CB-CG	6.59	119.19	112.60
2	E	156	GLY	N-CA-C	-6.59	104.51	112.48
1	C	328	GLU	CB-CG-CD	-6.58	101.41	112.60
2	D	400	ASP	CA-CB-CG	6.58	119.18	112.60
1	C	164	ARG	CD-NE-CZ	-6.58	115.19	124.40
1	C	215	GLN	OE1-CD-NE2	6.57	129.17	122.60
2	E	432	VAL	CA-C-N	6.57	127.10	120.14
2	E	432	VAL	C-N-CA	6.57	127.10	120.14
1	C	235	THR	N-CA-C	6.56	118.99	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	GLY	CA-C-N	6.54	126.56	119.89
1	B	119	GLY	C-N-CA	6.54	126.56	119.89
1	B	209	LYS	CA-C-O	-6.54	113.55	120.80
2	E	394	ASP	CA-CB-CG	-6.53	106.07	112.60
2	E	41	ARG	CD-NE-CZ	6.51	133.51	124.40
1	B	258	ARG	CD-NE-CZ	6.51	133.51	124.40
1	A	80	LYS	N-CA-C	-6.51	104.38	112.90
2	E	125	GLU	N-CA-C	-6.46	105.70	113.97
2	F	143	LEU	N-CA-C	6.46	121.37	112.90
2	D	84	ILE	N-CA-C	6.45	115.00	107.84
1	A	172	GLN	N-CA-CB	-6.44	102.41	111.62
2	F	225	PRO	CA-C-N	6.44	127.89	119.84
2	F	225	PRO	C-N-CA	6.44	127.89	119.84
2	D	144	ALA	CA-C-N	6.42	126.45	119.90
2	D	144	ALA	C-N-CA	6.42	126.45	119.90
2	F	313	PRO	N-CA-CB	6.42	109.05	103.27
2	D	113	PHE	CA-CB-CG	-6.41	107.39	113.80
3	G	221	THR	N-CA-CB	6.40	119.10	110.59
2	D	420	VAL	N-CA-CB	-6.40	104.01	112.26
2	F	193	GLY	N-CA-C	-6.40	105.08	112.50
2	E	394	ASP	N-CA-C	6.39	123.66	114.39
3	G	32	ALA	N-CA-C	-6.39	103.93	111.03
1	A	230	ILE	CA-C-N	-6.38	114.61	123.10
1	A	230	ILE	C-N-CA	-6.38	114.61	123.10
1	B	279	ARG	CD-NE-CZ	6.38	133.33	124.40
1	A	78	ASN	CA-CB-CG	6.38	118.97	112.60
1	B	299	PHE	N-CA-C	-6.38	104.41	111.36
1	A	231	VAL	CA-C-N	-6.34	114.94	122.93
1	A	231	VAL	C-N-CA	-6.34	114.94	122.93
2	D	221	GLN	N-CA-C	6.32	118.19	110.41
2	F	275	ILE	N-CA-C	-6.32	102.75	108.95
1	A	337	TYR	CA-C-N	6.28	124.19	120.24
1	A	337	TYR	C-N-CA	6.28	124.19	120.24
2	E	145	PRO	N-CA-CB	6.26	108.83	103.19
1	A	157	VAL	CA-C-N	6.26	126.63	119.93
1	A	157	VAL	C-N-CA	6.26	126.63	119.93
2	E	416	GLN	CA-C-N	6.26	127.20	120.13
2	E	416	GLN	C-N-CA	6.26	127.20	120.13
1	B	142	VAL	N-CA-CB	6.24	118.50	110.13
2	F	403	THR	N-CA-C	-6.24	104.40	111.14
1	A	371	VAL	CB-CA-C	-6.23	99.27	110.48
2	F	64	ASP	CA-C-O	-6.23	114.79	121.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	PRO	N-CA-CB	6.21	108.78	103.19
2	F	59	ARG	NE-CZ-NH2	6.21	124.79	119.20
1	C	164	ARG	NE-CZ-NH1	-6.20	115.30	121.50
1	C	291	ARG	NE-CZ-NH2	-6.18	113.64	119.20
1	B	93	ALA	N-CA-C	6.18	118.48	108.41
1	C	288	PRO	N-CA-CB	6.17	109.07	103.08
1	C	70	ASN	CA-C-O	-6.17	114.84	121.38
2	F	26	ASP	CA-CB-CG	-6.16	106.44	112.60
1	A	292	GLU	CB-CG-CD	6.15	123.06	112.60
2	E	94	ILE	N-CA-CB	6.14	119.61	111.25
2	F	144	ALA	CA-C-N	6.10	126.12	119.90
2	F	144	ALA	C-N-CA	6.10	126.12	119.90
2	E	225	PRO	N-CA-CB	6.09	108.99	103.08
2	E	422	GLU	N-CA-C	-6.09	105.87	113.55
2	E	106	GLY	CA-C-N	6.09	126.03	119.76
2	E	106	GLY	C-N-CA	6.09	126.03	119.76
1	C	157	VAL	CA-C-N	6.08	126.10	119.90
1	C	157	VAL	C-N-CA	6.08	126.10	119.90
1	B	287	ARG	CB-CA-C	6.08	118.19	109.26
2	F	261	PHE	CA-C-O	6.08	126.99	120.55
2	D	422	GLU	N-CA-C	-6.05	104.80	111.82
1	C	400	VAL	N-CA-CB	6.05	118.03	110.47
2	D	120	ALA	CA-C-N	6.04	126.07	119.90
2	D	120	ALA	C-N-CA	6.04	126.07	119.90
1	B	210	ARG	N-CA-CB	6.04	118.77	110.01
1	C	45	ARG	N-CA-C	6.04	118.66	111.71
1	B	374	VAL	N-CA-C	6.03	120.01	113.43
2	E	90	THR	N-CA-C	-6.03	106.06	113.41
2	F	432	VAL	CB-CA-C	-6.03	104.14	110.53
1	A	162	GLY	N-CA-C	-6.02	106.78	114.37
2	F	206	ILE	N-CA-CB	6.02	119.05	111.46
1	C	405	GLN	CA-C-N	6.01	133.03	121.54
1	C	405	GLN	C-N-CA	6.01	133.03	121.54
2	D	139	VAL	N-CA-CB	6.01	116.93	110.62
2	F	80	ALA	CA-C-N	6.01	126.20	120.31
2	F	80	ALA	C-N-CA	6.01	126.20	120.31
1	A	94	ILE	CB-CA-C	6.00	119.78	111.38
1	C	507	GLY	N-CA-C	-6.00	105.53	112.73
2	F	342	LEU	N-CA-C	-5.99	105.93	113.18
2	D	247	GLU	N-CA-C	-5.99	106.61	114.04
2	D	402	LEU	N-CA-C	-5.99	105.06	112.90
3	G	39	LYS	CA-C-N	5.98	125.69	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	39	LYS	C-N-CA	5.98	125.69	119.05
1	B	423	ARG	CD-NE-CZ	5.98	132.77	124.40
1	C	341	ASN	CA-C-O	-5.97	114.51	120.90
1	B	167	ILE	N-CA-CB	5.97	118.20	111.21
1	C	162	GLY	N-CA-C	-5.96	107.17	114.92
1	A	75	VAL	N-CA-C	5.94	116.73	109.30
1	B	371	VAL	CB-CA-C	-5.94	99.78	110.48
3	G	221	THR	N-CA-C	-5.94	106.57	113.88
1	C	336	ALA	O-C-N	-5.94	115.99	123.12
1	C	406	PHE	CA-CB-CG	5.92	119.72	113.80
1	B	162	GLY	N-CA-C	-5.92	106.81	115.63
1	C	109	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	106	ARG	CD-NE-CZ	5.91	132.68	124.40
1	B	91	THR	N-CA-C	-5.91	105.41	114.16
1	C	69	ASP	CA-CB-CG	-5.91	106.69	112.60
3	G	258	ILE	CB-CA-C	-5.91	104.16	112.14
2	F	96	ASN	N-CA-CB	-5.91	102.00	110.44
2	F	229	ARG	NE-CZ-NH1	-5.91	115.59	121.50
2	F	461	GLY	CA-C-N	5.90	126.24	119.92
2	F	461	GLY	C-N-CA	5.90	126.24	119.92
2	D	143	LEU	N-CA-C	5.90	120.61	113.41
1	C	345	ILE	N-CA-C	-5.89	106.97	111.62
1	A	98	PRO	N-CA-CB	5.89	108.92	103.39
1	B	477	GLN	CA-C-N	5.88	128.16	120.28
1	B	477	GLN	C-N-CA	5.88	128.16	120.28
2	F	370	VAL	N-CA-C	-5.88	105.00	110.53
1	C	46	ASN	CA-CB-CG	5.87	118.47	112.60
1	A	67	GLU	CA-C-N	5.87	125.34	119.24
1	A	67	GLU	C-N-CA	5.87	125.34	119.24
1	C	422	VAL	CB-CA-C	-5.87	104.22	112.14
1	C	91	THR	N-CA-C	-5.86	107.12	114.56
2	E	349	ASP	CA-C-N	5.86	125.97	119.87
2	E	349	ASP	C-N-CA	5.86	125.97	119.87
2	E	229	ARG	N-CA-C	-5.85	105.99	113.01
2	F	426	GLY	N-CA-C	-5.85	107.17	115.30
1	B	136	ILE	CA-C-N	5.85	125.01	120.33
1	B	136	ILE	C-N-CA	5.85	125.01	120.33
2	F	221	GLN	CA-C-N	5.85	130.04	120.63
2	F	221	GLN	C-N-CA	5.85	130.04	120.63
1	B	109	ASP	CA-CB-CG	5.84	118.44	112.60
2	F	388	ILE	CB-CA-C	-5.83	104.40	112.04
2	E	461	GLY	CA-C-N	5.83	125.74	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	461	GLY	C-N-CA	5.83	125.74	119.85
2	F	236	GLY	N-CA-C	-5.83	105.73	112.73
2	F	210	ASP	CB-CA-C	-5.83	100.34	111.48
1	B	351	PHE	N-CA-CB	5.83	119.92	110.42
1	B	45	ARG	CB-CG-CD	-5.82	97.91	111.30
1	A	373	ARG	NE-CZ-NH2	5.82	124.44	119.20
1	B	79	ASP	CA-CB-CG	5.82	118.42	112.60
1	C	93	ALA	N-CA-C	5.82	118.44	109.07
1	C	379	GLN	N-CA-C	5.82	118.96	109.59
1	A	370	SER	CA-C-O	-5.82	114.95	121.81
1	C	241	PRO	N-CA-CB	5.82	109.67	103.39
2	D	225	PRO	N-CA-CB	5.82	106.24	103.22
2	D	454	GLU	CA-CB-CG	5.79	125.68	114.10
1	C	341	ASN	O-C-N	5.78	128.11	122.09
1	C	100	GLY	N-CA-C	5.78	117.92	112.08
2	D	96	ASN	N-CA-CB	-5.77	101.67	110.49
2	F	389	ALA	N-CA-C	5.75	118.32	111.71
1	C	120	PRO	N-CA-CB	5.74	108.79	103.39
1	B	304	ARG	NE-CZ-NH1	-5.72	115.78	121.50
2	E	133	LEU	CA-C-O	-5.72	114.23	120.36
2	E	36	LEU	CA-C-O	-5.72	114.70	121.16
2	E	97	VAL	CB-CA-C	-5.70	102.87	112.16
1	C	303	SER	CA-C-N	5.69	129.35	120.82
1	C	303	SER	C-N-CA	5.69	129.35	120.82
2	D	145	PRO	N-CA-CB	5.69	108.26	103.25
2	F	157	GLY	CA-C-O	-5.68	115.53	122.75
2	F	84	ILE	N-CA-C	5.67	113.84	109.19
2	F	229	ARG	NE-CZ-NH2	5.67	124.30	119.20
2	D	163	THR	N-CA-C	5.66	117.45	111.28
1	A	335	SER	CB-CA-C	-5.65	99.83	110.01
2	D	145	PRO	CA-C-O	-5.65	114.97	121.36
2	D	225	PRO	CA-C-N	5.65	126.91	119.84
2	D	225	PRO	C-N-CA	5.65	126.91	119.84
3	G	237	LYS	CB-CA-C	5.65	121.52	110.67
1	B	245	LEU	N-CA-C	5.65	117.11	111.07
2	D	368	TYR	N-CA-C	5.64	117.43	111.28
1	C	230	ILE	CA-C-N	-5.64	115.33	123.11
1	C	230	ILE	C-N-CA	-5.64	115.33	123.11
1	B	103	LEU	N-CA-C	-5.62	106.55	113.41
1	A	194	ASP	CA-CB-CG	5.61	118.21	112.60
1	B	304	ARG	NE-CZ-NH2	5.61	124.25	119.20
1	B	433	TYR	CA-C-N	-5.61	116.36	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	433	TYR	C-N-CA	-5.61	116.36	122.59
2	E	120	ALA	CA-C-N	5.61	126.85	119.84
2	E	120	ALA	C-N-CA	5.61	126.85	119.84
2	F	113	PHE	CA-CB-CG	-5.60	108.20	113.80
2	D	356	ARG	CD-NE-CZ	-5.60	116.56	124.40
1	B	127	ARG	CD-NE-CZ	5.59	132.22	124.40
1	C	362	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	C	381	ARG	CD-NE-CZ	5.58	132.22	124.40
2	F	282	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	B	151	LYS	N-CA-C	5.57	117.79	111.11
2	F	96	ASN	N-CA-C	5.57	117.71	110.53
2	E	219	TYR	N-CA-C	5.56	118.47	109.40
1	A	200	TYR	CA-CB-CG	-5.56	103.89	113.90
2	E	336	SER	N-CA-C	5.56	117.96	108.90
2	F	473	LEU	N-CA-C	-5.56	106.00	112.89
1	C	74	VAL	CB-CA-C	5.56	117.80	110.91
1	A	271	LEU	CA-C-O	5.55	125.77	119.27
1	A	164	ARG	CA-C-O	-5.55	113.57	120.57
2	D	30	PRO	N-CA-CB	5.55	108.47	103.08
2	E	96	ASN	CA-CB-CG	5.55	118.15	112.60
2	E	95	MET	CA-C-N	5.54	132.12	121.54
2	E	95	MET	C-N-CA	5.54	132.12	121.54
1	A	420	ARG	NE-CZ-NH1	-5.54	115.96	121.50
2	E	216	ALA	CA-C-N	-5.54	115.36	123.00
2	E	216	ALA	C-N-CA	-5.54	115.36	123.00
2	F	95	MET	O-C-N	-5.51	116.50	123.17
2	F	88	PRO	N-CA-CB	5.51	108.80	103.51
2	E	239	VAL	N-CA-CB	-5.50	104.84	110.62
1	C	366	ASN	CA-C-O	5.50	126.64	120.92
1	A	233	SER	N-CA-CB	-5.50	102.13	110.77
2	F	215	VAL	N-CA-C	5.50	116.04	108.12
1	B	141	SER	CA-C-O	-5.49	114.97	120.96
2	D	164	VAL	N-CA-C	-5.48	105.16	110.42
2	D	179	GLY	CA-C-O	-5.48	116.24	121.83
1	A	92	GLY	N-CA-C	-5.48	108.46	115.42
2	D	215	VAL	CA-C-O	-5.47	113.94	120.78
1	A	367	VAL	CB-CA-C	5.47	119.53	112.14
2	E	260	ARG	NE-CZ-NH1	-5.47	116.03	121.50
1	A	235	THR	N-CA-C	5.46	118.51	110.59
1	C	423	ARG	CD-NE-CZ	5.46	132.05	124.40
2	E	83	ARG	NE-CZ-NH1	-5.45	116.06	121.50
1	A	263	HIS	CA-CB-CG	-5.44	108.36	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	GLN	N-CA-C	5.44	118.70	111.30
2	E	127	SER	N-CA-C	-5.44	101.67	110.32
1	A	466	ASN	OD1-CG-ND2	5.44	128.04	122.60
1	C	106	ARG	CA-CB-CG	-5.43	103.23	114.10
2	E	272	LEU	N-CA-C	-5.43	106.96	113.21
2	D	155	PHE	CA-CB-CG	5.43	119.23	113.80
1	A	74	VAL	N-CA-CB	-5.43	105.47	111.66
2	F	12	ARG	CD-NE-CZ	-5.42	116.81	124.40
1	B	40	ARG	NE-CZ-NH1	5.41	126.91	121.50
1	C	285	LEU	N-CA-C	-5.40	106.47	113.16
2	E	331	ALA	CA-C-O	5.40	128.23	120.51
1	A	93	ALA	CA-C-N	-5.39	114.85	122.34
1	A	93	ALA	C-N-CA	-5.39	114.85	122.34
2	E	257	ASN	CA-CB-CG	5.38	117.98	112.60
2	E	83	ARG	CD-NE-CZ	-5.38	116.87	124.40
2	E	282	GLN	CA-C-N	5.38	125.02	119.05
2	E	282	GLN	C-N-CA	5.38	125.02	119.05
2	D	119	GLU	CA-C-O	-5.38	115.70	121.56
2	E	196	LEU	N-CA-C	-5.38	105.08	111.69
3	G	222	THR	N-CA-C	-5.38	105.50	111.36
2	D	232	VAL	N-CA-CB	5.37	120.10	111.23
1	C	33	SER	CA-C-O	-5.37	115.48	121.23
2	D	198	HIS	CA-CB-CG	-5.37	108.43	113.80
2	E	297	THR	CB-CA-C	-5.36	101.16	111.78
2	E	200	MET	N-CA-C	-5.36	105.09	111.69
2	F	408	ARG	NE-CZ-NH2	5.36	124.02	119.20
2	F	121	PRO	N-CA-CB	5.36	107.96	103.25
1	C	123	SER	N-CA-C	5.35	117.99	109.96
2	E	137	ILE	CA-C-O	5.35	126.95	120.74
2	D	222	MET	CB-CA-C	-5.35	98.50	110.21
2	F	366	GLU	N-CA-C	-5.34	105.36	111.07
2	E	417	PRO	CB-CA-C	-5.33	104.87	111.11
1	A	372	SER	N-CA-CB	5.33	120.18	110.95
1	A	398	ARG	NE-CZ-NH1	-5.33	116.17	121.50
2	E	96	ASN	N-CA-CB	-5.33	101.48	110.49
1	C	304	ARG	NE-CZ-NH2	5.32	123.99	119.20
2	E	393	MET	N-CA-C	5.32	122.13	110.80
2	F	393	MET	N-CA-C	5.32	119.82	113.23
2	F	330	ASP	CA-CB-CG	-5.32	107.28	112.60
1	C	299	PHE	N-CA-C	-5.31	105.18	110.97
2	F	41	ARG	CG-CD-NE	5.31	123.68	112.00
2	E	398	GLU	N-CA-C	-5.30	105.44	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	309	ALA	N-CA-C	-5.30	102.01	109.96
1	A	134	PRO	N-CA-C	-5.29	102.88	111.14
1	B	478	ALA	N-CA-C	5.29	117.05	111.28
1	B	259	ASP	CA-CB-CG	-5.29	107.31	112.60
2	F	87	GLY	CA-C-N	5.29	124.90	119.56
2	F	87	GLY	C-N-CA	5.29	124.90	119.56
2	F	76	LEU	N-CA-C	5.29	117.14	108.52
2	D	327	ALA	CA-C-O	-5.29	113.09	119.49
2	F	423	VAL	CB-CA-C	-5.28	101.70	111.79
2	F	387	ILE	CB-CA-C	-5.28	105.10	112.02
1	C	75	VAL	N-CA-C	5.28	115.69	107.99
1	C	48	GLN	CA-C-O	-5.27	115.20	121.16
1	A	52	MET	CA-C-N	-5.27	115.33	122.92
1	A	52	MET	C-N-CA	-5.27	115.33	122.92
1	C	136	ILE	CA-C-N	5.27	124.55	120.33
1	C	136	ILE	C-N-CA	5.27	124.55	120.33
2	D	118	ALA	CA-C-O	-5.27	115.59	121.23
2	D	160	VAL	N-CA-CB	5.27	118.01	112.21
1	B	279	ARG	NE-CZ-NH1	5.27	126.77	121.50
2	D	411	GLN	CA-C-O	5.27	126.32	120.63
2	D	432	VAL	CA-C-N	5.27	125.17	119.85
2	D	432	VAL	C-N-CA	5.27	125.17	119.85
1	C	411	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	318	GLY	N-CA-C	-5.26	108.58	115.47
1	B	148	THR	N-CA-C	-5.26	107.00	113.41
1	C	127	ARG	NE-CZ-NH1	-5.25	116.25	121.50
2	E	72	GLY	N-CA-C	-5.25	108.44	114.69
2	E	358	MET	N-CA-CB	5.25	116.93	110.53
1	B	116	ASP	N-CA-C	-5.25	106.66	113.16
2	D	322	PRO	N-CA-C	-5.24	105.98	113.47
1	C	336	ALA	CA-C-O	5.24	126.72	121.07
2	E	122	GLU	CA-CB-CG	5.24	124.57	114.10
1	B	287	ARG	CA-C-N	5.23	125.77	120.38
1	B	287	ARG	C-N-CA	5.23	125.77	120.38
1	C	336	ALA	N-CA-C	5.23	117.67	110.35
1	C	405	GLN	CA-C-O	5.22	127.98	120.51
3	G	237	LYS	N-CA-C	-5.22	105.76	111.82
2	E	171	ASN	OD1-CG-ND2	5.20	127.80	122.60
2	F	100	GLU	CA-C-O	-5.20	115.82	120.19
2	E	330	ASP	CA-CB-CG	-5.20	107.40	112.60
2	F	19	ALA	CA-C-N	-5.20	116.04	123.11
2	F	19	ALA	C-N-CA	-5.20	116.04	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	59	ARG	CD-NE-CZ	-5.20	117.12	124.40
1	B	309	ALA	CA-C-O	-5.20	115.90	121.56
2	D	354	THR	CA-C-O	-5.19	115.53	121.40
2	F	178	GLY	CA-C-N	-5.19	114.30	122.92
2	F	178	GLY	C-N-CA	-5.19	114.30	122.92
2	E	173	VAL	N-CA-C	-5.19	105.35	111.00
2	F	416	GLN	CA-C-N	5.18	125.98	120.13
2	F	416	GLN	C-N-CA	5.18	125.98	120.13
2	F	225	PRO	N-CA-C	-5.18	104.38	110.70
1	B	397	TYR	N-CA-C	-5.17	107.52	113.88
1	B	149	GLY	N-CA-C	-5.17	108.49	115.21
3	G	250	PHE	CA-CB-CG	-5.16	108.64	113.80
1	B	130	GLY	O-C-N	-5.16	116.00	122.70
2	D	224	GLU	CA-C-N	5.16	123.37	119.66
2	D	224	GLU	C-N-CA	5.16	123.37	119.66
2	F	418	PHE	CA-CB-CG	5.16	118.96	113.80
2	F	257	ASN	OD1-CG-ND2	5.15	127.75	122.60
1	B	230	ILE	CA-C-O	-5.15	115.90	121.92
2	D	268	VAL	CA-C-O	5.14	123.42	118.90
2	D	165	LEU	N-CA-CB	5.14	117.67	110.12
2	E	400	ASP	CA-CB-CG	-5.14	107.46	112.60
2	F	281	TYR	CA-C-N	5.14	127.78	120.49
2	F	281	TYR	C-N-CA	5.14	127.78	120.49
2	F	170	ILE	N-CA-C	-5.13	105.38	110.62
2	F	200	MET	CA-C-O	5.13	125.86	120.42
2	F	200	MET	N-CA-CB	-5.13	102.57	110.16
2	D	475	GLU	N-CA-CB	5.12	119.21	110.50
1	A	219	ARG	CD-NE-CZ	5.12	131.57	124.40
2	E	250	ASP	CA-CB-CG	-5.11	107.49	112.60
2	F	388	ILE	N-CA-CB	5.11	116.86	110.47
2	E	226	PRO	CA-C-N	5.11	125.75	120.03
2	E	226	PRO	C-N-CA	5.11	125.75	120.03
2	D	175	LYS	N-CA-C	5.11	116.85	111.28
2	E	439	LYS	O-C-N	5.10	127.33	122.07
1	B	219	ARG	NE-CZ-NH1	-5.10	116.40	121.50
2	E	56	SER	CA-C-N	-5.10	115.29	122.94
2	E	56	SER	C-N-CA	-5.10	115.29	122.94
2	F	330	ASP	N-CA-C	-5.10	107.19	113.41
1	C	296	GLY	N-CA-C	-5.09	109.07	114.67
2	E	251	VAL	CB-CA-C	-5.09	105.99	111.59
1	C	483	ILE	N-CA-C	-5.09	105.54	110.42
2	D	454	GLU	CB-CA-C	-5.08	102.83	110.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	415	SER	CA-C-O	-5.08	115.95	121.89
3	G	44	TYR	CA-CB-CG	5.08	123.04	113.90
2	F	433	PRO	N-CA-CB	5.07	108.06	103.34
1	A	101	GLU	N-CA-C	5.07	118.93	112.34
2	D	357	ILE	N-CA-CB	5.07	119.60	112.15
2	D	361	ASN	CA-CB-CG	-5.07	107.53	112.60
1	A	400	VAL	N-CA-C	5.07	119.49	112.35
2	F	101	PRO	N-CA-CB	5.06	107.75	103.35
1	B	457	GLU	N-CA-C	5.06	116.27	109.24
2	E	125	GLU	CA-C-O	5.06	124.38	118.97
1	B	274	GLN	N-CA-C	-5.05	105.85	111.36
2	D	170	ILE	N-CA-C	-5.05	105.62	110.72
2	E	107	PRO	N-CA-CB	5.05	107.80	103.31
1	B	349	GLN	N-CA-CB	5.05	120.47	111.69
1	B	487	GLY	N-CA-C	-5.05	108.36	115.32
1	A	178	ILE	CB-CA-C	-5.03	105.44	111.88
1	B	94	ILE	N-CA-C	-5.03	102.58	109.37
1	B	222	ASP	CA-C-N	-5.03	114.24	122.54
1	B	222	ASP	C-N-CA	-5.03	114.24	122.54
2	F	85	PRO	N-CA-CB	5.03	107.65	103.17
1	B	141	SER	CB-CA-C	-5.03	102.30	109.84
2	E	64	ASP	O-C-N	-5.03	117.98	123.26
1	B	374	VAL	CB-CA-C	-5.03	104.56	110.84
2	E	161	GLY	N-CA-C	5.03	125.09	113.18
1	C	145	PRO	N-CA-CB	5.02	108.11	103.39
1	C	270	ASP	CA-CB-CG	5.02	117.62	112.60
2	F	417	PRO	CB-CA-C	-5.02	105.24	111.11
1	A	508	PHE	N-CA-C	5.01	117.40	111.33
1	B	391	LYS	N-CA-C	-5.01	106.00	111.82
1	A	224	ASP	CA-CB-CG	5.01	117.61	112.60
1	B	167	ILE	CA-C-N	-5.01	115.98	122.94
1	B	167	ILE	C-N-CA	-5.01	115.98	122.94
1	C	136	ILE	N-CA-C	5.01	115.24	110.53
1	A	191	ASP	N-CA-C	-5.00	107.22	113.38
1	C	209	LYS	N-CA-CB	-5.00	102.72	110.57

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3715	0	3813	172	0
1	B	3656	0	3764	153	0
1	C	3748	0	3843	165	0
2	D	3539	0	3593	155	0
2	E	3530	0	3587	200	0
2	F	3530	0	3587	124	0
3	G	945	0	1019	49	0
4	D	27	0	12	1	0
All	All	22690	0	23218	979	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (979) 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	1.07
3:G:39:LYS:HB2	3:G:40:PRO:HD3	1.35	1.05
1:C:404:ALA:C	1:C:406:PHE:H	1.64	0.95
2:E:223:ASN:HD22	2:E:223:ASN:H	1.00	0.95
2:F:223:ASN:HD22	2:F:223:ASN:H	1.07	0.94
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.48	0.92
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.52	0.92
1:C:127:ARG:NH1	1:C:255:GLU:HB2	1.84	0.91
1:C:215:GLN:HG3	2:F:356:ARG:HH22	1.34	0.90
1:C:30:ARG:HE	1:C:87:ILE:HD11	1.37	0.89
2:E:89:GLU:HG2	2:E:110:THR:HG22	1.56	0.88
2:D:84:ILE:HD12	2:D:95:MET:HE1	1.57	0.87
1:A:215:GLN:HG3	2:D:356:ARG:NH1	1.92	0.85
2:E:223:ASN:H	2:E:223:ASN:ND2	1.72	0.83
1:A:400:VAL:HG12	1:A:418:LEU:HD21	1.60	0.83
1:B:456:LEU:HD12	1:B:457:GLU:H	1.43	0.82
1:C:211:SER:HB3	2:F:126:MET:HE2	1.61	0.82
2:E:132:ILE:HD12	2:E:145:PRO:HB3	1.61	0.81
1:B:141:SER:O	1:B:143:ARG:HD2	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:GLN:HG3	1:B:199:LEU:HB3	1.65	0.78
2:D:282:GLN:H	2:D:282:GLN:HE21	1.30	0.78
2:D:136:GLY:HA3	2:D:431:LEU:HD13	1.66	0.78
1:A:215:GLN:HG3	2:D:356:ARG:HH12	1.48	0.78
2:D:139:VAL:HG13	2:D:414:LEU:HD22	1.65	0.77
2:D:404:VAL:O	2:D:408:ARG:HG3	1.84	0.77
2:E:370:VAL:HG21	2:E:438:ILE:HG22	1.65	0.77
2:F:130:GLN:HB3	2:F:357:ILE:HD11	1.67	0.77
2:D:53:LEU:HD12	2:D:57:THR:HG22	1.66	0.76
2:E:394:ASP:C	2:E:396:LEU:H	1.93	0.76
1:B:379:GLN:HB3	1:B:384:LYS:HE2	1.68	0.76
1:A:392:LEU:HG	1:A:396:GLN:HE21	1.50	0.76
1:C:52:MET:HE3	1:C:95:VAL:HG22	1.68	0.75
3:G:2:THR:HG22	3:G:4:LYS:H	1.51	0.75
2:E:89:GLU:HG3	2:E:109:LYS:O	1.87	0.74
2:E:96:ASN:HB3	2:E:100:GLU:H	1.52	0.74
2:D:433:PRO:HG2	2:D:436:GLU:HG2	1.70	0.74
2:D:223:ASN:H	2:D:223:ASN:HD22	1.35	0.74
2:E:390:ILE:HG22	2:E:391:LEU:HD23	1.70	0.73
1:B:283:LEU:CD1	2:E:277:SER:HB3	2.19	0.72
2:F:89:GLU:HG3	2:F:109:LYS:O	1.89	0.72
2:E:345:TYR:HA	2:E:346:PRO:C	2.13	0.72
1:B:283:LEU:HD12	2:E:277:SER:HB3	1.72	0.72
2:E:139:VAL:HG13	2:E:414:LEU:HD22	1.71	0.72
1:B:180:ILE:HD11	1:B:216:LEU:HD21	1.71	0.71
2:E:38:VAL:HG21	2:E:45:LEU:HD23	1.71	0.71
2:D:96:ASN:HB2	2:D:100:GLU:H	1.56	0.70
1:C:34:ILE:HD11	1:C:79:ASP:HB2	1.72	0.70
2:E:183:PHE:HB3	2:E:217:LEU:HD22	1.73	0.70
1:A:479:LEU:HA	1:A:482:LYS:HE3	1.73	0.70
1:C:211:SER:O	1:C:215:GLN:HG2	1.91	0.70
2:D:200:MET:HE3	2:D:215:VAL:HG21	1.74	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	1.73	0.70
1:A:97:VAL:HA	1:A:126:ARG:HH21	1.56	0.70
1:B:452:TYR:OH	1:B:498:LYS:HG3	1.92	0.70
2:F:223:ASN:HD22	2:F:223:ASN:N	1.85	0.69
2:E:321:ALA:HB3	2:E:322:PRO:HD3	1.75	0.69
1:A:211:SER:N	2:D:126:MET:HE2	2.07	0.69
2:E:105:ARG:CZ	2:E:208:LEU:HD23	2.23	0.69
2:F:89:GLU:HG2	2:F:110:THR:HG22	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:433:PRO:HD2	2:E:436:GLU:HB2	1.74	0.68
1:C:385:GLN:OE1	1:C:488:LYS:HG2	1.93	0.68
1:C:418:LEU:O	1:C:422:VAL:HG23	1.94	0.68
2:E:313:PRO:HD2	2:E:322:PRO:HG3	1.76	0.68
2:F:252:LEU:HD23	2:F:305:THR:HB	1.75	0.68
1:A:440:GLU:O	1:A:444:VAL:HG13	1.94	0.67
2:F:409:LYS:HD3	2:F:457:PHE:CE2	2.30	0.67
1:B:156:LEU:HD22	1:B:391:LYS:HD2	1.77	0.67
1:A:44:LEU:O	1:A:47:VAL:HG22	1.94	0.67
1:C:59:LEU:HD23	1:C:82:ILE:HD11	1.77	0.67
2:E:136:GLY:HA3	2:E:431:LEU:HD13	1.77	0.67
1:C:48:GLN:HB3	2:D:68:GLY:HA2	1.77	0.67
2:D:223:ASN:HD22	2:D:223:ASN:N	1.89	0.67
2:F:314:ALA:O	2:F:315:ASP:HB2	1.95	0.66
1:C:173:THR:HG22	1:C:354:THR:HG22	1.77	0.66
3:G:23:MET:SD	3:G:232:MET:HE2	2.35	0.66
3:G:39:LYS:CB	3:G:40:PRO:HD3	2.15	0.66
1:A:134:PRO:O	1:A:139:ARG:NH2	2.27	0.66
1:A:376:SER:HB3	1:A:384:LYS:HE2	1.78	0.66
3:G:24:LYS:HE3	3:G:233:ASP:HB2	1.78	0.66
1:A:97:VAL:HB	1:A:98:PRO:HD2	1.76	0.65
2:F:344:ILE:HG23	2:F:415:SER:HB3	1.79	0.65
1:B:44:LEU:HB3	1:B:47:VAL:HG22	1.77	0.65
1:C:362:ARG:HA	1:C:363:PRO:C	2.21	0.65
1:A:383:MET:HE2	1:A:438:ILE:HD11	1.77	0.65
2:E:359:ASP:OD2	2:E:361:ASN:HB2	1.96	0.65
2:F:200:MET:HG3	2:F:205:VAL:CG2	2.27	0.65
2:F:80:ALA:HB1	2:F:81:PRO:CD	2.26	0.65
1:C:44:LEU:O	1:C:47:VAL:HG22	1.97	0.65
2:D:167:MET:HB3	2:D:420:VAL:HG11	1.78	0.65
2:F:136:GLY:HA3	2:F:431:LEU:CD1	2.26	0.65
1:B:437:ALA:O	1:B:440:GLU:N	2.30	0.64
3:G:20:THR:HA	3:G:232:MET:HE3	1.77	0.64
1:B:362:ARG:HA	1:B:363:PRO:C	2.22	0.64
1:A:376:SER:C	1:A:378:ALA:H	2.03	0.64
2:F:200:MET:HG3	2:F:205:VAL:HG23	1.80	0.64
2:F:223:ASN:H	2:F:223:ASN:ND2	1.85	0.64
2:D:223:ASN:H	2:D:223:ASN:ND2	1.93	0.64
1:C:202:ILE:HG12	1:C:230:ILE:HD12	1.80	0.64
2:F:275:ILE:HD13	3:G:271:ALA:CB	2.28	0.64
1:A:471:HIS:CE1	1:A:475:GLN:HG3	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:94:ILE:HG22	2:F:102:ILE:HD11	1.80	0.64
1:B:188:ARG:HH21	1:B:437:ALA:HB2	1.62	0.64
1:C:99:VAL:HG22	1:C:253:MET:HA	1.78	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:F:136:GLY:HA3	2:F:431:LEU:HD12	1.80	0.63
1:C:436:MET:HE3	1:C:469:LEU:HD21	1.79	0.63
2:D:200:MET:HB3	2:D:206:ILE:HG13	1.79	0.63
1:C:419:SER:O	1:C:423:ARG:HG2	1.98	0.63
2:E:346:PRO:HG3	2:E:418:PHE:CZ	2.33	0.63
2:E:425:THR:O	2:E:427:HIS:ND1	2.20	0.63
2:E:443:GLN:HG2	2:E:448:GLU:OE2	1.98	0.63
2:F:363:VAL:HG23	2:F:367:HIS:HB3	1.81	0.63
1:B:389:THR:HA	1:B:392:LEU:CD1	2.29	0.63
1:C:52:MET:HE2	1:C:76:PHE:HE2	1.62	0.63
2:E:394:ASP:C	2:E:396:LEU:N	2.54	0.63
1:B:390:MET:HE1	1:B:428:LEU:HD21	1.80	0.63
2:E:298:THR:HG23	2:E:303:SER:HB3	1.81	0.63
2:E:139:VAL:CG1	2:E:414:LEU:HD22	2.28	0.63
2:E:316:ASP:OD2	3:G:254:ARG:NH1	2.31	0.62
2:E:400:ASP:O	2:E:404:VAL:HG23	1.98	0.62
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.34	0.62
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.34	0.62
2:E:204:GLY:O	2:E:206:ILE:N	2.32	0.62
1:A:341:ASN:O	1:A:345:ILE:HG13	1.99	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	1.80	0.62
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.63	0.62
1:B:184:ILE:HG22	1:B:435:PRO:HG2	1.81	0.62
1:C:404:ALA:C	1:C:406:PHE:N	2.44	0.62
1:C:151:LYS:HE3	1:C:430:GLN:HG3	1.82	0.62
1:C:292:GLU:O	1:C:293:ALA:HB3	2.00	0.62
2:D:473:LEU:C	2:D:475:GLU:H	2.08	0.62
1:A:376:SER:C	1:A:378:ALA:N	2.55	0.61
2:E:422:GLU:HG2	2:E:427:HIS:O	1.99	0.61
2:D:396:LEU:HD22	2:D:400:ASP:CB	2.30	0.61
1:C:408:SER:O	1:C:409:ASP:C	2.44	0.61
2:E:158:ALA:C	2:E:160:VAL:H	2.08	0.61
1:A:439:GLU:HG2	1:A:484:ARG:HB2	1.83	0.61
2:E:201:ILE:HD13	2:E:208:LEU:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:397:SER:C	2:E:399:GLU:N	2.57	0.61
1:A:270:ASP:OD1	1:A:273:LYS:HG3	2.01	0.61
2:D:63:MET:HE3	2:D:228:ALA:HA	1.83	0.61
2:D:89:GLU:HG2	2:D:110:THR:HG22	1.83	0.61
1:A:394:LEU:HD11	1:A:428:LEU:HD11	1.82	0.61
1:B:422:VAL:O	1:B:426:GLU:HG2	2.00	0.61
2:F:275:ILE:HD13	3:G:271:ALA:HB2	1.81	0.61
1:A:121:ILE:HD13	1:A:121:ILE:H	1.66	0.60
1:B:389:THR:HA	1:B:392:LEU:HD12	1.82	0.60
1:A:283:LEU:HD21	1:A:289:PRO:HB3	1.82	0.60
2:D:93:ARG:HG3	2:D:93:ARG:HH11	1.66	0.60
1:A:40:ARG:HH11	1:A:40:ARG:HG3	1.67	0.60
2:E:397:SER:H	2:E:400:ASP:HB2	1.66	0.60
1:B:479:LEU:HD11	1:B:497:LEU:HD13	1.83	0.60
2:E:149:GLY:HA2	2:E:304:ILE:O	2.02	0.60
1:B:51:GLU:HA	1:B:94:ILE:HA	1.83	0.60
1:B:102:GLU:HG3	1:B:122:GLY:O	2.00	0.60
1:C:99:VAL:HG13	1:C:256:TYR:HB2	1.83	0.60
1:C:313:ASN:OD1	1:C:316:PHE:HD1	1.85	0.60
2:E:32:ILE:O	2:E:33:LEU:HB2	2.02	0.60
1:A:157:VAL:N	1:A:158:PRO:CD	2.65	0.60
1:A:166:LEU:HA	1:A:325:PRO:HD2	1.83	0.60
3:G:239:ALA:O	3:G:243:ILE:HG13	2.02	0.60
1:A:52:MET:O	1:A:91:THR:HG23	2.01	0.60
2:F:63:MET:HE1	2:F:97:VAL:HG11	1.82	0.60
1:C:407:GLY:HA2	1:C:410:LEU:HD11	1.84	0.60
1:C:433:TYR:C	1:C:435:PRO:HD3	2.26	0.60
1:A:457:GLU:CB	1:A:460:LYS:HD3	2.32	0.59
2:D:317:LEU:HD22	2:D:326:PHE:HZ	1.67	0.59
2:E:200:MET:HB3	2:E:205:VAL:HG23	1.84	0.59
2:E:226:PRO:HB3	2:E:267:GLU:HB2	1.84	0.59
2:F:122:GLU:HB2	2:F:125:GLU:HG3	1.84	0.59
1:A:432:GLN:HB3	1:A:433:TYR:CD2	2.37	0.59
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.37	0.59
1:C:215:GLN:HG3	2:F:356:ARG:NH2	2.11	0.59
2:D:393:MET:HE3	2:D:404:VAL:HG21	1.83	0.59
1:B:136:ILE:HG13	2:F:190:THR:HG23	1.84	0.59
1:B:499:GLU:O	1:B:502:THR:HB	2.03	0.59
2:D:263:GLN:O	2:D:267:GLU:HG3	2.03	0.59
2:E:408:ARG:O	2:E:412:ARG:HG3	2.02	0.59
1:B:391:LYS:O	1:B:395:ALA:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:13:ILE:HG22	3:G:243:ILE:HG12	1.84	0.59
1:B:411:ASP:HB3	1:B:414:THR:OG1	2.02	0.59
2:E:419:GLN:HG3	2:E:429:GLY:HA3	1.84	0.59
2:F:29:LEU:HD12	2:F:30:PRO:HD2	1.85	0.59
1:A:472:VAL:HG23	1:A:480:LEU:HD11	1.85	0.59
1:B:452:TYR:O	1:B:453:LEU:HD23	2.03	0.59
1:C:406:PHE:O	1:C:408:SER:N	2.36	0.59
2:E:223:ASN:ND2	2:E:223:ASN:N	2.46	0.59
3:G:39:LYS:HB2	3:G:40:PRO:CD	2.24	0.59
1:C:140:ILE:HD11	1:C:143:ARG:NH2	2.18	0.58
1:B:400:VAL:HB	1:B:418:LEU:HD21	1.85	0.58
1:B:434:SER:N	1:B:435:PRO:HD3	2.18	0.58
1:C:464:PHE:CE1	1:C:505:LEU:HD23	2.39	0.58
2:D:186:VAL:HG13	2:D:232:VAL:HG23	1.85	0.58
1:B:170:ASP:O	1:B:175:LYS:HE2	2.03	0.58
2:F:105:ARG:NH1	2:F:208:LEU:HD23	2.18	0.58
1:B:438:ILE:O	1:B:442:VAL:HG22	2.02	0.58
1:C:102:GLU:OE2	1:C:123:SER:HA	2.03	0.58
1:C:344:SER:O	2:D:222:MET:HE1	2.04	0.58
2:E:95:MET:CG	2:E:99:GLY:HA2	2.34	0.58
2:F:395:GLU:OE2	3:G:77:LEU:HA	2.03	0.58
2:E:85:PRO:HD2	2:E:95:MET:HE2	1.85	0.58
1:B:352:LEU:HA	1:B:364:ALA:O	2.04	0.58
1:A:219:ARG:HH11	1:A:219:ARG:HB2	1.69	0.57
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.86	0.57
1:C:78:ASN:ND2	1:C:80:LYS:HD3	2.19	0.57
2:E:267:GLU:O	2:E:271:LEU:HG	2.05	0.57
1:C:215:GLN:HE22	2:F:128:VAL:HA	1.68	0.57
1:C:374:VAL:HG11	1:C:378:ALA:HB2	1.85	0.57
2:E:105:ARG:NH2	2:E:208:LEU:HA	2.20	0.57
2:E:126:MET:HE1	2:E:297:THR:HG21	1.86	0.57
3:G:17:GLN:HB2	3:G:239:ALA:HB1	1.85	0.57
1:C:107:VAL:HG12	1:C:115:ILE:HD11	1.86	0.57
2:E:246:GLN:HA	2:E:246:GLN:NE2	2.19	0.57
2:F:96:ASN:HD22	2:F:100:GLU:HB2	1.68	0.57
1:C:405:GLN:C	1:C:406:PHE:HD1	2.11	0.57
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.85	0.57
2:E:138:LYS:O	2:E:142:LEU:HB3	2.04	0.57
1:B:357:PHE:CE1	1:B:362:ARG:HD3	2.40	0.57
1:C:156:LEU:HD13	1:C:367:VAL:HG22	1.86	0.57
1:C:173:THR:CG2	1:C:354:THR:HG22	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:440:GLY:O	2:F:444:ILE:HG13	2.04	0.57
1:A:185:ASN:O	1:A:188:ARG:HG3	2.05	0.57
1:B:51:GLU:OE2	1:B:90:ARG:HB3	2.05	0.57
1:C:211:SER:HB3	2:F:126:MET:CE	2.34	0.57
1:C:187:LYS:HE2	1:C:191:ASP:OD2	2.05	0.56
1:B:62:MET:HE3	1:B:64:LEU:HD13	1.87	0.56
1:C:52:MET:HE2	1:C:76:PHE:CE2	2.41	0.56
2:D:431:LEU:C	2:D:431:LEU:HD12	2.29	0.56
2:E:155:PHE:CE1	2:E:310:ILE:HD12	2.40	0.56
2:F:324:THR:O	2:F:324:THR:HG22	2.05	0.56
1:A:450:ARG:NH2	1:A:494:ASP:OD2	2.38	0.56
2:E:122:GLU:N	2:E:125:GLU:OE2	2.37	0.56
1:B:351:PHE:CE1	1:B:369:LEU:HB3	2.40	0.56
1:C:184:ILE:HG22	1:C:435:PRO:HG2	1.87	0.56
1:C:218:LYS:HD2	2:F:128:VAL:HG21	1.88	0.56
2:E:433:PRO:HG2	2:E:436:GLU:HG2	1.86	0.56
1:B:393:GLU:OE1	1:B:424:LEU:HD11	2.05	0.56
2:E:174:ALA:CB	2:E:214:LYS:HD3	2.35	0.56
1:A:159:ILE:HD12	1:A:165:GLU:HG2	1.88	0.56
1:B:358:TYR:C	1:B:360:GLY:H	2.12	0.56
2:E:92:GLY:N	2:E:215:VAL:O	2.29	0.56
3:G:20:THR:HG21	3:G:236:SER:N	2.21	0.56
1:A:224:ASP:CG	1:A:227:LYS:HE3	2.31	0.56
1:A:347:ASP:OD1	2:E:191:ARG:NH1	2.39	0.56
2:D:366:GLU:HG3	2:D:442:GLN:HE22	1.71	0.56
2:F:10:THR:HG23	2:F:76:LEU:HD12	1.88	0.56
2:E:138:LYS:HG3	2:E:416:GLN:OE1	2.06	0.56
1:C:394:LEU:HD22	1:C:398:ARG:HH21	1.71	0.55
2:E:224:GLU:O	2:E:229:ARG:NH1	2.32	0.55
1:A:99:VAL:CG2	1:A:253:MET:HA	2.37	0.55
1:A:107:VAL:HG12	1:A:115:ILE:HD11	1.87	0.55
2:D:255:ILE:HG21	2:D:258:ILE:HD13	1.87	0.55
1:C:102:GLU:HG2	1:C:122:GLY:O	2.06	0.55
1:C:219:ARG:HD3	1:C:433:TYR:CE1	2.41	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
1:C:442:VAL:CG1	1:C:489:ILE:HD11	2.36	0.55
2:E:263:GLN:O	2:E:267:GLU:HG3	2.07	0.55
1:B:423:ARG:HE	1:B:458:PRO:HD3	1.72	0.55
1:B:482:LYS:O	1:B:486:ASP:N	2.37	0.55
1:C:52:MET:HG3	1:C:61:GLY:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:14:VAL:O	2:F:71:ARG:HG2	2.05	0.55
2:F:98:ILE:HG13	2:F:100:GLU:HG3	1.88	0.55
2:D:83:ARG:HA	2:D:114:ALA:O	2.07	0.55
1:B:270:ASP:OD1	1:B:273:LYS:HG3	2.07	0.55
1:B:423:ARG:HE	1:B:458:PRO:HG3	1.71	0.55
2:D:142:LEU:HD22	2:D:441:PHE:CD2	2.42	0.55
2:E:244:ARG:HG3	2:E:303:SER:N	2.22	0.54
2:F:63:MET:CE	2:F:97:VAL:HG11	2.37	0.54
1:A:209:LYS:HE3	1:A:211:SER:HB2	1.88	0.54
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.89	0.54
2:D:471:ASP:O	2:D:474:ALA:N	2.39	0.54
2:E:201:ILE:CD1	2:E:208:LEU:HD11	2.38	0.54
2:E:396:LEU:HB3	2:E:401:LYS:HG2	1.88	0.54
1:B:80:LYS:HG3	1:B:81:LEU:HD23	1.88	0.54
1:C:404:ALA:O	1:C:406:PHE:N	2.37	0.54
2:D:473:LEU:O	2:D:475:GLU:N	2.40	0.54
2:E:397:SER:O	2:E:401:LYS:HG3	2.08	0.54
1:B:180:ILE:O	1:B:181:ASP:C	2.47	0.54
1:B:347:ASP:HB3	1:B:374:VAL:HG22	1.88	0.54
1:B:441:GLN:O	1:B:445:ILE:HG12	2.08	0.54
1:C:390:MET:HE3	1:C:424:LEU:HD22	1.89	0.54
2:D:167:MET:CB	2:D:420:VAL:HG11	2.38	0.54
1:A:452:TYR:OH	1:A:498:LYS:HG3	2.08	0.54
1:C:91:THR:HG22	1:C:93:ALA:H	1.72	0.54
2:E:218:VAL:HG11	2:E:235:THR:CG2	2.38	0.54
1:B:114:ALA:HB2	1:B:121:ILE:HD11	1.89	0.54
2:D:412:ARG:HH11	2:D:412:ARG:HG3	1.73	0.54
2:E:77:ASP:OD1	2:E:79:GLY:N	2.34	0.54
1:A:170:ASP:O	1:A:175:LYS:HE2	2.08	0.54
2:E:174:ALA:HB2	2:E:214:LYS:HD3	1.90	0.54
1:A:150:ILE:HA	1:A:430:GLN:OE1	2.08	0.54
1:A:373:ARG:HG3	1:A:373:ARG:HH11	1.72	0.54
1:C:239:ALA:HB1	1:C:241:PRO:HD2	1.90	0.54
2:F:32:ILE:O	2:F:33:LEU:HB2	2.06	0.54
1:A:479:LEU:HD21	1:A:493:SER:HB3	1.89	0.54
3:G:81:ILE:HG22	3:G:82:HIS:HD2	1.73	0.54
2:D:381:TYR:HE2	2:D:411:GLN:HE22	1.56	0.54
2:D:388:ILE:HD12	2:D:393:MET:SD	2.48	0.54
2:D:396:LEU:HD22	2:D:400:ASP:HB3	1.89	0.54
1:A:463:LYS:HD3	1:A:508:PHE:HZ	1.73	0.53
1:C:211:SER:CB	2:F:126:MET:HE2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:TYR:CD2	1:B:497:LEU:HD23	2.43	0.53
2:D:122:GLU:OE1	2:D:122:GLU:HA	2.07	0.53
1:B:44:LEU:O	1:B:47:VAL:HG22	2.08	0.53
2:F:292:MET:CE	2:F:296:ILE:HD11	2.39	0.53
1:A:100:GLY:HA2	1:A:256:TYR:CE1	2.42	0.53
1:A:457:GLU:HB3	1:A:460:LYS:HD3	1.89	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
1:C:156:LEU:HD11	1:C:428:LEU:HD13	1.91	0.53
2:F:439:LYS:HE3	2:F:443:GLN:HE22	1.73	0.53
1:A:468:PHE:CE1	1:A:501:VAL:HG12	2.43	0.53
2:D:282:GLN:H	2:D:282:GLN:NE2	2.01	0.53
1:C:180:ILE:CD1	1:C:216:LEU:HD21	2.34	0.53
1:C:190:ASN:HA	1:C:198:LYS:HG2	1.91	0.53
2:D:31:PRO:HD2	2:D:34:ASN:ND2	2.24	0.53
2:F:210:ASP:HB2	2:F:212:THR:HG23	1.91	0.53
1:B:456:LEU:HD12	1:B:457:GLU:N	2.20	0.53
2:D:412:ARG:HD2	2:D:454:GLU:HB3	1.90	0.53
2:E:220:GLY:HA3	2:E:232:VAL:HG21	1.91	0.53
1:B:383:MET:O	1:B:384:LYS:C	2.52	0.52
1:C:270:ASP:OD1	1:C:273:LYS:HG3	2.09	0.52
2:D:136:GLY:CA	2:D:431:LEU:HD13	2.37	0.52
2:D:473:LEU:C	2:D:475:GLU:N	2.62	0.52
2:E:97:VAL:HG13	2:E:232:VAL:CG1	2.39	0.52
1:A:161:ARG:HH11	1:A:263:HIS:CG	2.25	0.52
2:E:80:ALA:HB1	2:E:81:PRO:HD2	1.92	0.52
2:E:218:VAL:HG11	2:E:235:THR:HG22	1.92	0.52
2:F:96:ASN:HB2	2:F:100:GLU:H	1.74	0.52
3:G:14:LYS:HG2	3:G:243:ILE:HD13	1.91	0.52
1:B:69:ASP:O	1:B:70:ASN:HB3	2.08	0.52
1:B:423:ARG:HD2	1:B:461:ILE:HD11	1.91	0.52
2:E:334:VAL:HG23	2:E:353:SER:HA	1.92	0.52
3:G:214:TYR:CZ	3:G:218:LYS:HG3	2.45	0.52
1:A:140:ILE:HG21	1:A:313:ASN:HA	1.91	0.52
1:B:214:ALA:HB2	2:E:123:PHE:CE1	2.44	0.52
3:G:37:GLU:OE1	3:G:218:LYS:HE3	2.10	0.52
2:D:96:ASN:CB	2:D:100:GLU:H	2.22	0.52
2:D:422:GLU:HG2	2:D:427:HIS:O	2.09	0.52
2:E:81:PRO:HG2	2:E:115:ALA:HB1	1.91	0.52
1:B:140:ILE:HG23	1:B:311:LYS:HG3	1.92	0.52
1:B:479:LEU:HA	1:B:482:LYS:HE3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LEU:O	1:A:246:ALA:C	2.51	0.52
1:B:386:VAL:HG22	1:B:442:VAL:HG12	1.91	0.52
2:E:9:THR:HG21	2:E:28:GLY:O	2.09	0.52
2:E:254:PHE:CD1	2:E:307:VAL:HB	2.45	0.52
1:A:137:ILE:HG13	2:E:104:GLU:HG3	1.92	0.52
1:B:157:VAL:N	1:B:158:PRO:HD3	2.25	0.52
2:F:257:ASN:HB3	2:F:260:ARG:HG2	1.92	0.52
1:A:179:ALA:HB1	1:A:267:ILE:HG12	1.91	0.51
2:E:377:ILE:HG21	2:E:410:ILE:CD1	2.40	0.51
3:G:1:ALA:HB1	3:G:6:ILE:HD11	1.92	0.51
3:G:6:ILE:HG23	3:G:246:LEU:HD22	1.92	0.51
1:C:267:ILE:N	1:C:267:ILE:HD12	2.25	0.51
2:E:443:GLN:O	2:E:446:ALA:HB3	2.10	0.51
2:F:234:LEU:O	2:F:237:LEU:HB3	2.10	0.51
1:B:214:ALA:HA	2:E:123:PHE:CZ	2.45	0.51
1:C:140:ILE:HD11	1:C:143:ARG:HH22	1.74	0.51
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.75	0.51
2:E:279:VAL:HG12	2:E:279:VAL:O	2.10	0.51
1:A:457:GLU:HB2	1:A:460:LYS:HD3	1.92	0.51
1:B:210:ARG:O	1:B:211:SER:C	2.53	0.51
2:E:204:GLY:O	2:E:205:VAL:C	2.54	0.51
2:F:360:PRO:HD3	2:F:368:TYR:CD2	2.45	0.51
3:G:17:GLN:HB2	3:G:239:ALA:CB	2.39	0.51
1:C:45:ARG:NH2	1:C:68:PRO:O	2.44	0.51
1:C:105:GLY:HA2	1:C:226:MET:HE3	1.93	0.51
1:C:164:ARG:HD2	1:C:306:LEU:O	2.11	0.51
2:D:356:ARG:O	2:D:356:ARG:HG2	2.09	0.51
3:G:38:LEU:HD11	3:G:42:ARG:NE	2.26	0.51
2:E:41:ARG:O	2:E:42:GLU:C	2.53	0.51
2:E:444:ILE:HD11	2:E:463:ILE:HD11	1.93	0.51
2:F:421:ALA:O	2:F:425:THR:HG23	2.11	0.51
1:B:157:VAL:N	1:B:158:PRO:CD	2.73	0.51
1:C:102:GLU:HG2	1:C:122:GLY:C	2.36	0.51
1:C:406:PHE:N	1:C:406:PHE:CD1	2.79	0.51
2:D:366:GLU:CG	2:D:442:GLN:HE22	2.23	0.51
2:E:25:PHE:O	2:E:56:SER:HB3	2.10	0.51
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.41	0.51
3:G:209:LEU:O	3:G:210:ALA:C	2.52	0.51
2:E:142:LEU:HD21	2:E:374:VAL:HG21	1.93	0.51
1:B:386:VAL:CG2	1:B:442:VAL:HG12	2.41	0.51
2:D:84:ILE:CD1	2:D:95:MET:HE1	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:154:LEU:HD22	2:D:165:LEU:HD23	1.92	0.51
2:F:455:GLN:H	2:F:455:GLN:CD	2.18	0.51
2:E:241:GLU:HA	2:E:304:ILE:HD11	1.93	0.51
1:A:245:LEU:C	1:A:247:PRO:HD2	2.36	0.50
1:A:344:SER:O	2:E:222:MET:HE1	2.11	0.50
1:B:489:ILE:HG22	1:B:494:ASP:HB2	1.93	0.50
2:E:382:LYS:O	2:E:385:GLN:HB2	2.11	0.50
2:F:96:ASN:ND2	2:F:100:GLU:HB2	2.26	0.50
1:C:436:MET:CE	1:C:469:LEU:HD21	2.41	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:E:242:TYR:C	2:E:244:ARG:H	2.18	0.50
2:F:345:TYR:HA	2:F:346:PRO:C	2.36	0.50
1:A:187:LYS:HE2	1:A:191:ASP:OD2	2.11	0.50
2:E:293:GLN:HG3	2:E:328:HIS:CG	2.46	0.50
1:A:140:ILE:HD11	1:A:143:ARG:NE	2.26	0.50
1:A:294:TYR:HB2	1:A:337:TYR:HE2	1.76	0.50
1:A:380:THR:O	1:A:384:LYS:HG3	2.12	0.50
1:C:23:VAL:HG12	1:C:23:VAL:O	2.11	0.50
1:C:443:ALA:O	1:C:446:TYR:HB3	2.10	0.50
2:E:155:PHE:HE1	2:E:310:ILE:HD12	1.77	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
1:A:137:ILE:N	1:A:138:PRO:CD	2.75	0.50
1:B:99:VAL:HG21	1:B:127:ARG:HB3	1.94	0.50
1:C:64:LEU:HD23	1:C:74:VAL:HG21	1.92	0.50
1:C:402:ALA:O	1:C:405:GLN:HG3	2.12	0.50
2:D:406:ARG:O	2:D:410:ILE:HG13	2.11	0.50
2:E:204:GLY:C	2:E:206:ILE:N	2.68	0.50
2:E:377:ILE:HG21	2:E:410:ILE:HD12	1.92	0.50
1:A:240:ALA:N	1:A:241:PRO:HD2	2.27	0.50
1:C:96:ASP:O	1:C:97:VAL:HG13	2.12	0.50
1:C:331:ALA:O	1:C:333:ASP:N	2.44	0.50
2:D:168:GLU:HG3	2:D:168:GLU:O	2.11	0.50
3:G:30:LYS:HA	3:G:33:ARG:HE	1.76	0.50
3:G:82:HIS:H	3:G:82:HIS:CD2	2.29	0.50
1:B:390:MET:CE	1:B:428:LEU:HD21	2.42	0.50
2:D:345:TYR:HA	2:D:346:PRO:C	2.37	0.50
2:E:275:ILE:O	2:E:283:PRO:HG3	2.12	0.50
2:F:163:THR:O	2:F:167:MET:HG2	2.12	0.50
1:B:27:GLU:O	1:B:90:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:TYR:O	1:C:247:PRO:HD2	2.11	0.49
2:E:463:ILE:O	2:E:467:VAL:HG23	2.12	0.49
1:A:85:GLY:O	1:A:86:ASP:C	2.53	0.49
1:C:434:SER:N	1:C:435:PRO:HD3	2.27	0.49
2:E:462:PRO:HD2	2:E:465:GLU:HG3	1.94	0.49
1:B:49:ALA:O	1:B:50:GLU:HB2	2.12	0.49
1:B:151:LYS:NZ	1:B:429:LYS:O	2.45	0.49
1:C:225:ALA:HA	1:C:228:TYR:CE1	2.47	0.49
2:D:136:GLY:HA2	2:D:432:VAL:O	2.12	0.49
2:D:390:ILE:HD13	3:G:16:ILE:CD1	2.42	0.49
2:D:397:SER:O	2:D:400:ASP:N	2.45	0.49
2:F:168:GLU:OE1	2:F:418:PHE:HB3	2.12	0.49
1:C:338:ILE:O	1:C:339:PRO:C	2.51	0.49
1:B:300:TYR:O	1:B:304:ARG:HG2	2.13	0.49
2:E:134:VAL:HG13	2:E:141:ASP:OD2	2.13	0.49
3:G:210:ALA:HA	3:G:213:ILE:HB	1.93	0.49
1:C:245:LEU:O	1:C:246:ALA:C	2.56	0.49
2:D:83:ARG:HA	2:D:115:ALA:HA	1.95	0.49
2:F:386:ASP:O	2:F:389:ALA:HB3	2.12	0.49
1:B:358:TYR:C	1:B:360:GLY:N	2.69	0.49
2:F:339:ILE:HG22	2:F:344:ILE:HB	1.95	0.49
1:A:300:TYR:O	1:A:304:ARG:HG2	2.13	0.49
1:A:373:ARG:HG3	1:A:373:ARG:NH1	2.28	0.49
1:B:423:ARG:HE	1:B:458:PRO:CD	2.25	0.49
1:C:399:GLU:OE2	2:D:408:ARG:NH2	2.46	0.49
1:B:107:VAL:HG12	1:B:115:ILE:CG1	2.43	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
2:D:93:ARG:HG3	2:D:93:ARG:NH1	2.27	0.49
1:B:180:ILE:CD1	1:B:216:LEU:HD21	2.39	0.48
1:C:334:VAL:HG13	1:C:351:PHE:CE1	2.48	0.48
2:D:319:ASP:O	2:D:320:PRO:C	2.55	0.48
3:G:20:THR:HG22	3:G:236:SER:HB3	1.94	0.48
2:E:54:GLY:O	2:E:55:GLU:HB2	2.13	0.48
2:E:393:MET:HE3	2:E:396:LEU:HD12	1.95	0.48
2:F:86:VAL:HG11	2:F:114:ALA:HB3	1.94	0.48
1:A:94:ILE:HG12	1:A:95:VAL:N	2.27	0.48
1:B:24:ASP:O	1:B:28:THR:HB	2.12	0.48
1:B:96:ASP:HB2	1:B:127:ARG:O	2.12	0.48
1:B:351:PHE:HE1	1:B:369:LEU:O	1.96	0.48
1:B:427:LEU:HD11	1:B:448:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:LEU:HB3	1:C:47:VAL:HG22	1.95	0.48
2:E:227:GLY:O	2:E:230:ALA:HB3	2.13	0.48
2:E:416:GLN:HG3	2:E:417:PRO:HD2	1.96	0.48
1:A:389:THR:O	1:A:393:GLU:HG2	2.13	0.48
1:A:417:LEU:HD23	1:A:417:LEU:H	1.77	0.48
1:B:463:LYS:HE2	1:B:508:PHE:CZ	2.48	0.48
2:F:221:GLN:HE21	2:F:221:GLN:HA	1.78	0.48
1:A:127:ARG:HE	1:A:131:LEU:CD1	2.27	0.48
1:B:218:LYS:HB2	2:E:128:VAL:HG12	1.95	0.48
2:D:84:ILE:N	2:D:114:ALA:O	2.42	0.48
2:F:321:ALA:HB3	2:F:322:PRO:HD3	1.94	0.48
2:E:404:VAL:O	2:E:408:ARG:HG3	2.14	0.48
2:E:444:ILE:HD11	2:E:463:ILE:CD1	2.43	0.48
1:B:211:SER:O	1:B:215:GLN:HG3	2.13	0.48
1:A:453:LEU:HD13	1:A:461:ILE:HG23	1.96	0.48
2:E:161:GLY:O	2:E:162:LYS:C	2.57	0.48
2:F:360:PRO:HD3	2:F:368:TYR:CE2	2.48	0.48
1:A:100:GLY:HA2	1:A:256:TYR:CD1	2.49	0.48
2:F:319:ASP:O	2:F:322:PRO:HD2	2.14	0.48
1:A:67:GLU:O	2:E:71:ARG:NH1	2.41	0.48
1:A:166:LEU:HD13	1:A:342:VAL:HG12	1.95	0.48
1:A:180:ILE:O	1:A:181:ASP:C	2.56	0.48
1:C:30:ARG:HA	1:C:86:ASP:O	2.13	0.48
2:E:360:PRO:HD3	2:E:368:TYR:CD1	2.49	0.48
2:E:397:SER:C	2:E:399:GLU:H	2.20	0.48
2:F:63:MET:HE1	2:F:231:ARG:HB2	1.95	0.48
2:F:96:ASN:HD22	2:F:100:GLU:CB	2.27	0.48
1:B:225:ALA:HA	1:B:228:TYR:CE2	2.49	0.47
2:D:32:ILE:O	2:D:33:LEU:HB2	2.14	0.47
2:E:116:ILE:HA	2:E:238:THR:OG1	2.14	0.47
2:E:158:ALA:C	2:E:160:VAL:N	2.72	0.47
2:F:88:PRO:HD2	2:F:89:GLU:OE2	2.14	0.47
1:B:45:ARG:HH11	1:B:45:ARG:HD3	1.53	0.47
1:B:311:LYS:HD2	1:B:312:MET:O	2.13	0.47
1:B:443:ALA:O	1:B:446:TYR:HB3	2.14	0.47
1:C:34:ILE:HD11	1:C:79:ASP:CB	2.41	0.47
1:B:151:LYS:NZ	1:B:427:LEU:O	2.47	0.47
1:B:240:ALA:N	1:B:241:PRO:CD	2.77	0.47
1:C:481:SER:O	1:C:485:THR:HB	2.14	0.47
2:D:14:VAL:HG11	2:D:24:GLN:HB2	1.95	0.47
2:D:360:PRO:HD3	2:D:368:TYR:CE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:36:LEU:N	2:F:36:LEU:HD23	2.30	0.47
2:F:289:MET:HE3	2:F:289:MET:HB2	1.73	0.47
2:F:357:ILE:HD12	2:F:362:ILE:HG21	1.95	0.47
1:A:188:ARG:HE	1:A:437:ALA:HB2	1.79	0.47
1:A:444:VAL:CG1	1:A:469:LEU:HD13	2.44	0.47
1:C:187:LYS:HE3	1:C:224:ASP:HB3	1.96	0.47
2:D:129:GLU:OE1	2:D:129:GLU:HA	2.14	0.47
2:D:425:THR:HB	2:D:459:MET:HE2	1.96	0.47
2:F:82:ILE:HD13	2:F:98:ILE:HG22	1.96	0.47
1:B:481:SER:O	1:B:485:THR:HB	2.14	0.47
1:C:313:ASN:OD1	1:C:315:ALA:HB3	2.15	0.47
2:F:93:ARG:NH2	2:F:106:GLY:O	2.48	0.47
2:F:275:ILE:HD13	3:G:271:ALA:HB1	1.97	0.47
3:G:210:ALA:O	3:G:213:ILE:N	2.47	0.47
2:E:33:LEU:HD13	2:E:117:HIS:CG	2.50	0.47
2:E:374:VAL:O	2:E:377:ILE:HG22	2.14	0.47
2:F:80:ALA:HB1	2:F:81:PRO:HD2	1.94	0.47
1:A:40:ARG:HH11	1:A:40:ARG:CG	2.28	0.47
1:A:52:MET:HE1	1:A:60:LYS:HD3	1.97	0.47
1:A:107:VAL:HB	1:A:116:ASP:HB3	1.97	0.47
1:A:485:THR:C	1:A:487:GLY:H	2.23	0.47
1:C:441:GLN:O	1:C:445:ILE:HG12	2.15	0.47
2:D:432:VAL:HG13	2:D:433:PRO:HD2	1.97	0.47
2:E:189:ARG:O	2:E:190:THR:C	2.58	0.47
2:E:253:LEU:O	2:E:306:SER:HA	2.14	0.47
2:E:259:PHE:CE2	2:E:263:GLN:HG2	2.50	0.47
2:E:438:ILE:O	2:E:442:GLN:HB2	2.15	0.47
2:F:346:PRO:HG3	2:F:418:PHE:HZ	1.80	0.47
1:A:376:SER:O	1:A:378:ALA:N	2.48	0.47
1:C:59:LEU:HD23	1:C:82:ILE:CD1	2.44	0.47
2:D:393:MET:HE1	2:D:404:VAL:HG11	1.96	0.47
1:A:209:LYS:HE3	1:A:211:SER:CB	2.44	0.47
1:B:496:LYS:O	1:B:500:ILE:HG13	2.15	0.47
1:C:445:ILE:HG22	1:C:449:VAL:CG2	2.44	0.47
2:E:95:MET:HE2	2:E:99:GLY:CA	2.45	0.47
2:F:467:VAL:O	2:F:470:ALA:HB3	2.14	0.47
2:D:368:TYR:CE1	2:D:372:ARG:HG3	2.50	0.47
1:C:292:GLU:O	1:C:293:ALA:CB	2.63	0.46
2:E:409:LYS:NZ	2:E:450:ASP:HA	2.30	0.46
2:F:205:VAL:HG23	2:F:215:VAL:HG21	1.96	0.46
1:A:313:ASN:OD1	1:A:316:PHE:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:ILE:H	1:A:461:ILE:HG12	1.60	0.46
1:B:171:ARG:HG3	1:B:171:ARG:HH11	1.79	0.46
2:D:417:PRO:HA	2:D:459:MET:HE1	1.96	0.46
2:F:462:PRO:HG2	2:F:465:GLU:HG3	1.96	0.46
1:A:485:THR:HG22	1:A:486:ASP:N	2.29	0.46
1:B:27:GLU:OE1	1:B:90:ARG:HD3	2.16	0.46
1:B:400:VAL:HB	1:B:418:LEU:CD2	2.45	0.46
1:B:433:TYR:C	1:B:435:PRO:HD3	2.40	0.46
1:B:469:LEU:HG	1:B:473:ILE:HD11	1.98	0.46
1:B:485:THR:O	1:B:486:ASP:C	2.58	0.46
1:C:30:ARG:HE	1:C:87:ILE:CD1	2.18	0.46
1:C:91:THR:HG22	1:C:93:ALA:HB3	1.97	0.46
1:A:49:ALA:O	1:A:50:GLU:HB2	2.13	0.46
1:C:251:CYS:O	1:C:255:GLU:HG3	2.16	0.46
2:D:397:SER:O	2:D:398:GLU:C	2.58	0.46
2:D:412:ARG:C	2:D:414:LEU:N	2.73	0.46
2:E:77:ASP:C	2:E:79:GLY:H	2.24	0.46
3:G:22:SER:HA	3:G:25:MET:HE3	1.97	0.46
1:A:78:ASN:OD1	1:A:80:LYS:HB3	2.15	0.46
1:B:179:ALA:O	1:B:182:THR:HB	2.14	0.46
2:D:469:LYS:O	2:D:473:LEU:HG	2.15	0.46
2:E:63:MET:CE	2:E:228:ALA:HA	2.46	0.46
2:E:431:LEU:HD12	2:E:431:LEU:O	2.15	0.46
3:G:259:THR:O	3:G:263:ILE:HG13	2.16	0.46
1:A:51:GLU:OE2	1:A:90:ARG:HB3	2.15	0.46
1:A:139:ARG:C	1:A:140:ILE:HG22	2.40	0.46
1:A:485:THR:C	1:A:487:GLY:N	2.73	0.46
2:E:61:ILE:HG13	2:E:61:ILE:O	2.14	0.46
2:E:146:TYR:O	2:E:357:ILE:HD11	2.16	0.46
1:A:142:VAL:HG22	1:A:161:ARG:O	2.16	0.46
1:B:34:ILE:HD12	1:B:35:GLY:H	1.81	0.46
1:B:381:ARG:HG2	1:B:488:LYS:HG3	1.98	0.46
1:C:180:ILE:HG22	1:C:184:ILE:HD12	1.96	0.46
2:D:237:LEU:HD21	2:D:295:ARG:HB2	1.98	0.46
2:E:82:ILE:HB	2:E:116:ILE:CD1	2.45	0.46
1:A:353:GLU:CD	1:A:366:ASN:HD22	2.24	0.46
1:C:67:GLU:HB3	1:C:68:PRO:HD2	1.98	0.46
2:D:154:LEU:HD13	2:D:165:LEU:HD23	1.96	0.46
2:F:151:LYS:HD3	2:F:328:HIS:O	2.15	0.46
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.98	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:A:213:VAL:O	1:A:216:LEU:HB3	2.16	0.46
2:F:310:ILE:HD13	2:F:325:THR:HG21	1.97	0.46
1:C:476:HIS:ND1	1:C:476:HIS:N	2.64	0.46
2:D:289:MET:SD	2:D:324:THR:HG22	2.56	0.46
2:D:440:GLY:O	2:D:444:ILE:HG13	2.16	0.46
2:E:112:GLN:NE2	2:E:242:TYR:HE2	2.13	0.46
2:E:343:GLY:O	2:E:345:TYR:HD1	1.99	0.46
2:E:405:SER:OG	2:E:406:ARG:N	2.49	0.46
2:F:221:GLN:HA	2:F:221:GLN:NE2	2.31	0.46
3:G:23:MET:HB3	3:G:23:MET:HE2	1.72	0.46
1:A:403:PHE:O	1:A:404:ALA:C	2.59	0.45
2:E:120:ALA:HB1	2:E:121:PRO:HD2	1.98	0.45
2:F:339:ILE:CG2	2:F:344:ILE:HB	2.46	0.45
2:F:469:LYS:O	2:F:473:LEU:HG	2.16	0.45
1:A:240:ALA:HB3	1:A:241:PRO:HD3	1.97	0.45
1:C:432:GLN:O	1:C:433:TYR:HB2	2.16	0.45
2:D:35:ALA:HB1	2:D:46:VAL:CG1	2.47	0.45
2:D:130:GLN:HE22	2:D:356:ARG:HD3	1.82	0.45
2:D:231:ARG:O	2:D:234:LEU:N	2.50	0.45
2:D:391:LEU:CD1	3:G:19:ILE:HG21	2.46	0.45
2:F:29:LEU:HD11	2:F:58:VAL:HG13	1.98	0.45
2:F:81:PRO:O	2:F:82:ILE:C	2.58	0.45
1:A:313:ASN:O	1:A:316:PHE:N	2.37	0.45
1:A:339:PRO:O	1:A:343:ILE:HG13	2.16	0.45
2:D:190:THR:O	2:D:191:ARG:C	2.60	0.45
2:D:201:ILE:HD13	2:D:208:LEU:HD11	1.98	0.45
2:E:388:ILE:HG23	2:E:393:MET:CG	2.43	0.45
2:F:200:MET:CG	2:F:206:ILE:HG12	2.45	0.45
1:B:389:THR:HA	1:B:392:LEU:HG	1.97	0.45
1:C:340:THR:O	1:C:341:ASN:C	2.59	0.45
1:C:474:SER:OG	1:C:475:GLN:N	2.49	0.45
1:B:465:GLU:O	1:B:469:LEU:HB2	2.17	0.45
1:C:390:MET:HE1	1:C:428:LEU:HD21	1.99	0.45
2:D:417:PRO:HB3	2:D:459:MET:HE3	1.99	0.45
2:E:443:GLN:HA	2:E:446:ALA:HB3	1.99	0.45
2:F:243:PHE:O	2:F:249:GLN:HB2	2.16	0.45
1:A:179:ALA:O	1:A:182:THR:HB	2.17	0.45
1:A:385:GLN:OE1	1:A:488:LYS:HB2	2.17	0.45
1:A:412:ALA:HA	1:A:415:GLN:HB3	1.98	0.45
1:A:413:ALA:O	1:A:416:GLN:HB3	2.17	0.45
1:B:141:SER:HB2	1:B:143:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:LEU:HD12	1:B:325:PRO:HB2	1.98	0.45
1:C:156:LEU:HD11	1:C:428:LEU:CD1	2.45	0.45
1:C:219:ARG:HD3	1:C:433:TYR:HE1	1.80	0.45
2:D:231:ARG:O	2:D:232:VAL:C	2.60	0.45
2:D:412:ARG:O	2:D:415:SER:OG	2.33	0.45
2:E:402:LEU:O	2:E:406:ARG:HG3	2.16	0.45
2:F:409:LYS:HD3	2:F:457:PHE:HE2	1.77	0.45
3:G:234:ASN:HA	3:G:237:LYS:HB2	1.98	0.45
1:A:45:ARG:HD3	1:A:45:ARG:HA	1.67	0.45
1:A:59:LEU:HD11	1:A:81:LEU:HD12	1.99	0.45
1:B:76:PHE:HB3	1:B:242:LEU:HD21	1.98	0.45
2:D:452:LEU:HD12	2:D:457:PHE:CZ	2.52	0.45
2:D:471:ASP:O	2:D:472:LYS:C	2.57	0.45
2:E:281:TYR:CZ	2:E:321:ALA:HB2	2.52	0.45
3:G:210:ALA:O	3:G:211:ASN:C	2.59	0.45
1:B:353:GLU:HG3	1:B:366:ASN:HB2	1.98	0.45
2:E:85:PRO:HD2	2:E:95:MET:CE	2.46	0.45
2:E:321:ALA:N	2:E:322:PRO:HD2	2.32	0.45
1:A:97:VAL:HG11	1:A:249:SER:HB2	1.99	0.45
2:D:96:ASN:HB2	2:D:100:GLU:N	2.27	0.45
2:D:170:ILE:O	2:D:174:ALA:HB3	2.17	0.45
1:B:212:THR:O	1:B:216:LEU:HB2	2.18	0.44
1:C:158:PRO:HB3	1:C:379:GLN:HG3	1.99	0.44
1:A:133:ALA:HB1	1:A:134:PRO:HD2	1.99	0.44
1:A:166:LEU:HD13	1:A:342:VAL:CG1	2.47	0.44
1:A:244:TYR:HE1	1:A:301:LEU:HD11	1.82	0.44
1:B:94:ILE:O	1:B:95:VAL:C	2.61	0.44
1:C:404:ALA:HB1	1:C:410:LEU:HD11	1.99	0.44
1:C:485:THR:O	1:C:486:ASP:C	2.57	0.44
2:D:108:ILE:HG22	2:D:110:THR:HG23	1.99	0.44
2:D:425:THR:HG21	2:D:459:MET:HE1	1.99	0.44
2:E:35:ALA:HB2	2:E:82:ILE:HG13	1.99	0.44
2:F:96:ASN:HB2	2:F:100:GLU:N	2.31	0.44
2:F:359:ASP:OD1	2:F:360:PRO:HD2	2.17	0.44
1:A:140:ILE:CG2	1:A:313:ASN:HA	2.47	0.44
1:B:300:TYR:HA	1:B:303:SER:OG	2.17	0.44
1:C:210:ARG:NH1	2:F:121:PRO:O	2.50	0.44
1:C:311:LYS:HE3	1:C:318:GLY:O	2.17	0.44
1:C:488:LYS:HG2	1:C:489:ILE:N	2.28	0.44
3:G:2:THR:O	3:G:3:LEU:C	2.57	0.44
3:G:82:HIS:CD2	3:G:82:HIS:N	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ILE:HG13	1:B:143:ARG:NH1	2.32	0.44
1:C:26:GLU:HB3	1:C:46:ASN:ND2	2.31	0.44
2:D:433:PRO:HG2	2:D:436:GLU:CG	2.44	0.44
2:D:470:ALA:O	2:D:474:ALA:N	2.51	0.44
1:A:379:GLN:HB2	1:A:384:LYS:HE3	2.00	0.44
2:D:95:MET:HG2	2:D:99:GLY:HA2	1.99	0.44
2:D:461:GLY:HA3	2:D:462:PRO:HD3	1.74	0.44
2:E:77:ASP:CG	2:E:79:GLY:H	2.23	0.44
2:F:50:ALA:O	2:F:51:GLN:HB3	2.17	0.44
3:G:13:ILE:HD13	3:G:242:MET:SD	2.57	0.44
1:A:55:PHE:O	1:A:56:SER:C	2.61	0.44
1:A:460:LYS:N	1:A:460:LYS:HD2	2.32	0.44
1:B:420:ARG:O	1:B:423:ARG:N	2.50	0.44
1:B:423:ARG:HE	1:B:458:PRO:CG	2.31	0.44
1:C:185:ASN:HB2	1:C:435:PRO:HB3	2.00	0.44
2:D:366:GLU:O	2:D:370:VAL:HG23	2.17	0.44
2:E:433:PRO:HG2	2:E:436:GLU:CG	2.48	0.44
1:A:492:GLU:C	1:A:494:ASP:N	2.73	0.44
2:D:400:ASP:O	2:D:404:VAL:HG23	2.18	0.44
1:A:482:LYS:O	1:A:483:ILE:C	2.61	0.44
1:C:269:ASP:HA	1:C:270:ASP:HA	1.78	0.44
2:D:462:PRO:HD2	2:D:465:GLU:HG3	2.00	0.44
2:E:166:ILE:O	2:E:170:ILE:HG13	2.18	0.44
2:F:407:ALA:O	2:F:411:GLN:HB2	2.18	0.44
1:A:392:LEU:O	1:A:396:GLN:HG3	2.18	0.44
1:C:489:ILE:HG22	1:C:494:ASP:HB2	1.99	0.44
2:E:147:ALA:HB2	2:E:357:ILE:HD13	1.98	0.44
2:F:105:ARG:CZ	2:F:208:LEU:HD23	2.47	0.44
1:A:107:VAL:HG11	2:D:123:PHE:CE2	2.53	0.43
1:B:400:VAL:HG12	1:B:418:LEU:HD11	2.00	0.43
1:C:290:GLY:O	1:C:291:ARG:C	2.61	0.43
2:E:72:GLY:O	2:E:73:GLN:C	2.60	0.43
2:E:432:VAL:HA	2:E:433:PRO:HD3	1.81	0.43
2:F:348:VAL:O	2:F:350:PRO:HD3	2.17	0.43
1:A:151:LYS:HE2	1:A:427:LEU:O	2.17	0.43
1:A:420:ARG:HA	1:A:420:ARG:HD3	1.78	0.43
1:A:463:LYS:HD3	1:A:508:PHE:CZ	2.52	0.43
1:B:389:THR:HA	1:B:392:LEU:CG	2.49	0.43
1:C:51:GLU:HG2	1:C:52:MET:N	2.33	0.43
2:D:298:THR:HG23	2:D:303:SER:HA	1.98	0.43
2:E:425:THR:C	2:E:427:HIS:N	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:GLN:NE2	2:D:128:VAL:CB	2.82	0.43
1:B:32:LEU:HD21	1:B:42:HIS:HB2	2.00	0.43
1:B:400:VAL:CG1	1:B:418:LEU:HD11	2.47	0.43
1:C:208:GLN:HE21	1:C:208:GLN:HB2	1.38	0.43
1:C:209:LYS:HE3	1:C:211:SER:OG	2.18	0.43
1:C:285:LEU:C	1:C:286:ARG:HG2	2.43	0.43
2:D:412:ARG:HG3	2:D:412:ARG:NH1	2.33	0.43
2:E:136:GLY:HA2	2:E:432:VAL:O	2.18	0.43
2:E:439:LYS:O	2:E:440:GLY:C	2.61	0.43
1:A:215:GLN:NE2	2:D:128:VAL:HB	2.33	0.43
1:A:283:LEU:HD11	1:A:293:ALA:HB1	1.98	0.43
1:B:215:GLN:HE22	2:E:130:GLN:NE2	2.16	0.43
1:C:187:LYS:O	1:C:188:ARG:C	2.61	0.43
2:D:63:MET:HE1	2:D:231:ARG:HB2	1.99	0.43
2:F:319:ASP:O	2:F:320:PRO:C	2.60	0.43
1:A:471:HIS:ND1	1:A:475:GLN:HG3	2.32	0.43
1:B:389:THR:HG22	1:B:392:LEU:HD12	2.00	0.43
1:C:107:VAL:O	1:C:115:ILE:HG12	2.18	0.43
1:C:180:ILE:O	1:C:181:ASP:C	2.61	0.43
1:C:193:THR:O	1:C:195:GLU:OE1	2.36	0.43
2:D:189:ARG:O	2:D:192:GLU:HB2	2.18	0.43
2:E:310:ILE:HD11	2:E:329:LEU:HD11	2.00	0.43
2:E:376:LYS:O	2:E:379:GLN:HB2	2.18	0.43
2:F:31:PRO:O	2:F:34:ASN:HB2	2.18	0.43
2:F:188:GLU:H	2:F:221:GLN:NE2	2.15	0.43
2:F:257:ASN:OD1	2:F:259:PHE:HB3	2.17	0.43
2:F:346:PRO:HG3	2:F:418:PHE:CZ	2.52	0.43
2:F:439:LYS:HG2	2:F:443:GLN:NE2	2.33	0.43
1:B:132:LYS:NZ	2:F:64:ASP:OD1	2.47	0.43
2:D:103:ASP:O	2:D:104:GLU:HB2	2.18	0.43
2:E:242:TYR:C	2:E:242:TYR:CD1	2.97	0.43
1:A:24:ASP:OD1	1:A:24:ASP:C	2.60	0.43
1:A:52:MET:CG	1:A:95:VAL:HG22	2.48	0.43
1:A:397:TYR:CD1	1:A:421:GLY:HA3	2.54	0.43
1:B:55:PHE:O	1:B:56:SER:C	2.62	0.43
1:C:116:ASP:O	1:C:117:GLY:C	2.60	0.43
1:C:457:GLU:O	1:C:458:PRO:C	2.62	0.43
2:E:29:LEU:HA	2:E:30:PRO:HD2	1.92	0.43
2:E:105:ARG:NE	2:E:208:LEU:HD23	2.33	0.43
2:E:409:LYS:HZ2	2:E:450:ASP:HA	1.83	0.43
2:F:47:LEU:HD23	2:F:62:ALA:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:141:ASP:HB3	2:F:434:LEU:HD13	2.01	0.43
2:F:270:ALA:O	2:F:273:GLY:N	2.44	0.43
1:C:32:LEU:HD21	1:C:42:HIS:HB2	2.00	0.43
1:C:49:ALA:N	1:C:66:LEU:HD11	2.34	0.43
1:C:147:GLN:OE1	1:C:438:ILE:HD13	2.19	0.43
2:D:410:ILE:HG23	2:D:441:PHE:CE1	2.54	0.43
2:E:114:ALA:HB3	2:E:238:THR:CG2	2.47	0.43
2:E:231:ARG:O	2:E:232:VAL:C	2.60	0.43
2:F:144:ALA:N	2:F:145:PRO:CD	2.82	0.43
3:G:209:LEU:O	3:G:212:ILE:N	2.51	0.43
1:A:210:ARG:HH11	1:A:210:ARG:HD2	1.69	0.43
1:A:251:CYS:O	1:A:255:GLU:HG3	2.18	0.43
1:C:169:GLY:O	1:C:175:LYS:HE2	2.19	0.43
1:C:423:ARG:CD	1:C:461:ILE:HD11	2.49	0.43
2:D:209:LYS:HA	2:D:209:LYS:HD3	1.83	0.43
2:D:345:TYR:HB3	4:D:1476:ADP:C6	2.54	0.43
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.48	0.43
1:C:78:ASN:HD21	1:C:80:LYS:HD3	1.84	0.43
2:D:38:VAL:HG11	2:D:69:LEU:CD2	2.49	0.43
2:E:397:SER:O	2:E:398:GLU:C	2.62	0.43
2:E:422:GLU:C	2:E:424:PHE:N	2.74	0.43
1:A:99:VAL:HG23	1:A:253:MET:HA	2.01	0.42
1:A:383:MET:O	1:A:386:VAL:HG23	2.19	0.42
1:B:213:VAL:O	1:B:217:VAL:HG13	2.18	0.42
2:D:93:ARG:NH1	2:D:108:ILE:HG12	2.33	0.42
2:D:95:MET:HE2	2:D:235:THR:CG2	2.49	0.42
2:E:242:TYR:C	2:E:244:ARG:N	2.77	0.42
2:F:136:GLY:HA3	2:F:431:LEU:HD11	1.99	0.42
2:F:400:ASP:O	2:F:404:VAL:HG23	2.19	0.42
3:G:38:LEU:O	3:G:39:LYS:C	2.62	0.42
1:B:255:GLU:HG2	1:B:258:ARG:CZ	2.49	0.42
1:B:294:TYR:CE2	1:B:338:ILE:HD13	2.53	0.42
1:B:385:GLN:NE2	1:B:489:ILE:HB	2.34	0.42
1:C:219:ARG:HH11	1:C:219:ARG:HD2	1.71	0.42
2:D:94:ILE:HG22	2:D:102:ILE:HD11	2.01	0.42
1:A:288:PRO:HA	1:A:289:PRO:HD3	1.88	0.42
1:A:340:THR:O	1:A:344:SER:HB3	2.19	0.42
1:B:107:VAL:HG12	1:B:115:ILE:HD11	2.00	0.42
1:B:165:GLU:O	1:B:325:PRO:HD2	2.19	0.42
1:C:164:ARG:HD2	1:C:164:ARG:HH11	1.41	0.42
1:C:353:GLU:O	1:C:364:ALA:HB1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:122:GLU:OE1	2:F:122:GLU:HA	2.19	0.42
1:A:74:VAL:HG13	1:A:241:PRO:HG3	1.99	0.42
1:A:96:ASP:HA	1:A:128:ARG:HA	2.01	0.42
1:C:299:PHE:O	1:C:300:TYR:C	2.62	0.42
2:D:266:SER:CB	2:D:282:GLN:NE2	2.82	0.42
2:E:296:ILE:HD13	2:E:306:SER:HB2	2.02	0.42
2:F:89:GLU:HG2	2:F:110:THR:CG2	2.44	0.42
2:F:95:MET:HG3	2:F:99:GLY:HA2	2.01	0.42
2:F:196:LEU:O	2:F:200:MET:HB2	2.19	0.42
1:A:78:ASN:ND2	1:A:80:LYS:HD2	2.35	0.42
1:A:184:ILE:HD12	1:A:223:ALA:CB	2.50	0.42
1:C:49:ALA:O	1:C:50:GLU:HB2	2.19	0.42
1:C:485:THR:C	1:C:487:GLY:N	2.75	0.42
1:A:56:SER:O	1:A:58:GLY:N	2.53	0.42
1:B:434:SER:N	1:B:435:PRO:CD	2.82	0.42
1:C:331:ALA:O	1:C:332:GLY:C	2.63	0.42
2:D:279:VAL:HG12	2:D:279:VAL:O	2.20	0.42
2:D:449:TYR:C	2:D:451:HIS:N	2.78	0.42
2:E:189:ARG:HB2	2:E:192:GLU:HG3	2.02	0.42
1:A:267:ILE:HA	1:A:324:LEU:O	2.20	0.42
1:B:430:GLN:HE21	1:B:430:GLN:HB3	1.50	0.42
2:D:112:GLN:NE2	2:D:242:TYR:HE1	2.18	0.42
2:E:12:ARG:NH2	2:E:24:GLN:OE1	2.50	0.42
2:E:95:MET:HA	2:E:100:GLU:O	2.20	0.42
2:F:452:LEU:HD22	2:F:470:ALA:CB	2.49	0.42
2:D:35:ALA:HB1	2:D:46:VAL:HG13	2.02	0.42
2:D:475:GLU:OE1	2:D:475:GLU:HA	2.20	0.42
2:E:425:THR:C	2:E:427:HIS:H	2.28	0.42
2:F:385:GLN:HA	2:F:388:ILE:HG12	2.01	0.42
3:G:254:ARG:O	3:G:258:ILE:HG13	2.20	0.42
1:A:32:LEU:HD21	1:A:42:HIS:HB2	2.02	0.42
1:A:383:MET:HG3	1:A:387:ALA:HB2	2.02	0.42
1:C:224:ASP:OD1	1:C:227:LYS:HE3	2.19	0.42
1:C:405:GLN:C	1:C:406:PHE:CD1	2.96	0.42
2:E:366:GLU:O	2:E:367:HIS:C	2.63	0.42
2:E:388:ILE:HD12	2:E:396:LEU:HD11	2.01	0.42
2:F:387:ILE:H	2:F:387:ILE:HG13	1.61	0.42
1:A:247:PRO:HG2	1:A:274:GLN:NE2	2.35	0.41
1:A:338:ILE:N	1:A:339:PRO:CD	2.83	0.41
1:A:356:LEU:O	1:A:357:PHE:C	2.63	0.41
1:A:506:ALA:O	1:A:507:GLY:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:ARG:HA	1:B:384:LYS:HB2	2.01	0.41
2:D:145:PRO:HB2	2:D:357:ILE:HD11	2.01	0.41
2:E:122:GLU:HB2	2:E:125:GLU:HG3	2.01	0.41
2:E:387:ILE:HG22	2:E:388:ILE:HD13	2.02	0.41
1:A:292:GLU:HB2	1:A:294:TYR:HD2	1.85	0.41
1:C:151:LYS:HE2	1:C:436:MET:SD	2.60	0.41
1:C:177:SER:O	1:C:178:ILE:C	2.60	0.41
2:D:201:ILE:CD1	2:D:208:LEU:HD11	2.50	0.41
2:D:396:LEU:HD22	2:D:400:ASP:HB2	2.01	0.41
2:E:396:LEU:CB	2:E:401:LYS:HG2	2.50	0.41
2:E:412:ARG:NH1	2:E:454:GLU:OE1	2.53	0.41
2:E:461:GLY:HA3	2:E:462:PRO:HD3	1.73	0.41
1:A:103:LEU:O	1:A:106:ARG:HB2	2.20	0.41
1:A:206:ILE:O	1:A:273:LYS:HD2	2.21	0.41
1:B:75:VAL:HG21	1:B:82:ILE:HD12	2.02	0.41
1:B:78:ASN:ND2	1:B:80:LYS:HE2	2.35	0.41
1:B:249:SER:O	1:B:250:GLY:C	2.61	0.41
1:B:336:ALA:HB3	1:B:339:PRO:HD2	2.02	0.41
1:C:467:ALA:O	1:C:470:SER:HB2	2.20	0.41
2:E:182:VAL:HG21	2:E:240:ALA:HB2	2.01	0.41
2:E:360:PRO:HD3	2:E:368:TYR:CG	2.56	0.41
1:A:105:GLY:HA2	1:A:226:MET:O	2.21	0.41
1:B:103:LEU:O	1:B:104:LEU:C	2.63	0.41
1:B:423:ARG:HH21	1:B:458:PRO:HD3	1.86	0.41
1:C:151:LYS:HG3	1:C:430:GLN:OE1	2.21	0.41
2:D:13:ILE:HD12	2:D:73:GLN:HB3	2.03	0.41
2:D:86:VAL:HG11	2:D:114:ALA:HB3	2.02	0.41
2:E:95:MET:HE2	2:E:99:GLY:HA2	2.01	0.41
2:E:340:ALA:O	2:E:343:GLY:N	2.42	0.41
2:E:346:PRO:HG3	2:E:418:PHE:HZ	1.83	0.41
2:E:387:ILE:HG22	2:E:388:ILE:N	2.36	0.41
2:E:441:PHE:O	2:E:445:LEU:HG	2.19	0.41
2:F:423:VAL:O	2:F:423:VAL:HG12	2.20	0.41
1:B:206:ILE:HA	1:B:234:ALA:O	2.21	0.41
1:C:442:VAL:HG11	1:C:489:ILE:HD11	2.01	0.41
2:D:27:GLU:H	2:D:27:GLU:HG3	1.77	0.41
2:D:38:VAL:HG22	2:D:75:VAL:HG22	2.02	0.41
2:D:139:VAL:O	2:D:140:VAL:C	2.63	0.41
2:E:282:GLN:H	2:E:282:GLN:NE2	2.19	0.41
1:A:498:LYS:O	1:A:502:THR:HG23	2.21	0.41
1:B:30:ARG:HA	1:B:86:ASP:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:VAL:CG1	1:C:378:ALA:HB2	2.51	0.41
1:C:465:GLU:O	1:C:469:LEU:HB2	2.21	0.41
2:D:64:ASP:CG	2:D:65:GLY:H	2.28	0.41
2:D:112:GLN:NE2	2:D:242:TYR:CE1	2.88	0.41
2:D:274:ARG:HH11	2:D:274:ARG:HD2	1.50	0.41
2:D:401:LYS:H	2:D:401:LYS:HG2	1.72	0.41
2:E:35:ALA:C	2:E:36:LEU:HD23	2.46	0.41
2:E:88:PRO:C	2:E:90:THR:H	2.28	0.41
2:F:38:VAL:HG11	2:F:69:LEU:CD2	2.50	0.41
1:A:74:VAL:CG1	1:A:241:PRO:HG3	2.51	0.41
1:A:400:VAL:O	1:A:401:ALA:C	2.64	0.41
1:B:340:THR:O	1:B:341:ASN:C	2.63	0.41
1:C:139:ARG:HB3	1:C:311:LYS:O	2.19	0.41
2:D:360:PRO:HD3	2:D:368:TYR:CD2	2.56	0.41
1:A:129:VAL:HG12	1:A:249:SER:HA	2.03	0.41
1:A:398:ARG:HH11	1:A:398:ARG:HD2	1.53	0.41
1:C:19:ALA:O	1:C:21:THR:HG23	2.21	0.41
1:C:104:LEU:HD21	1:C:257:PHE:CZ	2.56	0.41
2:D:52:HIS:CD2	2:D:58:VAL:HG12	2.56	0.41
2:D:398:GLU:HA	2:D:401:LYS:CG	2.51	0.41
2:E:358:MET:HE3	2:E:358:MET:HB3	1.93	0.41
2:F:251:VAL:HG12	2:F:252:LEU:N	2.35	0.41
2:F:434:LEU:O	2:F:438:ILE:HG12	2.21	0.41
3:G:217:LEU:O	3:G:221:THR:HG23	2.20	0.41
3:G:241:GLU:O	3:G:245:LYS:HB2	2.21	0.41
1:A:67:GLU:HB3	1:A:68:PRO:HD2	2.03	0.41
1:A:102:GLU:HG3	1:A:122:GLY:C	2.46	0.41
1:A:294:TYR:CE2	1:A:338:ILE:HD13	2.56	0.41
1:A:390:MET:HE1	1:A:428:LEU:HD21	2.02	0.41
1:B:99:VAL:HG13	1:B:256:TYR:HB2	2.02	0.41
1:B:201:CYS:O	1:B:229:THR:HA	2.21	0.41
1:B:361:ILE:HD13	1:B:429:LYS:HE2	2.02	0.41
1:B:423:ARG:O	1:B:426:GLU:N	2.51	0.41
1:C:342:VAL:HA	1:C:345:ILE:HD12	2.03	0.41
1:C:468:PHE:CZ	1:C:501:VAL:HG12	2.56	0.41
2:D:203:SER:OG	2:D:205:VAL:HG23	2.21	0.41
2:D:397:SER:C	2:D:399:GLU:N	2.77	0.41
2:E:97:VAL:HG13	2:E:232:VAL:HG12	2.02	0.41
2:E:165:LEU:HD22	2:E:335:LEU:HD21	2.02	0.41
2:E:231:ARG:O	2:E:234:LEU:N	2.50	0.41
2:F:228:ALA:O	2:F:232:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:357:ILE:O	2:F:359:ASP:N	2.48	0.41
2:F:442:GLN:O	2:F:445:LEU:HB2	2.21	0.41
3:G:13:ILE:HD13	3:G:242:MET:HG2	2.02	0.41
1:B:209:LYS:NZ	2:E:356:ARG:NH1	2.69	0.41
1:B:452:TYR:CD2	1:B:501:VAL:HG21	2.56	0.41
1:C:484:ARG:HH11	1:C:484:ARG:HD3	1.76	0.41
2:D:65:GLY:HA3	2:D:67:GLU:OE2	2.21	0.41
2:D:349:ASP:HA	2:D:350:PRO:HD2	1.85	0.41
2:E:210:ASP:OD1	2:E:211:ALA:N	2.55	0.41
2:E:345:TYR:CA	2:E:346:PRO:C	2.89	0.41
2:F:95:MET:HE3	2:F:108:ILE:HD13	2.03	0.41
1:A:268:TYR:HB2	1:A:325:PRO:HA	2.03	0.40
1:A:440:GLU:HG2	1:A:473:ILE:HD11	2.03	0.40
1:A:485:THR:O	1:A:487:GLY:N	2.55	0.40
1:B:187:LYS:HE3	1:B:227:LYS:NZ	2.37	0.40
2:E:139:VAL:HG21	2:E:348:VAL:HB	2.02	0.40
2:E:329:LEU:O	2:E:356:ARG:CZ	2.70	0.40
2:F:167:MET:HB2	2:F:420:VAL:HG11	2.02	0.40
1:A:347:ASP:C	1:A:373:ARG:HH11	2.28	0.40
1:B:221:THR:HG22	1:B:222:ASP:N	2.36	0.40
1:C:142:VAL:C	1:C:143:ARG:HG3	2.46	0.40
1:C:390:MET:HE2	1:C:428:LEU:HD11	2.02	0.40
2:D:97:VAL:HG11	2:D:231:ARG:HB2	2.03	0.40
2:D:368:TYR:O	2:D:372:ARG:HG2	2.22	0.40
2:E:82:ILE:CG2	2:E:116:ILE:HD13	2.50	0.40
1:A:294:TYR:HB2	1:A:337:TYR:CE2	2.54	0.40
1:A:441:GLN:O	1:A:445:ILE:HG12	2.21	0.40
1:B:107:VAL:O	1:B:115:ILE:HG12	2.20	0.40
1:B:239:ALA:HB1	1:B:241:PRO:HD2	2.03	0.40
1:B:366:ASN:ND2	1:B:369:LEU:HG	2.36	0.40
1:B:376:SER:O	1:B:384:LYS:HE2	2.22	0.40
1:C:129:VAL:HG21	1:C:245:LEU:HD11	2.02	0.40
1:C:335:SER:O	2:D:314:ALA:HA	2.22	0.40
2:D:63:MET:CE	2:D:97:VAL:HG11	2.51	0.40
2:D:95:MET:HE3	2:D:99:GLY:HA2	2.02	0.40
2:D:281:TYR:HB3	2:D:285:LEU:HD12	2.03	0.40
1:A:147:GLN:OE1	1:A:438:ILE:HD13	2.21	0.40
1:B:62:MET:HE3	1:B:64:LEU:CD1	2.51	0.40
2:D:67:GLU:H	2:D:67:GLU:CD	2.30	0.40
2:E:55:GLU:O	2:E:56:SER:HB2	2.21	0.40
2:E:185:GLY:HA3	2:E:188:GLU:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:434:LEU:O	2:E:437:THR:HB	2.20	0.40
2:E:434:LEU:CD1	2:E:438:ILE:HD11	2.52	0.40
3:G:10:LEU:O	3:G:14:LYS:HG3	2.20	0.40
1:A:383:MET:HE2	1:A:438:ILE:CD1	2.48	0.40
1:A:408:SER:O	1:A:409:ASP:HB2	2.20	0.40
1:A:444:VAL:HG12	1:A:469:LEU:HD13	2.03	0.40
1:A:479:LEU:O	1:A:482:LYS:HB2	2.22	0.40
1:B:209:LYS:NZ	2:E:356:ARG:HH12	2.19	0.40
1:B:413:ALA:O	1:B:414:THR:C	2.64	0.40
1:C:45:ARG:HA	1:C:45:ARG:HD3	1.29	0.40
1:C:45:ARG:HH11	1:C:45:ARG:HD2	1.68	0.40
2:D:381:TYR:O	2:D:385:GLN:HG3	2.22	0.40
2:E:454:GLU:C	2:E:456:ALA:H	2.29	0.40
2:E:454:GLU:O	2:E:456:ALA:N	2.55	0.40
2:F:471:ASP:O	2:F:474:ALA:N	2.53	0.40
3:G:2:THR:HB	3:G:5:ASP:CG	2.46	0.40
3:G:42:ARG:HG2	3:G:219:GLU:OE2	2.20	0.40

There are no symmetry-related clashes.

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%)	442 (91%)	36 (7%)	7 (1%)	9	40
1	B	475/553 (86%)	426 (90%)	42 (9%)	7 (2%)	8	40
1	C	490/553 (89%)	445 (91%)	37 (8%)	8 (2%)	7	38
2	D	465/528 (88%)	419 (90%)	43 (9%)	3 (1%)	21	59
2	E	464/528 (88%)	408 (88%)	47 (10%)	9 (2%)	6	32
2	F	464/528 (88%)	432 (93%)	30 (6%)	2 (0%)	30	67
3	G	116/298 (39%)	97 (84%)	18 (16%)	1 (1%)	14	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2959/3541 (84%)	2669 (90%)	253 (9%)	37 (1%)	9	42

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
1	C	476	HIS
2	D	28	GLY
2	E	161	GLY
2	E	205	VAL
3	G	81	ILE
1	A	364	ALA
1	A	404	ALA
1	B	236	ALA
1	B	452	TYR
2	E	121	PRO
2	E	455	GLN
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%)	335 (86%)	53 (14%)	3	14
1	C	397/444 (89%)	359 (90%)	38 (10%)	8	25
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	102/251 (41%)	90 (88%)	12 (12%)	5	18
All	All	2409/2834 (85%)	2149 (89%)	260 (11%)	6	21

All (260) 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

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

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Mol	Chain	Res	Type
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
1	B	298	VAL
1	B	327	ILE
1	B	334	VAL
1	B	335	SER
1	B	349	GLN
1	B	351	PHE
1	B	361	ILE
1	B	371	VAL
1	B	374	VAL
1	B	376	SER
1	B	380	THR
1	B	381	ARG
1	B	398	ARG
1	B	399	GLU
1	B	400	VAL
1	B	416	GLN
1	B	423	ARG
1	B	430	GLN
1	B	442	VAL
1	B	444	VAL
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

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

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Mol	Chain	Res	Type
2	D	95	MET
2	D	97	VAL
2	D	112	GLN
2	D	137	ILE
2	D	139	VAL
2	D	166	ILE
2	D	199	GLU
2	D	205	VAL
2	D	223	ASN
2	D	232	VAL
2	D	249	GLN
2	D	258	ILE
2	D	266	SER
2	D	279	VAL
2	D	282	GLN
2	D	306	SER
2	D	336	SER
2	D	361	ASN
2	D	365	SER
2	D	388	ILE
2	D	397	SER
2	D	401	LYS
2	D	423	VAL
2	D	428	LEU
2	D	431	LEU
2	D	439	LYS
2	D	452	LEU
2	D	475	GLU
2	E	9	THR
2	E	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

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

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Mol	Chain	Res	Type
2	F	210	ASP
2	F	223	ASN
2	F	232	VAL
2	F	279	VAL
2	F	292	MET
2	F	357	ILE
2	F	386	ASP
2	F	387	ILE
2	F	393	MET
2	F	397	SER
2	F	405	SER
2	F	410	ILE
2	F	423	VAL
2	F	428	LEU
2	F	435	LYS
2	F	438	ILE
2	F	455	GLN
2	F	467	VAL
3	G	4	LYS
3	G	11	LYS
3	G	13	ILE
3	G	20	THR
3	G	22	SER
3	G	77	LEU
3	G	82	HIS
3	G	85	VAL
3	G	209	LEU
3	G	214	TYR
3	G	221	THR
3	G	254	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	GLN
1	A	349	GLN
1	A	396	GLN
1	A	476	HIS
1	B	42	HIS
1	B	215	GLN
1	B	330	GLN
1	B	415	GLN

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Mol	Chain	Res	Type
1	B	466	ASN
1	C	48	GLN
1	C	208	GLN
1	C	215	GLN
1	C	260	ASN
1	C	396	GLN
1	C	416	GLN
1	C	432	GLN
2	D	24	GLN
2	D	130	GLN
2	D	171	ASN
2	D	221	GLN
2	D	223	ASN
2	D	282	GLN
2	D	411	GLN
2	D	442	GLN
2	D	455	GLN
2	E	130	GLN
2	E	194	ASN
2	E	223	ASN
2	E	246	GLN
2	E	282	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	249	GLN
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	211	ASN
3	G	225	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADP	D	1476	-	28,29,29	0.92	1 (3%)	43,45,45	1.19	4 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	D	1476	-	-	2/16/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1476	ADP	PA-O3A	2.34	1.62	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1476	ADP	N6-C6-N1	2.61	124.19	118.38
4	D	1476	ADP	O3'-C3'-C2'	-2.14	104.97	111.82
4	D	1476	ADP	O4'-C1'-N9	-2.13	104.00	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1476	ADP	O4'-C4'-C3'	-2.02	101.14	105.15

There are no chirality outliers.

All (2) torsion outliers are listed below:

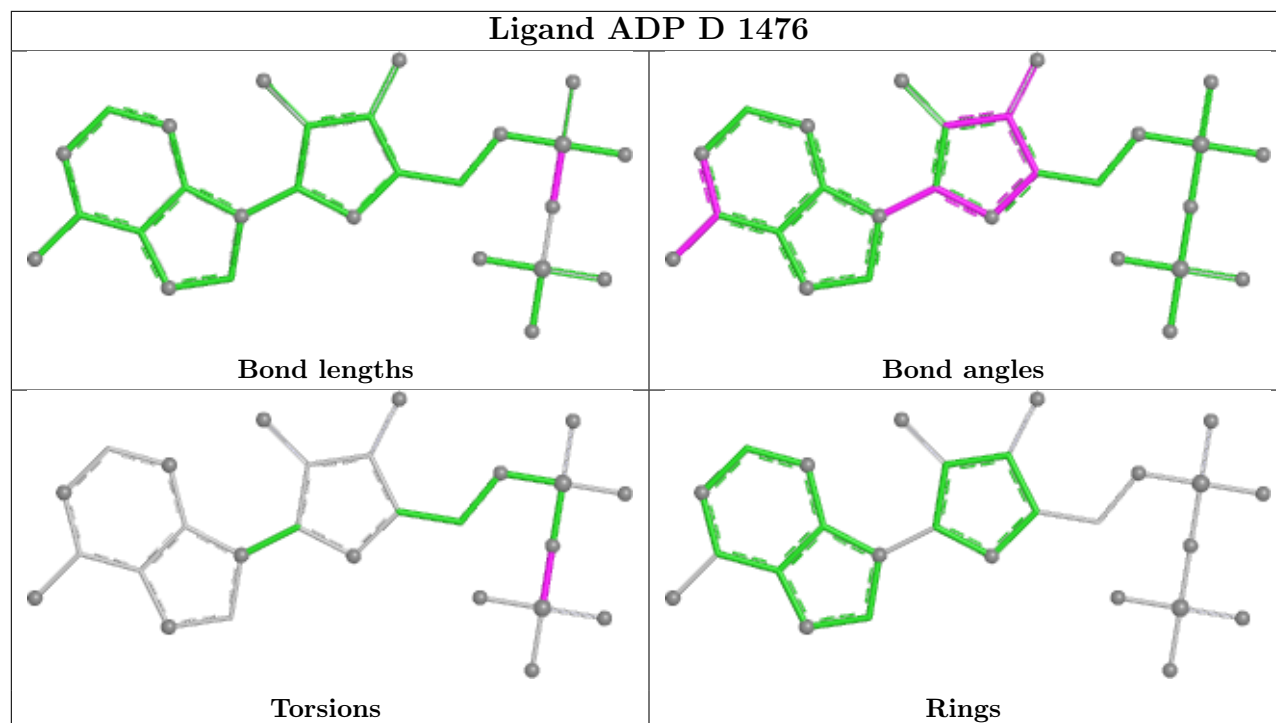
Mol	Chain	Res	Type	Atoms
4	D	1476	ADP	PA-O3A-PB-O2B
4	D	1476	ADP	PA-O3A-PB-O3B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1476	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	487/553 (88%)	0.03	18 (3%) 45 43	20, 20, 20, 20	0
1	B	479/553 (86%)	0.00	12 (2%) 58 50	20, 20, 20, 20	0
1	C	492/553 (88%)	0.03	15 (3%) 52 46	20, 20, 20, 20	0
2	D	467/528 (88%)	0.04	15 (3%) 50 45	20, 20, 20, 20	0
2	E	466/528 (88%)	-0.04	4 (0%) 81 70	20, 20, 20, 20	0
2	F	466/528 (88%)	0.05	18 (3%) 43 42	20, 20, 20, 20	0
3	G	122/298 (40%)	0.04	1 (0%) 82 72	20, 20, 20, 20	0
All	All	2979/3541 (84%)	0.02	83 (2%) 55 48	20, 20, 20, 20	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	166	ILE	5.0
1	A	269	ASP	4.7
1	A	203	TYR	4.6
2	F	117	HIS	4.1
1	B	351	PHE	4.0
1	C	270	ASP	3.9
2	F	116	ILE	3.9
1	A	201	CYS	3.9
2	D	102	ILE	3.8
1	A	176	THR	3.7
2	F	470	ALA	3.6
1	B	76	PHE	3.5
1	C	285	LEU	3.4
2	D	170	ILE	3.3
2	F	163	THR	3.2
1	C	254	GLY	3.2
1	A	414	THR	3.2

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Mol	Chain	Res	Type	RSRZ
2	F	340	ALA	3.2
1	C	501	VAL	3.1
1	A	283	LEU	3.1
2	D	466	ALA	3.1
1	B	380	THR	3.0
1	B	373	ARG	2.9
1	C	251	CYS	2.9
2	E	66	THR	2.9
1	A	167	ILE	2.9
2	D	233	ALA	2.9
1	B	493	SER	2.9
1	C	147	GLN	2.8
2	F	191	ARG	2.8
1	B	167	ILE	2.8
1	B	216	LEU	2.8
1	A	174	GLY	2.8
2	F	296	ILE	2.7
2	F	159	GLY	2.6
2	F	161	GLY	2.6
1	B	449	VAL	2.6
2	E	403	THR	2.6
2	F	197	TYR	2.6
1	A	350	ILE	2.6
1	C	167	ILE	2.6
1	A	246	ALA	2.5
1	A	173	THR	2.5
2	D	188	GLU	2.5
1	B	152	ALA	2.5
1	A	328	GLU	2.5
1	A	406	PHE	2.5
1	B	174	GLY	2.5
2	D	167	MET	2.5
2	F	162	LYS	2.4
1	A	172	GLN	2.4
2	D	19	ALA	2.4
1	B	469	LEU	2.4
2	D	256	ASP	2.4
2	F	127	SER	2.3
2	F	272	LEU	2.3
2	F	438	ILE	2.3
1	A	175	LYS	2.3
2	E	460	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	215	GLN	2.3
1	C	175	LYS	2.3
2	F	81	PRO	2.2
2	F	63	MET	2.2
1	C	364	ALA	2.2
2	F	466	ALA	2.2
1	C	44	LEU	2.2
2	F	368	TYR	2.2
2	D	317	LEU	2.2
2	D	289	MET	2.2
1	C	296	GLY	2.1
1	A	267	ILE	2.1
3	G	211	ASN	2.1
1	C	173	THR	2.1
2	D	444	ILE	2.1
1	C	103	LEU	2.1
2	D	410	ILE	2.1
1	A	480	LEU	2.0
1	B	56	SER	2.0
1	A	424	LEU	2.0
1	C	407	GLY	2.0
2	D	291	THR	2.0
2	D	275	ILE	2.0
2	E	19	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

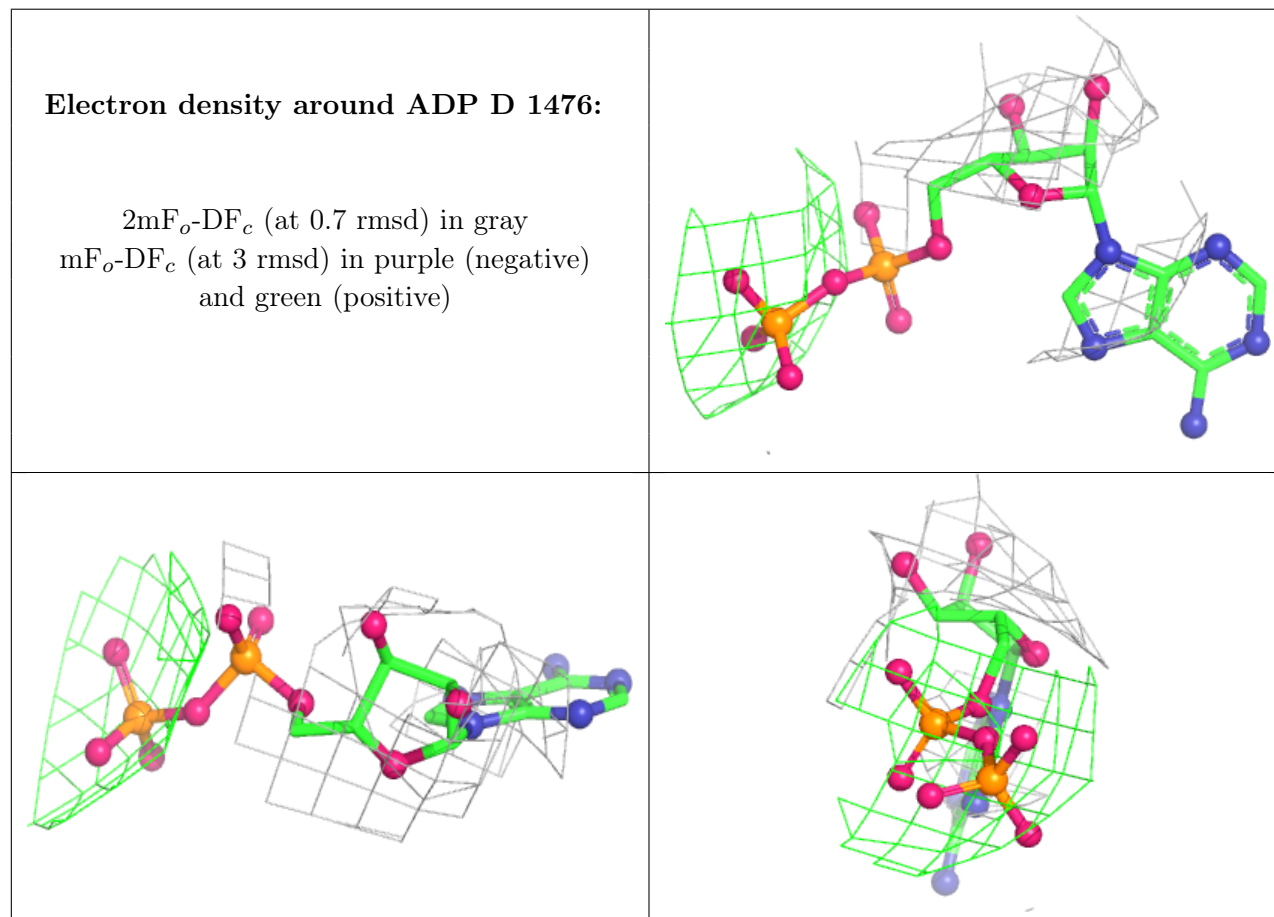
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ADP	D	1476	27/27	0.76	0.15	20,20,20,20	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.