Full wwPDB X-ray Structure Validation Report (i)

Dec 9, 2023 – 03:37 pm GMT

PDB ID	:	2W6E
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 (i) 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 (i)) were used in the production of this report:

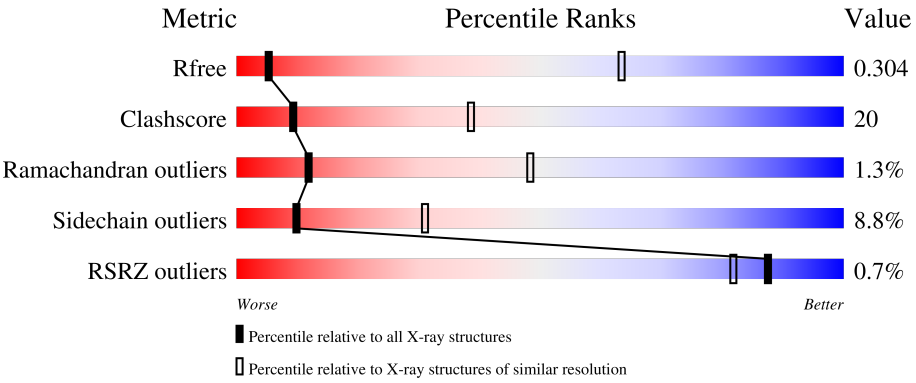
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	1000 (9.00-3.90)
Clashscore	141614	1064 (9.00-3.90)
Ramachandran outliers	138981	1012 (9.00-3.88)
Sidechain outliers	138945	1010 (9.00-3.84)
RSRZ outliers	127900	1002 (9.00-3.80)

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 <=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	% 47% 33% 7% • 12%
1	B	553	% 48% 31% 6% • 13%
1	C	553	53% 31% • • 11%
2	D	528	54% 29% 5% • 12%

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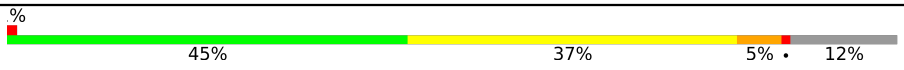
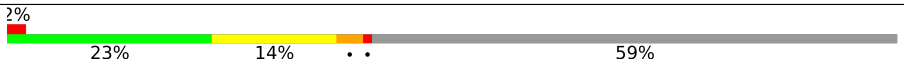
Mol	Chain	Length	Quality of chain
2	E	528	
2	F	528	
3	G	298	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ADP	D	1476	-	-	-	X

2 Entry composition (i)

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			

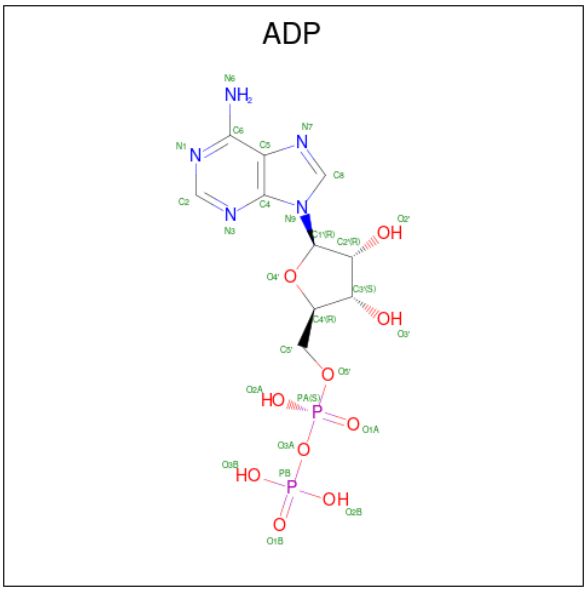
- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

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 (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



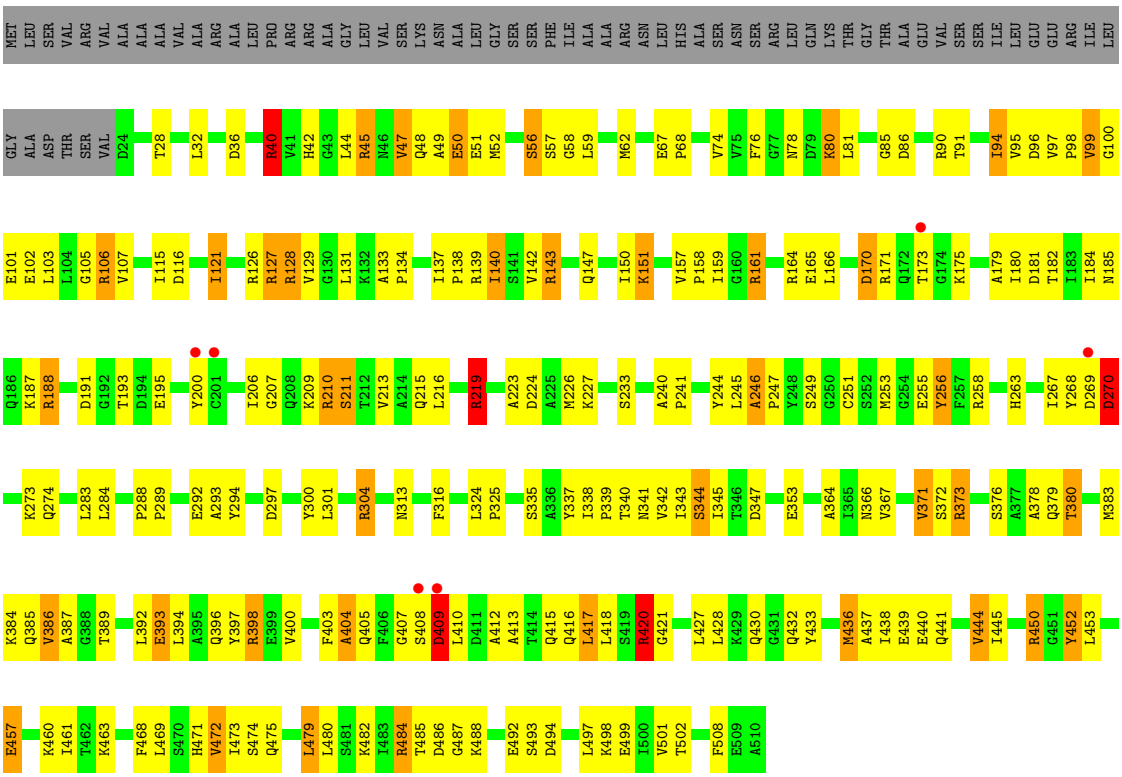
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	D	1	27	10	5	10	2	0	0

3 Residue-property plots (i)

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.

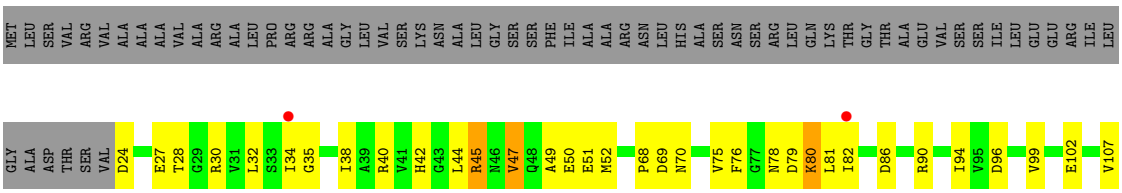
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL

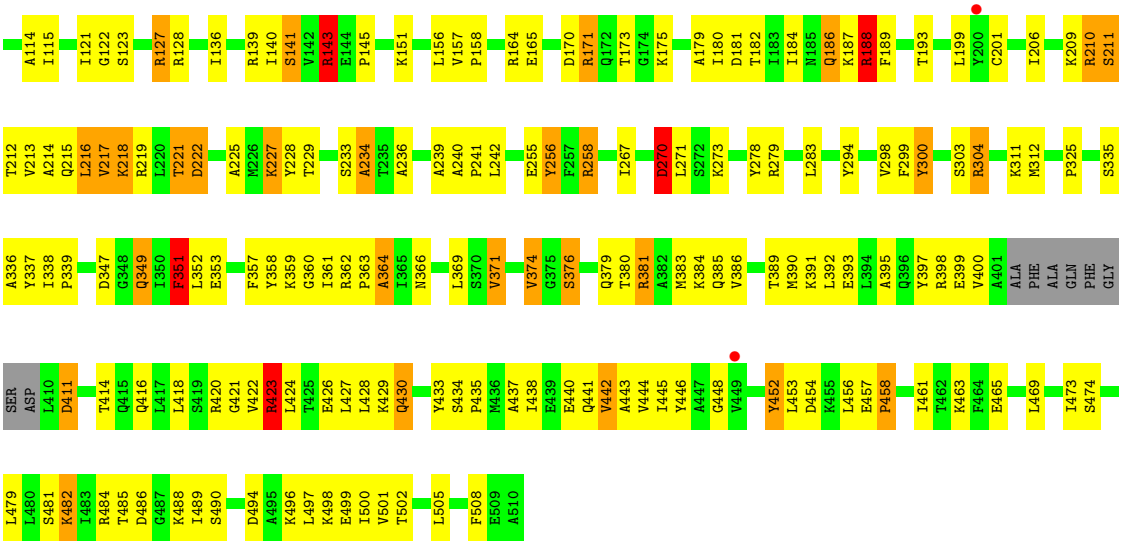
Chain A:



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

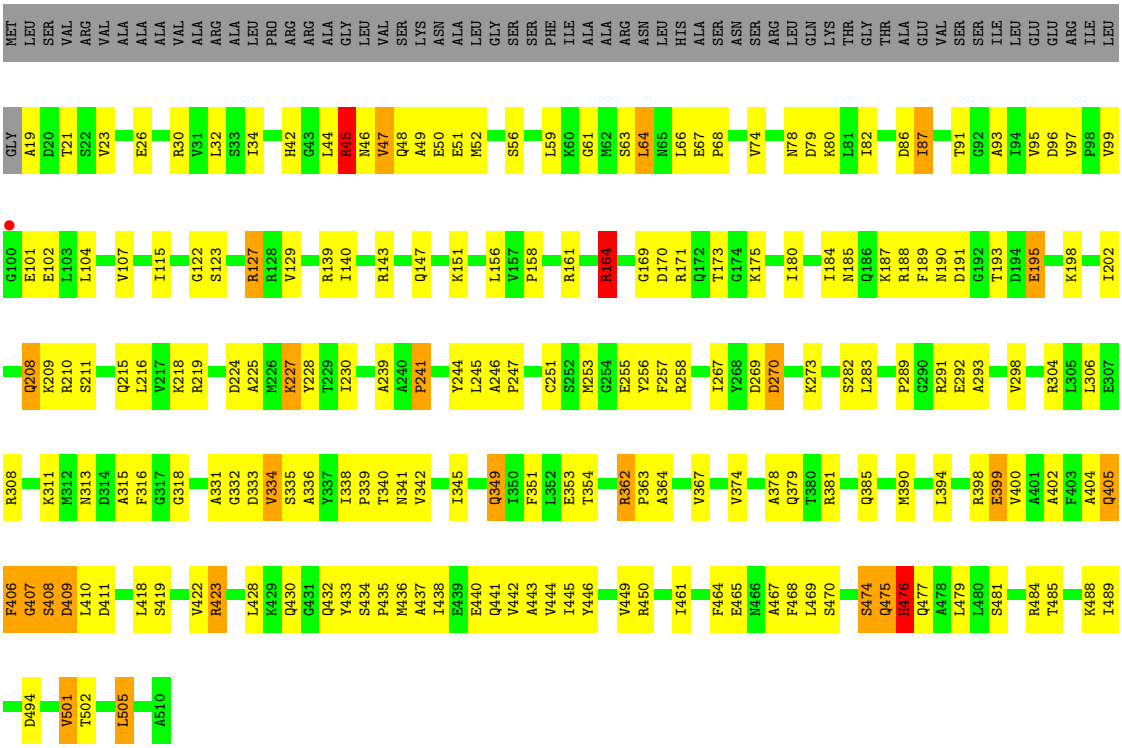
Chain B:





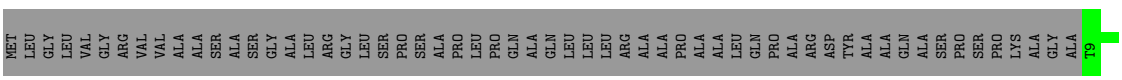
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL

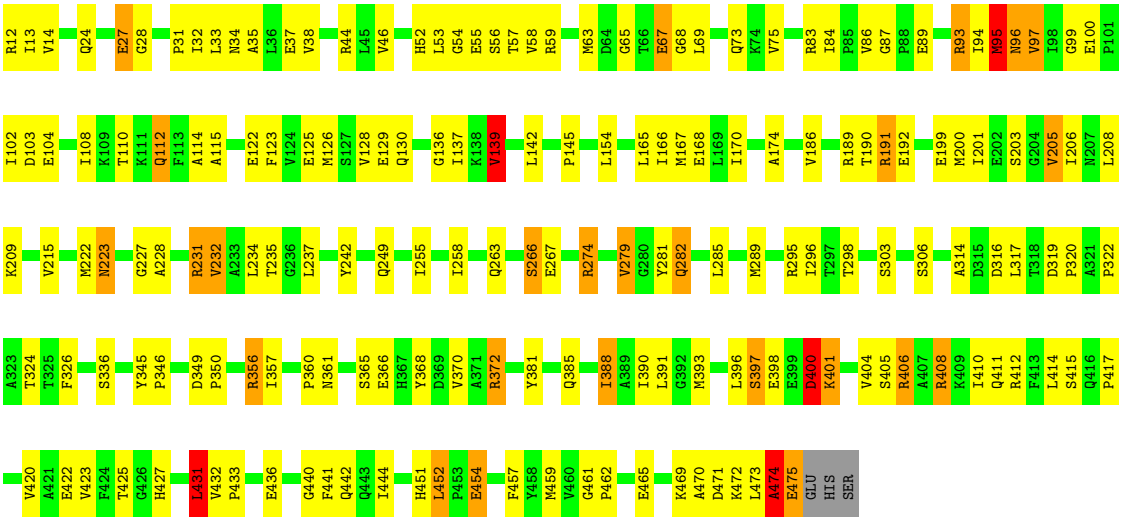
Chain C:



• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

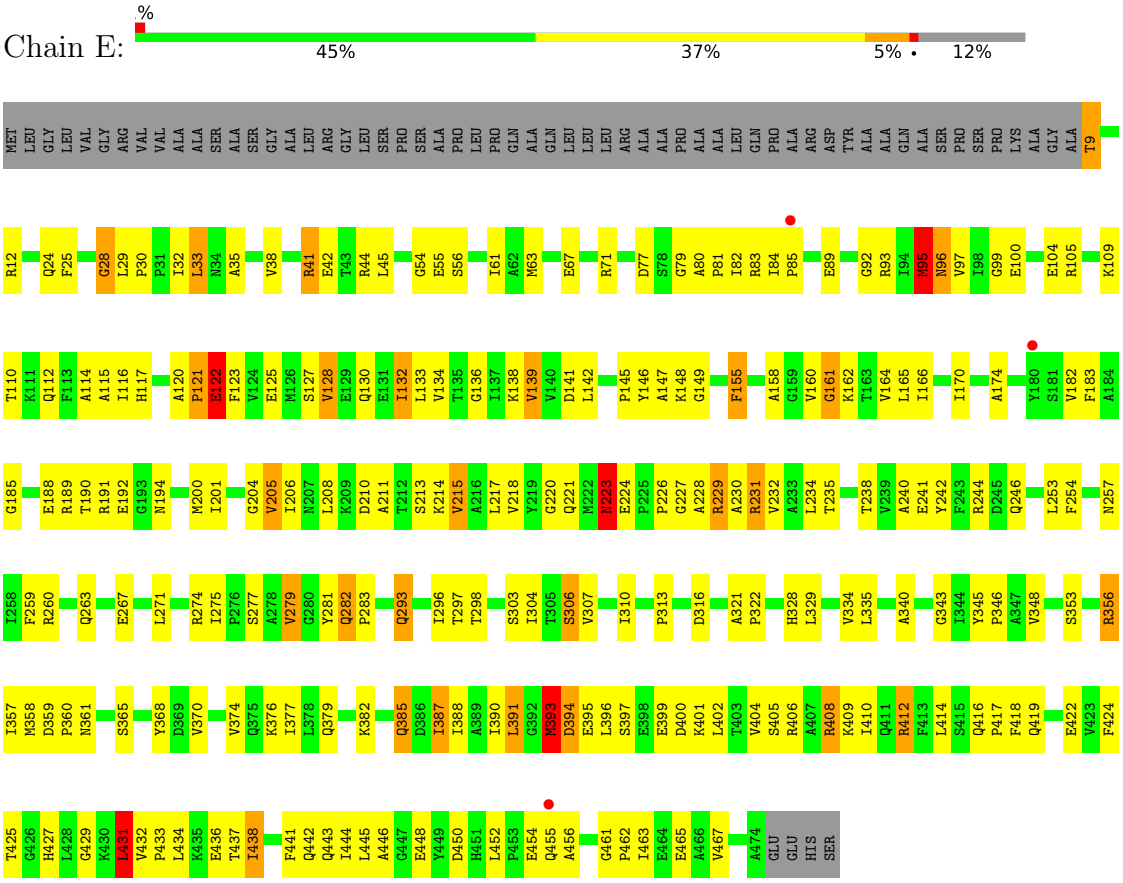
Chain D:





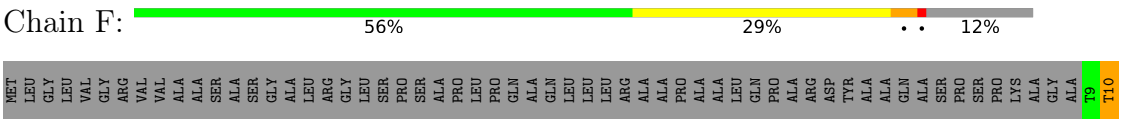
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

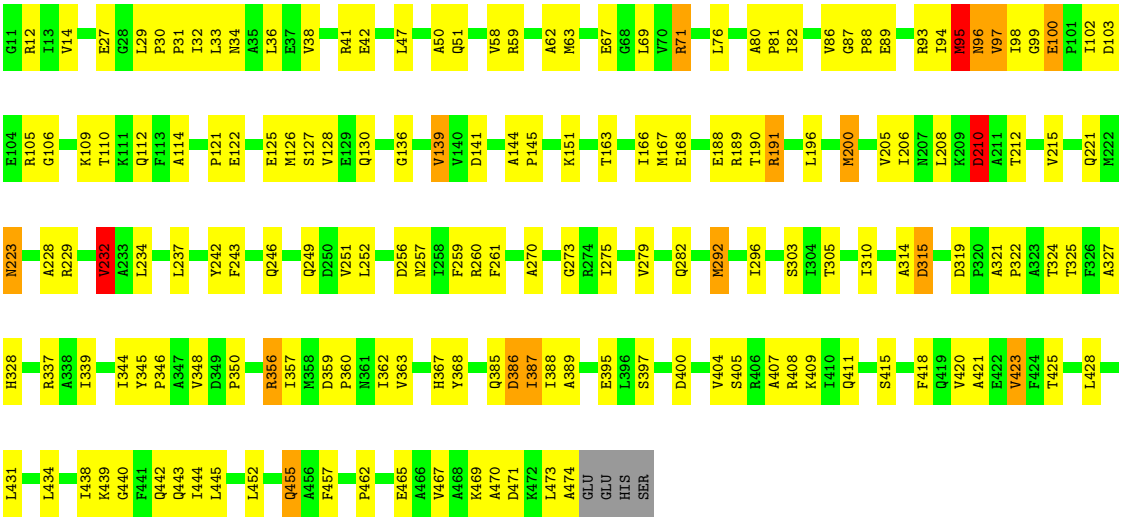
Chain E:



• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

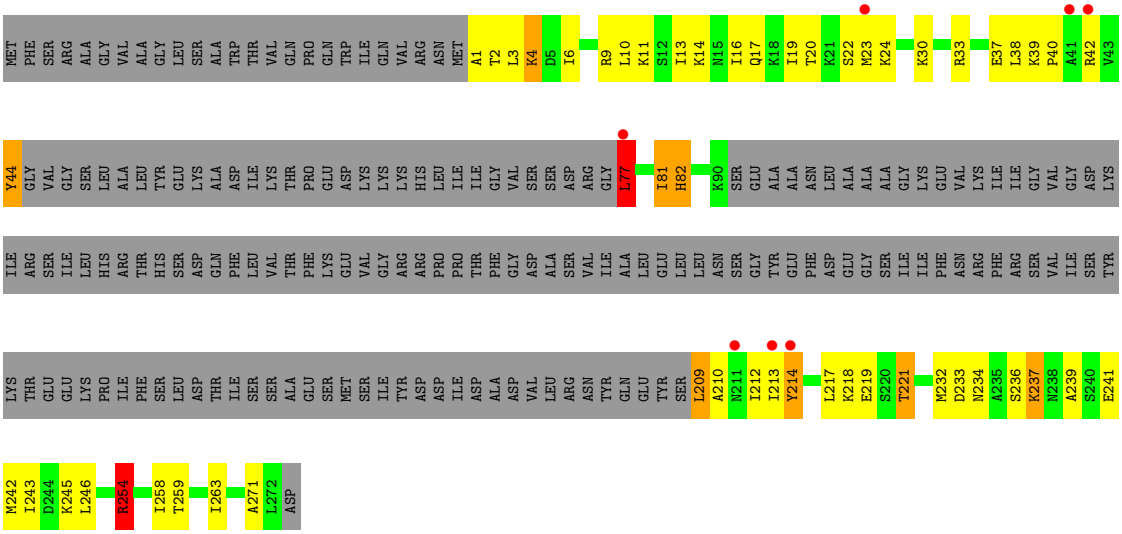
Chain F:





• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL

Chain G:



4 Data and refinement statistics (i)

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 50.70 – 6.50	Depositor EDS
% Data completeness (in resolution range)	86.9 (30.00-6.50) 86.8 (50.70-6.50)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 6.68Å)	Xtriage
Refinement program	REFMAC 5.5.0038	Depositor
R, R_{free}	0.290 , 0.285 0.303 , 0.304	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)	0.29 , 66.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.34$, $< L^2 > = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.79	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.60	0/3766	1.31	29/5080 (0.6%)
1	B	0.61	0/3704	1.36	33/4995 (0.7%)
1	C	0.62	0/3799	1.38	24/5126 (0.5%)
2	D	0.62	0/3596	1.36	23/4879 (0.5%)
2	E	0.60	0/3587	1.32	18/4867 (0.4%)
2	F	0.62	0/3587	1.36	28/4867 (0.6%)
3	G	0.52	0/949	1.15	5/1266 (0.4%)
All	All	0.61	0/22988	1.34	160/31080 (0.5%)

There are no bond length outliers.

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	408	ARG	CD-NE-CZ	23.29	156.21	123.60
2	E	408	ARG	CD-NE-CZ	14.03	143.24	123.60
1	C	291	ARG	NE-CZ-NH2	-13.33	113.64	120.30
1	B	40	ARG	NE-CZ-NH1	13.22	126.91	120.30
1	B	279	ARG	NE-CZ-NH1	12.94	126.77	120.30
2	F	356	ARG	NE-CZ-NH1	11.55	126.08	120.30
2	D	406	ARG	NE-CZ-NH1	-11.34	114.63	120.30
2	F	59	ARG	NE-CZ-NH1	-11.26	114.67	120.30
3	G	254	ARG	NE-CZ-NH2	-11.00	114.80	120.30
2	D	408	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	B	219	ARG	NE-CZ-NH2	10.33	125.47	120.30
2	F	282	GLN	CB-CG-CD	10.31	138.42	111.60
1	C	258	ARG	NE-CZ-NH1	10.02	125.31	120.30
1	C	164	ARG	NE-CZ-NH1	-10.01	115.30	120.30
1	B	40	ARG	CD-NE-CZ	9.89	137.45	123.60
2	F	229	ARG	NE-CZ-NH1	-9.41	115.59	120.30
2	F	356	ARG	NE-CZ-NH2	-9.36	115.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	95	MET	CA-CB-CG	9.26	129.04	113.30
2	D	44	ARG	NE-CZ-NH2	-9.17	115.72	120.30
1	C	161	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	B	304	ARG	NE-CZ-NH1	-9.05	115.78	120.30
2	F	59	ARG	NE-CZ-NH2	8.97	124.79	120.30
1	A	420	ARG	NE-CZ-NH1	-8.67	115.96	120.30
2	F	96	ASN	CB-CA-C	-8.56	93.28	110.40
2	E	260	ARG	NE-CZ-NH1	-8.54	116.03	120.30
2	E	95	MET	CA-CB-CG	8.52	127.78	113.30
2	E	83	ARG	NE-CZ-NH1	-8.49	116.06	120.30
1	C	450	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	A	373	ARG	NE-CZ-NH2	8.28	124.44	120.30
1	A	398	ARG	NE-CZ-NH1	-8.27	116.17	120.30
1	A	450	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	C	127	ARG	NE-CZ-NH1	-8.11	116.25	120.30
2	E	229	ARG	NE-CZ-NH1	8.08	124.34	120.30
2	F	229	ARG	NE-CZ-NH2	8.00	124.30	120.30
2	D	125	GLU	OE1-CD-OE2	-7.94	113.77	123.30
1	B	304	ARG	NE-CZ-NH2	7.90	124.25	120.30
1	C	362	ARG	NE-CZ-NH2	7.85	124.22	120.30
1	B	219	ARG	NE-CZ-NH1	-7.80	116.40	120.30
1	B	279	ARG	NE-CZ-NH2	-7.52	116.54	120.30
2	F	408	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	C	450	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	C	304	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	B	270	ASP	CB-CA-C	-7.37	95.67	110.40
2	D	93	ARG	NE-CZ-NH1	-7.18	116.71	120.30
1	C	161	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	C	45	ARG	NE-CZ-NH2	-7.13	116.73	120.30
2	E	356	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	450	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	270	ASP	CB-CA-C	-7.11	96.18	110.40
1	B	258	ARG	CD-NE-CZ	7.08	133.51	123.60
2	E	41	ARG	CD-NE-CZ	7.08	133.51	123.60
2	F	139	VAL	CB-CA-C	-7.04	98.03	111.40
2	E	356	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	B	279	ARG	CD-NE-CZ	6.95	133.33	123.60
3	G	77	LEU	CA-CB-CG	6.90	131.17	115.30
2	F	95	MET	C-N-CA	6.77	138.61	121.70
1	C	308	ARG	NE-CZ-NH1	-6.68	116.96	120.30
2	D	96	ASN	CB-CA-C	-6.68	97.04	110.40
2	D	95	MET	C-N-CA	6.64	138.29	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	349	GLN	CA-CB-CG	6.63	127.99	113.40
2	D	274	ARG	NE-CZ-NH1	-6.61	116.99	120.30
2	D	59	ARG	NE-CZ-NH1	-6.56	117.02	120.30
2	E	44	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	B	423	ARG	CD-NE-CZ	6.55	132.77	123.60
1	A	127	ARG	NE-CZ-NH2	-6.52	117.04	120.30
2	D	231	ARG	NE-CZ-NH1	6.52	123.56	120.30
2	F	256	ASP	CB-CG-OD1	6.50	124.15	118.30
1	B	270	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	106	ARG	CD-NE-CZ	6.48	132.68	123.60
1	A	372	SER	N-CA-CB	6.45	120.18	110.50
2	F	189	ARG	NE-CZ-NH2	6.44	123.52	120.30
2	D	191	ARG	NE-CZ-NH1	-6.43	117.08	120.30
2	E	431	LEU	CA-CB-CG	6.39	130.00	115.30
1	A	371	VAL	CB-CA-C	-6.38	99.27	111.40
1	A	210	ARG	NE-CZ-NH2	-6.35	117.12	120.30
2	F	12	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	A	170	ASP	CB-CG-OD1	6.31	123.98	118.30
1	B	300	TYR	CB-CG-CD2	-6.29	117.23	121.00
1	A	398	ARG	NE-CZ-NH2	6.27	123.44	120.30
1	C	308	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	C	291	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	171	ARG	NE-CZ-NH2	6.22	123.41	120.30
2	D	372	ARG	NE-CZ-NH2	6.19	123.39	120.30
1	C	476	HIS	N-CA-C	6.16	127.64	111.00
1	B	127	ARG	CD-NE-CZ	6.16	132.22	123.60
1	C	381	ARG	CD-NE-CZ	6.16	132.22	123.60
1	B	371	VAL	CB-CA-C	-6.11	99.78	111.40
2	F	97	VAL	CB-CA-C	-6.11	99.79	111.40
1	B	128	ARG	NE-CZ-NH1	6.11	123.35	120.30
2	E	274	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	C	423	ARG	CD-NE-CZ	6.03	132.05	123.60
1	C	164	ARG	CD-NE-CZ	-6.01	115.19	123.60
1	A	40	ARG	NE-CZ-NH2	5.98	123.29	120.30
2	D	222	MET	CB-CA-C	-5.95	98.50	110.40
1	A	269	ASP	C-N-CA	5.91	136.46	121.70
3	G	9	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	B	337	TYR	CB-CG-CD1	5.79	124.47	121.00
1	A	304	ARG	NE-CZ-NH1	-5.78	117.41	120.30
2	F	103	ASP	CB-CG-OD2	-5.73	113.14	118.30
2	F	191	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	219	ARG	CD-NE-CZ	5.69	131.57	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	41	ARG	CG-CD-NE	5.66	123.68	111.80
1	A	297	ASP	CB-CG-OD1	5.65	123.39	118.30
2	D	139	VAL	CB-CA-C	-5.65	100.67	111.40
2	D	474	ALA	C-N-CA	5.63	135.78	121.70
1	A	297	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	B	139	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	B	423	ARG	NE-CZ-NH1	5.58	123.09	120.30
2	D	454	GLU	CA-CB-CG	5.58	125.68	113.40
1	A	233	SER	N-CA-CB	-5.58	102.13	110.50
3	G	237	LYS	CB-CA-C	5.56	121.52	110.40
1	B	210	ARG	NE-CZ-NH1	-5.56	117.52	120.30
2	D	431	LEU	CA-CB-CG	5.56	128.08	115.30
1	B	398	ARG	NE-CZ-NH1	-5.54	117.53	120.30
2	E	93	ARG	NE-CZ-NH1	-5.51	117.54	120.30
2	D	12	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	B	349	GLN	N-CA-CB	5.48	120.47	110.60
1	B	143	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	A	335	SER	CB-CA-C	-5.40	99.83	110.10
1	C	349	GLN	CB-CA-C	-5.38	99.64	110.40
1	C	170	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	222	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	B	40	ARG	NE-CZ-NH2	-5.33	117.63	120.30
2	D	372	ARG	NE-CZ-NH1	-5.33	117.63	120.30
2	F	191	ARG	CD-NE-CZ	5.32	131.04	123.60
1	C	241	PRO	N-CA-CB	5.31	109.67	103.30
2	F	71	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	B	45	ARG	CB-CG-CD	-5.27	97.91	111.60
1	B	188	ARG	CG-CD-NE	5.25	122.83	111.80
1	C	171	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	270	ASP	CB-CG-OD1	5.23	123.01	118.30
1	C	336	ALA	N-CA-CB	-5.23	102.78	110.10
1	B	278	TYR	CB-CG-CD1	-5.22	117.87	121.00
1	A	258	ARG	CD-NE-CZ	5.18	130.86	123.60
1	B	351	PHE	N-CA-CB	5.18	119.92	110.60
2	D	316	ASP	CB-CG-OD2	-5.17	113.64	118.30
2	E	260	ARG	NE-CZ-NH2	5.16	122.88	120.30
2	E	408	ARG	NE-CZ-NH1	5.16	122.88	120.30
2	F	100	GLU	OE1-CD-OE2	5.14	129.47	123.30
2	F	423	VAL	CB-CA-C	-5.11	101.70	111.40
1	C	127	ARG	NH1-CZ-NH2	5.10	125.00	119.40
1	A	161	ARG	NE-CZ-NH2	-5.09	117.75	120.30
2	E	122	GLU	CA-CB-CG	5.08	124.57	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	128	ARG	NE-CZ-NH1	-5.08	117.76	120.30
2	D	400	ASP	CB-CG-OD1	5.08	122.87	118.30
3	G	44	TYR	CA-CB-CG	5.07	123.04	113.40
2	E	96	ASN	N-CA-CB	-5.07	101.48	110.60
2	F	337	ARG	CD-NE-CZ	5.05	130.67	123.60
1	A	40	ARG	CG-CD-NE	5.05	122.40	111.80
2	F	303	SER	N-CA-CB	-5.05	102.92	110.50
1	A	452	TYR	CB-CG-CD1	-5.05	117.97	121.00
2	F	232	VAL	CB-CA-C	-5.05	101.81	111.40
1	B	171	ARG	NE-CZ-NH2	-5.03	117.78	120.30
2	E	223	ASN	CB-CA-C	-5.03	100.34	110.40
2	F	315	ASP	CB-CG-OD1	5.03	122.83	118.30
2	D	356	ARG	CD-NE-CZ	-5.03	116.56	123.60
2	F	210	ASP	CB-CA-C	-5.03	100.34	110.40
2	E	231	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	B	234	ALA	N-CA-C	-5.02	97.46	111.00
1	A	200	TYR	CA-CB-CG	-5.00	103.89	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	162	0
1	B	3656	0	3764	143	0
1	C	3748	0	3843	145	0
2	D	3539	0	3593	150	0
2	E	3530	0	3587	184	0
2	F	3530	0	3586	117	0
3	G	945	0	1019	43	0
4	D	27	0	12	1	0
All	All	22690	0	23217	908	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 20.

All (908) 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
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:404:ALA:C	1:C:406:PHE:H	1.64	0.91
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
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
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
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
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
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
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
2:E:394:ASP:C	2:E:396:LEU:H	1.93	0.72
1:B:180:ILE:HD11	1:B:216:LEU:HD21	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:84:ILE:HB	2:D:95:MET:HE3	1.74	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: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
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
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
2:E:345:TYR:HA	2:E:346:PRO:C	2.13	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:D:393:MET:HE3	2:D:404:VAL:HG21	1.75	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
2:F:223:ASN:H	2:F:223:ASN:ND2	1.85	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:D:54:GLY:O	2:D:55:GLU:HB2	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:223:ASN:H	2:D:223:ASN:ND2	1.93	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
1:C:404:ALA:C	1:C:406:PHE:N	2.44	0.64
2:F:200:MET:HG3	2:F:205:VAL:HG23	1.80	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
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:F:136:GLY:HA3	2:F:431:LEU:HD12	1.80	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
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: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:E:394:ASP:C	2:E:396:LEU:N	2.54	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:270:ASP:OD1	1:A:273:LYS:HG3	2.01	0.61
1:C:211:SER:HB3	2:F:126:MET:HE3	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:C:362:ARG:HA	1:C:363:PRO:C	2.21	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
1:A:376:SER:C	1:A:378:ALA:H	2.03	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
1:C:407:GLY:HA2	1:C:410:LEU:HD11	1.84	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:362:ARG:HA	1:B:363:PRO:C	2.22	0.59
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.37	0.59
1:A:376:SER:C	1:A:378:ALA:N	2.55	0.59
1:C:215:GLN:HG3	2:F:356:ARG:NH2	2.11	0.59
1:B:136:ILE:HG13	2:F:190:THR:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
2:D:473:LEU:C	2:D:475:GLU:H	2.08	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:THR:CG2	1:C:354:THR:HG22	2.35	0.57
2: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
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
1:C:408:SER:O	1:C:409:ASP:C	2.44	0.56
2:E:122:GLU:N	2:E:125:GLU:OE2	2.37	0.56
2:E:158:ALA:C	2:E:160:VAL:H	2.08	0.56
2:F:32:ILE:O	2:F:33:LEU:HB2	2.06	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:397:SER:C	2:E:399:GLU:N	2.57	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
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: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
1:C:433:TYR:C	1:C:435:PRO:HD3	2.26	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: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
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:D:84:ILE:HD12	2:D:95:MET:HE1	1.88	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:69:ASP:O	1:B:70:ASN:HB3	2.08	0.53
1:C:156:LEU:HD11	1:C:428:LEU:HD13	1.91	0.53
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:D:431:LEU:C	2:D:431:LEU:HD12	2.29	0.53
1:B:358:TYR:C	1:B:360:GLY:H	2.12	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:D:473:LEU:C	2:D:475:GLU:N	2.62	0.53
2:E:84:ILE:HB	2:E:95:MET:HE1	1.91	0.53
2:E:220:GLY:HA3	2:E:232:VAL:HG21	1.91	0.53
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: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:423:ARG:HD2	1:B:461:ILE:HD11	1.91	0.52
1:C:405:GLN:C	1:C:406:PHE:HD1	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:LEU:HA	1:B:482:LYS:HE3	1.90	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
1:C:436:MET:CE	1:C:469:LEU:HD21	2.41	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
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: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: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: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
2:E:63:MET:HE3	2:E:228:ALA:HA	1.92	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:154:LEU:HD22	2:D:165:LEU:HD23	1.92	0.51
2:D:425:THR:HG21	2:D:459:MET:HE1	1.93	0.51
2:E:241:GLU:HA	2:E:304:ILE:HD11	1.93	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:96:ASN:ND2	2:F:100:GLU:HB2	2.26	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
1:A:187:LYS:HE2	1:A:191:ASP:OD2	2.11	0.50
1:B:390:MET:CE	1:B:428:LEU:HD21	2.42	0.50
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:B:180:ILE:O	1:B:181:ASP:C	2.47	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:A:224:ASP:CG	1:A:227:LYS:HE3	2.31	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: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:C:52:MET:HE3	1:C:95:VAL:HG13	1.92	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:417:PRO:HB3	2:D:459:MET:HE3	1.94	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
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
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: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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:383:MET:O	1:B:384:LYS:C	2.52	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: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:F:96:ASN:HD22	2:F:100:GLU:CB	2.27	0.48
1:A:245:LEU:O	1:A:246:ALA:C	2.51	0.47
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: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: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
2:F:36:LEU:N	2:F:36:LEU:HD23	2.30	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: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:107:VAL:HB	1:A:116:ASP:HB3	1.97	0.47
1:C:436:MET:HE1	1:C:469:LEU:HD21	1.96	0.47
1:C:441:GLN:O	1:C:445:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:63:MET:HE3	2:D:228:ALA:HA	1.96	0.47
2:D:432:VAL:HG13	2:D:433:PRO:HD2	1.97	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
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: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
2:E:204:GLY:C	2:E:206:ILE:N	2.68	0.47
1:B:210:ARG:O	1:B:211:SER:C	2.53	0.46
1:C:292:GLU:O	1:C:293:ALA:CB	2.63	0.46
2:E:204:GLY:O	2:E:205:VAL:C	2.54	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
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: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:358:TYR:C	1:B:360:GLY:N	2.69	0.46
1:B:400:VAL:HB	1:B:418:LEU:CD2	2.45	0.46
1:B:469:LEU:HG	1:B:473:ILE:HD11	1.98	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
2:E:41:ARG:O	2:E:42:GLU:C	2.53	0.46
1:A:49:ALA:O	1:A:50:GLU:HB2	2.13	0.46
1:C:102:GLU:HG2	1:C:122:GLY:C	2.36	0.46
1:C:251:CYS:O	1:C:255:GLU:HG3	2.16	0.46
2:F:455:GLN:H	2:F:455:GLN:CD	2.18	0.46
3:G:209:LEU:O	3:G:210:ALA:C	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:A:213:VAL:O	1:A:216:LEU:HB3	2.16	0.46
2:E:242:TYR:C	2:E:244:ARG:H	2.18	0.46
2:F:310:ILE:HD13	2:F:325:THR:HG21	1.97	0.46
2:F:345:TYR:HA	2:F:346:PRO:C	2.36	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
1:A:211:SER:HA	2:D:126:MET:HE3	1.98	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:474:SER:OG	1:C:475:GLN:N	2.49	0.45
1:A:245:LEU:C	1:A:247:PRO:HD2	2.36	0.45
1:B:465:GLU:O	1:B:469:LEU:HB2	2.17	0.45
2:D:345:TYR:HA	2:D:346:PRO:C	2.37	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:62:MET:HE2	1:A:76:PHE:HZ	1.81	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
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: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:A:85:GLY:O	1:A:86:ASP:C	2.53	0.45
1:B:76:PHE:HB3	1:B:242:LEU:HD21	1.98	0.45
2:D:319:ASP:O	2:D:320:PRO:C	2.55	0.45
2:D:452:LEU:HD12	2:D:457:PHE:CZ	2.52	0.45
2:E:85:PRO:HD2	2:E:95:MET:CE	2.46	0.45
2:E:281:TYR:CZ	2:E:321:ALA:HB2	2.52	0.45
1:B:353:GLU:HG3	1:B:366:ASN:HB2	1.98	0.45
2: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:C:338:ILE:O	1:C:339:PRO:C	2.51	0.44
2:D:63:MET:HE1	2:D:227:GLY:O	2.17	0.44
2:E:393:MET:HE2	2:E:393:MET:O	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:ALA:HB1	1:C:410:LEU:HD11	1.99	0.44
2:D:108:ILE:HG22	2:D:110:THR:HG23	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:245:LEU:O	1:C:246:ALA:C	2.56	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:82:HIS:CD2	3:G:82:HIS:N	2.85	0.44
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: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: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:B:437:ALA:O	1:B:438:ILE:C	2.54	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
2:D:400:ASP:O	2:D:404:VAL:HG23	2.18	0.44
1:C:269:ASP:HA	1:C:270:ASP:HA	1.78	0.44
1:C:390:MET:HE2	1:C:428:LEU:HD11	1.99	0.44
2:D:412:ARG:O	2:D:415:SER:OG	2.33	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:62:MET:HE2	1:A:76:PHE:CZ	2.53	0.43
1:A:107:VAL:HG11	2:D:123:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:VAL:HG12	1:B:418:LEU:HD11	2.00	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:103:ASP:O	2:D:104:GLU:HB2	2.18	0.43
2:D:298:THR:HG23	2:D:303:SER:HA	1.98	0.43
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
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
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
3:G:23:MET:HB2	3:G:232:MET:HE2	2.00	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: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:161:GLY:O	2:E:162:LYS:C	2.57	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
2:E:397:SER:C	2:E:399:GLU:H	2.20	0.43
1:A:52:MET:CG	1:A:95:VAL:HG22	2.48	0.43
1:A:180:ILE:O	1:A:181:ASP:C	2.56	0.43
1:A:397:TYR:CD1	1:A:421:GLY:HA3	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:47:LEU:HD23	2:F:62:ALA:HA	2.01	0.43
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:B:151:LYS:NZ	1:B:427:LEU:O	2.47	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: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:211:SER:CA	2:D:126:MET:HE3	2.48	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:D:425:THR:HB	2:D:459:MET:HE2	2.00	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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ASP:HA	1:A:128:ARG:HA	2.01	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:485:THR:C	1:A:487:GLY:H	2.23	0.42
2:E:189:ARG:O	2:E:190:THR:C	2.58	0.42
2:E:425:THR:C	2:E:427:HIS:N	2.71	0.42
1:A:184:ILE:HD12	1:A:223:ALA:CB	2.50	0.42
1:B:433:TYR:C	1:B:435:PRO:HD3	2.40	0.42
1:C:49:ALA:O	1:C:50:GLU:HB2	2.19	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
2:D:279:VAL:HG12	2:D:279:VAL:O	2.20	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
1:A:139:ARG:C	1:A:140:ILE:HG22	2.40	0.42
2:D:35:ALA:HB1	2:D:46:VAL:HG13	2.02	0.42
2:D:63:MET:CE	2:D:228:ALA:HA	2.50	0.42
2:D:475:GLU:OE1	2:D:475:GLU:HA	2.20	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
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:B:381:ARG:HA	1:B:384:LYS:HB2	2.01	0.41
1:B:485:THR:O	1:B:486:ASP:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:397:SER:O	2:D:398:GLU:C	2.58	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: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:D:200:MET:CE	2:D:215:VAL:HG21	2.50	0.41
2:D:412:ARG:C	2:D:414:LEU:N	2.73	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:A:485:THR:C	1:A:487:GLY:N	2.73	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: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:A:492:GLU:C	1:A:494:ASP:N	2.73	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:E:282:GLN:H	2:E:282:GLN:NE2	2.19	0.41
1:A:353:GLU:CD	1:A:366:ASN:HD22	2.24	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
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:112:GLN:NE2	2:D:242:TYR:CE1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:158:ALA:C	2:E:160:VAL:N	2.72	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: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
2:D:417:PRO:HA	2:D:459:MET:HE1	2.02	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:397:SER:O	2:E:399:GLU:N	2.54	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:294:TYR:CE2	1:A:338:ILE:HD13	2.56	0.41
1:A:403:PHE:O	1:A:404:ALA:C	2.59	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:84:ILE:HD12	2:D:95:MET:CE	2.50	0.41
2:D:203:SER:OG	2:D:205:VAL:HG23	2.21	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:81:PRO:O	2:F:82:ILE:C	2.58	0.41
2:F:228:ALA:O	2:F:232:VAL:HG22	2.21	0.41
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:2:THR:O	3:G:3:LEU:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:190:THR:O	2:D:191:ARG:C	2.60	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:422:GLU:C	2:E:424:PHE:N	2.74	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:B:221:THR:HG22	1:B:222:ASP:N	2.36	0.40
1:C:340:THR:O	1:C:341:ASN:C	2.59	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:281:TYR:HB3	2:D:285:LEU:HD12	2.03	0.40
2:D:471:ASP:O	2:D:472:LYS:C	2.57	0.40
1:A:147:GLN:OE1	1:A:438:ILE:HD13	2.21	0.40
2:E:55:GLU:O	2:E:56:SER:HB2	2.21	0.40
2:E:77:ASP:C	2:E:79:GLY:H	2.24	0.40
2:E:185:GLY:HA3	2:E:188:GLU:HG3	2.02	0.40
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: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:C:45:ARG:HA	1:C:45:ARG:HD3	1.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:ARG:HH11	1:C:45:ARG:HD2	1.68	0.40
2:D:200:MET:HE3	2:D:215:VAL:HG21	2.03	0.40
2:D:231:ARG:O	2:D:232:VAL:C	2.60	0.40
2:D:381:TYR:O	2:D:385:GLN:HG3	2.22	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:42:ARG:HG2	3:G:219:GLU:OE2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	485/553 (88%)	442 (91%)	36 (7%)	7 (1%)	11 46
1	B	475/553 (86%)	426 (90%)	42 (9%)	7 (2%)	10 46
1	C	490/553 (89%)	445 (91%)	37 (8%)	8 (2%)	9 44
2	D	465/528 (88%)	419 (90%)	43 (9%)	3 (1%)	25 66
2	E	464/528 (88%)	408 (88%)	47 (10%)	9 (2%)	8 38
2	F	464/528 (88%)	432 (93%)	30 (6%)	2 (0%)	34 72
3	G	116/298 (39%)	97 (84%)	18 (16%)	1 (1%)	17 57
All	All	2959/3541 (84%)	2669 (90%)	253 (9%)	37 (1%)	12 48

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

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	393/444 (88%)	351 (89%)	42 (11%)	6 24
1	B	388/444 (87%)	342 (88%)	46 (12%)	5 20
1	C	397/444 (89%)	369 (93%)	28 (7%)	14 39
2	D	377/417 (90%)	346 (92%)	31 (8%)	11 34
2	E	376/417 (90%)	344 (92%)	32 (8%)	10 33
2	F	376/417 (90%)	354 (94%)	22 (6%)	19 45
3	G	102/251 (41%)	92 (90%)	10 (10%)	8 27
All	All	2409/2834 (85%)	2198 (91%)	211 (9%)	10 31

All (211) 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
1	A	256	TYR
1	A	270	ASP
1	A	344	SER
1	A	367	VAL
1	A	371	VAL
1	A	380	THR

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Mol	Chain	Res	Type
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
1	B	270	ASP
1	B	298	VAL
1	B	299	PHE
1	B	335	SER
1	B	349	GLN
1	B	351	PHE

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Mol	Chain	Res	Type
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	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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	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
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

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Mol	Chain	Res	Type
2	F	397	SER
2	F	405	SER
2	F	428	LEU
2	F	455	GLN
3	G	4	LYS
3	G	11	LYS
3	G	22	SER
3	G	44	TYR
3	G	77	LEU
3	G	82	HIS
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 (31) 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
1	C	208	GLN
1	C	260	ASN
1	C	349	GLN
1	C	432	GLN
2	D	130	GLN
2	D	194	ASN
2	D	221	GLN
2	D	223	ASN
2	D	282	GLN
2	D	442	GLN
2	E	39	GLN
2	E	130	GLN
2	E	194	ASN
2	E	223	ASN
2	E	246	GLN
2	E	367	HIS

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Mol	Chain	Res	Type
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

5.3.3 RNA (i)

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 monosaccharides 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	-	24,29,29	0.90	0	29,45,45	1.26	4 (13%)

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	-	-	2/12/32/32	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1476	ADP	C4-C5-N7	2.73	112.24	109.40
4	D	1476	ADP	N6-C6-N1	2.70	124.19	118.57
4	D	1476	ADP	O3'-C3'-C2'	-2.12	104.97	111.82
4	D	1476	ADP	O4'-C4'-C3'	-2.01	101.14	105.11

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

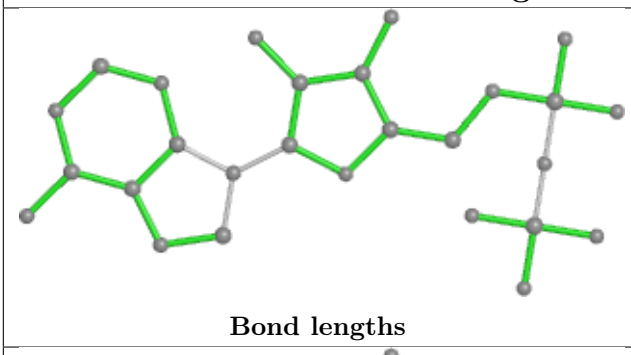
There are no ring outliers.

1 monomer is involved in 1 short contact:

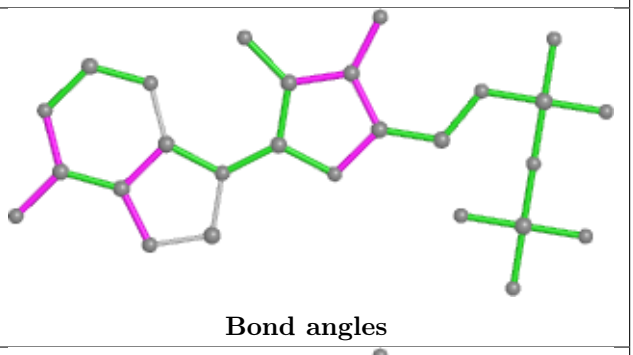
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1476	ADP	1	0

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 then 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.

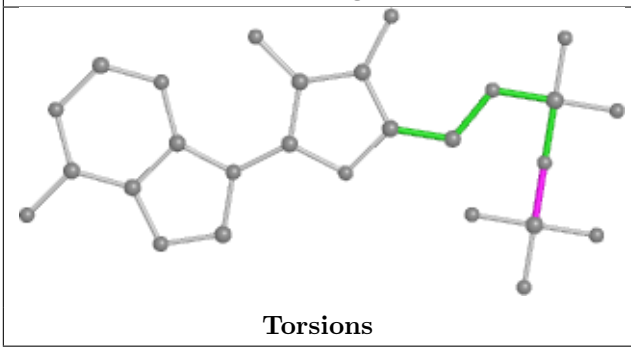
Ligand ADP D 1476



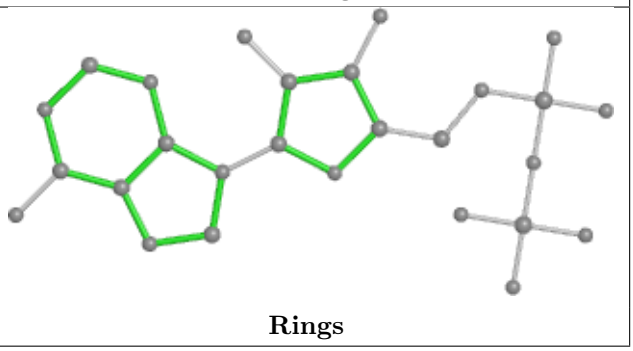
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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%)	-0.05	6 (1%) 79 71	20, 20, 20, 20	0
1	B	479/553 (86%)	-0.03	4 (0%) 86 79	20, 20, 20, 20	0
1	C	492/553 (88%)	-0.08	1 (0%) 95 93	20, 20, 20, 20	0
2	D	467/528 (88%)	0.02	0 100 100	20, 20, 20, 20	0
2	E	466/528 (88%)	0.05	3 (0%) 89 83	20, 20, 20, 20	0
2	F	466/528 (88%)	-0.09	0 100 100	20, 20, 20, 20	0
3	G	122/298 (40%)	0.29	7 (5%) 23 23	20, 20, 20, 20	0
All	All	2979/3541 (84%)	-0.02	21 (0%) 87 82	20, 20, 20, 20	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	409	ASP	3.4
3	G	77	LEU	2.7
1	A	173	THR	2.6
3	G	211	ASN	2.5
1	A	269	ASP	2.4
3	G	23	MET	2.3
1	B	449	VAL	2.3
2	E	85	PRO	2.2
1	B	200	TYR	2.2
1	A	408	SER	2.2
1	C	100	GLY	2.2
2	E	180	TYR	2.1
3	G	42	ARG	2.1
2	E	455	GLN	2.1
1	A	200	TYR	2.1
3	G	41	ALA	2.1
3	G	214	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	34	ILE	2.0
1	A	201	CYS	2.0
3	G	213	ILE	2.0
1	B	82	ILE	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 monosaccharides in this entry.

6.4 Ligands (i)

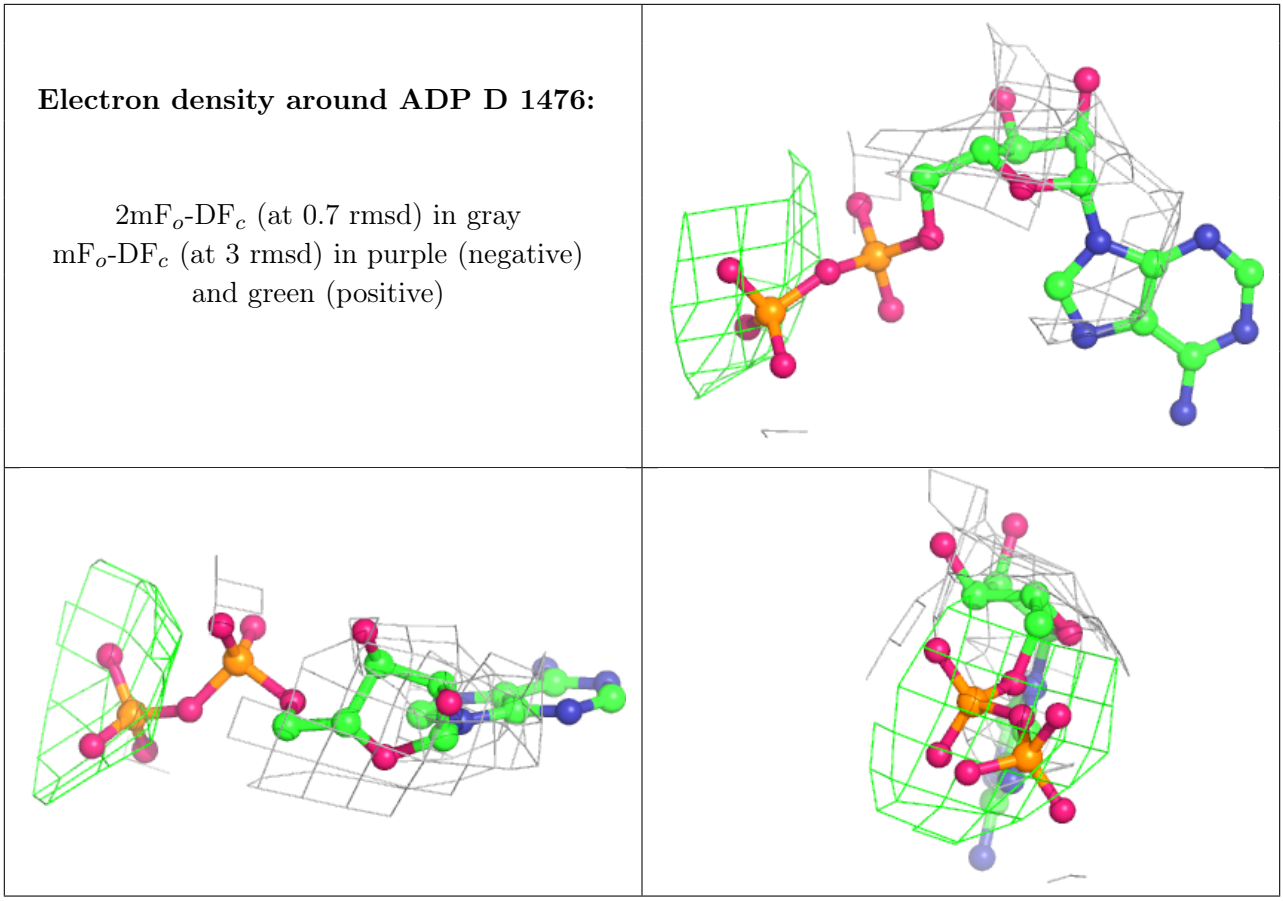
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ADP	D	1476	27/27	0.64	0.43	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.

Electron density around ADP D 1476:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.