



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:33 PM UTC

PDB ID : 4XD7 / pdb_00004xd7
Title : Structure of thermophilic F1-ATPase inhibited by epsilon subunit
Authors : SHIRAKIHARA, Y.; SHIRATORI, A.; TANIKAWA, H.; NAKASAKO, M.;
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Deposited on : 2014-12-19
Resolution : 3.90 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

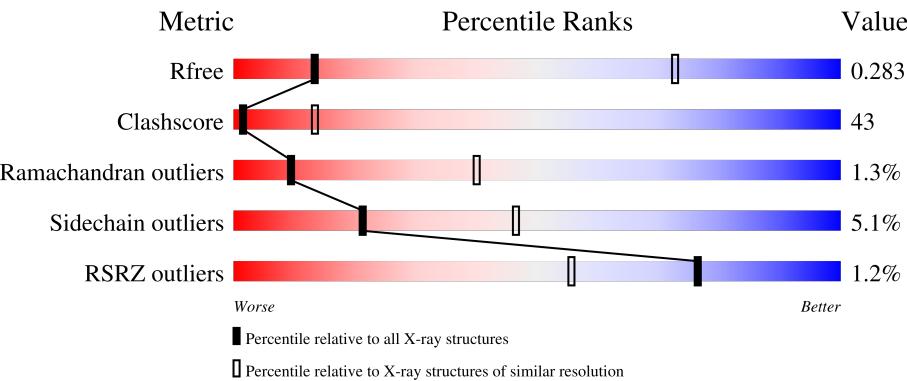
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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	502	% 35% 55% • 5%
1	B	502	2% 40% 42% • 16%
1	C	502	41% 48% 5% • 5%
2	D	483	% 46% 49% • •
2	E	483	% 42% 51% 5% •

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Mol	Chain	Length	Quality of chain
2	F	483	
3	G	285	
4	H	133	

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
5	SO4	A	700	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22656 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	Se	0	0	0
			3462	2189	606	658	9			
1	B	423	Total	C	N	O	Se	0	0	0
			2833	1786	484	554	9			
1	C	475	Total	C	N	O	Se	1	0	0
			3329	2109	577	634	9			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	193	SER	CYS	conflict	UNP Q5KUJ1
A	254	LYS	GLN	conflict	UNP Q5KUJ1
A	463	PHE	TRP	conflict	UNP Q5KUJ1
B	193	SER	CYS	conflict	UNP Q5KUJ1
B	254	LYS	GLN	conflict	UNP Q5KUJ1
B	463	PHE	TRP	conflict	UNP Q5KUJ1
C	193	SER	CYS	conflict	UNP Q5KUJ1
C	254	LYS	GLN	conflict	UNP Q5KUJ1
C	463	PHE	TRP	conflict	UNP Q5KUJ1

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	470	Total	C	N	O	Se	1	0	0
			3480	2199	599	669	13			
2	E	469	Total	C	N	O	Se	0	0	0
			3484	2198	598	676	12			
2	F	464	Total	C	N	O	Se	4	0	0
			3334	2097	580	644	13			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	MSE	-	initiating methionine	UNP Q5KUJ3
D	-8	HIS	-	expression tag	UNP Q5KUJ3
D	-7	HIS	-	expression tag	UNP Q5KUJ3
D	-6	HIS	-	expression tag	UNP Q5KUJ3
D	-5	HIS	-	expression tag	UNP Q5KUJ3
D	-4	HIS	-	expression tag	UNP Q5KUJ3
D	-3	HIS	-	expression tag	UNP Q5KUJ3
D	-2	HIS	-	expression tag	UNP Q5KUJ3
D	-1	HIS	-	expression tag	UNP Q5KUJ3
D	0	HIS	-	expression tag	UNP Q5KUJ3
D	1	HIS	-	expression tag	UNP Q5KUJ3
E	-9	MSE	-	initiating methionine	UNP Q5KUJ3
E	-8	HIS	-	expression tag	UNP Q5KUJ3
E	-7	HIS	-	expression tag	UNP Q5KUJ3
E	-6	HIS	-	expression tag	UNP Q5KUJ3
E	-5	HIS	-	expression tag	UNP Q5KUJ3
E	-4	HIS	-	expression tag	UNP Q5KUJ3
E	-3	HIS	-	expression tag	UNP Q5KUJ3
E	-2	HIS	-	expression tag	UNP Q5KUJ3
E	-1	HIS	-	expression tag	UNP Q5KUJ3
E	0	HIS	-	expression tag	UNP Q5KUJ3
E	1	HIS	-	expression tag	UNP Q5KUJ3
F	-9	MSE	-	initiating methionine	UNP Q5KUJ3
F	-8	HIS	-	expression tag	UNP Q5KUJ3
F	-7	HIS	-	expression tag	UNP Q5KUJ3
F	-6	HIS	-	expression tag	UNP Q5KUJ3
F	-5	HIS	-	expression tag	UNP Q5KUJ3
F	-4	HIS	-	expression tag	UNP Q5KUJ3
F	-3	HIS	-	expression tag	UNP Q5KUJ3
F	-2	HIS	-	expression tag	UNP Q5KUJ3
F	-1	HIS	-	expression tag	UNP Q5KUJ3
F	0	HIS	-	expression tag	UNP Q5KUJ3
F	1	HIS	-	expression tag	UNP Q5KUJ3

- Molecule 3 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	G	254	Total	C	N	O	S	Se	0	0	0
			1797	1142	308	339	1	7			

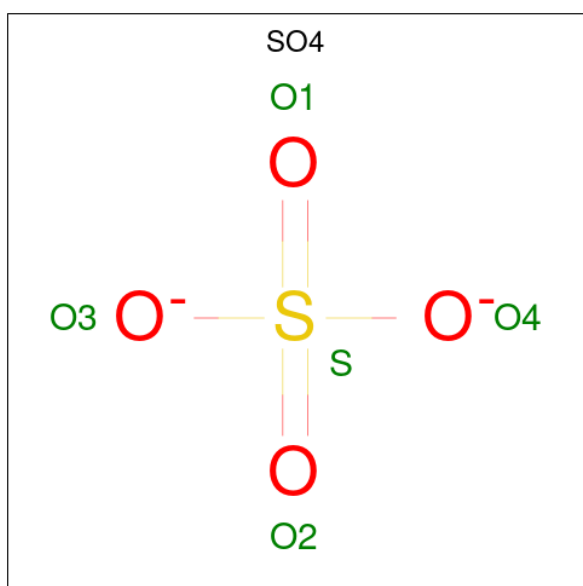
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	109	CYS	SER	conflict	UNP Q5KUJ2

- Molecule 4 is a protein called ATP synthase epsilon chain.

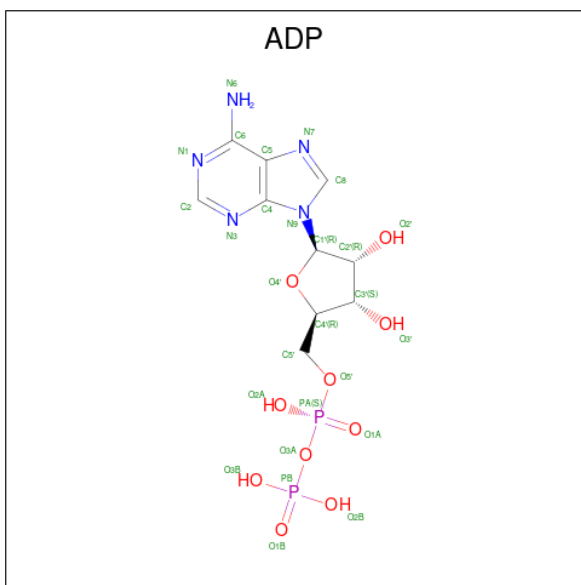
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	129	Total	C	N	O	Se	0	0	0
			890	563	148	175	4			

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

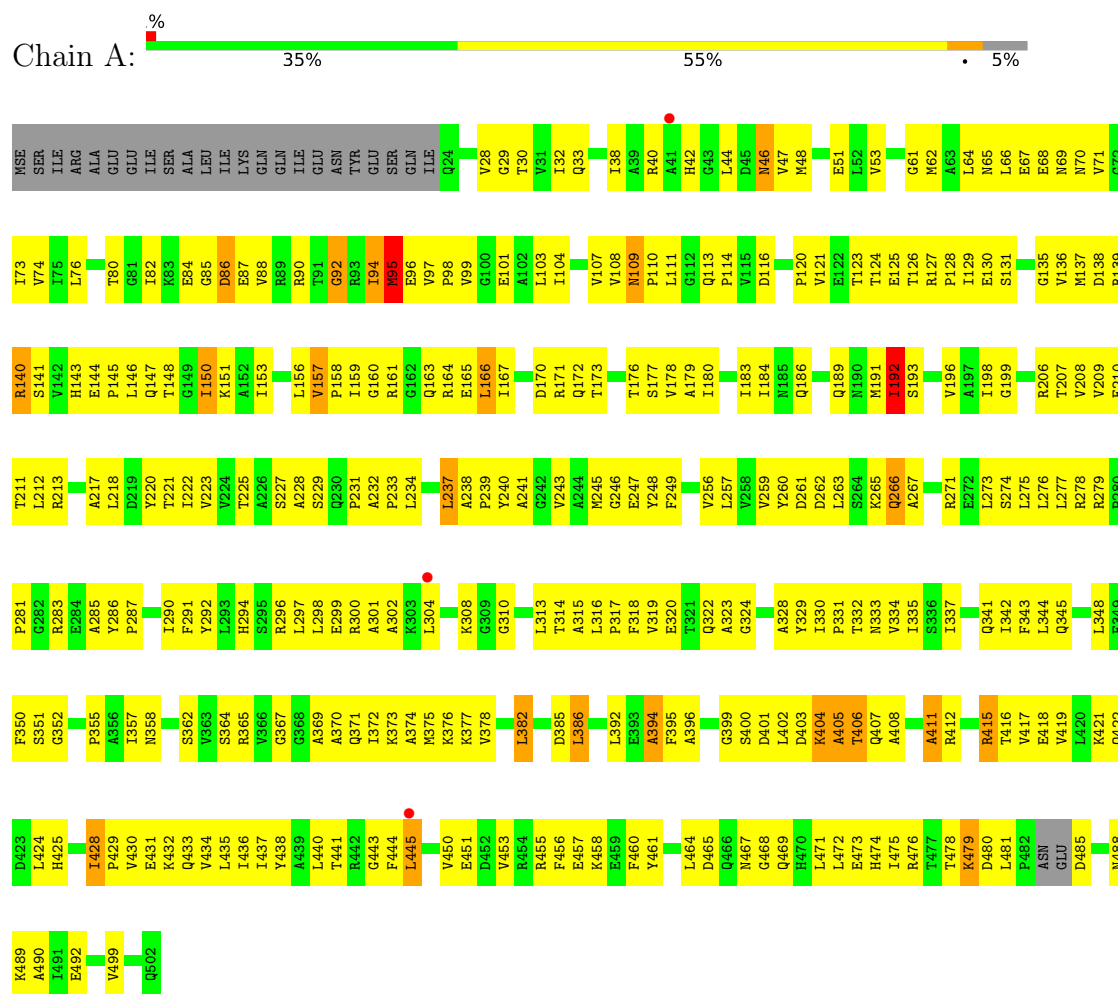


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	F	1	Total 27	C 10	N 5	O 10	P 2	0	0

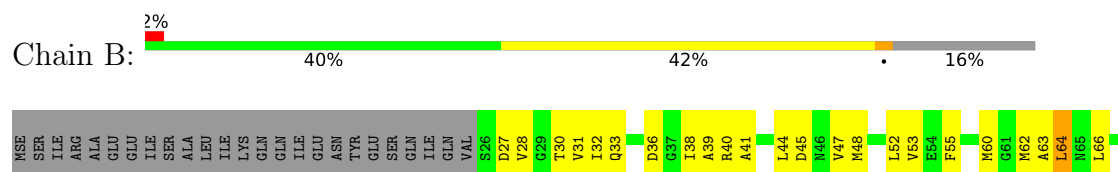
3 Residue-property plots

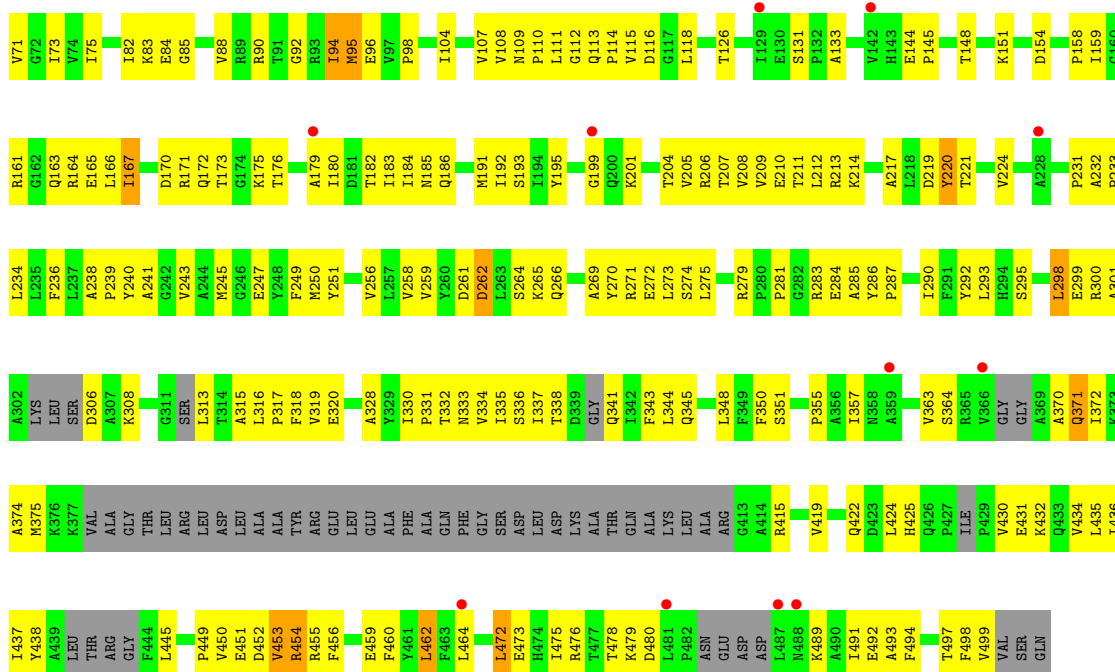
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

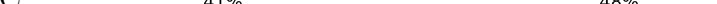


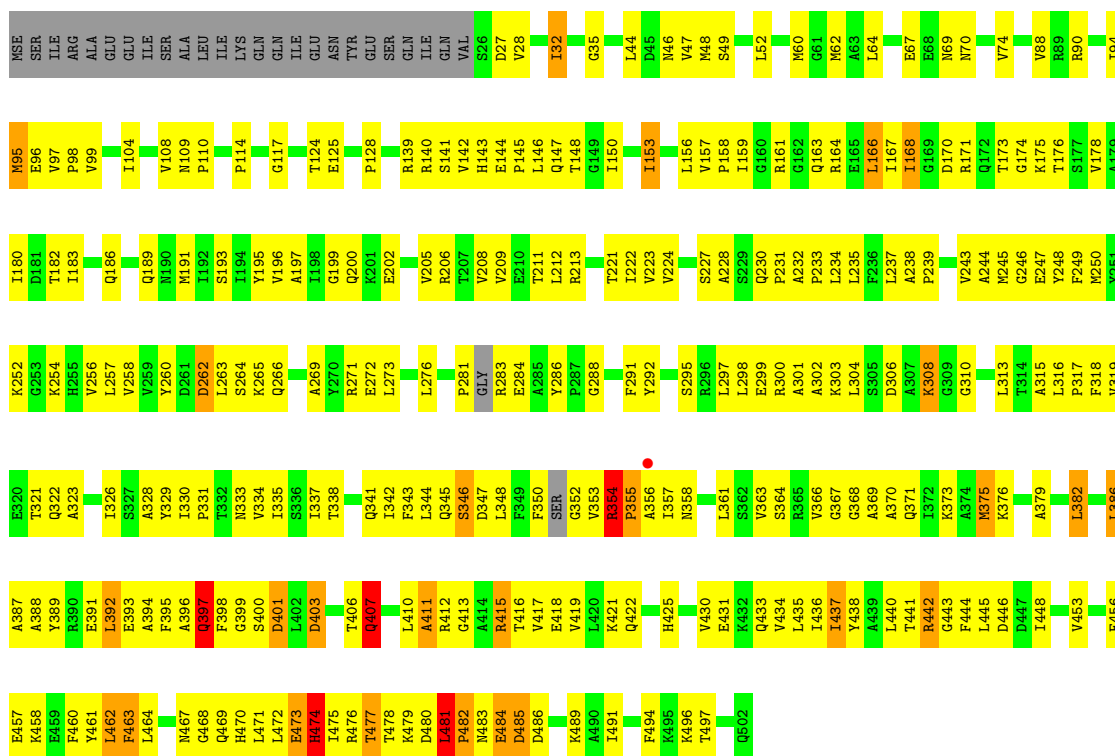
• Molecule 1: ATP synthase subunit alpha



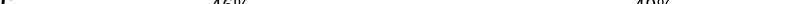


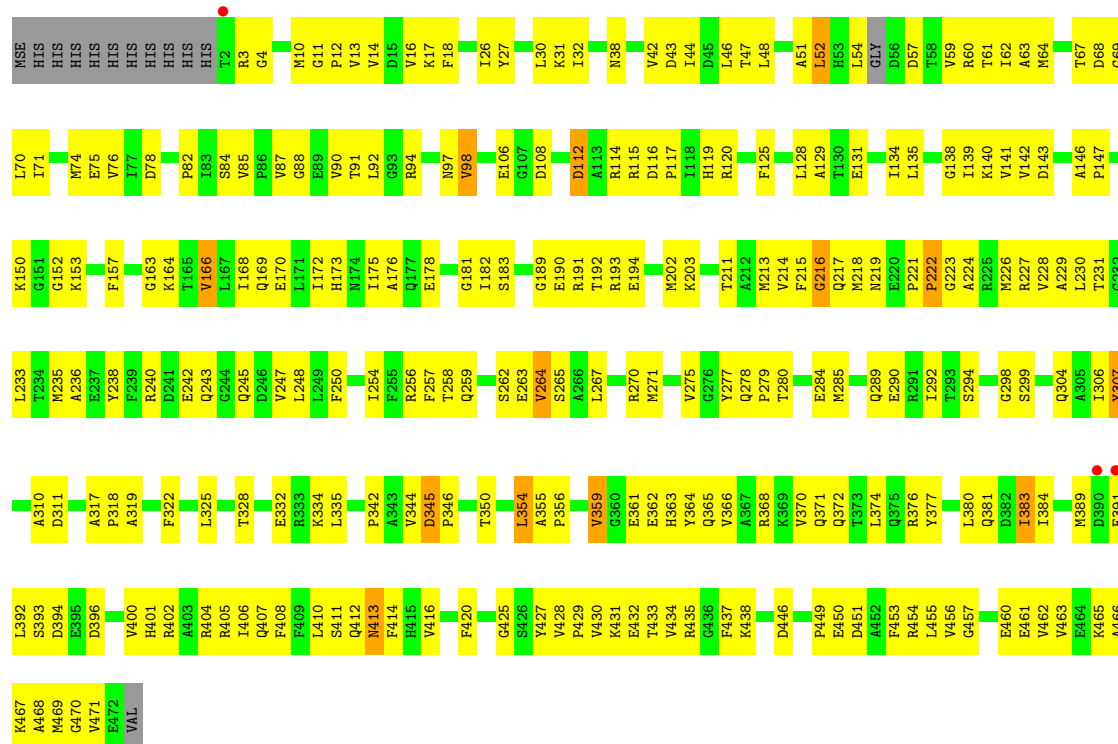
- Molecule 1: ATP synthase subunit alpha

Chain C:  41% 48% 5% • 5%

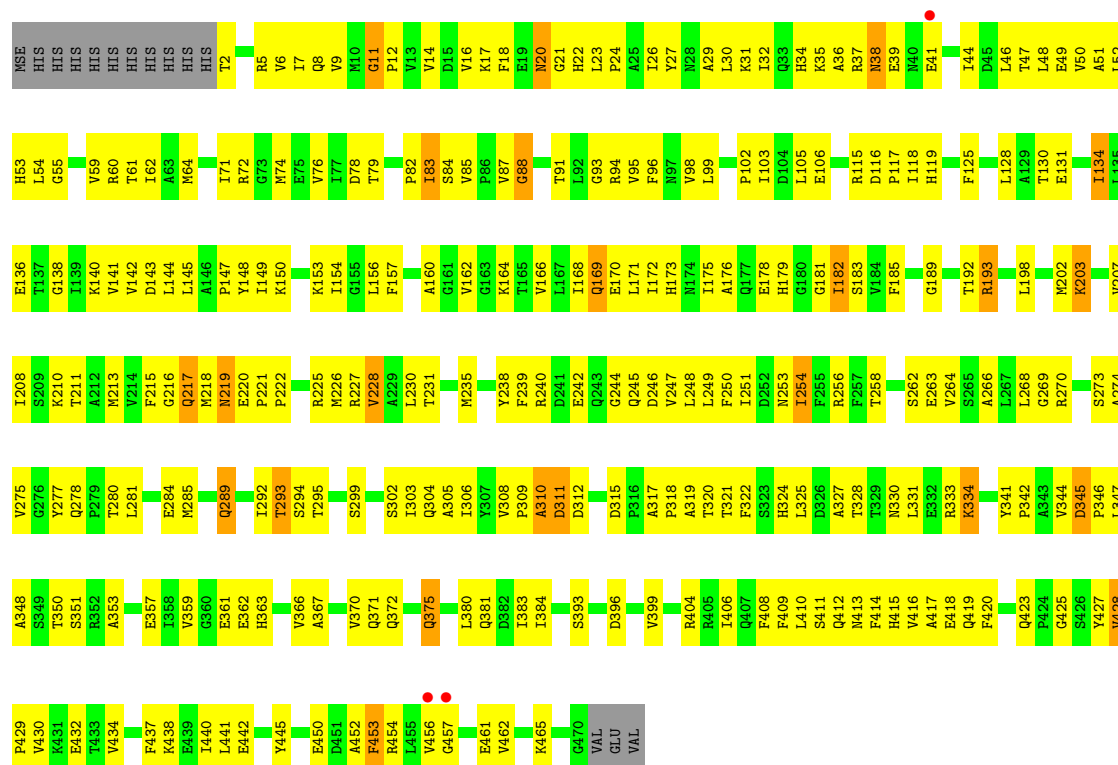


- Molecule 2: ATP synthase subunit beta

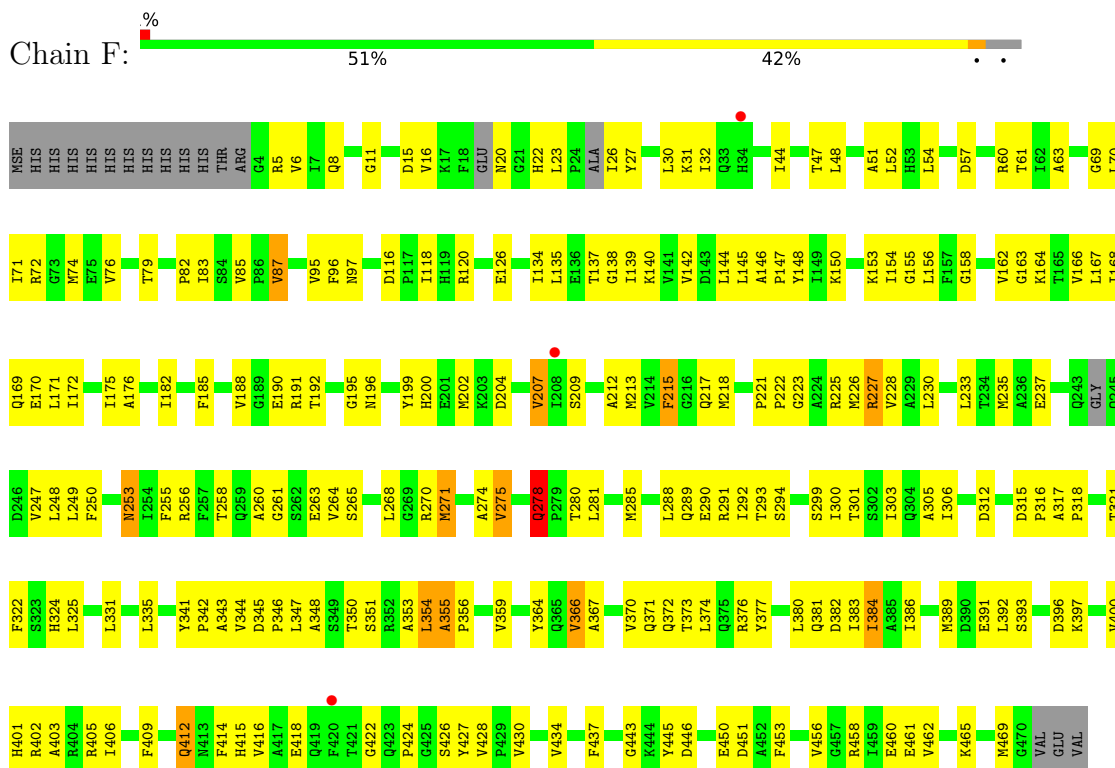
Chain D:  46% 49% %



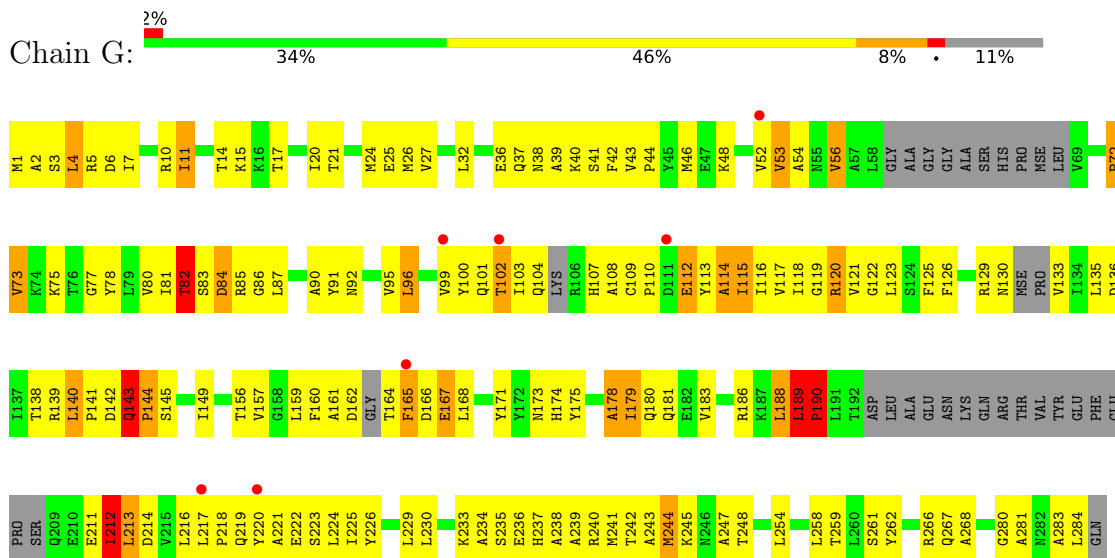
• Molecule 2: ATP synthase subunit beta



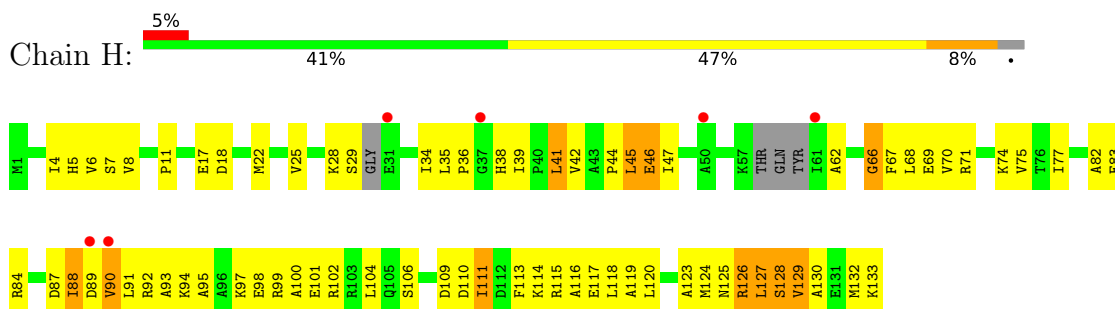
• Molecule 2: ATP synthase subunit beta



- Molecule 3: ATP synthase gamma chain



- Molecule 4: ATP synthase epsilon chain



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	233.40Å 233.40Å 303.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.90 19.99 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.99-3.90) 98.9 (19.99-3.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.71Å)	Xtriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.250 , 0.282 0.252 , 0.283	Depositor DCC
R_{free} test set	2247 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	123.5	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 75.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	22656	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% 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: SO4, 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	0.71	0/3496	1.15	16/4711 (0.3%)
1	B	0.64	0/2853	1.10	7/3840 (0.2%)
1	C	0.68	0/3367	1.15	22/4526 (0.5%)
2	D	0.69	0/3519	1.07	7/4735 (0.1%)
2	E	0.69	0/3524	1.11	13/4751 (0.3%)
2	F	0.59	0/3362	1.03	12/4504 (0.3%)
3	G	0.82	0/1808	1.28	22/2435 (0.9%)
4	H	0.82	0/895	1.28	9/1202 (0.7%)
All	All	0.69	0/22824	1.12	108/30704 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
2	D	0	2
2	F	0	1
3	G	0	1
All	All	0	6

There are no bond length outliers.

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	115	ILE	N-CA-C	13.32	125.93	108.35
3	G	189	LEU	CA-C-N	11.65	134.40	119.84
3	G	189	LEU	C-N-CA	11.65	134.40	119.84
3	G	186	ARG	N-CA-C	-10.86	95.89	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	114	ALA	N-CA-C	9.13	121.51	110.19
3	G	188	LEU	N-CA-C	8.88	122.94	107.49
2	E	11	GLY	CA-C-N	8.70	128.35	119.82
2	E	11	GLY	C-N-CA	8.70	128.35	119.82
4	H	66	GLY	N-CA-C	8.46	119.99	111.95
1	C	473	GLU	N-CA-C	8.45	124.62	113.30
1	A	369	ALA	N-CA-C	-8.07	102.88	112.89
1	C	484	GLU	N-CA-C	-7.90	93.97	110.80
1	C	69	ASN	N-CA-C	7.73	122.42	112.92
2	D	243	GLN	N-CA-C	7.69	122.37	112.92
2	F	207	VAL	N-CA-C	7.57	119.40	112.29
3	G	178	ALA	CA-C-N	-7.12	114.12	122.95
3	G	178	ALA	C-N-CA	-7.12	114.12	122.95
1	C	442	ARG	N-CA-C	7.02	122.71	113.30
1	C	397	GLN	N-CA-C	-7.01	95.87	110.80
2	E	308	VAL	CA-C-N	6.86	128.42	119.84
2	E	308	VAL	C-N-CA	6.86	128.42	119.84
1	C	346	SER	N-CA-C	-6.81	104.97	113.28
4	H	111	ILE	N-CA-C	6.63	119.34	111.05
1	C	407	GLN	N-CA-C	-6.62	105.21	113.28
2	F	11	GLY	CA-C-N	6.58	126.21	119.56
2	F	11	GLY	C-N-CA	6.58	126.21	119.56
2	E	423	GLN	CA-C-N	6.54	127.06	119.47
2	E	423	GLN	C-N-CA	6.54	127.06	119.47
1	A	308	LYS	N-CA-C	6.52	121.29	112.88
1	A	157	VAL	CA-C-N	6.51	126.42	119.85
1	A	157	VAL	C-N-CA	6.51	126.42	119.85
4	H	46	GLU	N-CA-C	-6.45	99.61	109.41
1	B	92	GLY	N-CA-C	-6.34	106.39	115.64
1	C	28	VAL	CB-CA-C	-6.30	104.66	111.59
1	B	258	VAL	N-CA-C	6.25	116.86	108.11
1	C	369	ALA	N-CA-C	-6.24	105.15	112.89
2	D	359	VAL	N-CA-C	6.24	119.77	113.47
2	D	345	ASP	CA-C-N	6.22	126.34	119.87
2	D	345	ASP	C-N-CA	6.22	126.34	119.87
3	G	180	GLN	N-CA-C	-6.17	98.55	108.55
1	A	150	ILE	CB-CA-C	-6.17	102.62	111.19
2	E	345	ASP	CA-C-N	6.11	125.67	119.19
2	E	345	ASP	C-N-CA	6.11	125.67	119.19
2	F	324	HIS	N-CA-C	6.10	120.42	112.92
2	E	6	VAL	CB-CA-C	-6.09	103.17	111.33
2	E	88	GLY	N-CA-C	6.08	118.17	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	308	LYS	N-CA-C	6.08	120.39	112.92
2	D	166	VAL	CB-CA-C	-5.98	104.31	111.97
1	A	92	GLY	N-CA-C	-5.97	106.70	115.72
1	A	394	ALA	N-CA-C	-5.96	105.97	113.72
1	C	394	ALA	N-CA-C	-5.93	106.05	113.28
3	G	190	PRO	N-CA-C	5.92	124.67	112.47
2	D	264	VAL	CB-CA-C	-5.92	104.05	112.22
3	G	212	ILE	N-CA-C	5.90	117.16	111.91
4	H	71	ARG	CA-C-N	5.88	126.03	119.32
4	H	71	ARG	C-N-CA	5.88	126.03	119.32
4	H	75	VAL	CB-CA-C	-5.87	103.74	110.73
1	A	467	ASN	N-CA-C	5.83	120.67	113.50
1	A	445	LEU	N-CA-C	-5.79	106.14	113.43
2	E	210	LYS	N-CA-C	5.78	120.02	112.92
2	F	227	ARG	N-CA-C	5.77	121.22	113.72
1	C	392	LEU	N-CA-C	-5.75	106.26	113.28
1	A	405	ALA	N-CA-C	-5.75	105.92	113.17
1	B	308	LYS	N-CA-C	5.70	120.23	112.88
1	A	189	GLN	CA-C-N	-5.70	114.93	122.85
1	A	189	GLN	C-N-CA	-5.70	114.93	122.85
1	C	46	ASN	N-CA-C	5.69	120.33	113.17
1	B	113	GLN	CA-C-N	5.67	125.96	119.83
1	B	113	GLN	C-N-CA	5.67	125.96	119.83
2	F	355	ALA	N-CA-C	5.64	117.00	109.83
1	C	221	THR	N-CA-C	5.63	118.07	108.90
1	C	481	LEU	CA-C-N	5.60	126.84	119.84
1	C	481	LEU	C-N-CA	5.60	126.84	119.84
4	H	117	GLU	N-CA-C	-5.60	105.55	112.38
1	C	262	ASP	N-CA-C	5.59	117.45	110.91
1	B	454	ARG	N-CA-C	-5.58	104.58	111.33
4	H	123	ALA	N-CA-C	-5.58	106.32	113.23
1	B	220	TYR	N-CA-C	5.54	120.02	112.88
3	G	112	GLU	N-CA-C	-5.52	100.61	108.23
3	G	82	THR	N-CA-C	5.50	115.38	108.45
2	D	471	VAL	N-CA-C	5.49	116.88	108.71
2	F	278	GLN	CA-C-N	5.49	125.20	119.82
2	F	278	GLN	C-N-CA	5.49	125.20	119.82
3	G	144	PRO	CA-C-N	-5.47	115.24	122.85
3	G	144	PRO	C-N-CA	-5.47	115.24	122.85
3	G	120	ARG	N-CA-C	-5.46	104.56	111.11
1	A	46	ASN	N-CA-C	5.46	120.04	113.17
3	G	178	ALA	CB-CA-C	-5.44	110.32	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	437	ILE	N-CA-C	-5.42	106.21	112.98
2	F	426	SER	N-CA-C	5.39	117.29	108.55
1	C	32	ILE	N-CA-C	5.38	119.29	113.43
3	G	108	ALA	CA-C-N	-5.34	116.83	122.28
3	G	108	ALA	C-N-CA	-5.34	116.83	122.28
2	E	375	GLN	N-CA-C	-5.32	106.76	113.20
3	G	56	VAL	N-CA-C	5.31	117.11	109.51
1	C	28	VAL	N-CA-C	5.29	115.81	110.05
2	F	253	ASN	N-CA-C	5.26	117.06	110.91
2	F	366	VAL	CB-CA-C	-5.12	105.32	111.88
2	E	445	TYR	N-CA-C	5.12	120.16	113.30
1	C	474	HIS	N-CA-C	-5.10	105.61	111.07
1	C	153	ILE	N-CA-C	5.08	116.53	111.00
1	A	192	ILE	N-CA-C	-5.04	99.91	107.37
1	A	404	LYS	CB-CA-C	-5.04	109.24	115.89
1	A	428	ILE	N-CA-C	5.03	115.66	107.71
2	F	428	VAL	N-CA-C	5.03	112.84	107.76
3	G	140	LEU	CA-C-N	-5.03	114.73	119.76
3	G	140	LEU	C-N-CA	-5.03	114.73	119.76
4	H	129	VAL	N-CA-CB	-5.02	105.67	112.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	354	ARG	Peptide
1	C	401	ASP	Peptide
2	D	216	GLY	Peptide
2	D	391	GLU	Peptide
2	F	215	PHE	Peptide
3	G	188	LEU	Peptide

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	3462	0	3344	336	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2833	0	2533	253	0
1	C	3329	0	3032	297	0
2	D	3480	0	3309	284	0
2	E	3484	0	3345	274	0
2	F	3334	0	3069	213	0
3	G	1797	0	1665	207	0
4	H	890	0	833	90	0
5	A	5	0	0	3	0
5	B	5	0	0	1	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0
6	F	27	0	12	1	0
All	All	22656	0	21142	1873	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 43.

All (1873) 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:262:ASP:H	1:C:318:PHE:HB2	1.05	1.13
1:A:404:LYS:HG3	1:A:405:ALA:H	1.06	1.11
4:H:129:VAL:HG13	4:H:132:MSE:HA	1.33	1.09
2:F:139:ILE:HA	2:F:412:GLN:NE2	1.69	1.07
1:A:32:ILE:HG22	1:A:33:GLN:HG3	1.40	1.04
3:G:189:LEU:H	3:G:190:PRO:CD	1.71	1.02
2:D:31:LYS:HD2	2:D:47:THR:HG22	1.38	1.02
1:C:419:VAL:HG21	1:C:440:LEU:HD13	1.38	1.01
1:B:62:MSE:HE3	1:B:95:MSE:HG3	1.43	1.01
2:F:139:ILE:HA	2:F:412:GLN:HE22	0.86	1.01
4:H:38:HIS:CE1	4:H:41:LEU:HD23	1.96	1.00
1:C:109:ASN:HB2	1:C:110:PRO:HD2	1.43	1.00
1:A:145:PRO:HB3	1:A:370:ALA:O	1.61	1.00
1:B:109:ASN:HB2	1:B:110:PRO:HD2	1.42	1.00
1:C:319:VAL:HG21	1:C:334:VAL:HG11	1.42	0.99
1:A:196:VAL:HG12	1:A:198:ILE:HD11	1.45	0.99
1:B:64:LEU:HD21	1:B:279:ARG:NH2	1.76	0.98
3:G:82:THR:HG22	3:G:83:SER:H	1.27	0.98
2:F:190:GLU:HG3	2:F:191:ARG:H	1.25	0.98
1:A:262:ASP:H	1:A:318:PHE:HB2	1.24	0.97
3:G:82:THR:HG21	3:G:92:ASN:OD1	1.64	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:38:ASN:HD21	2:E:41:GLU:HG3	1.29	0.97
2:D:10:MSE:HB2	2:D:13:VAL:CG1	1.95	0.96
2:D:143:ASP:HB3	2:D:430:VAL:HG22	1.46	0.96
2:F:139:ILE:CA	2:F:412:GLN:HE22	1.78	0.96
1:A:239:PRO:HG2	1:A:266:GLN:HE21	1.29	0.96
1:B:472:LEU:O	1:B:475:ILE:HG22	1.65	0.95
1:A:404:LYS:HG3	1:A:405:ALA:N	1.82	0.95
1:A:233:PRO:HG3	1:A:273:LEU:HD12	1.46	0.94
2:D:271:MSE:HE2	3:G:281:ALA:HB1	1.46	0.94
2:F:253:ASN:H	2:F:305:ALA:HB3	1.31	0.94
1:B:27:ASP:O	1:B:44:LEU:HD23	1.65	0.94
1:C:476:ARG:O	1:C:479:LYS:HG3	1.68	0.94
2:F:6:VAL:HG22	2:F:16:VAL:HG22	1.50	0.94
3:G:173:ASN:OD1	3:G:183:VAL:HG22	1.67	0.93
3:G:189:LEU:N	3:G:190:PRO:CD	2.29	0.93
2:D:10:MSE:HB2	2:D:13:VAL:HG13	1.49	0.93
2:D:216:GLY:HA3	2:D:228:VAL:HG21	1.49	0.93
1:A:104:ILE:HD13	1:A:222:ILE:HD11	1.50	0.92
2:F:31:LYS:HG3	2:F:47:THR:HG22	1.51	0.92
1:A:419:VAL:HG21	1:A:440:LEU:HD13	1.51	0.91
2:D:383:ILE:H	2:D:383:ILE:HD12	1.33	0.91
2:F:154:ILE:HD12	2:F:303:ILE:HG12	1.50	0.91
1:A:148:THR:HG22	1:A:150:ILE:HG13	1.53	0.91
1:A:319:VAL:HG21	1:A:334:VAL:HG11	1.51	0.91
2:F:147:PRO:HG2	2:F:353:ALA:HB3	1.53	0.91
2:E:53:HIS:CD2	2:E:59:VAL:HG12	2.06	0.90
2:F:199:TYR:HD2	2:F:200:HIS:CE1	1.89	0.90
1:C:481:LEU:CB	1:C:482:PRO:HD2	2.01	0.90
1:B:64:LEU:HD21	1:B:279:ARG:HH22	1.32	0.90
1:C:443:GLY:HA2	1:C:446:ASP:OD2	1.72	0.89
1:B:319:VAL:HG21	1:B:334:VAL:HG11	1.54	0.89
3:G:112:GLU:CD	3:G:113:TYR:H	1.80	0.89
1:A:170:ASP:O	1:A:173:THR:HG23	1.73	0.89
2:E:328:THR:HG23	2:E:350:THR:H	1.37	0.89
1:A:198:ILE:HG21	1:A:266:GLN:HB2	1.53	0.88
2:E:181:GLY:HA2	2:E:245:GLN:NE2	1.89	0.88
2:F:168:ILE:HD11	2:F:305:ALA:HB2	1.56	0.88
2:E:289:GLN:HE21	2:E:289:GLN:HA	1.38	0.88
1:B:52:LEU:HD21	1:B:60:MSE:HB3	1.55	0.87
3:G:179:ILE:HD13	3:G:242:THR:HB	1.56	0.87
1:A:440:LEU:HB3	1:A:445:LEU:HD13	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:193:ARG:HB3	2:D:193:ARG:HH11	1.39	0.86
2:E:408:PHE:CE1	2:E:454:ARG:HD2	2.11	0.86
1:C:262:ASP:N	1:C:318:PHE:HB2	1.89	0.86
2:D:71:ILE:H	2:D:74:MSE:SE	2.10	0.85
2:E:94:ARG:NH1	2:E:106:GLU:HB2	1.90	0.85
3:G:179:ILE:HD13	3:G:242:THR:CB	2.07	0.84
1:B:166:LEU:HB2	1:B:338:THR:HG21	1.58	0.84
1:B:176:THR:O	1:B:180:ILE:HG12	1.77	0.84
1:C:477:THR:HG23	1:C:478:THR:H	1.42	0.84
1:C:146:LEU:HG	1:C:191:MSE:HE2	1.59	0.84
2:E:62:ILE:HD11	2:E:268:LEU:HD21	1.58	0.84
2:F:453:PHE:CD1	2:F:462:VAL:HG11	2.13	0.84
4:H:132:MSE:O	4:H:133:LYS:HG3	1.78	0.84
1:A:109:ASN:HB2	1:A:110:PRO:HD2	1.60	0.83
1:C:96:GLU:HB3	1:C:128:PRO:HA	1.59	0.83
1:A:42:HIS:CA	1:A:42:HIS:CG	2.61	0.83
2:D:181:GLY:HA2	2:D:245:GLN:OE1	1.77	0.83
2:D:405:ARG:HD3	2:D:453:PHE:CZ	2.14	0.83
1:B:107:VAL:HB	1:B:116:ASP:HB3	1.59	0.83
2:F:223:GLY:O	2:F:226:MSE:HB2	1.78	0.83
1:C:444:PHE:CG	1:C:444:PHE:CA	2.62	0.83
3:G:99:VAL:HG11	3:G:126:PHE:CZ	2.13	0.82
3:G:10:ARG:HD2	4:H:129:VAL:HA	1.61	0.82
2:F:415:HIS:CA	2:F:415:HIS:CG	2.62	0.82
2:E:289:GLN:HG3	2:E:324:HIS:CG	2.14	0.82
2:F:96:PHE:CG	2:F:96:PHE:CA	2.62	0.82
1:B:53:VAL:HG21	1:B:73:ILE:CD1	2.09	0.82
2:D:401:HIS:CD2	2:D:405:ARG:HH12	1.98	0.82
2:D:383:ILE:HD12	2:D:383:ILE:N	1.95	0.81
1:B:199:GLY:HA3	1:B:265:LYS:HD3	1.62	0.81
2:E:181:GLY:HA2	2:E:245:GLN:HE21	1.42	0.81
1:A:243:VAL:CG1	1:A:260:TYR:OH	2.29	0.81
1:C:476:ARG:O	1:C:479:LYS:CG	2.28	0.81
2:D:414:PHE:CG	2:D:414:PHE:CA	2.63	0.81
2:E:315:ASP:O	2:E:318:PRO:HD2	1.80	0.81
1:A:395:PHE:CE2	3:G:26:MSE:HE1	2.14	0.81
2:D:64:MSE:HE1	2:D:227:ARG:HB2	1.61	0.81
2:E:53:HIS:HD2	2:E:59:VAL:HG12	1.41	0.81
1:C:412:ARG:O	1:C:416:THR:HG23	1.79	0.81
3:G:82:THR:CG2	3:G:92:ASN:OD1	2.28	0.81
1:C:425:HIS:CA	1:C:425:HIS:CG	2.64	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:ILE:O	1:C:479:LYS:HA	1.80	0.81
1:C:355:PRO:O	1:C:357:ILE:HG12	1.81	0.80
2:D:141:VAL:HG11	2:D:344:VAL:HB	1.63	0.80
3:G:10:ARG:CD	4:H:129:VAL:HA	2.11	0.80
2:D:10:MSE:O	2:D:13:VAL:HG12	1.81	0.80
1:B:370:ALA:O	1:B:371:GLN:O	2.00	0.79
2:D:31:LYS:CD	2:D:47:THR:HG22	2.12	0.79
3:G:78:TYR:CD1	3:G:171:TYR:CE1	2.69	0.79
4:H:127:LEU:O	4:H:129:VAL:N	2.16	0.79
1:A:376:LYS:CD	1:A:376:LYS:CB	2.59	0.79
2:D:271:MSE:HE2	3:G:281:ALA:CB	2.12	0.79
2:E:216:GLY:HA3	2:E:228:VAL:HG21	1.64	0.79
3:G:1:MSE:HG2	3:G:2:ALA:H	1.48	0.79
1:A:239:PRO:HG2	1:A:266:GLN:NE2	1.98	0.79
1:B:350:PHE:CD1	1:B:350:PHE:CB	2.66	0.79
1:C:231:PRO:HG2	1:C:234:LEU:HG	1.65	0.79
2:E:46:LEU:HD21	2:E:48:LEU:HD21	1.65	0.79
1:C:391:GLU:O	1:C:391:GLU:HG2	1.82	0.79
1:A:172:GLN:N	5:A:700:SO4:O4	2.15	0.78
1:B:453:VAL:O	1:B:456:PHE:HB3	1.81	0.78
2:E:143:ASP:HB3	2:E:430:VAL:HG22	1.65	0.78
2:E:428:VAL:HG23	2:E:432:GLU:HB2	1.66	0.78
4:H:8:VAL:HG22	4:H:77:ILE:HB	1.64	0.78
1:B:53:VAL:HG21	1:B:73:ILE:HD12	1.65	0.78
1:A:488:ASN:O	1:A:492:GLU:HG2	1.83	0.78
2:F:315:ASP:O	2:F:318:PRO:HD2	1.82	0.78
1:A:375:MSE:HG2	1:A:434:VAL:HG12	1.66	0.78
1:B:161:ARG:HH12	1:B:191:MSE:HG3	1.48	0.78
2:F:233:LEU:HD23	2:F:291:ARG:HD2	1.64	0.78
4:H:129:VAL:HG13	4:H:132:MSE:CA	2.13	0.78
2:D:193:ARG:HB3	2:D:193:ARG:NH1	1.98	0.78
4:H:38:HIS:HE1	4:H:41:LEU:HD23	1.48	0.78
1:C:382:LEU:HG	1:C:437:ILE:HD11	1.64	0.78
2:D:262:SER:HB3	2:D:278:GLN:OE1	1.84	0.78
2:D:258:THR:HG21	2:D:285:MSE:HE2	1.66	0.78
1:C:431:GLU:HG2	1:C:473:GLU:HG2	1.64	0.78
1:C:230:GLN:HB3	1:C:234:LEU:HD12	1.67	0.77
2:E:85:VAL:HG12	2:E:99:LEU:O	1.84	0.77
2:E:253:ASN:H	2:E:305:ALA:HB3	1.48	0.77
1:C:140:ARG:CZ	1:C:143:HIS:NE2	2.47	0.77
2:D:175:ILE:HG13	2:D:248:LEU:HD11	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:141:VAL:HG22	2:E:410:LEU:HB3	1.67	0.77
1:A:44:LEU:HB3	1:A:47:VAL:HG13	1.65	0.77
1:C:460:PHE:CA	1:C:460:PHE:CG	2.68	0.77
3:G:78:TYR:HD1	3:G:171:TYR:CE1	2.02	0.77
1:B:195:TYR:CE1	1:B:259:VAL:HG11	2.20	0.77
1:C:95:MSE:HE2	1:C:96:GLU:H	1.50	0.77
1:C:263:LEU:CD1	1:C:317:PRO:HB3	2.15	0.76
2:F:8:GLN:HB2	2:F:15:ASP:HB2	1.67	0.76
4:H:125:ASN:C	4:H:127:LEU:H	1.93	0.76
1:C:250:MSE:HG2	1:C:304:LEU:HD11	1.64	0.76
1:A:416:THR:HA	1:A:440:LEU:CD1	2.15	0.76
1:B:262:ASP:H	1:B:318:PHE:HB2	1.48	0.76
2:F:51:ALA:O	2:F:52:LEU:HD23	1.85	0.76
1:A:53:VAL:CG1	1:A:88:VAL:HG12	2.15	0.76
1:B:64:LEU:CD2	1:B:279:ARG:NH2	2.48	0.76
2:D:3:ARG:CD	2:D:3:ARG:CZ	2.64	0.76
1:A:65:ASN:ND2	1:A:277:LEU:HB3	2.01	0.75
4:H:130:ALA:HB3	4:H:133:LYS:CE	2.16	0.75
2:D:140:LYS:CG	2:D:140:LYS:CA	2.65	0.75
2:D:153:LYS:N	2:D:153:LYS:HD2	2.02	0.75
1:A:29:GLY:HA3	1:A:42:HIS:O	1.86	0.75
2:D:377:TYR:CE1	2:D:400:VAL:HG13	2.21	0.75
2:D:383:ILE:H	2:D:383:ILE:CD1	1.99	0.75
3:G:112:GLU:CD	3:G:113:TYR:N	2.44	0.75
1:A:109:ASN:C	1:A:109:ASN:HD22	1.93	0.75
2:D:404:ARG:HD3	2:D:450:GLU:OE2	1.87	0.75
3:G:10:ARG:HD2	4:H:128:SER:O	1.87	0.75
2:E:348:ALA:O	2:E:350:THR:HG23	1.87	0.74
1:C:288:GLY:O	2:D:263:GLU:HG3	1.86	0.74
1:B:372:ILE:O	1:B:479:LYS:O	2.05	0.74
1:C:243:VAL:CG1	1:C:260:TYR:OH	2.35	0.74
3:G:78:TYR:HE1	3:G:171:TYR:HH	1.34	0.74
1:B:108:VAL:HG12	1:B:114:PRO:HA	1.68	0.74
2:D:178:GLU:HG3	2:D:427:TYR:CE2	2.23	0.74
3:G:87:LEU:HD23	3:G:244:MSE:HE1	1.70	0.74
1:B:39:ALA:O	1:B:73:ILE:HG22	1.87	0.74
2:D:271:MSE:CE	3:G:281:ALA:HB1	2.16	0.74
2:D:401:HIS:CE1	2:D:405:ARG:HH12	2.06	0.74
2:F:401:HIS:HD2	2:F:405:ARG:NH2	1.84	0.74
3:G:82:THR:HG22	3:G:83:SER:N	2.03	0.74
4:H:91:LEU:O	4:H:94:LYS:N	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:LYS:CD	1:B:83:LYS:CB	2.65	0.73
1:C:395:PHE:O	1:C:397:GLN:HG3	1.88	0.73
2:E:162:VAL:HG11	2:E:331:LEU:HB3	1.70	0.73
1:A:480:ASP:O	1:A:481:LEU:HD23	1.86	0.73
1:B:53:VAL:CG2	1:B:73:ILE:HD11	2.18	0.73
2:F:87:VAL:HG21	2:F:116:ASP:OD2	1.88	0.73
1:C:262:ASP:H	1:C:318:PHE:CB	1.95	0.73
1:C:434:VAL:HA	1:C:437:ILE:HG22	1.70	0.73
2:D:431:LYS:CD	2:D:431:LYS:CB	2.66	0.73
2:D:26:ILE:O	2:D:27:TYR:HB2	1.86	0.73
2:F:212:ALA:HB1	2:F:235:MSE:HE3	1.68	0.73
1:C:27:ASP:O	1:C:90:ARG:HG3	1.89	0.73
1:C:166:LEU:HB2	1:C:338:THR:HG21	1.69	0.73
2:E:428:VAL:HG23	2:E:432:GLU:CB	2.19	0.73
1:A:243:VAL:HG12	1:A:260:TYR:OH	1.89	0.73
2:E:240:ARG:HD2	2:E:295:THR:HG23	1.71	0.73
2:F:405:ARG:CB	2:F:405:ARG:CD	2.66	0.73
1:A:186:GLN:OE1	1:A:191:MSE:HG3	1.89	0.73
1:C:104:ILE:HD13	1:C:222:ILE:HD11	1.71	0.73
1:A:372:ILE:HD12	1:A:375:MSE:H	1.54	0.73
2:E:262:SER:HB3	2:E:278:GLN:OE1	1.89	0.73
2:E:318:PRO:HB2	2:E:322:PHE:CE1	2.24	0.73
1:A:231:PRO:HD2	1:A:234:LEU:HD12	1.71	0.72
1:B:271:ARG:CD	1:B:271:ARG:CB	2.67	0.72
1:C:99:VAL:HG11	1:C:248:TYR:HB2	1.71	0.72
1:C:474:HIS:HA	1:C:477:THR:HG22	1.71	0.72
2:D:466:ALA:O	2:D:469:MSE:N	2.22	0.72
2:E:419:GLN:CA	2:E:419:GLN:CG	2.67	0.72
2:D:202:MSE:HE2	2:D:211:THR:HG21	1.69	0.72
2:E:14:VAL:O	2:E:61:THR:HG22	1.89	0.72
1:B:472:LEU:HD23	1:B:473:GLU:N	2.05	0.72
1:C:263:LEU:HD11	1:C:317:PRO:HB3	1.71	0.72
2:F:192:THR:OG1	2:F:217:GLN:HG3	1.88	0.72
2:D:254:ILE:HD12	2:D:304:GLN:NE2	2.04	0.72
2:F:443:GLY:HA2	2:F:446:ASP:OD1	1.90	0.72
1:A:450:VAL:HA	1:A:453:VAL:HG23	1.70	0.72
1:C:144:GLU:CG	1:C:144:GLU:CA	2.66	0.72
3:G:53:VAL:HG22	3:G:216:LEU:HD13	1.70	0.72
2:D:226:MSE:HG2	2:D:227:ARG:HH11	1.53	0.72
2:E:94:ARG:CB	2:E:94:ARG:CD	2.68	0.72
1:C:166:LEU:HD22	1:C:334:VAL:HG22	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:294:SER:HA	2:E:299:SER:HA	1.71	0.72
2:D:342:PRO:HG3	2:D:414:PHE:CZ	2.25	0.71
2:E:138:GLY:HA3	2:E:427:TYR:CD1	2.25	0.71
2:E:342:PRO:HG3	2:E:414:PHE:CZ	2.25	0.71
3:G:20:ILE:HD13	4:H:119:ALA:HB1	1.69	0.71
3:G:36:GLU:HA	3:G:39:ALA:HB3	1.71	0.71
1:A:161:ARG:HH12	1:A:191:MSE:HG2	1.56	0.71
1:C:156:LEU:O	1:C:158:PRO:HD3	1.90	0.71
1:C:235:LEU:H	1:C:235:LEU:HD12	1.55	0.71
1:A:32:ILE:O	1:A:84:GLU:HG2	1.90	0.71
1:B:195:TYR:HD1	1:B:259:VAL:HB	1.56	0.71
1:C:308:LYS:CE	1:C:308:LYS:CG	2.68	0.71
1:C:345:GLN:O	1:C:356:ALA:HB1	1.91	0.71
1:A:32:ILE:CG2	1:A:33:GLN:HG3	2.19	0.71
1:C:238:ALA:HB3	1:C:239:PRO:HD3	1.72	0.71
2:F:306:ILE:HD13	2:F:321:THR:HG21	1.71	0.71
3:G:96:LEU:CD2	3:G:125:PHE:HB3	2.20	0.71
2:F:72:ARG:CG	2:F:72:ARG:CA	2.69	0.71
3:G:4:LEU:HD21	3:G:262:TYR:CE1	2.26	0.71
1:C:96:GLU:CB	1:C:128:PRO:HA	2.20	0.70
2:D:411:SER:HB2	2:D:455:LEU:HD23	1.72	0.70
3:G:87:LEU:HD23	3:G:244:MSE:CE	2.20	0.70
1:A:62:MSE:CE	1:A:95:MSE:HB2	2.21	0.70
1:A:163:GLN:HG2	1:A:164:ARG:N	2.06	0.70
2:E:35:LYS:CA	2:E:36:ALA:N	2.54	0.70
4:H:83:GLU:OE1	4:H:95:ALA:CB	2.38	0.70
1:A:121:VAL:O	1:A:121:VAL:HG23	1.91	0.70
1:A:167:ILE:HD11	1:A:318:PHE:CE2	2.26	0.70
1:A:196:VAL:CG1	1:A:198:ILE:HD11	2.20	0.70
1:B:161:ARG:HH12	1:B:191:MSE:CG	2.04	0.70
2:E:31:LYS:HD2	2:E:47:THR:HG22	1.74	0.70
1:B:372:ILE:HD11	1:B:434:VAL:HG11	1.72	0.70
2:E:182:ILE:O	2:E:247:VAL:HG13	1.92	0.70
1:B:44:LEU:O	1:B:47:VAL:HG22	1.90	0.70
2:E:277:TYR:CE2	2:E:317:ALA:HB2	2.26	0.70
2:E:408:PHE:HE1	2:E:454:ARG:HD2	1.56	0.70
1:C:271:ARG:HD3	1:C:286:TYR:CD2	2.27	0.70
1:C:52:LEU:HG	1:C:60:MSE:HE3	1.73	0.70
1:A:345:GLN:HG2	1:A:358:ASN:HB2	1.73	0.69
1:C:458:LYS:CB	1:C:458:LYS:CD	2.70	0.69
2:E:258:THR:CG2	2:E:285:MSE:HE2	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:80:VAL:CG1	3:G:117:VAL:HG22	2.22	0.69
1:B:330:ILE:HB	1:B:331:PRO:HD3	1.73	0.69
1:C:257:LEU:HD23	1:C:257:LEU:C	2.17	0.69
1:C:482:PRO:C	1:C:484:GLU:H	2.00	0.69
2:E:141:VAL:HG11	2:E:344:VAL:HB	1.74	0.69
1:B:145:PRO:HB3	1:B:370:ALA:O	1.91	0.69
1:B:328:ALA:HB3	1:B:331:PRO:HG2	1.73	0.69
2:D:384:ILE:HG23	2:D:389:MSE:SE	2.41	0.69
2:D:457:GLY:HA3	2:D:461:GLU:OE2	1.92	0.69
1:C:167:ILE:HG22	1:C:342:ILE:HB	1.72	0.69
3:G:52:VAL:HG13	4:H:42:VAL:HG11	1.73	0.69
1:B:163:GLN:HG2	1:B:164:ARG:N	2.08	0.69
1:C:463:PHE:O	1:C:467:ASN:HB2	1.92	0.69
2:D:256:ARG:NH1	2:D:259:GLN:HE22	1.90	0.69
3:G:86:GLY:O	3:G:240:ARG:NH1	2.26	0.69
1:A:196:VAL:HG12	1:A:198:ILE:CD1	2.21	0.69
1:C:419:VAL:CG2	1:C:440:LEU:HD13	2.18	0.69
1:C:474:HIS:C	1:C:474:HIS:CD2	2.70	0.69
2:F:253:ASN:HA	2:F:305:ALA:O	1.92	0.69
2:D:401:HIS:CE1	2:D:446:ASP:HB3	2.28	0.69
2:F:171:LEU:HD13	2:F:303:ILE:HD13	1.75	0.69
2:F:172:ILE:HD11	2:F:185:PHE:CE2	2.28	0.69
1:A:148:THR:HG21	1:A:153:ILE:HD12	1.73	0.69
2:E:147:PRO:HB2	2:E:353:ALA:HB3	1.74	0.69
3:G:179:ILE:HD13	3:G:242:THR:OG1	1.93	0.69
2:D:214:VAL:HG12	2:D:228:VAL:HG13	1.74	0.68
2:E:46:LEU:CD2	2:E:48:LEU:HD21	2.23	0.68
2:F:249:LEU:HD23	2:F:292:ILE:HG23	1.75	0.68
2:F:23:LEU:HD21	2:F:57:ASP:HA	1.75	0.68
2:F:48:LEU:HB3	2:F:61:THR:HB	1.73	0.68
2:F:139:ILE:HD12	2:F:414:PHE:HE1	1.58	0.68
1:C:375:MSE:SE	1:C:379:ALA:HB2	2.44	0.68
2:D:214:VAL:CG1	2:D:228:VAL:HG13	2.23	0.68
2:D:377:TYR:HD1	2:D:400:VAL:HG22	1.58	0.68
1:B:241:ALA:O	1:B:245:MSE:HG3	1.93	0.68
1:C:249:PHE:HB3	1:C:254:LYS:HB2	1.74	0.68
2:E:381:GLN:O	2:E:384:ILE:HG22	1.94	0.68
2:D:318:PRO:O	2:D:322:PHE:HD1	1.77	0.68
1:A:110:PRO:HG2	1:A:234:LEU:HD22	1.74	0.68
1:A:382:LEU:HG	1:A:437:ILE:HD11	1.74	0.68
1:C:436:ILE:CB	1:C:461:TYR:OH	2.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:27:TYR:O	2:D:82:PRO:HB3	1.94	0.68
2:F:120:ARG:O	2:F:291:ARG:NH2	2.22	0.68
1:A:301:ALA:HB1	1:A:313:LEU:O	1.92	0.68
1:C:330:ILE:HB	1:C:331:PRO:HD3	1.76	0.68
2:E:253:ASN:HA	2:E:305:ALA:O	1.93	0.68
2:F:456:VAL:HG21	2:F:462:VAL:HG22	1.74	0.68
1:C:445:LEU:HD21	1:C:453:VAL:HG22	1.76	0.67
2:D:31:LYS:NZ	2:D:47:THR:CG2	2.57	0.67
2:D:182:ILE:HG23	2:D:183:SER:N	2.08	0.67
1:C:434:VAL:HA	1:C:437:ILE:CG2	2.24	0.67
1:C:231:PRO:HD2	1:C:234:LEU:HD12	1.75	0.67
1:A:163:GLN:HG2	1:A:164:ARG:H	1.60	0.67
2:D:98:VAL:HG21	2:D:224:ALA:HB1	1.77	0.67
2:D:435:ARG:CD	2:D:435:ARG:CB	2.73	0.67
1:B:53:VAL:CG2	1:B:73:ILE:CD1	2.73	0.67
1:C:315:ALA:C	1:C:317:PRO:HD3	2.19	0.67
1:B:52:LEU:HG	1:B:95:MSE:HE3	1.77	0.67
2:F:450:GLU:CA	2:F:450:GLU:CG	2.72	0.67
2:D:88:GLY:HA2	2:D:238:TYR:CE2	2.30	0.67
3:G:161:ALA:O	3:G:164:THR:HB	1.94	0.67
2:D:401:HIS:CE1	2:D:446:ASP:O	2.47	0.67
3:G:114:ALA:C	3:G:115:ILE:HG13	2.18	0.67
4:H:132:MSE:O	4:H:133:LYS:CG	2.43	0.67
1:A:53:VAL:HG11	1:A:88:VAL:HG12	1.75	0.67
3:G:254:LEU:O	3:G:258:LEU:HG	1.95	0.67
1:A:435:LEU:O	1:A:438:TYR:HB3	1.95	0.67
1:B:44:LEU:HB3	1:B:47:VAL:CG1	2.25	0.67
2:D:131:GLU:CB	2:D:131:GLU:CD	2.68	0.67
1:B:193:SER:HB2	1:B:221:THR:OG1	1.96	0.66
2:F:275:VAL:O	2:F:275:VAL:HG12	1.95	0.66
4:H:127:LEU:C	4:H:129:VAL:H	2.01	0.66
1:B:182:THR:O	1:B:186:GLN:HG2	1.95	0.66
1:B:209:VAL:HG11	2:E:125:PHE:HZ	1.59	0.66
2:F:370:VAL:HG13	2:F:406:ILE:HG21	1.77	0.66
1:A:465:ASP:CG	1:A:465:ASP:CA	2.68	0.66
1:C:354:ARG:O	1:C:355:PRO:C	2.38	0.66
1:C:388:ALA:O	1:C:392:LEU:N	2.28	0.66
2:E:48:LEU:HD13	2:E:61:THR:HG21	1.77	0.66
2:E:168:ILE:HG23	2:E:250:PHE:CE2	2.30	0.66
1:A:395:PHE:CD2	3:G:26:MSE:HE1	2.30	0.66
1:B:430:VAL:O	1:B:434:VAL:HG13	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:190:GLU:HG3	2:F:191:ARG:N	2.07	0.66
3:G:114:ALA:C	3:G:115:ILE:CG1	2.68	0.66
1:A:438:TYR:O	1:A:441:THR:HG22	1.96	0.66
1:C:191:MSE:HE3	1:C:257:LEU:HD12	1.78	0.66
2:D:62:ILE:HD13	2:D:226:MSE:HE1	1.78	0.66
2:D:116:ASP:HB3	2:D:117:PRO:HD2	1.77	0.66
4:H:111:ILE:O	4:H:115:ARG:HG3	1.96	0.66
1:C:199:GLY:O	1:C:228:ALA:HB2	1.95	0.66
2:E:372:GLN:CB	2:E:372:GLN:CD	2.69	0.66
1:B:434:VAL:O	1:B:437:ILE:HG22	1.96	0.66
1:C:300:ARG:CD	1:C:300:ARG:CB	2.74	0.66
2:F:155:GLY:HA3	2:F:325:LEU:HD13	1.78	0.66
2:F:199:TYR:CD2	2:F:200:HIS:CE1	2.80	0.66
2:F:372:GLN:OE1	2:F:376:ARG:NH2	2.29	0.66
1:A:404:LYS:HB3	1:A:406:THR:OG1	1.96	0.66
1:C:174:GLY:O	1:C:178:VAL:HG23	1.96	0.66
1:A:419:VAL:CG2	1:A:440:LEU:HD13	2.24	0.66
1:B:343:PHE:HD2	1:B:344:LEU:N	1.93	0.66
1:C:62:MSE:HE3	1:C:95:MSE:HG3	1.78	0.65
2:D:168:ILE:HG23	2:D:250:PHE:CD2	2.31	0.65
2:D:190:GLU:HA	2:D:218:MSE:HE3	1.78	0.65
1:A:210:GLU:O	1:A:213:ARG:N	2.30	0.65
1:C:350:PHE:CE2	2:F:347:LEU:O	2.49	0.65
1:A:90:ARG:CB	1:A:90:ARG:NE	2.59	0.65
1:C:67:GLU:CB	1:C:67:GLU:CD	2.69	0.65
1:C:186:GLN:OE1	1:C:191:MSE:HG3	1.97	0.65
1:B:243:VAL:O	1:B:247:GLU:HG3	1.97	0.65
2:F:137:THR:HG21	2:F:148:TYR:CD2	2.32	0.65
2:D:226:MSE:HG2	2:D:227:ARG:NH1	2.11	0.65
2:E:208:ILE:HA	2:E:211:THR:HG22	1.77	0.65
3:G:174:HIS:CG	3:G:175:TYR:H	2.15	0.65
1:A:137:MSE:HG3	2:E:105:LEU:HG	1.78	0.65
1:B:167:ILE:HD12	1:B:318:PHE:HE2	1.62	0.65
1:C:463:PHE:HD1	1:C:463:PHE:H	1.44	0.65
2:D:150:LYS:CD	2:D:150:LYS:CB	2.75	0.65
2:F:396:ASP:O	2:F:400:VAL:HG23	1.96	0.65
1:B:207:THR:O	1:B:211:THR:HG23	1.96	0.65
2:D:216:GLY:CA	2:D:228:VAL:HG21	2.23	0.65
2:E:430:VAL:O	2:E:434:VAL:HG23	1.96	0.65
1:C:301:ALA:HB1	1:C:313:LEU:O	1.96	0.65
2:D:392:LEU:O	2:D:394:ASP:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:HIS:O	1:C:474:HIS:HD2	1.81	0.64
1:A:38:ILE:CD1	1:A:74:VAL:HG12	2.27	0.64
1:B:497:THR:C	1:B:499:VAL:H	2.05	0.64
2:F:260:ALA:HA	2:F:263:GLU:OE2	1.97	0.64
3:G:179:ILE:CD1	3:G:242:THR:HB	2.27	0.64
1:A:233:PRO:CG	1:A:273:LEU:HD12	2.26	0.64
1:B:75:ILE:HD13	1:B:82:ILE:HD12	1.78	0.64
2:E:17:LYS:CA	2:E:18:PHE:N	2.60	0.64
2:F:135:LEU:HD12	2:F:150:LYS:HG2	1.79	0.64
2:F:142:VAL:HG13	2:F:146:ALA:O	1.97	0.64
2:F:453:PHE:CE1	2:F:462:VAL:HG11	2.31	0.64
1:A:416:THR:HA	1:A:440:LEU:HD12	1.78	0.64
1:B:261:ASP:HA	1:B:318:PHE:CD1	2.32	0.64
1:C:416:THR:HA	1:C:440:LEU:CD1	2.28	0.64
1:C:445:LEU:O	1:C:445:LEU:HD23	1.97	0.64
2:F:376:ARG:O	2:F:380:LEU:HG	1.96	0.64
3:G:103:ILE:O	3:G:107:HIS:HB3	1.96	0.64
1:A:87:GLU:CG	1:A:87:GLU:CA	2.76	0.64
1:A:146:LEU:HD12	1:A:314:THR:HG21	1.80	0.64
1:C:491:ILE:O	1:C:494:PHE:HB2	1.98	0.64
2:D:64:MSE:CE	2:D:227:ARG:HB2	2.28	0.64
2:D:277:TYR:CE2	2:D:317:ALA:HB2	2.33	0.64
1:A:104:ILE:HD11	1:A:249:PHE:CZ	2.33	0.64
1:A:213:ARG:HD2	1:A:218:LEU:HD12	1.79	0.64
1:B:435:LEU:O	1:B:438:TYR:HB3	1.98	0.64
1:C:371:GLN:HB3	1:C:375:MSE:HB3	1.80	0.64
2:D:120:ARG:CG	2:D:120:ARG:NE	2.60	0.64
3:G:179:ILE:HD12	3:G:238:ALA:C	2.23	0.64
2:E:251:ILE:HD12	2:E:304:GLN:HE21	1.63	0.64
1:C:139:ARG:NH1	2:D:192:THR:HB	2.12	0.64
2:D:335:LEU:HD11	2:D:345:ASP:HA	1.80	0.64
3:G:43:VAL:N	3:G:44:PRO:HD2	2.13	0.64
4:H:41:LEU:C	4:H:41:LEU:HD12	2.22	0.64
1:A:44:LEU:HB3	1:A:47:VAL:CG1	2.27	0.64
2:E:38:ASN:ND2	2:E:41:GLU:HG3	2.10	0.64
2:E:173:HIS:CD2	2:E:415:HIS:ND1	2.66	0.64
1:B:144:GLU:CA	1:B:144:GLU:CG	2.76	0.64
1:A:296:ARG:HA	2:E:219:ASN:HB2	1.79	0.63
2:E:94:ARG:HH11	2:E:106:GLU:HB2	1.64	0.63
2:F:354:LEU:O	2:F:364:TYR:HD2	1.80	0.63
2:F:382:ASP:OD1	4:H:128:SER:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:VAL:O	1:C:212:LEU:HG	1.98	0.63
2:F:6:VAL:CG2	2:F:16:VAL:HG22	2.27	0.63
2:F:294:SER:HB2	2:F:299:SER:HA	1.80	0.63
1:A:198:ILE:HD12	1:A:198:ILE:N	2.13	0.63
1:B:301:ALA:HB2	1:B:313:LEU:HD22	1.80	0.63
2:D:92:LEU:HD21	2:D:182:ILE:CG1	2.29	0.63
2:D:213:MSE:HE2	2:D:215:PHE:CZ	2.33	0.63
2:D:247:VAL:HG12	2:D:248:LEU:N	2.14	0.63
3:G:24:MSE:HE3	3:G:244:MSE:HE3	1.80	0.63
1:A:392:LEU:O	1:A:394:ALA:N	2.30	0.63
1:C:484:GLU:O	1:C:485:ASP:C	2.41	0.63
1:C:485:ASP:CG	1:C:486:ASP:H	2.07	0.63
2:D:182:ILE:CG2	2:D:183:SER:N	2.61	0.63
2:F:354:LEU:O	2:F:364:TYR:CD2	2.52	0.63
1:B:55:PHE:CZ	1:B:73:ILE:HD13	2.33	0.63
1:C:232:ALA:HA	1:C:235:LEU:HD13	1.79	0.63
3:G:78:TYR:HD1	3:G:171:TYR:HE1	1.43	0.63
1:A:304:LEU:O	1:A:310:GLY:HA2	1.98	0.63
2:D:362:GLU:O	2:D:366:VAL:HG23	1.99	0.63
1:B:39:ALA:O	1:B:73:ILE:CG2	2.47	0.63
1:C:260:TYR:HB2	1:C:317:PRO:HA	1.80	0.63
1:C:448:ILE:HD12	1:C:456:PHE:CD1	2.33	0.63
1:C:438:TYR:HE1	1:C:489:LYS:HB3	1.63	0.62
2:D:294:SER:HB3	2:D:299:SER:HB2	1.81	0.62
3:G:159:LEU:HD11	3:G:221:ALA:HB3	1.79	0.62
1:C:463:PHE:N	1:C:463:PHE:CD1	2.65	0.62
2:F:430:VAL:O	2:F:434:VAL:HG23	1.99	0.62
4:H:127:LEU:C	4:H:129:VAL:N	2.53	0.62
2:E:453:PHE:HD1	2:E:453:PHE:H	1.46	0.62
4:H:106:SER:HB2	4:H:109:ASP:OD2	1.99	0.62
2:D:191:ARG:HH11	2:D:191:ARG:HG3	1.64	0.62
2:F:294:SER:HB3	2:F:300:ILE:H	1.64	0.62
2:D:10:MSE:O	2:D:13:VAL:CG1	2.47	0.62
2:F:383:ILE:HA	4:H:124:MSE:HE2	1.82	0.62
1:B:116:ASP:HA	2:E:125:PHE:HD2	1.64	0.62
1:C:363:VAL:CG1	1:C:364:SER:N	2.62	0.62
1:C:463:PHE:HD1	1:C:463:PHE:N	1.97	0.62
1:C:481:LEU:CB	1:C:482:PRO:CD	2.75	0.62
2:E:26:ILE:HA	2:E:50:VAL:CG1	2.30	0.62
1:A:499:VAL:HG22	1:A:499:VAL:O	1.99	0.62
2:E:34:HIS:CB	2:E:74:MSE:HE3	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:134:ILE:HG13	2:E:148:TYR:O	2.00	0.62
2:E:240:ARG:O	2:E:244:GLY:HA2	1.99	0.62
2:E:250:PHE:CE2	2:E:303:ILE:HD12	2.34	0.62
2:E:341:TYR:HA	2:E:342:PRO:C	2.25	0.62
2:F:227:ARG:HD2	2:F:230:LEU:HD12	1.81	0.62
1:B:47:VAL:HG12	1:B:90:ARG:HG3	1.82	0.62
1:C:388:ALA:HB1	1:C:392:LEU:HD13	1.82	0.62
1:C:448:ILE:HD12	1:C:456:PHE:CE1	2.35	0.62
1:A:90:ARG:HH21	1:A:92:GLY:HA2	1.63	0.61
1:C:163:GLN:HG2	1:C:164:ARG:N	2.15	0.61
2:D:310:ALA:O	2:D:311:ASP:C	2.43	0.61
2:E:193:ARG:HB3	2:E:193:ARG:HH11	1.65	0.61
3:G:99:VAL:HG11	3:G:126:PHE:CE2	2.35	0.61
1:C:363:VAL:HG12	1:C:364:SER:N	2.12	0.61
2:E:51:ALA:O	2:E:52:LEU:HD23	2.00	0.61
1:C:438:TYR:HE2	1:C:442:ARG:CD	2.12	0.61
2:E:278:GLN:HG3	2:E:284:GLU:OE1	2.00	0.61
1:A:104:ILE:HD13	1:A:222:ILE:CD1	2.28	0.61
2:E:183:SER:O	2:E:211:THR:HA	1.99	0.61
2:F:373:THR:HG22	2:F:376:ARG:NH1	2.15	0.61
1:A:232:ALA:HB3	1:A:233:PRO:HD3	1.83	0.61
1:C:140:ARG:NH2	1:C:143:HIS:NE2	2.49	0.61
1:C:392:LEU:O	1:C:395:PHE:HB2	2.00	0.61
1:A:179:ALA:HB2	1:A:318:PHE:HZ	1.64	0.61
1:A:206:ARG:NH1	2:D:125:PHE:O	2.34	0.61
2:F:196:ASN:OD1	2:F:200:HIS:CE1	2.54	0.61
1:A:67:GLU:HA	2:E:8:GLN:HG2	1.82	0.61
2:D:258:THR:CG2	2:D:285:MSE:HE2	2.29	0.61
2:F:139:ILE:HD12	2:F:414:PHE:CE1	2.35	0.61
3:G:219:GLN:OE1	4:H:66:GLY:HA2	2.00	0.61
1:A:62:MSE:HE3	1:A:95:MSE:HB2	1.82	0.61
1:A:206:ARG:HD2	2:D:128:LEU:HB2	1.82	0.61
1:A:209:VAL:HG11	2:D:125:PHE:HZ	1.66	0.61
1:B:30:THR:O	1:B:41:ALA:HB1	1.99	0.61
1:B:33:GLN:OE1	1:B:40:ARG:CZ	2.49	0.61
1:A:401:ASP:O	1:A:402:LEU:C	2.44	0.61
1:A:457:GLU:CA	1:A:457:GLU:CG	2.79	0.61
1:A:488:ASN:C	1:A:492:GLU:HG2	2.25	0.61
1:C:395:PHE:O	1:C:397:GLN:N	2.33	0.61
2:F:26:ILE:HG22	2:F:27:TYR:CD1	2.36	0.61
1:A:209:VAL:HA	1:A:212:LEU:HD12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:153:LYS:N	2:E:153:LYS:HD2	2.16	0.61
3:G:83:SER:HB3	3:G:236:GLU:CD	2.25	0.61
2:E:115:ARG:HG3	2:E:115:ARG:HH11	1.65	0.60
1:C:474:HIS:HA	1:C:477:THR:CG2	2.31	0.60
2:F:147:PRO:HD2	2:F:351:SER:HB3	1.82	0.60
3:G:53:VAL:O	3:G:53:VAL:HG12	2.00	0.60
3:G:96:LEU:HG	3:G:126:PHE:HE1	1.66	0.60
1:C:347:ASP:O	1:C:348:LEU:HD23	2.01	0.60
1:A:139:ARG:NH1	1:A:302:ALA:HB2	2.16	0.60
2:F:148:TYR:CD2	2:F:154:ILE:HD13	2.37	0.60
3:G:212:ILE:HG12	4:H:44:PRO:HD3	1.82	0.60
4:H:45:LEU:HB2	4:H:66:GLY:O	2.00	0.60
1:A:124:THR:HG23	1:A:125:GLU:HG3	1.83	0.60
1:B:131:SER:HB3	1:B:300:ARG:HH21	1.67	0.60
1:B:195:TYR:CD1	1:B:259:VAL:HG11	2.37	0.60
1:B:275:LEU:HD21	1:B:281:PRO:HB3	1.82	0.60
2:E:157:PHE:HZ	2:E:322:PHE:HE2	1.50	0.60
2:D:166:VAL:HG13	2:D:416:VAL:HG23	1.84	0.60
2:E:47:THR:O	2:E:48:LEU:HD23	2.01	0.60
2:E:289:GLN:HA	2:E:289:GLN:NE2	2.14	0.60
2:F:195:GLY:HA2	2:F:215:PHE:HE2	1.65	0.60
1:A:345:GLN:CB	1:A:348:LEU:HD23	2.31	0.60
1:A:434:VAL:HA	1:A:437:ILE:HG22	1.83	0.60
2:E:34:HIS:HB3	2:E:74:MSE:HE3	1.82	0.60
1:B:44:LEU:HB3	1:B:47:VAL:HG13	1.83	0.60
1:B:195:TYR:HE1	1:B:259:VAL:HG11	1.63	0.60
2:E:289:GLN:HG3	2:E:324:HIS:CD2	2.35	0.60
2:E:318:PRO:HB2	2:E:322:PHE:HE1	1.66	0.60
1:B:262:ASP:H	1:B:318:PHE:CB	2.15	0.60
1:C:232:ALA:HB3	1:C:233:PRO:HD3	1.83	0.60
2:D:202:MSE:CE	2:D:211:THR:HG21	2.32	0.60
2:D:407:GLN:HA	2:D:410:LEU:HD12	1.84	0.60
2:E:138:GLY:HA3	2:E:427:TYR:CE1	2.37	0.60
1:A:109:ASN:HD21	1:A:113:GLN:H	1.49	0.60
4:H:7:SER:HA	4:H:17:GLU:HG3	1.84	0.60
2:E:453:PHE:N	2:E:453:PHE:CD1	2.70	0.59
2:F:26:ILE:O	2:F:27:TYR:HB2	2.02	0.59
1:B:84:GLU:OE1	2:E:55:GLY:HA2	2.02	0.59
1:B:208:VAL:O	1:B:212:LEU:HG	2.02	0.59
1:A:159:ILE:HA	1:A:163:GLN:OE1	2.02	0.59
1:A:239:PRO:HG2	1:A:266:GLN:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:LYS:CG	1:A:405:ALA:H	1.93	0.59
2:D:54:LEU:HD11	2:D:60:ARG:NE	2.17	0.59
2:E:413:ASN:CB	2:E:425:GLY:HA2	2.33	0.59
1:A:386:LEU:HD13	1:A:386:LEU:O	2.01	0.59
1:B:151:LYS:HB2	1:B:151:LYS:HZ3	1.66	0.59
1:C:205:VAL:O	1:C:209:VAL:HG12	2.02	0.59
2:D:84:SER:HB3	2:D:115:ARG:O	2.02	0.59
1:A:97:VAL:HB	1:A:98:PRO:HD2	1.83	0.59
1:A:156:LEU:HD21	1:A:382:LEU:HD12	1.85	0.59
2:D:152:GLY:C	2:D:153:LYS:HD2	2.27	0.59
2:F:213:MSE:HB3	2:F:215:PHE:HE1	1.68	0.59
4:H:89:ASP:O	4:H:91:LEU:N	2.36	0.59
1:C:373:LYS:HB2	1:C:480:ASP:CB	2.33	0.59
2:E:134:ILE:HD12	2:E:147:PRO:HB3	1.85	0.59
2:F:248:LEU:HD23	2:F:301:THR:HB	1.84	0.59
3:G:10:ARG:HD3	4:H:130:ALA:H	1.66	0.59
1:B:284:GLU:O	1:B:285:ALA:HB3	2.03	0.59
1:C:418:GLU:O	1:C:421:LYS:HB2	2.02	0.59
2:E:370:VAL:HG13	2:E:406:ILE:HG21	1.84	0.59
1:A:355:PRO:HB2	1:A:357:ILE:HG12	1.85	0.59
2:D:328:THR:HG22	2:D:350:THR:OG1	2.03	0.59
2:F:401:HIS:CD2	2:F:405:ARG:NH2	2.67	0.59
3:G:87:LEU:CD2	3:G:244:MSE:HE1	2.32	0.59
1:C:263:LEU:HD12	1:C:317:PRO:HB3	1.85	0.59
2:D:230:LEU:O	2:D:233:LEU:HB3	2.02	0.59
3:G:226:TYR:CZ	3:G:230:LEU:HD21	2.37	0.59
1:B:292:TYR:HA	1:B:295:SER:OG	2.02	0.59
1:C:62:MSE:HE3	1:C:95:MSE:CG	2.33	0.59
2:D:85:VAL:HG11	2:D:231:THR:HG23	1.85	0.59
2:D:401:HIS:HE1	2:D:446:ASP:O	1.85	0.59
2:F:289:GLN:O	2:F:292:ILE:N	2.35	0.59
2:F:341:TYR:HA	2:F:342:PRO:C	2.27	0.59
1:A:48:MSE:HG2	2:E:71:ILE:HD11	1.83	0.58
1:B:195:TYR:HD1	1:B:259:VAL:CB	2.15	0.58
3:G:72:PRO:CG	3:G:166:ASP:OD2	2.51	0.58
4:H:22:MSE:HB2	4:H:35:LEU:HD23	1.85	0.58
4:H:125:ASN:O	4:H:127:LEU:N	2.36	0.58
1:A:151:LYS:HA	1:A:433:GLN:OE1	2.02	0.58
1:C:202:GLU:OE1	1:C:227:SER:HB2	2.03	0.58
1:C:416:THR:HG22	1:C:440:LEU:CD1	2.33	0.58
2:D:98:VAL:HG11	2:D:224:ALA:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:212:ALA:HB1	2:F:235:MSE:CE	2.33	0.58
3:G:78:TYR:HE1	3:G:171:TYR:OH	1.85	0.58
3:G:96:LEU:HD21	3:G:125:PHE:HB3	1.83	0.58
1:A:74:VAL:HG11	1:A:273:LEU:HD21	1.86	0.58
1:C:438:TYR:O	1:C:441:THR:HG22	2.03	0.58
2:E:29:ALA:HB2	2:E:83:ILE:H	1.68	0.58
2:F:288:LEU:O	2:F:288:LEU:HG	2.03	0.58
3:G:143:GLN:O	3:G:144:PRO:C	2.44	0.58
4:H:129:VAL:HG22	4:H:132:MSE:SE	2.53	0.58
1:C:482:PRO:HB3	1:C:485:ASP:O	2.03	0.58
2:D:175:ILE:HG13	2:D:248:LEU:CD1	2.32	0.58
1:A:101:GLU:CG	1:A:101:GLU:CA	2.81	0.58
1:A:108:VAL:HG12	1:A:114:PRO:HA	1.84	0.58
1:A:294:HIS:O	1:A:298:LEU:HD13	2.03	0.58
1:A:403:ASP:O	1:A:407:GLN:HG3	2.04	0.58
1:B:167:ILE:HD11	1:B:316:LEU:HB3	1.85	0.58
1:C:148:THR:HG23	1:C:182:THR:OG1	2.01	0.58
2:E:44:ILE:HG13	2:E:74:MSE:HE1	1.85	0.58
1:B:239:PRO:HG2	1:B:266:GLN:CD	2.28	0.58
2:D:48:LEU:HD13	2:D:61:THR:OG1	2.04	0.58
3:G:174:HIS:CG	3:G:175:TYR:N	2.72	0.58
4:H:125:ASN:C	4:H:127:LEU:N	2.58	0.58
2:E:306:ILE:CD1	2:E:325:LEU:HD11	2.34	0.58
2:F:172:ILE:HD11	2:F:185:PHE:HE2	1.68	0.58
3:G:96:LEU:HD23	3:G:125:PHE:HB3	1.86	0.58
1:A:167:ILE:HD11	1:A:318:PHE:CZ	2.38	0.58
2:D:354:LEU:O	2:D:354:LEU:HD22	2.04	0.58
3:G:118:ILE:HA	3:G:138:THR:HB	1.84	0.58
1:B:55:PHE:CE1	1:B:73:ILE:HD11	2.38	0.58
1:B:96:GLU:HB3	1:B:126:THR:HG22	1.86	0.58
2:D:307:TYR:HD2	2:D:307:TYR:O	1.87	0.58
1:A:372:ILE:HD12	1:A:372:ILE:O	2.03	0.58
2:E:452:ALA:O	2:E:465:LYS:HD3	2.04	0.58
1:A:489:LYS:HA	1:A:492:GLU:HB2	1.86	0.57
1:B:492:GLU:CA	1:B:493:ALA:N	2.67	0.57
1:C:333:ASN:O	1:C:337:ILE:HG13	2.03	0.57
2:E:328:THR:CG2	2:E:350:THR:OG1	2.52	0.57
4:H:97:LYS:O	4:H:100:ALA:N	2.33	0.57
1:B:107:VAL:HG12	1:B:115:VAL:CG2	2.34	0.57
1:B:497:THR:C	1:B:499:VAL:N	2.60	0.57
2:D:254:ILE:O	2:D:254:ILE:HG12	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:3:SER:HB2	3:G:6:ASP:CB	2.34	0.57
1:B:64:LEU:CD2	1:B:279:ARG:HH21	2.17	0.57
1:C:407:GLN:HA	1:C:410:LEU:HD12	1.86	0.57
2:D:456:VAL:HG21	2:D:462:VAL:HG22	1.86	0.57
2:F:207:VAL:O	2:F:209:SER:N	2.36	0.57
2:F:237:GLU:OE1	2:F:291:ARG:HD3	2.04	0.57
1:A:143:HIS:ND1	1:A:144:GLU:N	2.51	0.57
1:B:55:PHE:CD2	1:B:82:ILE:HD13	2.39	0.57
1:B:452:ASP:O	1:B:455:ARG:HB2	2.03	0.57
2:E:24:PRO:HB3	2:E:78:ASP:OD1	2.04	0.57
2:E:48:LEU:CD1	2:E:61:THR:HG21	2.34	0.57
2:E:413:ASN:HB3	2:E:425:GLY:HA2	1.86	0.57
2:F:364:TYR:O	2:F:367:ALA:HB3	2.05	0.57
3:G:225:ILE:HD12	3:G:226:TYR:N	2.18	0.57
1:A:65:ASN:HD22	1:A:277:LEU:HB3	1.69	0.57
1:B:163:GLN:HG2	1:B:164:ARG:H	1.70	0.57
1:C:434:VAL:CA	1:C:437:ILE:HG22	2.35	0.57
2:D:213:MSE:HE2	2:D:215:PHE:CE1	2.38	0.57
3:G:100:TYR:HD1	3:G:129:ARG:HD2	1.70	0.57
1:A:104:ILE:HA	1:A:222:ILE:CD1	2.34	0.57
1:A:172:GLN:CA	5:A:700:SO4:O4	2.53	0.57
1:A:233:PRO:HG3	1:A:273:LEU:CD1	2.30	0.57
1:A:297:LEU:HG	1:A:298:LEU:HD12	1.87	0.57
2:E:366:VAL:HG13	2:E:441:LEU:HD12	1.85	0.57
3:G:109:CYS:N	3:G:110:PRO:CD	2.67	0.57
1:A:107:VAL:HB	1:A:116:ASP:HB3	1.85	0.57
3:G:216:LEU:HG	4:H:67:PHE:CE1	2.39	0.57
3:G:1:MSE:HG2	3:G:2:ALA:N	2.16	0.57
1:C:170:ASP:O	1:C:173:THR:HG23	2.05	0.57
1:C:354:ARG:CB	1:C:355:PRO:CD	2.83	0.57
3:G:1:MSE:CG	3:G:2:ALA:H	2.17	0.57
1:B:110:PRO:HB3	1:B:238:ALA:HA	1.86	0.57
1:B:272:GLU:CD	2:E:280:THR:HA	2.30	0.57
1:C:345:GLN:O	1:C:356:ALA:CB	2.52	0.57
2:D:135:LEU:HB2	2:D:150:LYS:CB	2.34	0.57
2:D:342:PRO:HG3	2:D:414:PHE:CE1	2.40	0.57
2:E:62:ILE:CD1	2:E:268:LEU:HD21	2.33	0.57
3:G:25:GLU:CD	3:G:245:LYS:HD3	2.30	0.57
1:A:109:ASN:ND2	1:A:113:GLN:H	2.03	0.56
1:B:133:ALA:CB	1:B:300:ARG:HA	2.35	0.56
1:B:231:PRO:HB2	1:B:233:PRO:HD2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:MSE:HB3	2:D:69:GLY:HA2	1.86	0.56
2:D:457:GLY:HA3	2:D:461:GLU:CD	2.30	0.56
3:G:87:LEU:N	3:G:87:LEU:HD12	2.19	0.56
3:G:133:VAL:O	3:G:133:VAL:HG12	2.05	0.56
3:G:139:ARG:C	3:G:141:PRO:HD3	2.29	0.56
1:B:133:ALA:HB2	1:B:300:ARG:HA	1.86	0.56
1:B:206:ARG:HA	1:B:209:VAL:HG12	1.87	0.56
2:F:83:ILE:HD12	2:F:118:ILE:HD11	1.86	0.56
1:B:98:PRO:HG2	1:B:112:GLY:HA3	1.87	0.56
1:B:432:LYS:O	1:B:436:ILE:HD13	2.05	0.56
1:B:445:LEU:HD21	1:B:453:VAL:HG22	1.86	0.56
1:C:191:MSE:CE	1:C:257:LEU:HB2	2.35	0.56
1:C:400:SER:O	1:C:401:ASP:C	2.47	0.56
1:C:485:ASP:N	1:C:485:ASP:OD1	2.38	0.56
2:D:463:VAL:O	2:D:466:ALA:HB3	2.05	0.56
1:A:97:VAL:O	1:A:126:THR:HG23	2.04	0.56
1:A:267:ALA:HB2	1:A:294:HIS:CE1	2.41	0.56
1:B:109:ASN:HB2	1:B:110:PRO:CD	2.24	0.56
1:B:210:GLU:OE1	2:E:130:THR:OG1	2.24	0.56
1:B:434:VAL:C	1:B:437:ILE:HG22	2.30	0.56
2:F:384:ILE:HD12	2:F:392:LEU:HD11	1.86	0.56
1:C:109:ASN:HB2	1:C:110:PRO:CD	2.27	0.56
2:D:94:ARG:NH1	2:D:106:GLU:HB2	2.21	0.56
2:D:178:GLU:HG3	2:D:427:TYR:CD2	2.40	0.56
2:E:64:MSE:HE1	2:E:227:ARG:HB2	1.87	0.56
1:B:148:THR:HG23	1:B:182:THR:OG1	2.05	0.56
1:B:232:ALA:HB3	1:B:233:PRO:HD3	1.88	0.56
1:C:148:THR:HA	1:C:182:THR:HG23	1.87	0.56
1:C:292:TYR:HA	1:C:295:SER:OG	2.06	0.56
2:D:307:TYR:C	2:D:307:TYR:CD2	2.84	0.56
2:E:26:ILE:HA	2:E:50:VAL:HG12	1.88	0.56
2:E:48:LEU:HD13	2:E:61:THR:CG2	2.35	0.56
2:F:265:SER:HB2	2:F:278:GLN:HB3	1.87	0.56
1:A:145:PRO:HA	1:A:160:GLY:HA2	1.87	0.56
1:A:159:ILE:HD11	1:A:165:GLU:HG2	1.86	0.56
1:A:365:ARG:C	1:A:367:GLY:H	2.14	0.56
1:A:455:ARG:NH2	1:A:458:LYS:HZ2	2.04	0.56
1:B:55:PHE:CE1	1:B:73:ILE:CD1	2.89	0.56
1:B:337:ILE:HA	2:F:218:MSE:HE1	1.87	0.56
2:D:14:VAL:HB	2:D:61:THR:OG1	2.05	0.56
2:D:46:LEU:HD11	2:D:63:ALA:HB1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:353:ALA:O	2:F:359:VAL:HG13	2.05	0.56
1:A:274:SER:OG	1:A:279:ARG:HD2	2.05	0.56
1:A:450:VAL:HA	1:A:453:VAL:CG2	2.36	0.56
1:C:283:ARG:HD2	1:C:329:TYR:CD1	2.41	0.56
1:C:386:LEU:O	1:C:386:LEU:HD13	2.05	0.56
1:C:477:THR:HG23	1:C:478:THR:N	2.19	0.56
2:F:253:ASN:HB3	2:F:256:ARG:HG2	1.87	0.56
1:A:66:LEU:HD23	1:A:71:VAL:HG13	1.88	0.56
1:C:335:ILE:C	1:C:337:ILE:H	2.14	0.56
2:D:91:THR:HG21	2:D:235:MSE:HE2	1.88	0.56
2:D:401:HIS:CD2	2:D:405:ARG:NH1	2.71	0.56
2:E:37:ARG:HG2	2:E:41:GLU:OE1	2.06	0.56
2:F:6:VAL:HG23	2:F:76:VAL:CG2	2.36	0.56
2:F:71:ILE:H	2:F:74:MSE:SE	2.39	0.56
2:F:237:GLU:OE2	2:F:291:ARG:HG3	2.06	0.56
2:F:384:ILE:CD1	2:F:392:LEU:HD11	2.35	0.56
4:H:25:VAL:HG21	4:H:68:LEU:HD22	1.86	0.56
1:A:455:ARG:CZ	1:A:458:LYS:HZ2	2.19	0.55
1:B:193:SER:O	1:B:221:THR:HA	2.06	0.55
1:B:262:ASP:OD2	1:B:265:LYS:HG3	2.06	0.55
1:C:145:PRO:HB3	1:C:370:ALA:O	2.06	0.55
1:C:346:SER:C	1:C:348:LEU:H	2.13	0.55
3:G:4:LEU:HD21	3:G:262:TYR:HE1	1.70	0.55
3:G:112:GLU:CG	3:G:113:TYR:H	2.20	0.55
1:A:412:ARG:O	1:A:416:THR:HG23	2.06	0.55
1:B:179:ALA:O	1:B:183:ILE:HG13	2.06	0.55
2:D:223:GLY:HA2	2:D:226:MSE:HE2	1.87	0.55
3:G:143:GLN:O	3:G:145:SER:N	2.39	0.55
4:H:28:LYS:O	4:H:29:SER:HB2	2.06	0.55
1:A:158:PRO:HD2	1:A:364:SER:HB3	1.89	0.55
1:B:110:PRO:HG2	1:B:234:LEU:HD22	1.88	0.55
1:C:243:VAL:HG12	1:C:260:TYR:OH	2.07	0.55
1:C:335:ILE:HG23	1:C:341:GLN:OE1	2.06	0.55
2:E:93:GLY:HA2	2:E:208:ILE:HG12	1.88	0.55
3:G:36:GLU:O	3:G:39:ALA:N	2.39	0.55
3:G:85:ARG:H	3:G:85:ARG:HD2	1.71	0.55
1:A:396:ALA:O	1:A:399:GLY:N	2.39	0.55
2:D:182:ILE:O	2:D:247:VAL:HG13	2.07	0.55
2:F:137:THR:HG22	2:F:175:ILE:HD11	1.88	0.55
3:G:24:MSE:SE	4:H:116:ALA:HB1	2.56	0.55
3:G:36:GLU:O	3:G:40:LYS:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:109:CYS:N	3:G:110:PRO:HD3	2.22	0.55
3:G:123:LEU:HD23	3:G:123:LEU:O	2.06	0.55
1:B:62:MSE:CE	1:B:95:MSE:HG3	2.28	0.55
1:C:395:PHE:O	1:C:397:GLN:CG	2.54	0.55
2:D:413:ASN:HB2	2:D:425:GLY:HA2	1.86	0.55
3:G:142:ASP:O	3:G:143:GLN:HB2	2.05	0.55
2:D:190:GLU:C	2:D:217:GLN:HE22	2.14	0.55
2:D:191:ARG:H	2:D:218:MSE:HE3	1.70	0.55
2:E:315:ASP:C	2:E:318:PRO:HD2	2.32	0.55
4:H:129:VAL:CG2	4:H:132:MSE:SE	3.04	0.55
1:A:319:VAL:CG2	1:A:334:VAL:HG11	2.33	0.55
1:B:107:VAL:O	1:B:115:VAL:HG22	2.06	0.55
1:B:171:ARG:HB2	1:B:320:GLU:OE2	2.07	0.55
1:C:140:ARG:NH1	1:C:306:ASP:OD1	2.40	0.55
2:D:224:ALA:O	2:D:228:VAL:HG23	2.06	0.55
2:E:94:ARG:HH12	2:E:106:GLU:HB2	1.67	0.55
2:E:275:VAL:O	2:E:275:VAL:HG12	2.06	0.55
2:F:393:SER:O	2:F:397:LYS:HG3	2.07	0.55
1:A:206:ARG:HD3	2:D:129:ALA:O	2.06	0.55
1:B:240:TYR:OH	1:B:293:LEU:HD12	2.07	0.55
2:E:202:MSE:HE2	2:E:207:VAL:HG23	1.89	0.55
1:A:51:GLU:OE2	1:A:90:ARG:NE	2.40	0.54
1:B:159:ILE:HA	1:B:163:GLN:OE1	2.07	0.54
2:D:262:SER:CB	2:D:278:GLN:OE1	2.53	0.54
2:D:275:VAL:O	2:D:275:VAL:HG12	2.06	0.54
2:D:453:PHE:CD2	2:D:462:VAL:HG11	2.42	0.54
3:G:181:GLN:HE22	3:G:239:ALA:HB2	1.72	0.54
2:E:366:VAL:O	2:E:370:VAL:HG23	2.07	0.54
1:B:452:ASP:O	1:B:456:PHE:N	2.38	0.54
2:D:91:THR:CG2	2:D:235:MSE:HE2	2.38	0.54
2:F:48:LEU:HD13	2:F:61:THR:OG1	2.07	0.54
1:C:99:VAL:HG13	1:C:245:MSE:HA	1.90	0.54
1:C:197:ALA:HB1	1:C:200:GLN:HB2	1.90	0.54
2:E:277:TYR:CZ	2:E:317:ALA:HB2	2.42	0.54
2:F:355:ALA:O	2:F:359:VAL:HG22	2.08	0.54
3:G:21:THR:HG21	3:G:248:THR:N	2.22	0.54
1:A:150:ILE:HD12	1:A:153:ILE:HD12	1.88	0.54
1:A:161:ARG:HH12	1:A:191:MSE:CG	2.20	0.54
1:A:431:GLU:O	1:A:434:VAL:HG22	2.08	0.54
2:D:176:ALA:HA	2:D:181:GLY:H	1.73	0.54
2:E:203:LYS:NZ	2:E:203:LYS:HB3	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:386:ILE:HB	4:H:124:MSE:CE	2.37	0.54
1:A:212:LEU:HB3	1:A:217:ALA:HB3	1.89	0.54
2:F:271:MSE:HE1	3:G:283:ALA:HB2	1.88	0.54
2:F:344:VAL:O	2:F:346:PRO:HD3	2.07	0.54
3:G:40:LYS:HG3	3:G:41:SER:N	2.21	0.54
3:G:52:VAL:HG22	4:H:69:GLU:HG2	1.89	0.54
3:G:87:LEU:CD2	3:G:244:MSE:CE	2.85	0.54
1:C:104:ILE:HD13	1:C:222:ILE:CD1	2.37	0.54
1:C:397:GLN:O	1:C:398:PHE:C	2.51	0.54
2:D:31:LYS:HD2	2:D:47:THR:CG2	2.24	0.54
1:A:206:ARG:O	1:A:209:VAL:HG12	2.08	0.54
2:D:67:THR:HB	2:D:70:LEU:HD12	1.89	0.54
2:E:35:LYS:O	2:E:36:ALA:N	2.41	0.54
2:E:322:PHE:HD2	2:E:325:LEU:HD12	1.73	0.54
2:F:95:VAL:HA	2:F:213:MSE:O	2.08	0.54
1:A:262:ASP:N	1:A:318:PHE:HB2	2.08	0.54
1:B:204:THR:O	1:B:208:VAL:HG23	2.08	0.54
2:D:17:LYS:HG3	2:D:57:ASP:O	2.07	0.54
2:D:430:VAL:O	2:D:434:VAL:HG23	2.08	0.54
1:A:94:ILE:O	1:A:95:MSE:C	2.51	0.53
1:B:195:TYR:CD1	1:B:259:VAL:CG1	2.90	0.53
1:C:124:THR:HG23	1:C:125:GLU:H	1.73	0.53
1:C:371:GLN:HB3	1:C:375:MSE:CB	2.38	0.53
1:C:481:LEU:O	1:C:483:ASN:N	2.41	0.53
2:D:191:ARG:HG3	2:D:191:ARG:NH1	2.23	0.53
2:E:262:SER:HA	2:E:278:GLN:HB3	1.91	0.53
3:G:84:ASP:N	3:G:84:ASP:OD1	2.41	0.53
1:B:171:ARG:O	1:B:172:GLN:HB3	2.08	0.53
1:C:322:GLN:O	1:C:323:ALA:HB3	2.07	0.53
2:F:268:LEU:CD1	2:F:270:ARG:CZ	2.86	0.53
1:B:250:MSE:HE2	1:B:251:TYR:CD1	2.43	0.53
2:E:32:ILE:HG12	2:E:76:VAL:HG22	1.89	0.53
2:F:135:LEU:HD23	2:F:135:LEU:C	2.33	0.53
2:F:140:LYS:H	2:F:412:GLN:CD	2.17	0.53
2:F:345:ASP:HB3	2:F:348:ALA:HB3	1.90	0.53
2:F:356:PRO:HD3	2:F:364:TYR:CE2	2.43	0.53
1:B:238:ALA:HB3	1:B:239:PRO:HD3	1.89	0.53
2:E:17:LYS:O	2:E:18:PHE:N	2.41	0.53
2:F:85:VAL:O	2:F:87:VAL:HG13	2.08	0.53
3:G:175:TYR:CE1	3:G:178:ALA:O	2.61	0.53
4:H:46:GLU:HG3	4:H:47:ILE:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ARG:HH12	1:B:299:GLU:CD	2.16	0.53
2:E:450:GLU:C	2:E:452:ALA:H	2.16	0.53
3:G:40:LYS:O	3:G:42:PHE:N	2.41	0.53
3:G:78:TYR:CD1	3:G:171:TYR:HE1	2.20	0.53
1:A:341:GLN:CD	1:A:341:GLN:N	2.67	0.53
1:B:175:LYS:CE	5:B:700:SO4:O4	2.56	0.53
1:B:450:VAL:O	1:B:451:GLU:C	2.50	0.53
1:B:452:ASP:HA	1:B:455:ARG:HB2	1.91	0.53
1:B:44:LEU:O	2:F:72:ARG:NH2	2.41	0.53
1:C:354:ARG:O	1:C:356:ALA:N	2.42	0.53
2:D:168:ILE:O	2:D:172:ILE:HG13	2.09	0.53
2:F:383:ILE:HA	4:H:124:MSE:CE	2.38	0.53
4:H:4:ILE:O	4:H:4:ILE:HG23	2.09	0.53
1:C:258:VAL:CG2	1:C:313:LEU:HD21	2.38	0.53
1:C:281:PRO:HG2	3:G:280:GLY:HA2	1.89	0.53
2:D:322:PHE:HA	2:D:325:LEU:HD12	1.90	0.53
2:E:7:ILE:O	2:E:72:ARG:HG2	2.09	0.53
2:E:128:LEU:HA	2:E:295:THR:HA	1.90	0.53
2:E:345:ASP:OD1	2:E:348:ALA:N	2.38	0.53
1:C:468:GLY:O	1:C:470:HIS:N	2.42	0.53
3:G:42:PHE:CZ	3:G:46:MSE:HE2	2.44	0.53
1:B:131:SER:HB3	1:B:300:ARG:NH2	2.24	0.53
1:C:144:GLU:O	1:C:161:ARG:HG3	2.09	0.53
1:C:163:GLN:HG2	1:C:164:ARG:H	1.74	0.53
2:D:140:LYS:HE2	2:D:457:GLY:O	2.08	0.53
1:A:104:ILE:HA	1:A:222:ILE:HD13	1.89	0.52
1:A:350:PHE:C	1:A:352:GLY:H	2.17	0.52
1:B:492:GLU:O	1:B:493:ALA:N	2.42	0.52
2:D:277:TYR:HE2	2:D:317:ALA:HB2	1.72	0.52
2:E:2:THR:HB	2:E:22:HIS:CE1	2.44	0.52
2:E:51:ALA:HB3	2:E:60:ARG:O	2.09	0.52
3:G:114:ALA:HB3	3:G:165:PHE:HE1	1.73	0.52
4:H:104:LEU:C	4:H:106:SER:H	2.16	0.52
1:A:38:ILE:HG13	1:A:276:LEU:HB3	1.91	0.52
2:D:361:GLU:O	2:D:365:GLN:N	2.41	0.52
2:D:410:LEU:HD23	2:D:437:PHE:CZ	2.45	0.52
2:F:356:PRO:HD3	2:F:364:TYR:CD2	2.44	0.52
4:H:89:ASP:C	4:H:91:LEU:N	2.67	0.52
4:H:97:LYS:O	4:H:99:ARG:N	2.43	0.52
1:B:472:LEU:O	1:B:475:ILE:CG2	2.49	0.52
2:D:401:HIS:CG	2:D:405:ARG:HH12	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:404:ARG:CD	2:D:450:GLU:OE2	2.57	0.52
1:B:453:VAL:O	1:B:456:PHE:CB	2.55	0.52
1:C:197:ALA:HB1	1:C:200:GLN:HG3	1.91	0.52
1:C:445:LEU:HD11	1:C:453:VAL:HG13	1.92	0.52
2:E:149:ILE:HD12	2:E:149:ILE:N	2.24	0.52
4:H:41:LEU:HD12	4:H:42:VAL:N	2.25	0.52
1:A:103:LEU:HB3	1:A:222:ILE:HD12	1.91	0.52
1:A:151:LYS:NZ	1:A:422:GLN:HB2	2.24	0.52
1:B:108:VAL:HG12	1:B:114:PRO:CA	2.38	0.52
1:C:161:ARG:HH22	1:C:189:GLN:HB3	1.74	0.52
3:G:20:ILE:CD1	4:H:119:ALA:HB1	2.38	0.52
3:G:56:VAL:HG21	3:G:211:GLU:OE2	2.08	0.52
1:A:166:LEU:HD12	1:A:167:ILE:N	2.25	0.52
1:A:291:PHE:HB3	2:E:263:GLU:OE1	2.09	0.52
1:C:176:THR:O	1:C:180:ILE:HG12	2.08	0.52
2:D:134:ILE:HG12	2:D:135:LEU:N	2.23	0.52
2:D:247:VAL:HG12	2:D:248:LEU:H	1.75	0.52
1:A:64:LEU:HD12	1:A:273:LEU:HD21	1.91	0.52
1:A:150:ILE:HA	1:A:422:GLN:OE1	2.10	0.52
1:C:222:ILE:HG22	1:C:223:VAL:H	1.75	0.52
2:D:370:VAL:HG13	2:D:406:ILE:HG21	1.92	0.52
2:F:30:LEU:HD12	2:F:61:THR:HG21	1.90	0.52
2:F:221:PRO:HB2	2:F:222:PRO:HD2	1.92	0.52
3:G:221:ALA:O	3:G:225:ILE:HG13	2.10	0.52
1:C:313:LEU:C	1:C:313:LEU:HD23	2.35	0.52
1:C:416:THR:HG22	1:C:440:LEU:HD11	1.91	0.52
1:C:444:PHE:CA	1:C:444:PHE:CD2	2.93	0.52
2:E:87:VAL:HG21	2:E:116:ASP:OD2	2.10	0.52
2:E:361:GLU:O	2:E:362:GLU:C	2.51	0.52
3:G:72:PRO:HG2	3:G:166:ASP:OD2	2.09	0.52
3:G:80:VAL:HG11	3:G:117:VAL:HG22	1.92	0.52
1:B:52:LEU:CG	1:B:95:MSE:HE3	2.40	0.52
1:C:496:LYS:N	1:C:496:LYS:HD2	2.25	0.52
2:D:94:ARG:HH11	2:D:106:GLU:HB2	1.74	0.52
2:D:280:THR:HG23	2:D:284:GLU:CD	2.35	0.52
2:E:150:LYS:HD2	2:E:246:ASP:OD1	2.10	0.52
2:F:237:GLU:OE2	2:F:291:ARG:CG	2.58	0.52
3:G:103:ILE:HG22	3:G:104:GLN:N	2.24	0.52
1:A:80:THR:C	1:A:82:ILE:H	2.17	0.52
2:D:32:ILE:HD11	2:D:76:VAL:HG22	1.92	0.52
2:F:258:THR:OG1	2:F:285:MSE:HE2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:20:ILE:HD13	4:H:119:ALA:CB	2.39	0.52
1:A:139:ARG:NH1	1:A:302:ALA:CB	2.73	0.51
1:A:180:ILE:O	1:A:184:ILE:HG13	2.10	0.51
1:A:275:LEU:HD21	1:A:281:PRO:HB3	1.92	0.51
1:A:276:LEU:C	1:A:278:ARG:H	2.17	0.51
1:A:371:GLN:O	1:A:376:LYS:HE3	2.10	0.51
1:C:354:ARG:CB	1:C:355:PRO:HD3	2.40	0.51
1:C:431:GLU:HB3	1:C:472:LEU:O	2.10	0.51
2:F:227:ARG:CD	2:F:230:LEU:HD12	2.41	0.51
3:G:216:LEU:HG	4:H:67:PHE:CZ	2.45	0.51
1:B:262:ASP:C	1:B:264:SER:N	2.67	0.51
1:B:372:ILE:HD11	1:B:434:VAL:CG1	2.40	0.51
1:C:209:VAL:HA	1:C:212:LEU:HD12	1.91	0.51
2:D:138:GLY:HA2	2:D:428:VAL:O	2.10	0.51
2:E:144:LEU:CD1	2:E:367:ALA:HB2	2.40	0.51
2:E:145:LEU:HD22	2:E:371:GLN:CG	2.40	0.51
2:E:238:TYR:CE1	2:E:242:GLU:HG2	2.46	0.51
2:F:32:ILE:HG12	2:F:76:VAL:HG22	1.92	0.51
1:A:207:THR:O	1:A:211:THR:HG22	2.10	0.51
1:B:345:GLN:HB2	1:B:348:LEU:HB2	1.93	0.51
1:A:283:ARG:HH22	2:E:275:VAL:HG12	1.76	0.51
2:F:140:LYS:N	2:F:412:GLN:OE1	2.44	0.51
1:A:131:SER:HB3	1:A:300:ARG:NH2	2.25	0.51
1:B:328:ALA:HB3	1:B:331:PRO:CG	2.41	0.51
1:C:206:ARG:HA	1:C:209:VAL:HG12	1.93	0.51
1:B:170:ASP:O	1:B:173:THR:HG23	2.10	0.51
2:D:264:VAL:O	2:D:265:SER:C	2.54	0.51
2:D:377:TYR:HE1	2:D:400:VAL:HG13	1.73	0.51
2:D:401:HIS:NE2	2:D:405:ARG:NH2	2.57	0.51
2:E:347:LEU:HD13	2:E:375:GLN:OE1	2.10	0.51
3:G:72:PRO:HG2	3:G:73:VAL:H	1.75	0.51
1:A:322:GLN:C	1:A:324:GLY:H	2.19	0.51
1:A:400:SER:OG	1:A:400:SER:CA	2.58	0.51
1:C:183:ILE:HG23	1:C:193:SER:OG	2.11	0.51
1:C:262:ASP:OD2	1:C:264:SER:HB2	2.11	0.51
2:D:30:LEU:HD23	2:D:78:ASP:HA	1.92	0.51
2:E:48:LEU:HB3	2:E:61:THR:OG1	2.10	0.51
2:E:370:VAL:HG21	2:E:437:PHE:HD2	1.75	0.51
1:A:415:ARG:O	1:A:418:GLU:HB2	2.11	0.51
1:C:474:HIS:CA	1:C:477:THR:HG22	2.40	0.51
2:F:225:ARG:HA	2:F:228:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:HD21	1:A:245:MSE:HE2	1.93	0.51
2:E:254:ILE:O	2:E:254:ILE:HG12	2.11	0.51
2:E:415:HIS:HD2	2:E:425:GLY:HA3	1.75	0.51
3:G:175:TYR:HE1	3:G:178:ALA:O	1.94	0.51
4:H:62:ALA:O	4:H:82:ALA:HA	2.11	0.51
4:H:83:GLU:O	4:H:84:ARG:C	2.53	0.51
4:H:89:ASP:C	4:H:91:LEU:H	2.17	0.51
1:A:331:PRO:O	1:A:335:ILE:HG13	2.10	0.51
1:B:195:TYR:CE1	1:B:259:VAL:CG1	2.93	0.51
1:B:491:ILE:O	1:B:494:PHE:N	2.33	0.51
1:C:32:ILE:HG22	1:C:32:ILE:O	2.10	0.51
2:E:96:PHE:CG	2:E:235:MSE:HE1	2.45	0.51
2:F:48:LEU:HD23	2:F:63:ALA:HA	1.91	0.51
1:A:345:GLN:HB3	1:A:348:LEU:HD23	1.92	0.50
1:B:161:ARG:NH1	1:B:191:MSE:SE	2.94	0.50
1:B:299:GLU:OE1	2:F:192:THR:HB	2.11	0.50
1:C:250:MSE:HG2	1:C:304:LEU:CD1	2.39	0.50
1:C:368:GLY:O	1:C:376:LYS:HE2	2.11	0.50
1:C:415:ARG:HG2	1:C:445:LEU:HD22	1.93	0.50
1:C:445:LEU:HG	1:C:456:PHE:CD1	2.47	0.50
2:D:4:GLY:O	2:D:76:VAL:N	2.38	0.50
2:D:429:PRO:HG2	2:D:432:GLU:HG2	1.92	0.50
1:A:172:GLN:HA	5:A:700:SO4:O4	2.10	0.50
1:B:66:LEU:HD23	1:B:71:VAL:HG13	1.92	0.50
1:B:161:ARG:HH12	1:B:191:MSE:SE	2.44	0.50
1:C:446:ASP:C	1:C:448:ILE:H	2.19	0.50
1:C:476:ARG:O	1:C:479:LYS:HG2	2.09	0.50
2:D:166:VAL:HG11	2:D:414:PHE:HD1	1.76	0.50
1:A:157:VAL:HG21	1:A:362:SER:HB3	1.94	0.50
2:E:84:SER:HA	2:E:116:ASP:O	2.11	0.50
2:E:172:ILE:HD12	2:E:202:MSE:CE	2.41	0.50
2:E:189:GLY:O	2:E:218:MSE:HE3	2.11	0.50
2:F:195:GLY:HA2	2:F:215:PHE:CE2	2.46	0.50
1:A:44:LEU:HD22	1:A:47:VAL:CG1	2.42	0.50
1:C:235:LEU:H	1:C:235:LEU:CD1	2.24	0.50
2:D:262:SER:CA	2:D:278:GLN:OE1	2.60	0.50
2:F:261:GLY:O	2:F:264:VAL:HG22	2.11	0.50
3:G:21:THR:HG21	3:G:247:ALA:HB3	1.92	0.50
4:H:6:VAL:HG12	4:H:18:ASP:O	2.10	0.50
1:C:74:VAL:CG1	1:C:233:PRO:HB3	2.41	0.50
1:C:460:PHE:CE2	1:C:464:LEU:HD11	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:153:LYS:N	2:D:153:LYS:CD	2.74	0.50
2:D:178:GLU:HG3	2:D:427:TYR:CZ	2.46	0.50
2:F:458:ARG:HG3	2:F:461:GLU:HG3	1.93	0.50
3:G:96:LEU:HG	3:G:126:PHE:CE1	2.44	0.50
1:B:262:ASP:C	1:B:264:SER:H	2.18	0.50
2:D:30:LEU:HB3	2:D:76:VAL:CG1	2.40	0.50
2:D:31:LYS:HZ3	2:D:47:THR:CG2	2.24	0.50
2:E:130:THR:HG23	2:E:131:GLU:N	2.27	0.50
2:F:44:ILE:HG21	2:F:70:LEU:HD21	1.93	0.50
3:G:123:LEU:HD23	3:G:123:LEU:C	2.37	0.50
1:A:292:TYR:CE2	1:A:296:ARG:HD3	2.47	0.50
1:B:33:GLN:OE1	1:B:40:ARG:NH2	2.45	0.50
2:E:309:PRO:O	2:E:311:ASP:N	2.45	0.50
2:F:391:GLU:CD	3:G:87:LEU:CD1	2.85	0.50
1:A:151:LYS:HE3	1:A:428:ILE:HD12	1.94	0.50
1:A:455:ARG:NH2	1:A:458:LYS:NZ	2.60	0.50
1:C:257:LEU:C	1:C:257:LEU:CD2	2.83	0.50
2:D:31:LYS:CE	2:D:47:THR:HG22	2.41	0.50
3:G:77:GLY:HA3	3:G:165:PHE:CZ	2.47	0.50
4:H:39:ILE:HD12	4:H:39:ILE:O	2.12	0.50
2:F:71:ILE:HG22	2:F:72:ARG:N	2.27	0.50
3:G:102:THR:O	3:G:107:HIS:HB2	2.12	0.50
3:G:242:THR:O	3:G:245:LYS:N	2.28	0.50
1:B:44:LEU:HB3	1:B:47:VAL:HG11	1.93	0.49
1:B:453:VAL:HG12	1:B:454:ARG:N	2.27	0.49
2:D:264:VAL:O	2:D:267:LEU:N	2.45	0.49
2:D:289:GLN:NE2	2:D:292:ILE:HD12	2.27	0.49
2:E:26:ILE:O	2:E:27:TYR:HB2	2.11	0.49
2:E:414:PHE:O	2:E:417:ALA:HB3	2.12	0.49
2:F:5:ARG:HA	2:F:74:MSE:O	2.12	0.49
1:A:151:LYS:HZ1	1:A:422:GLN:HB2	1.77	0.49
1:C:208:VAL:O	1:C:211:THR:HG22	2.12	0.49
2:E:226:MSE:HE3	2:E:227:ARG:NE	2.26	0.49
2:F:190:GLU:CG	2:F:191:ARG:H	2.05	0.49
3:G:96:LEU:CD2	3:G:125:PHE:CB	2.90	0.49
1:A:145:PRO:O	1:A:161:ARG:HG3	2.12	0.49
2:D:413:ASN:N	2:D:413:ASN:OD1	2.45	0.49
2:E:440:ILE:HD11	2:E:453:PHE:CD2	2.46	0.49
3:G:100:TYR:CD1	3:G:129:ARG:HD2	2.47	0.49
1:B:262:ASP:OD2	1:B:264:SER:HB2	2.13	0.49
2:D:51:ALA:C	2:D:52:LEU:HD23	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:290:GLU:O	2:F:293:THR:HG22	2.12	0.49
1:C:243:VAL:HG23	1:C:244:ALA:N	2.28	0.49
1:C:398:PHE:N	1:C:398:PHE:CD1	2.80	0.49
1:C:431:GLU:O	1:C:434:VAL:HG22	2.12	0.49
2:E:94:ARG:NH1	2:E:106:GLU:CB	2.70	0.49
2:E:428:VAL:HG23	2:E:432:GLU:HB3	1.94	0.49
3:G:96:LEU:HD23	3:G:125:PHE:CB	2.42	0.49
1:A:246:GLY:O	1:A:247:GLU:C	2.56	0.49
1:B:167:ILE:HD12	1:B:318:PHE:CE2	2.44	0.49
1:B:452:ASP:C	1:B:455:ARG:HB2	2.38	0.49
2:F:458:ARG:HH11	2:F:460:GLU:HB2	1.76	0.49
3:G:95:VAL:HG23	3:G:96:LEU:N	2.27	0.49
1:A:241:ALA:O	1:A:245:MSE:HG3	2.13	0.49
1:B:108:VAL:HB	1:B:112:GLY:C	2.37	0.49
1:B:206:ARG:O	1:B:209:VAL:HG12	2.12	0.49
2:D:414:PHE:CA	2:D:414:PHE:CD2	2.95	0.49
2:E:277:TYR:HD2	2:E:281:LEU:HD22	1.78	0.49
1:A:444:PHE:HE1	1:A:490:ALA:HA	1.77	0.49
1:B:270:TYR:CD2	1:B:293:LEU:HD22	2.48	0.49
1:B:492:GLU:CA	1:B:492:GLU:O	2.60	0.49
1:C:446:ASP:C	1:C:448:ILE:N	2.70	0.49
2:D:332:GLU:HG3	2:D:334:LYS:H	1.78	0.49
2:E:359:VAL:HB	2:E:363:HIS:HB3	1.95	0.49
2:E:362:GLU:HG3	2:E:434:VAL:HG11	1.95	0.49
1:A:206:ARG:HA	1:A:209:VAL:HG12	1.95	0.49
1:A:372:ILE:HB	1:A:479:LYS:HB3	1.93	0.49
1:A:396:ALA:C	1:A:399:GLY:H	2.21	0.49
1:A:151:LYS:NZ	1:A:151:LYS:HB2	2.28	0.49
1:B:295:SER:O	1:B:299:GLU:HB2	2.12	0.49
1:C:95:MSE:HE2	1:C:96:GLU:N	2.22	0.49
1:C:171:ARG:HD3	2:F:322:PHE:HB3	1.94	0.49
1:C:257:LEU:HD23	1:C:258:VAL:N	2.27	0.49
2:F:31:LYS:HD3	2:F:79:THR:CG2	2.43	0.49
2:F:188:VAL:HG13	2:F:228:VAL:HG23	1.95	0.49
2:F:250:PHE:HE1	2:F:303:ILE:HD12	1.76	0.49
2:F:397:LYS:NZ	2:F:397:LYS:HB3	2.28	0.49
2:F:465:LYS:O	2:F:469:MSE:HG2	2.13	0.49
1:A:109:ASN:C	1:A:109:ASN:ND2	2.63	0.48
1:A:408:ALA:O	1:A:411:ALA:HB3	2.12	0.48
1:B:355:PRO:HB2	1:B:357:ILE:HG12	1.95	0.48
1:C:95:MSE:SE	1:C:237:LEU:HD21	2.63	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ILE:O	1:C:157:VAL:O	2.30	0.48
2:D:138:GLY:HA3	2:D:427:TYR:CD1	2.48	0.48
2:D:401:HIS:NE2	2:D:405:ARG:NH1	2.55	0.48
2:E:47:THR:C	2:E:48:LEU:HD23	2.38	0.48
4:H:102:ARG:HH11	4:H:102:ARG:HG3	1.78	0.48
1:C:139:ARG:CZ	1:C:302:ALA:HB2	2.42	0.48
1:C:397:GLN:C	1:C:399:GLY:N	2.69	0.48
1:C:434:VAL:C	1:C:437:ILE:HG22	2.38	0.48
2:E:20:ASN:O	2:E:21:GLY:C	2.56	0.48
2:E:412:GLN:HG2	2:E:413:ASN:N	2.28	0.48
2:F:445:TYR:HB3	2:F:453:PHE:HZ	1.77	0.48
1:C:196:VAL:HG13	1:C:224:VAL:HB	1.95	0.48
1:C:346:SER:C	1:C:348:LEU:N	2.66	0.48
1:C:413:GLY:O	1:C:416:THR:OG1	2.31	0.48
2:D:54:LEU:HD11	2:D:60:ARG:HE	1.78	0.48
2:E:258:THR:HG23	2:E:285:MSE:HE2	1.94	0.48
1:A:385:ASP:OD2	1:A:412:ARG:HD2	2.14	0.48
1:B:159:ILE:HG23	1:B:163:GLN:OE1	2.13	0.48
1:B:217:ALA:HA	1:B:220:TYR:CE2	2.49	0.48
1:C:288:GLY:C	2:D:263:GLU:HG3	2.38	0.48
2:D:13:VAL:HG21	2:D:60:ARG:HD3	1.95	0.48
2:D:31:LYS:HZ3	2:D:47:THR:HG21	1.77	0.48
2:D:51:ALA:O	2:D:52:LEU:HD23	2.12	0.48
2:E:29:ALA:HB3	2:E:79:THR:OG1	2.13	0.48
2:E:82:PRO:HG2	2:E:117:PRO:HB2	1.95	0.48
2:E:309:PRO:HG2	2:E:318:PRO:HD3	1.95	0.48
2:F:348:ALA:O	2:F:350:THR:HG23	2.13	0.48
1:B:491:ILE:C	1:B:493:ALA:N	2.72	0.48
1:C:64:LEU:CD1	1:C:74:VAL:HG21	2.44	0.48
1:C:117:GLY:HA3	2:F:126:GLU:OE2	2.14	0.48
1:C:440:LEU:HD23	1:C:441:THR:H	1.78	0.48
2:D:16:VAL:HB	2:D:59:VAL:HG23	1.96	0.48
2:D:172:ILE:HD12	2:D:202:MSE:HE3	1.96	0.48
2:E:273:SER:HB3	2:E:277:TYR:O	2.14	0.48
2:F:156:LEU:HD13	2:F:167:LEU:HD23	1.94	0.48
1:A:30:THR:CG2	1:A:85:GLY:HA2	2.43	0.48
1:A:298:LEU:HD12	1:A:298:LEU:N	2.28	0.48
1:B:438:TYR:C	1:B:438:TYR:CD2	2.89	0.48
1:B:456:PHE:CE2	1:B:460:PHE:HB2	2.49	0.48
2:D:30:LEU:HB3	2:D:76:VAL:HG12	1.94	0.48
2:E:342:PRO:HB2	2:E:344:VAL:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:410:LEU:HD23	2:E:437:PHE:HZ	1.79	0.48
2:F:366:VAL:O	2:F:370:VAL:HG23	2.13	0.48
4:H:22:MSE:HG3	4:H:34:ILE:O	2.13	0.48
1:A:46:ASN:HB3	1:A:90:ARG:NH1	2.29	0.48
1:A:424:LEU:HD23	1:A:425:HIS:CG	2.49	0.48
2:D:64:MSE:HE3	2:D:224:ALA:HA	1.94	0.48
2:E:219:ASN:C	2:E:219:ASN:HD22	2.21	0.48
2:E:231:THR:O	2:E:235:MSE:HG3	2.13	0.48
1:B:154:ASP:C	1:B:375:MSE:HE3	2.38	0.48
1:C:161:ARG:HH12	1:C:191:MSE:HG2	1.78	0.48
1:C:197:ALA:HB1	1:C:200:GLN:CG	2.44	0.48
2:D:191:ARG:N	2:D:218:MSE:HE3	2.29	0.48
2:E:456:VAL:HG21	2:E:462:VAL:HG22	1.95	0.48
3:G:14:THR:OG1	3:G:254:LEU:HD23	2.14	0.48
1:A:62:MSE:O	1:A:73:ILE:HG23	2.14	0.48
1:C:326:ILE:HD11	1:C:343:PHE:CZ	2.49	0.48
2:D:119:HIS:HE1	2:D:227:ARG:NH2	2.12	0.48
2:E:53:HIS:CD2	2:E:59:VAL:CG1	2.88	0.48
2:E:309:PRO:O	2:E:310:ALA:C	2.54	0.48
2:F:163:GLY:HA2	6:F:600:ADP:O2A	2.14	0.48
2:F:253:ASN:N	2:F:305:ALA:HB3	2.13	0.48
3:G:42:PHE:HD1	4:H:11:PRO:HA	1.79	0.48
3:G:78:TYR:CE1	3:G:171:TYR:OH	2.65	0.48
1:A:286:TYR:CD2	1:A:290:ILE:HG12	2.49	0.48
1:A:299:GLU:HG3	2:E:219:ASN:HB3	1.95	0.48
2:D:240:ARG:HG3	2:D:299:SER:N	2.28	0.48
2:E:130:THR:HG23	2:E:131:GLU:H	1.79	0.48
2:E:408:PHE:O	2:E:411:SER:OG	2.28	0.48
2:F:6:VAL:HG23	2:F:76:VAL:HG21	1.96	0.48
3:G:80:VAL:HG21	3:G:99:VAL:HG21	1.95	0.48
1:A:432:LYS:O	1:A:461:TYR:HE2	1.97	0.47
1:C:440:LEU:HD23	1:C:441:THR:N	2.29	0.47
1:C:457:GLU:O	1:C:458:LYS:C	2.57	0.47
2:E:292:ILE:O	2:E:293:THR:HG23	2.13	0.47
2:F:144:LEU:HD21	2:F:370:VAL:HG21	1.95	0.47
2:F:391:GLU:CD	3:G:87:LEU:HD11	2.38	0.47
3:G:80:VAL:O	3:G:80:VAL:HG13	2.14	0.47
3:G:85:ARG:HB3	4:H:113:PHE:CE2	2.49	0.47
4:H:39:ILE:HD12	4:H:39:ILE:C	2.38	0.47
1:A:109:ASN:ND2	1:A:111:LEU:H	2.11	0.47
1:A:167:ILE:O	1:A:167:ILE:HG13	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:PHE:C	1:A:352:GLY:N	2.71	0.47
1:C:35:GLY:HA3	2:F:52:LEU:HD22	1.95	0.47
1:C:352:GLY:O	1:C:353:VAL:C	2.56	0.47
4:H:68:LEU:HG	4:H:70:VAL:HG23	1.94	0.47
4:H:88:ILE:HG23	4:H:90:VAL:N	2.28	0.47
4:H:91:LEU:O	4:H:92:ARG:C	2.55	0.47
1:A:38:ILE:HD11	1:A:74:VAL:HG12	1.95	0.47
1:A:48:MSE:HA	2:E:71:ILE:HG12	1.95	0.47
1:A:99:VAL:HG21	1:A:127:ARG:CB	2.45	0.47
1:A:146:LEU:HD21	1:A:257:LEU:HD12	1.96	0.47
1:A:429:PRO:HG2	1:A:432:LYS:HG2	1.96	0.47
1:B:33:GLN:CD	1:B:40:ARG:NH2	2.73	0.47
1:C:292:TYR:HB2	2:D:263:GLU:OE2	2.14	0.47
2:D:377:TYR:CD1	2:D:400:VAL:HG22	2.44	0.47
2:E:49:GLU:N	2:E:61:THR:OG1	2.46	0.47
2:E:88:GLY:HA2	2:E:238:TYR:CE2	2.48	0.47
2:E:162:VAL:CG1	2:E:331:LEU:HB3	2.42	0.47
2:F:418:GLU:O	2:F:422:GLY:N	2.47	0.47
1:A:53:VAL:HG12	1:A:88:VAL:HG12	1.94	0.47
1:A:443:GLY:C	1:A:445:LEU:H	2.21	0.47
1:B:217:ALA:HA	1:B:220:TYR:CZ	2.49	0.47
1:B:450:VAL:HA	1:B:453:VAL:HG23	1.96	0.47
1:C:108:VAL:HA	1:C:114:PRO:HA	1.96	0.47
1:C:167:ILE:HD11	1:C:318:PHE:CE2	2.49	0.47
1:C:345:GLN:HB3	1:C:347:ASP:HB3	1.97	0.47
1:C:382:LEU:CG	1:C:437:ILE:HD11	2.42	0.47
2:D:355:ALA:HB1	2:D:356:PRO:HD2	1.97	0.47
2:E:118:ILE:HG13	2:E:119:HIS:N	2.29	0.47
2:E:380:LEU:HA	2:E:383:ILE:HG22	1.96	0.47
2:E:429:PRO:HG2	2:E:432:GLU:HG2	1.96	0.47
2:F:54:LEU:HD21	2:F:60:ARG:HB2	1.97	0.47
2:F:249:LEU:HD23	2:F:292:ILE:CG2	2.42	0.47
3:G:46:MSE:CE	3:G:223:SER:O	2.62	0.47
3:G:52:VAL:C	3:G:54:ALA:H	2.22	0.47
1:A:64:LEU:CD1	1:A:273:LEU:HD21	2.45	0.47
1:A:99:VAL:CG1	1:A:248:TYR:HB2	2.45	0.47
1:A:431:GLU:H	1:A:431:GLU:CD	2.22	0.47
1:C:269:ALA:O	1:C:272:GLU:HB3	2.14	0.47
1:C:344:LEU:HA	1:C:356:ALA:O	2.13	0.47
2:D:318:PRO:O	2:D:322:PHE:CD1	2.65	0.47
2:E:140:LYS:HG2	2:E:428:VAL:HG11	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:145:LEU:HD22	2:F:371:GLN:HG3	1.96	0.47
3:G:90:ALA:O	3:G:91:TYR:C	2.58	0.47
3:G:235:SER:O	3:G:236:GLU:C	2.57	0.47
4:H:93:ALA:O	4:H:97:LYS:N	2.48	0.47
1:C:199:GLY:HA3	1:C:265:LYS:HD3	1.95	0.47
2:D:214:VAL:HG12	2:D:228:VAL:CG1	2.44	0.47
2:D:307:TYR:O	2:D:307:TYR:CD2	2.65	0.47
2:E:38:ASN:HD22	2:E:38:ASN:C	2.21	0.47
2:F:172:ILE:HD11	2:F:185:PHE:CD2	2.49	0.47
3:G:236:GLU:O	3:G:237:HIS:C	2.57	0.47
1:A:96:GLU:CB	1:A:128:PRO:HA	2.45	0.47
1:A:375:MSE:HG2	1:A:434:VAL:CG1	2.41	0.47
1:B:55:PHE:CZ	1:B:73:ILE:CD1	2.97	0.47
1:B:165:GLU:OE2	1:B:341:GLN:N	2.48	0.47
1:B:449:PRO:O	1:B:453:VAL:HG23	2.15	0.47
1:C:44:LEU:O	1:C:47:VAL:HG22	2.14	0.47
1:C:430:VAL:HA	1:C:433:GLN:HE21	1.79	0.47
2:E:17:LYS:CA	2:E:17:LYS:O	2.62	0.47
2:E:156:LEU:HD21	2:E:164:LYS:CG	2.44	0.47
2:E:277:TYR:CD2	2:E:281:LEU:HD22	2.50	0.47
2:E:285:MSE:HG2	2:E:320:THR:HG22	1.97	0.47
2:F:222:PRO:O	2:F:226:MSE:HG2	2.15	0.47
3:G:229:LEU:O	3:G:230:LEU:C	2.58	0.47
1:C:474:HIS:C	1:C:476:ARG:N	2.72	0.47
1:A:249:PHE:HB2	1:A:256:VAL:CG2	2.45	0.47
1:B:40:ARG:HA	1:B:71:VAL:O	2.14	0.47
1:B:301:ALA:HB1	1:B:313:LEU:O	2.15	0.47
1:B:315:ALA:C	1:B:317:PRO:HD3	2.40	0.47
1:C:48:MSE:SE	2:D:42:VAL:HG23	2.65	0.47
1:C:94:ILE:O	1:C:95:MSE:C	2.57	0.47
2:D:4:GLY:O	2:D:75:GLU:HA	2.15	0.47
3:G:80:VAL:HG13	3:G:117:VAL:HG13	1.97	0.47
1:A:315:ALA:C	1:A:317:PRO:HD3	2.40	0.47
1:A:480:ASP:O	1:A:481:LEU:CD2	2.62	0.47
1:B:31:VAL:HB	1:B:85:GLY:H	1.80	0.47
1:C:140:ARG:NH1	1:C:306:ASP:OD2	2.48	0.47
1:C:142:VAL:O	1:C:142:VAL:HG23	2.14	0.47
1:C:222:ILE:HG22	1:C:223:VAL:N	2.30	0.47
2:D:157:PHE:HE1	2:D:306:ILE:HB	1.79	0.47
1:A:126:THR:HG22	1:A:127:ARG:N	2.30	0.46
1:C:291:PHE:CZ	2:D:256:ARG:NH1	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:44:ILE:HG21	2:F:70:LEU:CD2	2.45	0.46
2:F:233:LEU:CD2	2:F:291:ARG:HD2	2.39	0.46
3:G:32:LEU:HD21	3:G:238:ALA:HB2	1.96	0.46
3:G:157:VAL:O	3:G:161:ALA:HB2	2.15	0.46
4:H:110:ASP:OD1	4:H:114:LYS:HE3	2.15	0.46
1:A:434:VAL:CA	1:A:437:ILE:HG22	2.45	0.46
1:A:474:HIS:CE1	1:A:478:THR:HG21	2.50	0.46
1:B:66:LEU:CD2	1:B:71:VAL:HG13	2.45	0.46
1:C:235:LEU:HD12	1:C:235:LEU:N	2.28	0.46
2:D:265:SER:OG	2:D:270:ARG:HB2	2.15	0.46
1:A:32:ILE:HG22	1:A:33:GLN:CG	2.28	0.46
1:A:62:MSE:CE	1:A:95:MSE:CB	2.90	0.46
1:A:271:ARG:HD2	1:A:285:ALA:HB3	1.98	0.46
1:B:166:LEU:HD11	1:B:319:VAL:HG23	1.97	0.46
1:B:337:ILE:HG12	2:F:218:MSE:SE	2.66	0.46
2:E:162:VAL:O	2:E:162:VAL:HG12	2.16	0.46
2:E:266:ALA:O	2:E:269:GLY:N	2.40	0.46
1:A:283:ARG:HD2	1:A:329:TYR:CD1	2.51	0.46
1:B:116:ASP:HA	2:E:125:PHE:CD2	2.47	0.46
1:B:171:ARG:O	1:B:172:GLN:CB	2.63	0.46
1:C:124:THR:HG23	1:C:125:GLU:N	2.29	0.46
2:D:317:ALA:HB3	2:D:318:PRO:CD	2.45	0.46
2:D:411:SER:O	2:D:412:GLN:HB2	2.15	0.46
2:E:95:VAL:O	2:E:102:PRO:HA	2.15	0.46
2:E:310:ALA:O	2:E:312:ASP:N	2.48	0.46
1:A:95:MSE:SE	1:A:237:LEU:HD21	2.66	0.46
1:A:210:GLU:O	1:A:213:ARG:HB3	2.15	0.46
1:A:298:LEU:N	1:A:298:LEU:CD1	2.78	0.46
1:B:453:VAL:O	1:B:454:ARG:C	2.58	0.46
1:C:97:VAL:HB	1:C:98:PRO:HD2	1.98	0.46
2:D:190:GLU:C	2:D:217:GLN:NE2	2.73	0.46
2:F:290:GLU:O	2:F:293:THR:CG2	2.63	0.46
3:G:165:PHE:CD2	3:G:168:LEU:HD21	2.51	0.46
1:A:170:ASP:O	1:A:173:THR:CG2	2.54	0.46
1:C:195:TYR:O	1:C:223:VAL:HA	2.16	0.46
1:C:316:LEU:N	1:C:317:PRO:HD3	2.30	0.46
2:D:392:LEU:C	2:D:394:ASP:H	2.24	0.46
3:G:179:ILE:HD12	3:G:238:ALA:O	2.16	0.46
1:A:103:LEU:CD1	1:A:123:THR:HG21	2.46	0.46
1:A:292:TYR:O	1:A:296:ARG:HG2	2.15	0.46
1:B:231:PRO:HD2	1:B:234:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:482:PRO:C	1:C:484:GLU:N	2.68	0.46
2:D:64:MSE:HE3	2:D:98:VAL:HG11	1.98	0.46
2:D:98:VAL:HG21	2:D:224:ALA:CB	2.45	0.46
2:D:402:ARG:O	2:D:406:ILE:HG13	2.15	0.46
2:D:449:PRO:O	2:D:450:GLU:C	2.58	0.46
2:F:83:ILE:HB	2:F:118:ILE:CD1	2.46	0.46
2:F:409:PHE:HD2	2:F:437:PHE:CE1	2.34	0.46
1:A:144:GLU:HG2	1:A:161:ARG:HD2	1.98	0.46
1:A:243:VAL:HG11	1:A:260:TYR:OH	2.13	0.46
1:A:468:GLY:O	1:A:471:LEU:N	2.48	0.46
1:B:36:ASP:C	1:B:38:ILE:H	2.23	0.46
1:B:286:TYR:CD2	1:B:290:ILE:HG12	2.51	0.46
1:C:388:ALA:O	1:C:391:GLU:N	2.48	0.46
1:C:474:HIS:CD2	1:C:474:HIS:O	2.63	0.46
2:D:294:SER:HB3	2:D:299:SER:CB	2.44	0.46
2:D:451:ASP:OD1	2:D:454:ARG:NH1	2.45	0.46
2:F:294:SER:CB	2:F:299:SER:HA	2.46	0.46
3:G:114:ALA:O	3:G:115:ILE:HG12	2.16	0.46
4:H:98:GLU:O	4:H:102:ARG:HD2	2.15	0.46
1:A:62:MSE:HE3	1:A:95:MSE:CG	2.45	0.46
1:A:148:THR:CG2	1:A:150:ILE:HG13	2.37	0.46
1:A:330:ILE:HB	1:A:331:PRO:HD3	1.97	0.46
1:A:333:ASN:O	1:A:337:ILE:HG13	2.15	0.46
1:C:343:PHE:CD2	1:C:344:LEU:N	2.84	0.46
1:C:435:LEU:O	1:C:438:TYR:HB3	2.15	0.46
2:D:97:ASN:O	2:D:98:VAL:C	2.58	0.46
2:E:11:GLY:HA3	2:E:12:PRO:HD2	1.70	0.46
3:G:101:GLN:O	3:G:103:ILE:N	2.49	0.46
3:G:118:ILE:N	3:G:118:ILE:HD12	2.31	0.46
1:A:40:ARG:CZ	1:A:40:ARG:CG	2.94	0.46
1:A:262:ASP:OD1	1:A:265:LYS:CD	2.64	0.46
1:C:62:MSE:HE3	1:C:95:MSE:HB2	1.98	0.46
1:C:146:LEU:C	1:C:146:LEU:HD23	2.41	0.46
1:C:230:GLN:HB3	1:C:231:PRO:HD2	1.98	0.46
2:E:145:LEU:HD13	2:E:346:PRO:O	2.15	0.46
2:E:258:THR:HG21	2:E:285:MSE:HE2	1.96	0.46
3:G:219:GLN:HE22	4:H:66:GLY:CA	2.29	0.46
1:A:479:LYS:HD2	1:A:479:LYS:N	2.30	0.45
1:B:199:GLY:CA	1:B:265:LYS:HD3	2.41	0.45
1:C:395:PHE:O	1:C:396:ALA:C	2.55	0.45
2:D:163:GLY:O	2:D:164:LYS:C	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:429:PRO:HG2	2:D:432:GLU:CG	2.46	0.45
2:E:169:GLN:CG	2:E:207:VAL:HG21	2.46	0.45
2:E:318:PRO:O	2:E:321:THR:N	2.49	0.45
2:F:134:ILE:HG22	2:F:135:LEU:N	2.32	0.45
3:G:43:VAL:N	3:G:44:PRO:CD	2.79	0.45
1:A:350:PHE:HE2	2:D:350:THR:HG21	1.81	0.45
2:D:88:GLY:C	2:D:90:VAL:H	2.24	0.45
2:E:46:LEU:HG	2:E:47:THR:N	2.31	0.45
3:G:42:PHE:HZ	3:G:46:MSE:HE2	1.82	0.45
3:G:101:GLN:C	3:G:103:ILE:H	2.25	0.45
1:A:435:LEU:HD13	1:A:464:LEU:HD13	1.98	0.45
1:B:201:LYS:O	1:B:205:VAL:HG23	2.16	0.45
1:B:372:ILE:HG13	1:B:374:ALA:H	1.81	0.45
1:C:303:LYS:NZ	1:C:310:GLY:O	2.49	0.45
1:A:166:LEU:HD12	1:A:166:LEU:C	2.41	0.45
1:B:283:ARG:HG2	1:B:284:GLU:N	2.30	0.45
1:B:489:LYS:O	1:B:493:ALA:N	2.50	0.45
2:D:401:HIS:HE1	2:D:446:ASP:HB3	1.75	0.45
2:F:221:PRO:CB	2:F:222:PRO:HD2	2.47	0.45
3:G:46:MSE:HE1	3:G:223:SER:C	2.41	0.45
4:H:5:HIS:O	4:H:74:LYS:HA	2.16	0.45
1:A:430:VAL:O	1:A:431:GLU:C	2.58	0.45
2:D:141:VAL:HG11	2:D:344:VAL:CB	2.42	0.45
2:F:188:VAL:HG13	2:F:228:VAL:CG2	2.45	0.45
2:F:253:ASN:C	2:F:255:PHE:N	2.75	0.45
3:G:83:SER:HB3	3:G:236:GLU:OE1	2.16	0.45
3:G:142:ASP:O	3:G:143:GLN:CB	2.65	0.45
4:H:104:LEU:C	4:H:106:SER:N	2.75	0.45
4:H:126:ARG:O	4:H:127:LEU:C	2.59	0.45
1:A:139:ARG:NE	2:E:192:THR:HG21	2.31	0.45
1:A:343:PHE:C	1:A:343:PHE:CD2	2.94	0.45
1:A:472:LEU:O	1:A:475:ILE:HB	2.16	0.45
1:B:96:GLU:OE1	1:B:126:THR:HG21	2.16	0.45
1:C:44:LEU:HD21	1:C:88:VAL:O	2.16	0.45
1:C:147:GLN:OE1	1:C:430:VAL:HG22	2.16	0.45
2:E:168:ILE:HG23	2:E:250:PHE:CD2	2.52	0.45
2:F:191:ARG:HA	2:F:218:MSE:HE3	1.98	0.45
4:H:97:LYS:C	4:H:99:ARG:N	2.74	0.45
1:A:147:GLN:OE1	1:A:430:VAL:HG22	2.17	0.45
1:A:157:VAL:HG11	1:A:342:ILE:HG12	1.98	0.45
1:A:440:LEU:HA	1:A:445:LEU:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:GLN:O	1:A:473:GLU:HG2	2.16	0.45
1:B:104:ILE:HG21	1:B:219:ASP:O	2.17	0.45
2:D:240:ARG:HG3	2:D:298:GLY:HA3	1.98	0.45
2:E:239:PHE:HB2	2:E:247:VAL:HG21	1.98	0.45
2:F:166:VAL:HG13	2:F:416:VAL:HG23	1.99	0.45
1:A:110:PRO:HB3	1:A:238:ALA:HA	1.99	0.45
1:B:295:SER:HA	1:B:337:ILE:HD13	1.98	0.45
1:B:343:PHE:C	1:B:343:PHE:CD2	2.93	0.45
2:D:88:GLY:C	2:D:90:VAL:N	2.75	0.45
2:D:112:ASP:OD1	2:D:112:ASP:N	2.48	0.45
1:A:278:ARG:CZ	3:G:284:LEU:HD13	2.47	0.45
1:B:333:ASN:O	1:B:336:SER:OG	2.35	0.45
2:D:396:ASP:O	2:D:400:VAL:HG23	2.16	0.45
2:D:437:PHE:O	2:D:438:LYS:C	2.58	0.45
3:G:80:VAL:CG2	3:G:99:VAL:HG21	2.47	0.45
1:A:322:GLN:C	1:A:324:GLY:N	2.73	0.45
1:B:195:TYR:CD1	1:B:259:VAL:HB	2.44	0.45
1:C:335:ILE:C	1:C:337:ILE:N	2.70	0.45
3:G:110:PRO:HG2	3:G:112:GLU:HB3	1.98	0.45
1:A:140:ARG:O	1:A:141:SER:C	2.60	0.44
1:A:445:LEU:HD21	1:A:453:VAL:HG13	1.98	0.44
1:C:168:ILE:HD11	1:C:321:THR:CG2	2.46	0.44
1:C:246:GLY:O	1:C:256:VAL:HG21	2.17	0.44
1:C:482:PRO:O	1:C:484:GLU:N	2.48	0.44
2:D:248:LEU:HB3	2:D:250:PHE:CE1	2.52	0.44
2:E:30:LEU:HB2	2:E:48:LEU:HB2	1.98	0.44
2:E:170:GLU:HG2	2:E:414:PHE:CE2	2.52	0.44
2:F:222:PRO:HB2	2:F:264:VAL:HG13	1.98	0.44
2:F:402:ARG:O	2:F:403:ALA:C	2.59	0.44
3:G:5:ARG:CB	3:G:5:ARG:NE	2.79	0.44
1:A:377:LYS:CG	1:A:378:VAL:H	2.29	0.44
1:B:236:PHE:HE1	1:B:293:LEU:CD1	2.29	0.44
2:F:145:LEU:HD22	2:F:371:GLN:CG	2.48	0.44
2:F:158:GLY:O	2:F:164:LYS:HD3	2.18	0.44
2:F:169:GLN:HB3	2:F:416:VAL:HG11	2.00	0.44
1:A:74:VAL:HG23	1:A:74:VAL:O	2.17	0.44
1:A:416:THR:HG22	1:A:440:LEU:CD1	2.48	0.44
1:B:179:ALA:HB1	1:B:259:VAL:HG21	2.00	0.44
1:C:417:VAL:HG23	1:C:418:GLU:N	2.32	0.44
1:C:431:GLU:HG2	1:C:473:GLU:CG	2.42	0.44
1:C:445:LEU:CD2	1:C:453:VAL:HG22	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:30:LEU:CD2	2:D:78:ASP:HA	2.47	0.44
2:D:189:GLY:HA2	2:D:217:GLN:C	2.43	0.44
2:E:144:LEU:HD11	2:E:367:ALA:HB2	1.99	0.44
2:F:202:MSE:HE3	2:F:207:VAL:HG23	2.00	0.44
3:G:221:ALA:O	3:G:222:GLU:C	2.60	0.44
4:H:132:MSE:O	4:H:133:LYS:CB	2.64	0.44
1:A:179:ALA:HB1	1:A:259:VAL:HG11	1.98	0.44
1:A:372:ILE:O	1:A:373:LYS:C	2.61	0.44
1:B:262:ASP:N	1:B:318:PHE:HB2	2.24	0.44
1:B:450:VAL:O	1:B:453:VAL:HB	2.17	0.44
1:B:472:LEU:HD23	1:B:472:LEU:C	2.42	0.44
1:C:343:PHE:HD2	1:C:344:LEU:N	2.15	0.44
1:C:343:PHE:HD1	1:C:361:LEU:HD12	1.82	0.44
2:E:2:THR:HB	2:E:22:HIS:HE1	1.80	0.44
2:E:141:VAL:HG23	2:E:410:LEU:O	2.18	0.44
2:E:457:GLY:HA3	2:E:461:GLU:OE2	2.17	0.44
3:G:220:TYR:O	3:G:224:LEU:HD12	2.18	0.44
1:A:429:PRO:HB2	1:A:431:GLU:OE1	2.18	0.44
1:A:440:LEU:HA	1:A:445:LEU:HB3	1.98	0.44
1:C:334:VAL:O	1:C:338:THR:HG23	2.17	0.44
2:D:31:LYS:HZ2	2:D:47:THR:CG2	2.29	0.44
2:E:16:VAL:CG1	2:E:18:PHE:CE1	3.01	0.44
2:E:185:PHE:CE2	2:E:198:LEU:CD2	3.00	0.44
2:E:249:LEU:O	2:E:302:SER:HA	2.17	0.44
2:F:148:TYR:CD2	2:F:154:ILE:CD1	3.00	0.44
2:F:274:ALA:O	2:F:275:VAL:HB	2.18	0.44
3:G:36:GLU:O	3:G:37:GLN:C	2.60	0.44
3:G:40:LYS:C	3:G:42:PHE:N	2.75	0.44
3:G:96:LEU:HD11	3:G:122:GLY:HA2	1.99	0.44
1:A:68:GLU:HG3	1:A:69:ASN:N	2.33	0.44
1:A:405:ALA:O	1:A:408:ALA:N	2.44	0.44
1:A:445:LEU:HD23	1:A:445:LEU:O	2.17	0.44
1:B:166:LEU:HB3	1:B:341:GLN:HB3	1.99	0.44
1:B:213:ARG:O	1:B:214:LYS:C	2.60	0.44
1:B:272:GLU:O	1:B:273:LEU:C	2.60	0.44
1:C:140:ARG:NH1	1:C:306:ASP:CG	2.76	0.44
1:C:250:MSE:C	1:C:252:LYS:N	2.75	0.44
2:E:213:MSE:HE2	2:E:215:PHE:CZ	2.53	0.44
2:E:270:ARG:HG3	2:E:270:ARG:HH11	1.81	0.44
2:F:6:VAL:HA	2:F:16:VAL:HA	1.99	0.44
2:F:30:LEU:HB3	2:F:76:VAL:CG1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:190:GLU:OE2	2:F:191:ARG:NH1	2.51	0.44
2:F:275:VAL:O	2:F:275:VAL:CG1	2.64	0.44
2:F:391:GLU:OE1	3:G:87:LEU:HD11	2.18	0.44
3:G:21:THR:CG2	3:G:247:ALA:HB3	2.47	0.44
1:A:157:VAL:O	1:A:157:VAL:HG12	2.18	0.44
1:C:403:ASP:O	1:C:406:THR:OG1	2.36	0.44
2:D:318:PRO:O	2:D:319:ALA:C	2.60	0.44
1:A:129:ILE:HG23	1:A:240:TYR:HB3	2.00	0.44
1:A:275:LEU:HD12	2:D:279:PRO:HB3	1.99	0.44
1:C:239:PRO:HG2	1:C:266:GLN:NE2	2.33	0.44
1:C:345:GLN:NE2	1:C:358:ASN:HD22	2.16	0.44
2:D:27:TYR:O	2:D:82:PRO:CB	2.63	0.44
2:E:35:LYS:CA	2:E:35:LYS:O	2.66	0.44
2:E:91:THR:HA	2:E:96:PHE:HZ	1.82	0.44
2:F:353:ALA:O	2:F:355:ALA:N	2.51	0.44
3:G:24:MSE:CE	4:H:116:ALA:HB1	2.47	0.44
3:G:166:ASP:OD1	3:G:167:GLU:CB	2.66	0.44
1:A:292:TYR:CD1	2:E:221:PRO:HA	2.53	0.44
1:A:355:PRO:HB2	1:A:357:ILE:CG1	2.47	0.44
1:B:32:ILE:CG1	1:B:41:ALA:HA	2.48	0.44
2:D:87:VAL:HG22	2:D:114:ARG:O	2.18	0.44
2:D:140:LYS:CG	2:D:428:VAL:HG11	2.48	0.44
2:D:146:ALA:N	2:D:147:PRO:HD3	2.33	0.44
2:D:214:VAL:HG11	2:D:228:VAL:HG13	1.98	0.44
2:D:294:SER:HA	2:D:299:SER:HA	1.99	0.44
2:E:250:PHE:CZ	2:E:303:ILE:HD12	2.53	0.44
1:B:274:SER:OG	1:B:287:PRO:HG3	2.18	0.43
1:B:424:LEU:O	1:B:425:HIS:HB2	2.18	0.43
1:C:62:MSE:CE	1:C:95:MSE:HB2	2.48	0.43
1:C:436:ILE:C	1:C:438:TYR:H	2.26	0.43
2:D:166:VAL:HG13	2:D:416:VAL:CG2	2.48	0.43
2:D:247:VAL:CG1	2:D:248:LEU:N	2.80	0.43
2:D:317:ALA:HB3	2:D:318:PRO:HD3	1.99	0.43
2:D:453:PHE:CD1	2:D:453:PHE:N	2.86	0.43
2:E:289:GLN:HE21	2:E:289:GLN:CA	2.09	0.43
3:G:77:GLY:O	3:G:168:LEU:HA	2.17	0.43
3:G:162:ASP:OD2	3:G:189:LEU:HD11	2.18	0.43
1:A:114:PRO:HG3	1:A:120:PRO:HA	2.01	0.43
1:A:163:GLN:C	1:A:164:ARG:HG3	2.43	0.43
1:A:322:GLN:O	1:A:323:ALA:HB3	2.18	0.43
1:A:431:GLU:CG	1:A:476:ARG:CG	2.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:PRO:HB2	1:B:370:ALA:HB3	1.99	0.43
2:D:254:ILE:O	2:D:257:PHE:HB3	2.18	0.43
2:D:328:THR:HG23	2:D:328:THR:O	2.18	0.43
2:D:354:LEU:HD22	2:D:364:TYR:HD1	1.83	0.43
2:D:392:LEU:C	2:D:394:ASP:N	2.73	0.43
2:E:14:VAL:O	2:E:61:THR:CG2	2.63	0.43
2:E:156:LEU:HD21	2:E:164:LYS:HG2	1.99	0.43
2:E:370:VAL:HG22	2:E:441:LEU:HD11	1.99	0.43
2:F:20:ASN:OD1	2:F:20:ASN:C	2.61	0.43
3:G:262:TYR:O	3:G:266:ARG:N	2.47	0.43
1:A:53:VAL:HG11	1:A:88:VAL:CG1	2.47	0.43
1:A:135:GLY:O	1:A:136:VAL:C	2.61	0.43
1:A:329:TYR:O	1:A:332:THR:OG1	2.30	0.43
1:B:331:PRO:O	1:B:335:ILE:HG13	2.18	0.43
1:B:453:VAL:O	1:B:456:PHE:N	2.52	0.43
1:C:49:SER:OG	2:D:68:ASP:HA	2.18	0.43
2:D:43:ASP:O	2:D:44:ILE:HD13	2.18	0.43
2:D:405:ARG:NH2	2:D:446:ASP:O	2.51	0.43
1:B:363:VAL:HG22	1:B:364:SER:N	2.33	0.43
1:C:52:LEU:HD22	1:C:95:MSE:HE3	2.01	0.43
1:C:297:LEU:HG	1:C:298:LEU:HD12	1.99	0.43
2:D:16:VAL:HG22	2:D:76:VAL:HG21	2.00	0.43
2:D:359:VAL:HG11	2:D:363:HIS:CE1	2.54	0.43
2:E:34:HIS:CE1	2:E:35:LYS:O	2.72	0.43
3:G:217:LEU:N	3:G:218:PRO:HD2	2.34	0.43
1:A:104:ILE:HA	1:A:222:ILE:HD11	2.01	0.43
1:A:345:GLN:CD	1:A:358:ASN:HD22	2.25	0.43
1:A:460:PHE:O	1:A:464:LEU:HG	2.18	0.43
1:B:96:GLU:HB3	1:B:126:THR:CG2	2.47	0.43
1:B:261:ASP:O	1:B:262:ASP:CB	2.65	0.43
1:B:434:VAL:HA	1:B:437:ILE:HG22	2.01	0.43
1:C:410:LEU:O	1:C:411:ALA:C	2.61	0.43
2:E:345:ASP:OD1	2:E:345:ASP:C	2.61	0.43
3:G:96:LEU:CG	3:G:126:PHE:HE1	2.31	0.43
1:A:101:GLU:CG	1:A:101:GLU:N	2.82	0.43
1:A:103:LEU:CD2	1:A:245:MSE:HE2	2.49	0.43
1:A:298:LEU:HD22	1:A:337:ILE:HG21	2.00	0.43
1:B:298:LEU:HD21	1:B:317:PRO:HG2	2.01	0.43
1:B:330:ILE:O	1:B:333:ASN:HB2	2.19	0.43
2:D:172:ILE:HG23	2:D:183:SER:OG	2.19	0.43
2:D:380:LEU:HA	2:D:383:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:173:HIS:NE2	2:E:415:HIS:ND1	2.66	0.43
1:A:399:GLY:O	1:A:402:LEU:N	2.52	0.43
1:B:48:MSE:HB3	2:F:69:GLY:HA2	2.01	0.43
1:B:348:LEU:HA	1:B:351:SER:OG	2.18	0.43
1:C:44:LEU:HB3	1:C:47:VAL:HG13	1.99	0.43
2:D:368:ARG:O	2:D:372:GLN:HG3	2.19	0.43
2:F:281:LEU:C	2:F:281:LEU:HD23	2.43	0.43
1:A:110:PRO:CG	1:A:234:LEU:HD22	2.48	0.43
1:A:150:ILE:O	1:A:151:LYS:C	2.62	0.43
1:A:328:ALA:O	1:A:332:THR:HG23	2.17	0.43
1:B:459:GLU:O	1:B:462:LEU:N	2.51	0.43
1:C:158:PRO:HG2	1:C:367:GLY:HA2	2.00	0.43
1:C:163:GLN:HG3	1:C:366:VAL:HG21	1.99	0.43
1:C:328:ALA:C	1:C:331:PRO:HD2	2.43	0.43
1:C:396:ALA:C	1:C:397:GLN:HG2	2.43	0.43
2:E:166:VAL:HG13	2:E:416:VAL:CG2	2.48	0.43
2:E:292:ILE:HD13	2:E:302:SER:HB2	1.99	0.43
2:E:440:ILE:HD11	2:E:453:PHE:CE2	2.54	0.43
2:F:138:GLY:HA3	2:F:427:TYR:CD1	2.53	0.43
2:F:373:THR:HG22	2:F:376:ARG:HH11	1.81	0.43
4:H:115:ARG:O	4:H:118:LEU:HB3	2.19	0.43
1:A:38:ILE:HD13	1:A:74:VAL:HA	2.00	0.43
1:B:45:ASP:HA	2:F:72:ARG:NH2	2.34	0.43
1:B:163:GLN:C	1:B:164:ARG:HG3	2.43	0.43
1:B:460:PHE:O	1:B:464:LEU:HG	2.18	0.43
1:B:475:ILE:HG23	1:B:476:ARG:N	2.33	0.43
1:C:496:LYS:O	1:C:497:THR:C	2.62	0.43
2:D:172:ILE:HG23	2:D:183:SER:CB	2.49	0.43
2:E:30:LEU:HB3	2:E:76:VAL:CG1	2.49	0.43
2:E:315:ASP:O	2:E:318:PRO:CD	2.58	0.43
2:F:22:HIS:O	2:F:23:LEU:C	2.61	0.43
2:F:225:ARG:HA	2:F:228:VAL:CG2	2.48	0.43
3:G:53:VAL:HG22	3:G:216:LEU:CD1	2.46	0.43
3:G:119:GLY:O	3:G:120:ARG:C	2.61	0.43
3:G:156:THR:HG23	3:G:160:PHE:CE1	2.53	0.43
1:A:150:ILE:CD1	1:A:178:VAL:HG13	2.49	0.43
1:B:450:VAL:HA	1:B:453:VAL:CG2	2.49	0.43
1:C:243:VAL:HG13	1:C:260:TYR:OH	2.16	0.43
1:C:387:ALA:O	1:C:388:ALA:C	2.62	0.43
1:C:435:LEU:HD21	1:C:475:ILE:HD11	2.01	0.43
3:G:72:PRO:C	3:G:73:VAL:CG2	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:80:VAL:HG11	3:G:126:PHE:CZ	2.54	0.43
1:A:294:HIS:O	1:A:297:LEU:HB3	2.19	0.42
1:A:343:PHE:HD2	1:A:344:LEU:N	2.17	0.42
1:A:417:VAL:O	1:A:421:LYS:HG3	2.19	0.42
1:A:434:VAL:O	1:A:438:TYR:HB2	2.19	0.42
1:B:317:PRO:C	1:B:318:PHE:HD2	2.27	0.42
1:C:373:LYS:HD3	1:C:376:LYS:HD2	2.00	0.42
2:D:221:PRO:O	2:D:222:PRO:C	2.62	0.42
2:D:405:ARG:CD	2:D:453:PHE:CZ	2.97	0.42
2:D:460:GLU:O	2:D:463:VAL:HB	2.18	0.42
2:E:381:GLN:C	2:E:384:ILE:HG22	2.43	0.42
2:E:418:GLU:O	2:E:419:GLN:C	2.62	0.42
2:F:346:PRO:HB2	2:F:374:LEU:HD13	2.01	0.42
3:G:14:THR:O	3:G:15:LYS:C	2.62	0.42
3:G:120:ARG:O	3:G:121:VAL:C	2.62	0.42
1:A:66:LEU:O	2:E:8:GLN:HA	2.19	0.42
1:A:247:GLU:CD	1:A:300:ARG:HH21	2.27	0.42
1:B:195:TYR:HD1	1:B:259:VAL:CG1	2.31	0.42
1:B:240:TYR:O	1:B:243:VAL:HG22	2.19	0.42
2:D:168:ILE:HG23	2:D:250:PHE:CE2	2.53	0.42
2:D:370:VAL:HG13	2:D:406:ILE:CG2	2.48	0.42
2:D:406:ILE:O	2:D:410:LEU:HG	2.18	0.42
2:E:96:PHE:CD1	2:E:235:MSE:HE1	2.54	0.42
2:E:408:PHE:CD1	2:E:454:ARG:HB2	2.53	0.42
2:E:410:LEU:HD23	2:E:437:PHE:CZ	2.54	0.42
3:G:225:ILE:HD12	3:G:225:ILE:C	2.44	0.42
3:G:242:THR:O	3:G:243:ALA:C	2.62	0.42
3:G:258:LEU:HA	3:G:261:SER:OG	2.19	0.42
1:B:55:PHE:HE1	1:B:73:ILE:HD11	1.80	0.42
1:B:334:VAL:O	1:B:338:THR:HG23	2.20	0.42
1:C:416:THR:HA	1:C:440:LEU:HD12	1.99	0.42
2:D:170:GLU:HG2	2:D:414:PHE:CE2	2.54	0.42
2:F:312:ASP:HA	3:G:1:MSE:HB2	2.00	0.42
3:G:25:GLU:OE2	3:G:245:LYS:HD3	2.18	0.42
1:A:61:GLY:HA2	1:A:76:LEU:HG	2.01	0.42
1:A:239:PRO:CG	1:A:266:GLN:HG3	2.46	0.42
1:B:185:ASN:O	1:B:185:ASN:ND2	2.53	0.42
1:B:298:LEU:HD11	1:B:317:PRO:HG3	2.02	0.42
1:C:150:ILE:HA	1:C:422:GLN:OE1	2.19	0.42
2:D:342:PRO:HB2	2:D:344:VAL:HG23	2.02	0.42
2:D:371:GLN:O	2:D:374:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:467:LYS:O	2:D:470:GLY:N	2.51	0.42
2:E:5:ARG:HA	2:E:74:MSE:O	2.20	0.42
2:E:103:ILE:HD11	2:E:215:PHE:HD1	1.85	0.42
2:E:157:PHE:HB2	2:E:330:ASN:HD22	1.84	0.42
2:E:409:PHE:HD2	2:E:437:PHE:CE1	2.37	0.42
2:E:409:PHE:CD2	2:E:437:PHE:CE1	3.07	0.42
2:F:280:THR:O	2:F:281:LEU:C	2.62	0.42
2:F:315:ASP:O	2:F:316:PRO:C	2.62	0.42
2:F:381:GLN:HA	2:F:384:ILE:HG12	2.01	0.42
2:F:384:ILE:HD13	2:F:384:ILE:N	2.35	0.42
3:G:156:THR:HG23	3:G:160:PHE:CD1	2.54	0.42
1:A:95:MSE:SE	1:A:237:LEU:CD2	3.16	0.42
1:A:192:ILE:HA	1:A:220:TYR:HB2	2.01	0.42
2:D:466:ALA:HA	2:D:469:MSE:HG2	2.01	0.42
3:G:7:ILE:O	3:G:11:ILE:HG13	2.19	0.42
3:G:10:ARG:HD3	4:H:129:VAL:HA	1.94	0.42
1:A:151:LYS:HE3	1:A:428:ILE:CD1	2.49	0.42
1:A:229:SER:HB3	2:D:290:GLU:CB	2.50	0.42
1:A:416:THR:HG22	1:A:440:LEU:HD12	2.01	0.42
1:B:233:PRO:O	1:B:236:PHE:HB3	2.20	0.42
1:B:343:PHE:CD2	1:B:344:LEU:N	2.79	0.42
2:D:256:ARG:HH11	2:D:259:GLN:HE22	1.67	0.42
2:E:154:ILE:HG13	2:E:327:ALA:HB3	2.02	0.42
3:G:52:VAL:CG2	4:H:69:GLU:HG2	2.49	0.42
3:G:116:ILE:HG23	3:G:136:ASP:HB2	2.02	0.42
1:A:99:VAL:HG21	1:A:127:ARG:HB2	2.02	0.42
1:A:193:SER:O	1:A:221:THR:HA	2.19	0.42
1:A:208:VAL:HA	1:A:211:THR:HG22	2.02	0.42
1:B:180:ILE:HG23	1:B:212:LEU:HD21	2.02	0.42
1:C:153:ILE:O	1:C:157:VAL:C	2.62	0.42
2:D:362:GLU:O	2:D:366:VAL:CG2	2.66	0.42
3:G:212:ILE:O	3:G:213:LEU:C	2.63	0.42
4:H:83:GLU:OE1	4:H:95:ALA:HB1	2.19	0.42
1:A:129:ILE:HG22	1:A:130:GLU:N	2.35	0.42
1:B:415:ARG:O	1:B:419:VAL:HG23	2.19	0.42
1:B:497:THR:O	1:B:499:VAL:N	2.53	0.42
2:E:147:PRO:HD2	2:E:351:SER:HB3	2.00	0.42
2:F:170:GLU:OE2	2:F:414:PHE:HA	2.20	0.42
3:G:112:GLU:CG	3:G:113:TYR:N	2.83	0.42
3:G:120:ARG:O	3:G:123:LEU:N	2.53	0.42
1:B:195:TYR:HA	1:B:259:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:LEU:HD13	1:C:464:LEU:HD13	2.01	0.42
2:E:171:LEU:HD13	2:E:303:ILE:HD13	2.02	0.42
2:F:144:LEU:HD22	2:F:437:PHE:CD2	2.55	0.42
3:G:233:LYS:HD3	3:G:236:GLU:OE1	2.20	0.42
1:C:159:ILE:HA	1:C:163:GLN:OE1	2.20	0.42
1:C:407:GLN:HA	1:C:410:LEU:HB2	2.01	0.42
2:D:18:PHE:N	2:D:18:PHE:CD1	2.87	0.42
2:E:175:ILE:HG13	2:E:248:LEU:HD11	2.01	0.42
2:E:270:ARG:HG3	2:E:270:ARG:NH1	2.35	0.42
2:E:285:MSE:HG3	2:E:324:HIS:CD2	2.55	0.42
2:E:328:THR:CG2	2:E:350:THR:H	2.19	0.42
2:F:30:LEU:O	2:F:47:THR:HA	2.20	0.42
2:F:162:VAL:CG1	2:F:331:LEU:HB3	2.49	0.42
3:G:212:ILE:H	3:G:212:ILE:HD12	1.84	0.42
4:H:28:LYS:O	4:H:29:SER:CB	2.68	0.42
4:H:116:ALA:C	4:H:118:LEU:N	2.77	0.42
4:H:130:ALA:O	4:H:132:MSE:O	2.37	0.42
1:A:319:VAL:HG11	1:A:331:PRO:HA	2.02	0.41
1:B:94:ILE:O	1:B:95:MSE:C	2.63	0.41
1:B:118:LEU:HD23	1:B:118:LEU:HA	1.83	0.41
1:B:298:LEU:C	1:B:300:ARG:H	2.27	0.41
1:B:452:ASP:CA	1:B:455:ARG:HB2	2.50	0.41
1:C:157:VAL:HG13	1:C:364:SER:HB2	2.02	0.41
1:C:343:PHE:CD2	1:C:343:PHE:C	2.95	0.41
2:D:10:MSE:O	2:D:11:GLY:C	2.62	0.41
2:D:26:ILE:O	2:D:27:TYR:CB	2.62	0.41
2:D:335:LEU:HD11	2:D:346:PRO:HD3	2.02	0.41
2:E:227:ARG:HD2	2:E:230:LEU:HD12	2.01	0.41
2:F:195:GLY:CA	2:F:215:PHE:HE2	2.31	0.41
3:G:212:ILE:O	3:G:214:ASP:N	2.53	0.41
4:H:90:VAL:O	4:H:90:VAL:HG12	2.20	0.41
1:A:240:TYR:O	1:A:243:VAL:HG22	2.20	0.41
1:A:286:TYR:HA	1:A:287:PRO:HD3	1.92	0.41
1:B:62:MSE:HE3	1:B:95:MSE:CG	2.31	0.41
1:B:165:GLU:OE2	1:B:341:GLN:CA	2.68	0.41
2:D:322:PHE:HA	2:D:325:LEU:CD1	2.49	0.41
2:D:345:ASP:OD1	2:D:345:ASP:C	2.62	0.41
2:E:273:SER:O	2:E:274:ALA:C	2.63	0.41
2:F:253:ASN:C	2:F:255:PHE:H	2.27	0.41
2:F:377:TYR:HE1	2:F:400:VAL:HG13	1.85	0.41
3:G:181:GLN:NE2	3:G:239:ALA:HB2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:191:ARG:HD2	2:D:194:GLU:CD	2.45	0.41
2:E:396:ASP:O	2:E:399:VAL:HB	2.19	0.41
2:F:182:ILE:O	2:F:247:VAL:HG13	2.21	0.41
2:F:317:ALA:HB3	2:F:318:PRO:HD3	2.00	0.41
1:A:329:TYR:CD2	1:A:329:TYR:C	2.98	0.41
1:A:355:PRO:HB2	1:A:357:ILE:CD1	2.50	0.41
1:A:434:VAL:HA	1:A:437:ILE:CG2	2.47	0.41
1:B:28:VAL:O	1:B:28:VAL:HG13	2.20	0.41
1:B:232:ALA:O	1:B:233:PRO:C	2.63	0.41
1:C:139:ARG:NH2	1:C:299:GLU:O	2.54	0.41
1:C:463:PHE:O	1:C:467:ASN:O	2.39	0.41
2:E:148:TYR:CE1	2:E:154:ILE:HG12	2.55	0.41
2:E:219:ASN:C	2:E:219:ASN:ND2	2.78	0.41
2:E:222:PRO:HB2	2:E:264:VAL:HG22	2.02	0.41
2:E:438:LYS:O	2:E:442:GLU:HG3	2.20	0.41
2:F:148:TYR:CG	2:F:154:ILE:CD1	3.04	0.41
2:F:265:SER:CB	2:F:278:GLN:HB3	2.51	0.41
2:F:354:LEU:HD23	2:F:354:LEU:HA	1.77	0.41
1:A:62:MSE:HE3	1:A:95:MSE:CB	2.47	0.41
1:A:263:LEU:HD12	1:A:317:PRO:HB3	2.03	0.41
1:A:319:VAL:HG21	1:A:334:VAL:CG1	2.35	0.41
1:A:434:VAL:C	1:A:437:ILE:HG22	2.45	0.41
1:A:481:LEU:HD22	1:A:485:ASP:CG	2.46	0.41
1:B:108:VAL:O	1:B:224:VAL:HA	2.20	0.41
1:B:109:ASN:OD1	1:B:111:LEU:HB2	2.20	0.41
1:B:328:ALA:O	1:B:332:THR:HG23	2.20	0.41
1:C:175:LYS:HB3	1:C:318:PHE:CE1	2.55	0.41
2:D:139:ILE:O	2:D:140:LYS:C	2.63	0.41
2:D:404:ARG:O	2:D:408:PHE:HB2	2.20	0.41
2:E:84:SER:HB3	2:E:115:ARG:HB3	2.02	0.41
2:E:217:GLN:O	2:E:220:GLU:CG	2.68	0.41
2:E:334:LYS:CE	2:E:334:LYS:HA	2.50	0.41
1:A:176:THR:O	1:A:177:SER:C	2.64	0.41
1:A:179:ALA:O	1:A:183:ILE:HG13	2.21	0.41
1:A:257:LEU:HD21	1:A:316:LEU:HD12	2.02	0.41
2:E:7:ILE:HG22	2:E:8:GLN:HG3	2.02	0.41
2:F:185:PHE:CD2	2:F:250:PHE:HB2	2.56	0.41
2:F:222:PRO:O	2:F:223:GLY:C	2.63	0.41
3:G:81:ILE:HD13	3:G:229:LEU:HD22	2.02	0.41
3:G:258:LEU:O	3:G:259:THR:C	2.63	0.41
4:H:101:GLU:HA	4:H:104:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:MSE:HG3	1:A:237:LEU:HD21	2.02	0.41
1:A:365:ARG:C	1:A:367:GLY:N	2.73	0.41
1:A:405:ALA:C	1:A:407:GLN:N	2.77	0.41
1:B:232:ALA:N	1:B:233:PRO:CD	2.83	0.41
1:C:273:LEU:HD23	1:C:273:LEU:C	2.45	0.41
1:C:373:LYS:HB2	1:C:480:ASP:CA	2.51	0.41
1:C:462:LEU:HD13	1:C:462:LEU:HA	1.83	0.41
2:D:12:PRO:HG2	2:D:267:LEU:CD1	2.50	0.41
2:D:376:ARG:O	2:D:380:LEU:HG	2.21	0.41
2:D:380:LEU:O	2:D:381:GLN:C	2.63	0.41
2:E:318:PRO:HG2	2:E:319:ALA:N	2.36	0.41
2:F:175:ILE:O	2:F:176:ALA:C	2.63	0.41
3:G:95:VAL:CG2	3:G:96:LEU:N	2.84	0.41
3:G:242:THR:C	3:G:244:MSE:N	2.78	0.41
1:A:171:ARG:NE	1:A:320:GLU:OE2	2.54	0.41
1:B:44:LEU:HD21	1:B:88:VAL:O	2.20	0.41
1:B:151:LYS:HZ1	1:B:422:GLN:CB	2.34	0.41
1:B:209:VAL:HG11	2:E:125:PHE:CZ	2.48	0.41
1:C:246:GLY:C	1:C:248:TYR:N	2.77	0.41
1:C:266:GLN:O	1:C:269:ALA:HB3	2.19	0.41
2:D:229:ALA:O	2:D:233:LEU:HB2	2.20	0.41
2:D:342:PRO:CG	2:D:414:PHE:CZ	3.01	0.41
2:D:433:THR:O	2:D:437:PHE:HD1	2.04	0.41
2:E:39:GLU:H	2:E:39:GLU:CD	2.29	0.41
2:E:136:GLU:HB3	2:E:179:HIS:HE2	1.86	0.41
2:E:144:LEU:HD12	2:E:367:ALA:HB2	2.02	0.41
2:E:328:THR:HG23	2:E:350:THR:N	2.20	0.41
3:G:72:PRO:HG3	3:G:166:ASP:OD2	2.21	0.41
3:G:129:ARG:O	3:G:130:ASN:CB	2.69	0.41
1:A:65:ASN:O	1:A:71:VAL:HA	2.20	0.41
1:A:377:LYS:CG	1:A:378:VAL:N	2.84	0.41
1:A:431:GLU:HB3	1:A:472:LEU:HB2	2.03	0.41
1:A:436:ILE:O	1:A:440:LEU:HD22	2.21	0.41
1:A:453:VAL:O	1:A:456:PHE:HB3	2.21	0.41
1:B:33:GLN:HG2	2:E:54:LEU:O	2.21	0.41
1:C:209:VAL:O	1:C:213:ARG:HG3	2.20	0.41
2:D:10:MSE:CB	2:D:13:VAL:HG13	2.36	0.41
2:D:233:LEU:O	2:D:236:ALA:N	2.54	0.41
2:D:465:LYS:O	2:D:468:ALA:HB3	2.21	0.41
2:E:9:VAL:HG13	2:E:14:VAL:HG22	2.01	0.41
2:E:95:VAL:HG12	2:E:103:ILE:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:157:PHE:HB2	2:E:330:ASN:ND2	2.36	0.41
2:E:216:GLY:O	2:E:225:ARG:HG2	2.21	0.41
2:F:142:VAL:O	2:F:146:ALA:C	2.64	0.41
2:F:353:ALA:C	2:F:355:ALA:H	2.29	0.41
3:G:21:THR:HB	3:G:248:THR:OG1	2.21	0.41
3:G:48:LYS:HD2	4:H:69:GLU:HG3	2.02	0.41
3:G:140:LEU:N	3:G:141:PRO:HD3	2.36	0.41
3:G:267:GLN:O	3:G:268:ALA:C	2.64	0.41
4:H:91:LEU:C	4:H:93:ALA:N	2.77	0.41
1:A:471:LEU:HD21	1:A:489:LYS:CG	2.50	0.41
1:B:265:LYS:O	1:B:269:ALA:HB2	2.21	0.41
1:B:301:ALA:CB	1:B:313:LEU:HD22	2.49	0.41
1:C:197:ALA:HB1	1:C:200:GLN:CB	2.50	0.41
1:C:474:HIS:C	1:C:474:HIS:HD2	2.17	0.41
2:D:213:MSE:HE2	2:D:215:PHE:HZ	1.80	0.41
2:D:256:ARG:HH11	2:D:259:GLN:NE2	2.17	0.41
2:D:364:TYR:O	2:D:365:GLN:C	2.64	0.41
2:D:404:ARG:NH1	2:D:408:PHE:CE2	2.89	0.41
2:E:87:VAL:O	2:E:87:VAL:HG23	2.21	0.41
2:E:203:LYS:HB3	2:E:203:LYS:HZ2	1.85	0.41
2:F:416:VAL:HG23	2:F:416:VAL:O	2.21	0.41
3:G:25:GLU:HG3	3:G:245:LYS:HG3	2.03	0.41
4:H:129:VAL:CG1	4:H:132:MSE:HA	2.24	0.41
1:A:62:MSE:CE	1:A:95:MSE:HG3	2.52	0.40
1:A:121:VAL:O	1:A:121:VAL:CG2	2.63	0.40
1:A:431:GLU:CG	1:A:476:ARG:HG3	2.51	0.40
1:B:62:MSE:HG2	1:B:63:ALA:N	2.36	0.40
1:B:249:PHE:HB2	1:B:256:VAL:CG2	2.51	0.40
1:B:478:THR:C	1:B:480:ASP:N	2.77	0.40
2:D:32:ILE:CD1	2:D:76:VAL:HG22	2.50	0.40
2:D:170:GLU:O	2:D:173:HIS:HB3	2.21	0.40
2:E:176:ALA:HA	2:E:181:GLY:H	1.86	0.40
2:F:401:HIS:HD2	2:F:405:ARG:HH21	1.64	0.40
3:G:78:TYR:CE1	3:G:171:TYR:CE1	3.07	0.40
3:G:164:THR:O	3:G:164:THR:HG22	2.21	0.40
3:G:233:LYS:O	3:G:234:ALA:C	2.63	0.40
1:A:95:MSE:SE	1:A:129:ILE:HD12	2.71	0.40
1:A:209:VAL:HG23	1:A:223:VAL:HG21	2.01	0.40
1:A:372:ILE:HD13	1:A:374:ALA:HB3	2.04	0.40
1:A:450:VAL:O	1:A:451:GLU:C	2.63	0.40
1:B:206:ARG:O	1:B:209:VAL:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:GLU:O	1:C:276:LEU:HD23	2.22	0.40
1:C:326:ILE:O	1:C:326:ILE:HG22	2.21	0.40
2:D:115:ARG:HG2	2:D:115:ARG:HH11	1.87	0.40
2:D:359:VAL:HB	2:D:363:HIS:ND1	2.36	0.40
2:E:91:THR:HA	2:E:96:PHE:CZ	2.56	0.40
2:E:450:GLU:O	2:E:452:ALA:N	2.54	0.40
3:G:114:ALA:HB3	3:G:165:PHE:CE1	2.54	0.40
1:A:84:GLU:C	1:A:86:ASP:H	2.29	0.40
1:C:99:VAL:CG1	1:C:245:MSE:HA	2.51	0.40
1:C:145:PRO:HB2	1:C:147:GLN:HE21	1.87	0.40
1:C:186:GLN:HB3	1:C:191:MSE:HB2	2.02	0.40
1:C:243:VAL:O	1:C:247:GLU:N	2.45	0.40
1:C:412:ARG:HA	1:C:415:ARG:HB2	2.03	0.40
2:D:173:HIS:CD2	2:D:173:HIS:C	2.99	0.40
2:D:256:ARG:NH1	2:D:259:GLN:NE2	2.62	0.40
2:E:453:PHE:CD2	2:E:462:VAL:HG11	2.56	0.40
2:F:153:LYS:NZ	2:F:289:GLN:HB3	2.37	0.40
2:F:335:LEU:HB2	2:F:343:ALA:HB1	2.02	0.40
3:G:14:THR:O	3:G:17:THR:HB	2.22	0.40
3:G:24:MSE:HA	3:G:27:VAL:HB	2.03	0.40
3:G:25:GLU:CD	3:G:245:LYS:CD	2.93	0.40
3:G:92:ASN:O	3:G:95:VAL:HG22	2.21	0.40
4:H:35:LEU:O	4:H:36:PRO:C	2.65	0.40
4:H:129:VAL:O	4:H:129:VAL:HG12	2.21	0.40
1:A:382:LEU:CG	1:A:437:ILE:HD11	2.46	0.40
1:A:480:ASP:OD2	1:A:481:LEU:N	2.55	0.40
1:B:241:ALA:O	1:B:245:MSE:HE3	2.20	0.40
1:C:389:TYR:O	1:C:393:GLU:HB2	2.20	0.40
2:D:317:ALA:N	2:D:318:PRO:HD2	2.36	0.40
2:D:466:ALA:C	2:D:468:ALA:N	2.78	0.40
2:E:98:VAL:HG13	2:E:228:VAL:HA	2.03	0.40
2:E:226:MSE:HE3	2:E:227:ARG:CZ	2.50	0.40
2:E:246:ASP:HA	2:E:299:SER:O	2.20	0.40
2:E:370:VAL:CG1	2:E:406:ILE:HG21	2.50	0.40
2:E:404:ARG:O	2:E:408:PHE:HD2	2.03	0.40
2:E:428:VAL:CG2	2:E:432:GLU:HB2	2.44	0.40
4:H:22:MSE:HB2	4:H:35:LEU:CD2	2.50	0.40
1:A:199:GLY:O	1:A:228:ALA:HB2	2.21	0.40
1:A:261:ASP:O	1:A:262:ASP:HB3	2.22	0.40
1:A:456:PHE:C	1:A:458:LYS:N	2.78	0.40
1:B:184:ILE:HA	1:B:220:TYR:OH	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:ILE:HA	1:B:220:TYR:O	2.22	0.40
1:B:445:LEU:HG	1:B:456:PHE:CD1	2.56	0.40
1:C:284:GLU:HG2	1:C:284:GLU:O	2.22	0.40
2:E:160:ALA:HB3	2:E:333:ARG:NH2	2.37	0.40
2:E:178:GLU:HG3	2:E:427:TYR:CE2	2.57	0.40
2:F:250:PHE:CE1	2:F:303:ILE:HD12	2.54	0.40
2:F:384:ILE:HG23	2:F:389:MSE:CG	2.52	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	473/502 (94%)	429 (91%)	42 (9%)	2 (0%)	30	64
1	B	403/502 (80%)	357 (89%)	42 (10%)	4 (1%)	12	45
1	C	469/502 (93%)	411 (88%)	51 (11%)	7 (2%)	8	37
2	D	466/483 (96%)	414 (89%)	50 (11%)	2 (0%)	30	64
2	E	463/483 (96%)	418 (90%)	39 (8%)	6 (1%)	9	40
2	F	456/483 (94%)	406 (89%)	46 (10%)	4 (1%)	14	47
3	G	242/285 (85%)	193 (80%)	38 (16%)	11 (4%)	2	19
4	H	123/133 (92%)	108 (88%)	12 (10%)	3 (2%)	4	29
All	All	3095/3373 (92%)	2736 (88%)	320 (10%)	39 (1%)	9	40

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	371	GLN
1	C	354	ARG
2	D	393	SER

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Mol	Chain	Res	Type
2	E	311	ASP
3	G	143	GLN
1	C	355	PRO
1	C	469	GLN
2	E	20	ASN
2	E	83	ILE
2	F	275	VAL
3	G	190	PRO
4	H	126	ARG
1	C	485	ASP
3	G	72	PRO
3	G	167	GLU
3	G	213	LEU
4	H	90	VAL
4	H	128	SER
1	A	95	MSE
1	C	482	PRO
3	G	102	THR
1	A	411	ALA
1	B	431	GLU
1	B	498	PHE
1	C	411	ALA
1	C	481	LEU
2	E	310	ALA
2	E	393	SER
2	F	424	PRO
3	G	189	LEU
2	F	354	LEU
3	G	149	ILE
2	D	142	VAL
1	B	453	VAL
2	F	82	PRO
3	G	11	ILE
3	G	53	VAL
3	G	73	VAL
2	E	142	VAL

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	332/402 (83%)	312 (94%)	20 (6%)	17	44
1	B	242/402 (60%)	233 (96%)	9 (4%)	30	53
1	C	291/402 (72%)	274 (94%)	17 (6%)	18	44
2	D	333/385 (86%)	318 (96%)	15 (4%)	24	49
2	E	349/385 (91%)	330 (95%)	19 (5%)	20	46
2	F	309/385 (80%)	301 (97%)	8 (3%)	40	60
3	G	157/231 (68%)	144 (92%)	13 (8%)	10	34
4	H	78/104 (75%)	72 (92%)	6 (8%)	12	37
All	All	2091/2696 (78%)	1984 (95%)	107 (5%)	21	46

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	70	ASN
1	A	86	ASP
1	A	94	ILE
1	A	95	MSE
1	A	109	ASN
1	A	138	ASP
1	A	140	ARG
1	A	166	LEU
1	A	192	ILE
1	A	225	THR
1	A	227	SER
1	A	237	LEU
1	A	266	GLN
1	A	351	SER
1	A	382	LEU
1	A	386	LEU
1	A	406	THR
1	A	415	ARG
1	A	479	LYS
1	B	64	LEU
1	B	94	ILE
1	B	95	MSE
1	B	167	ILE

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Mol	Chain	Res	Type
1	B	262	ASP
1	B	298	LEU
1	B	306	ASP
1	B	462	LEU
1	B	472	LEU
1	C	70	ASN
1	C	95	MSE
1	C	141	SER
1	C	166	LEU
1	C	168	ILE
1	C	375	MSE
1	C	382	LEU
1	C	386	LEU
1	C	397	GLN
1	C	403	ASP
1	C	407	GLN
1	C	415	ARG
1	C	462	LEU
1	C	463	PHE
1	C	471	LEU
1	C	474	HIS
1	C	477	THR
2	D	38	ASN
2	D	52	LEU
2	D	98	VAL
2	D	108	ASP
2	D	112	ASP
2	D	169	GLN
2	D	203	LYS
2	D	219	ASN
2	D	222	PRO
2	D	242	GLU
2	D	307	TYR
2	D	354	LEU
2	D	383	ILE
2	D	413	ASN
2	D	420	PHE
2	E	23	LEU
2	E	38	ASN
2	E	134	ILE
2	E	169	GLN
2	E	182	ILE

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Mol	Chain	Res	Type
2	E	193	ARG
2	E	203	LYS
2	E	217	GLN
2	E	219	ASN
2	E	228	VAL
2	E	254	ILE
2	E	256	ARG
2	E	289	GLN
2	E	293	THR
2	E	334	LYS
2	E	357	GLU
2	E	420	PHE
2	E	428	VAL
2	E	453	PHE
2	F	87	VAL
2	F	97	ASN
2	F	204	ASP
2	F	271	MSE
2	F	278	GLN
2	F	384	ILE
2	F	412	GLN
2	F	451	ASP
3	G	4	LEU
3	G	38	ASN
3	G	75	LYS
3	G	82	THR
3	G	84	ASP
3	G	96	LEU
3	G	135	LEU
3	G	143	GLN
3	G	165	PHE
3	G	179	ILE
3	G	212	ILE
3	G	241	MSE
3	G	244	MSE
4	H	41	LEU
4	H	45	LEU
4	H	87	ASP
4	H	88	ILE
4	H	120	LEU
4	H	127	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	109	ASN
1	A	113	GLN
1	A	266	GLN
1	A	371	GLN
1	A	433	GLN
1	B	322	GLN
1	B	425	HIS
1	C	322	GLN
1	C	345	GLN
1	C	397	GLN
1	C	407	GLN
1	C	433	GLN
1	C	467	ASN
1	C	474	HIS
2	D	259	GLN
2	D	289	GLN
2	D	304	GLN
2	D	372	GLN
2	E	22	HIS
2	E	28	ASN
2	E	38	ASN
2	E	245	GLN
2	E	253	ASN
2	E	304	GLN
2	E	324	HIS
2	F	8	GLN
2	F	173	HIS
2	F	200	HIS
2	F	324	HIS
2	F	401	HIS
3	G	252	ASN
3	G	263	ASN
4	H	80	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](#)

5 ligands are 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	$\# Z > 2$
5	SO4	D	700	-	4,4,4	0.26	0	6,6,6	0.20	0
5	SO4	B	700	-	4,4,4	0.28	0	6,6,6	0.23	0
5	SO4	E	700	-	4,4,4	0.28	0	6,6,6	0.21	0
5	SO4	A	700	-	4,4,4	0.27	0	6,6,6	0.34	0
6	ADP	F	600	-	28,29,29	1.50	5 (17%)	43,45,45	1.84	8 (18%)

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
6	ADP	F	600	-	-	8/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	600	ADP	C5-C4	4.93	1.47	1.39
6	F	600	ADP	PA-O3A	2.65	1.62	1.59
6	F	600	ADP	C5-C6	2.65	1.48	1.41
6	F	600	ADP	C8-N7	2.40	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	600	ADP	C5-N7	-2.18	1.35	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	600	ADP	C5-C4-N3	-6.00	118.46	126.72
6	F	600	ADP	N3-C4-N9	4.94	135.57	127.17
6	F	600	ADP	C2-N3-C4	3.75	120.98	111.83
6	F	600	ADP	N3-C2-N1	-3.21	123.72	128.58
6	F	600	ADP	C4-C5-N7	-2.92	107.24	110.58
6	F	600	ADP	C3'-C2'-C1'	2.68	106.53	101.46
6	F	600	ADP	C4-N9-C8	2.44	108.30	105.74
6	F	600	ADP	C5-N7-C8	2.09	106.73	103.45

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	600	ADP	PA-O3A-PB-O2B
6	F	600	ADP	PA-O3A-PB-O3B
6	F	600	ADP	C5'-O5'-PA-O2A
6	F	600	ADP	C5'-O5'-PA-O3A
6	F	600	ADP	O4'-C4'-C5'-O5'
6	F	600	ADP	C3'-C4'-C5'-O5'
6	F	600	ADP	C5'-O5'-PA-O1A
6	F	600	ADP	PA-O3A-PB-O1B

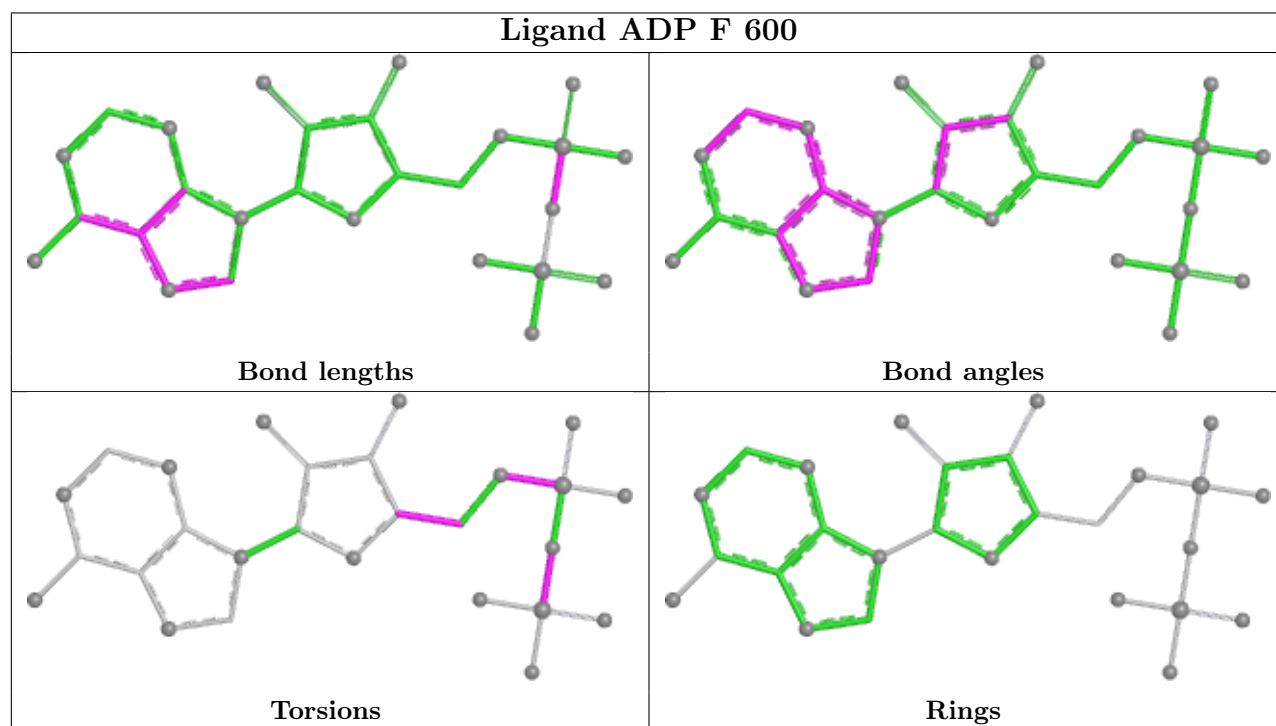
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	700	SO4	1	0
5	A	700	SO4	3	0
6	F	600	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	468/502 (93%)	-0.25	3 (0%) 85 69	63, 97, 156, 240	0
1	B	414/502 (82%)	0.12	11 (2%) 56 39	92, 129, 236, 263	0
1	C	466/502 (92%)	-0.02	1 (0%) 91 81	86, 124, 177, 215	0
2	D	457/483 (94%)	-0.23	3 (0%) 84 67	70, 107, 165, 212	0
2	E	456/483 (94%)	-0.20	3 (0%) 84 67	71, 103, 155, 210	0
2	F	451/483 (93%)	0.00	3 (0%) 84 67	95, 137, 164, 211	0
3	G	247/285 (86%)	0.33	7 (2%) 55 38	80, 134, 182, 199	0
4	H	125/133 (93%)	0.36	6 (4%) 35 27	114, 143, 168, 191	0
All	All	3084/3373 (91%)	-0.05	37 (1%) 76 55	63, 119, 180, 263	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	142	VAL	4.6
4	H	89	ASP	3.6
2	F	420	PHE	3.5
1	B	464	LEU	3.5
3	G	52	VAL	3.4
3	G	220	TYR	3.3
4	H	61	ILE	3.3
1	B	199	GLY	3.2
1	B	359	ALA	3.1
4	H	50	ALA	3.1
1	B	366	VAL	3.0
2	F	34	HIS	2.8
3	G	99	VAL	2.8
4	H	31	GLU	2.7
2	E	456	VAL	2.6
2	D	2	THR	2.6

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Mol	Chain	Res	Type	RSRZ
3	G	165	PHE	2.6
1	B	179	ALA	2.6
1	A	304	LEU	2.5
1	A	41	ALA	2.5
2	D	390	ASP	2.4
3	G	102	THR	2.3
2	F	208	ILE	2.3
2	E	41	GLU	2.3
1	C	356	ALA	2.2
1	B	129	ILE	2.2
1	B	228	ALA	2.2
4	H	37	GLY	2.2
1	A	445	LEU	2.2
2	D	391	GLU	2.2
1	B	488	ASN	2.2
3	G	217	LEU	2.2
4	H	90	VAL	2.1
1	B	487	LEU	2.1
3	G	111	ASP	2.1
2	E	457	GLY	2.1
1	B	481	LEU	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.

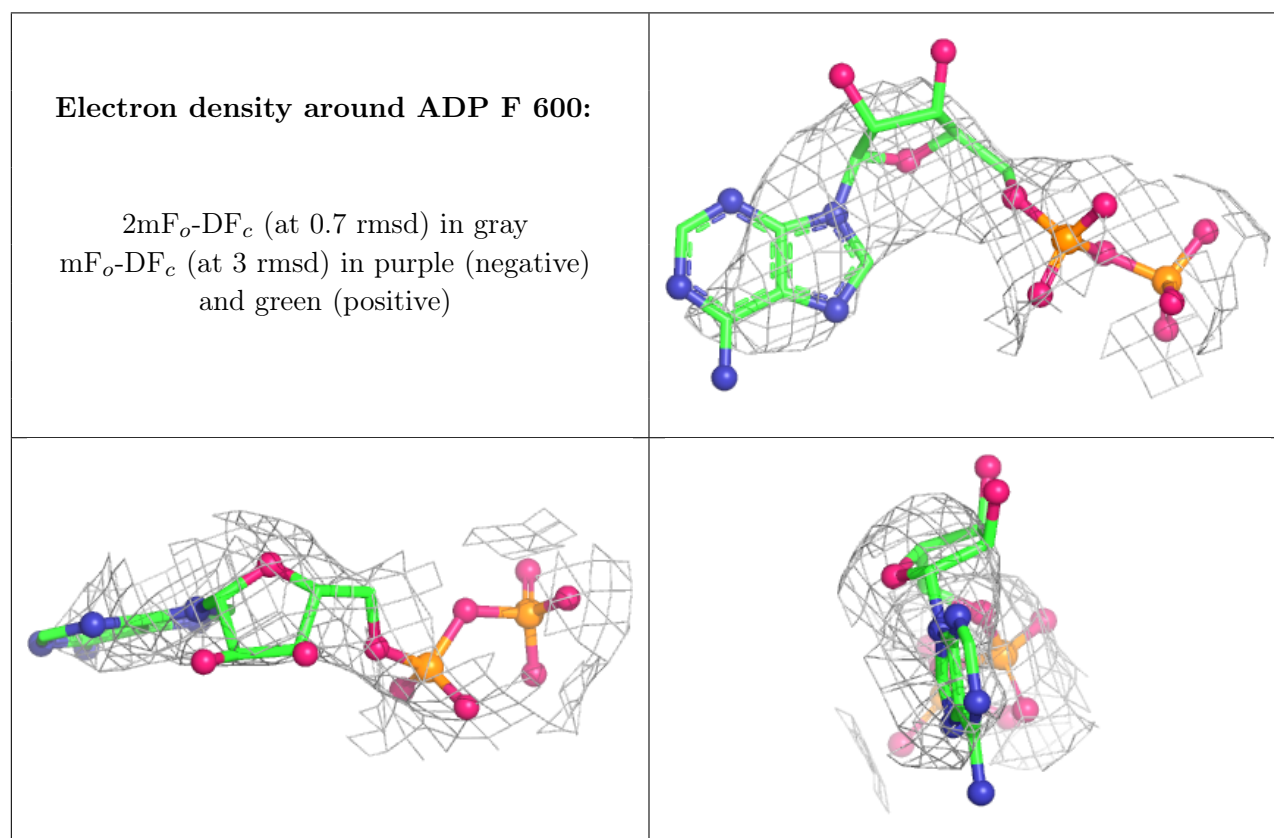
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	E	700	5/5	0.38	0.21	185,189,190,191	0
5	SO4	D	700	5/5	0.63	0.07	190,192,193,194	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	B	700	5/5	0.63	0.14	187,190,191,194	0
5	SO4	A	700	5/5	0.85	0.18	184,186,190,192	0
6	ADP	F	600	27/27	0.89	0.13	173,198,203,203	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.