Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:33 AM GMT

PDB ID	:	2DHR
Title	:	Whole cytosolic region of ATP-dependent metalloprotease FtsH (G399L)
Authors	:	Suno, R.; Niwa, H.; Tsuchiya, D.; Zhang, X.; Yoshida, M.; Morikawa, K.
Deposited on	:	2006-03-24
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

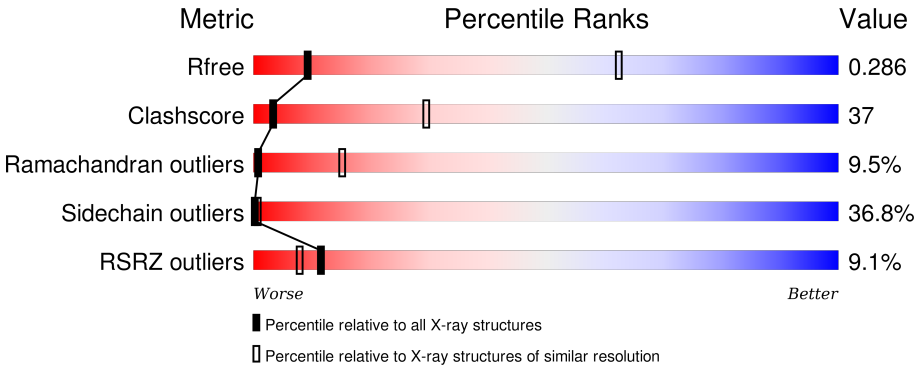
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	499	8% 34% 36% 19% • 8%
1	B	499	9% 29% 38% 18% • 11%
1	C	499	10% 34% 36% 19% • 8%
1	D	499	7% 30% 36% 19% • 11%
1	E	499	8% 34% 36% 19% • 8%

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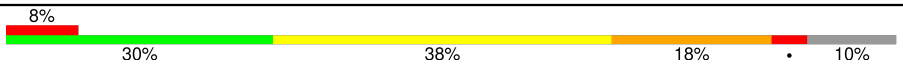
Mol	Chain	Length	Quality of chain
1	F	499	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21460 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.

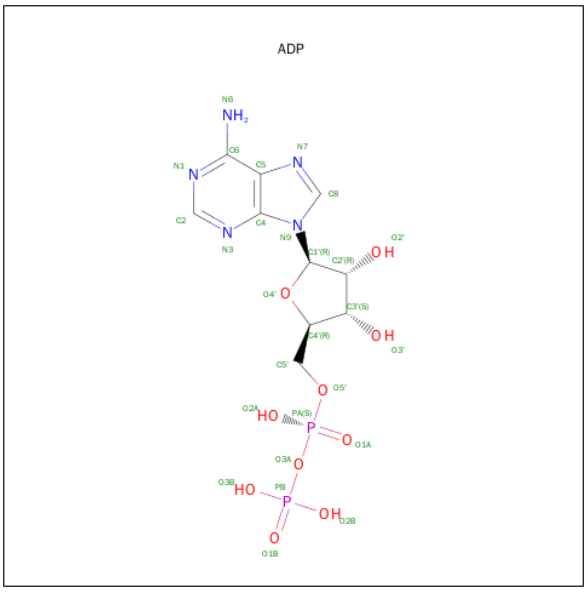
- Molecule 1 is a protein called FtsH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	0	0
			3579	2245	659	662	13			
1	B	446	Total	C	N	O	S	0	0	0
			3511	2206	641	651	13			
1	C	458	Total	C	N	O	S	0	0	0
			3583	2247	659	664	13			
1	D	445	Total	C	N	O	S	0	0	0
			3503	2200	640	650	13			
1	E	458	Total	C	N	O	S	0	0	0
			3583	2247	659	664	13			
1	F	450	Total	C	N	O	S	0	0	0
			3539	2223	648	655	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	399	LEU	GLY	ENGINEERED	UNP Q9LCZ4
B	399	LEU	GLY	ENGINEERED	UNP Q9LCZ4
C	399	LEU	GLY	ENGINEERED	UNP Q9LCZ4
D	399	LEU	GLY	ENGINEERED	UNP Q9LCZ4
E	399	LEU	GLY	ENGINEERED	UNP Q9LCZ4
F	399	LEU	GLY	ENGINEERED	UNP Q9LCZ4

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



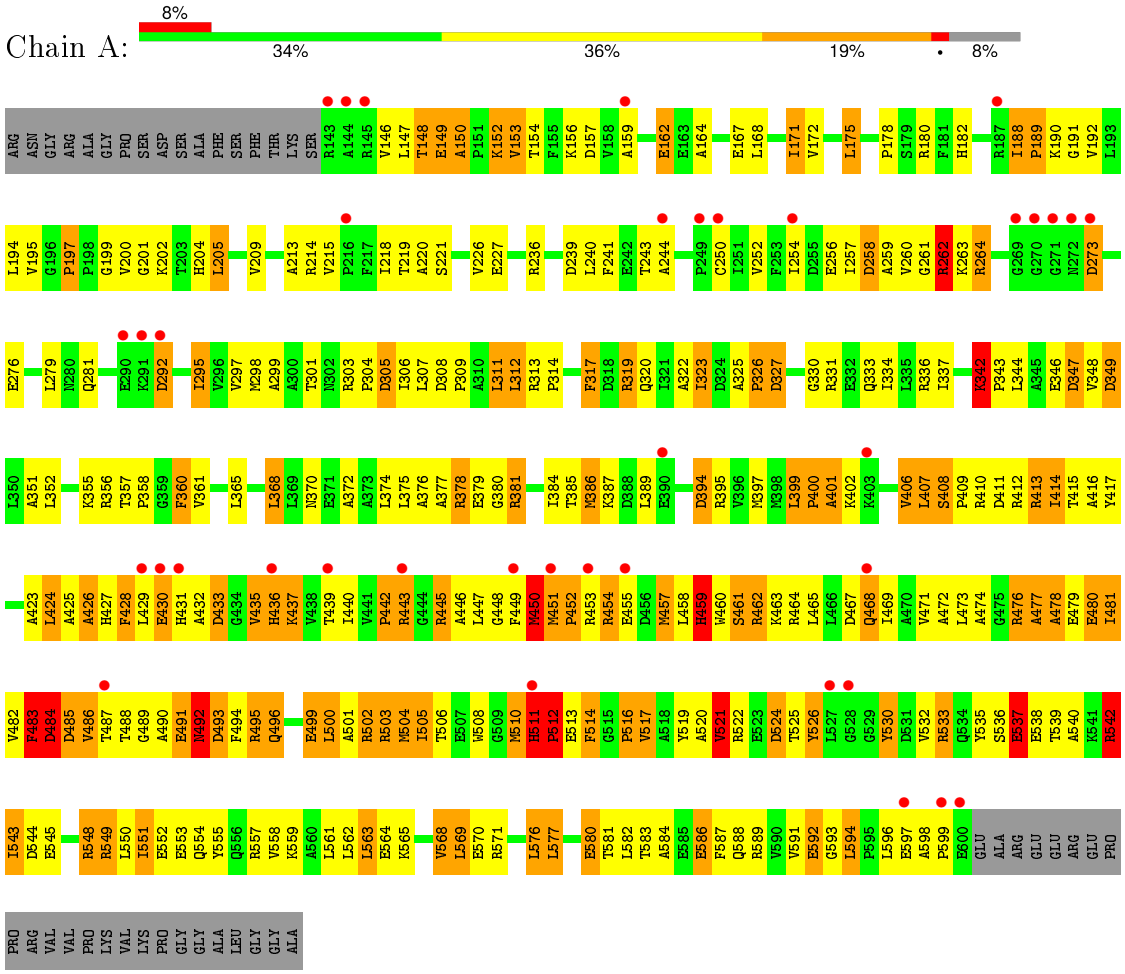
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

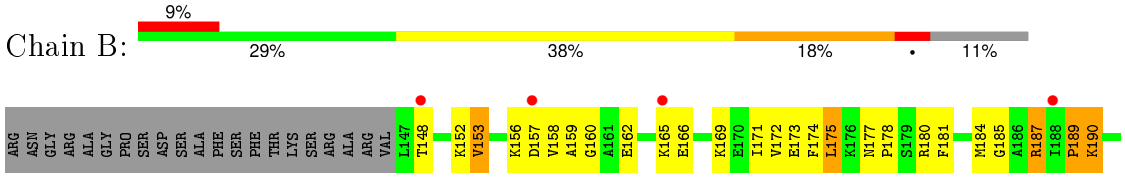
- Molecule 1: FtsH

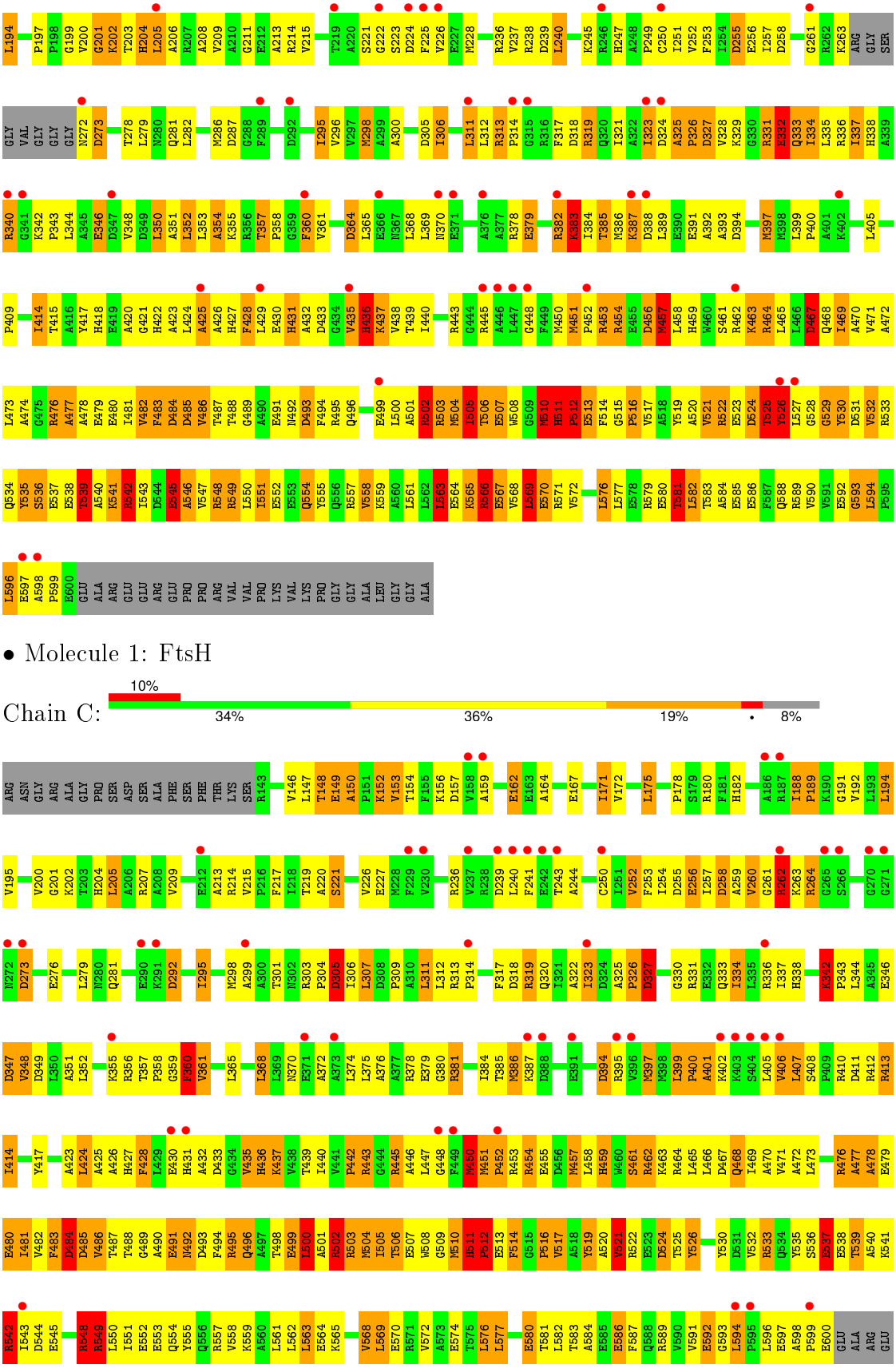
Chain A:



- Molecule 1: FtsH

Chain B:



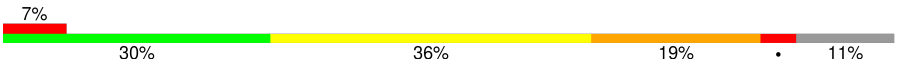


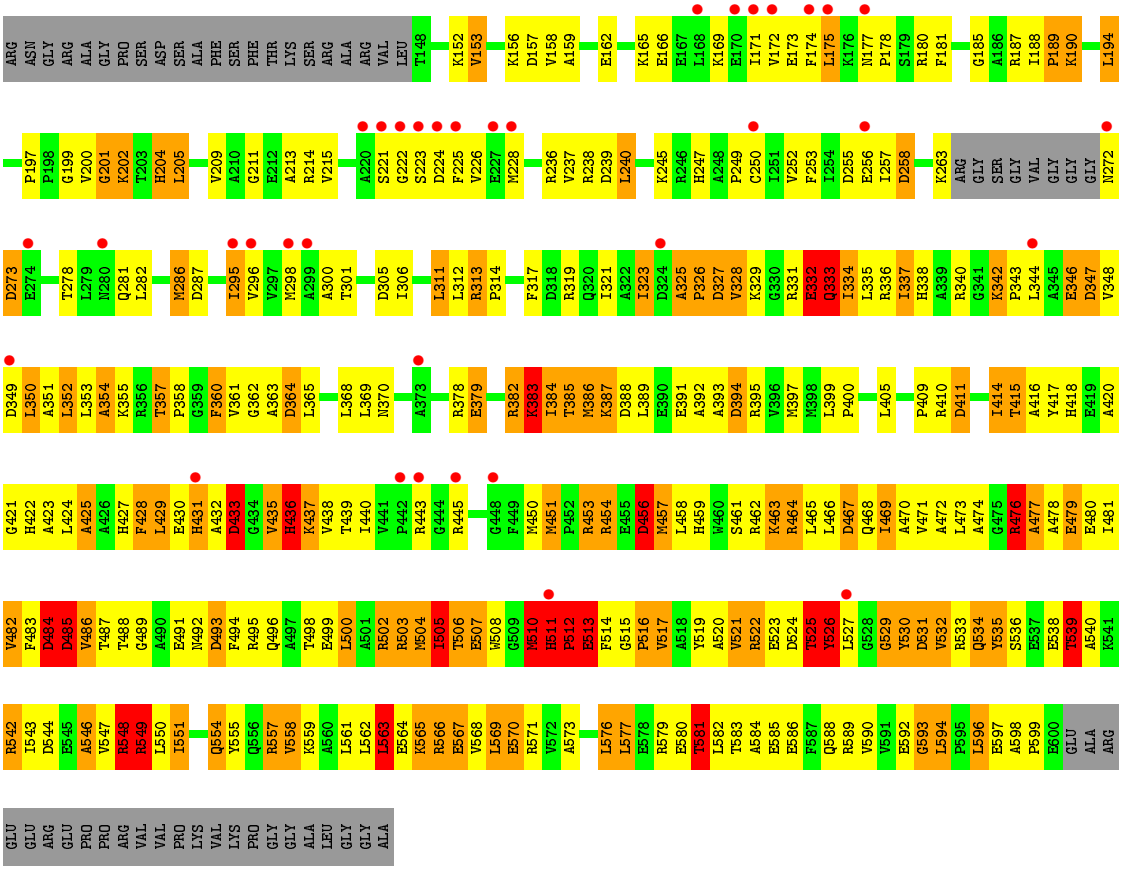
• Molecule 1: FtsH

Chain C:

- Molecule 1: FtsH

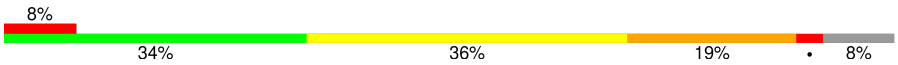
Chain D:

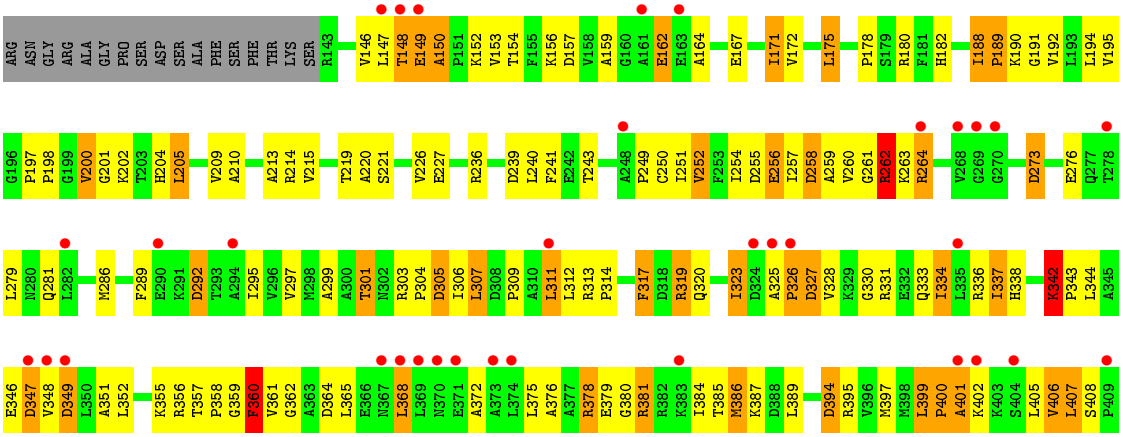


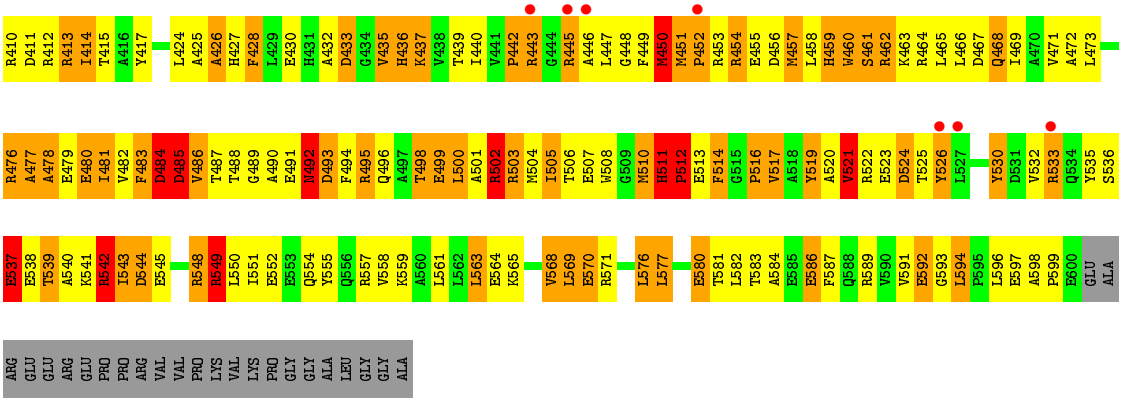


- Molecule 1: FtsH

Chain E:

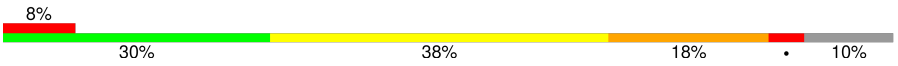


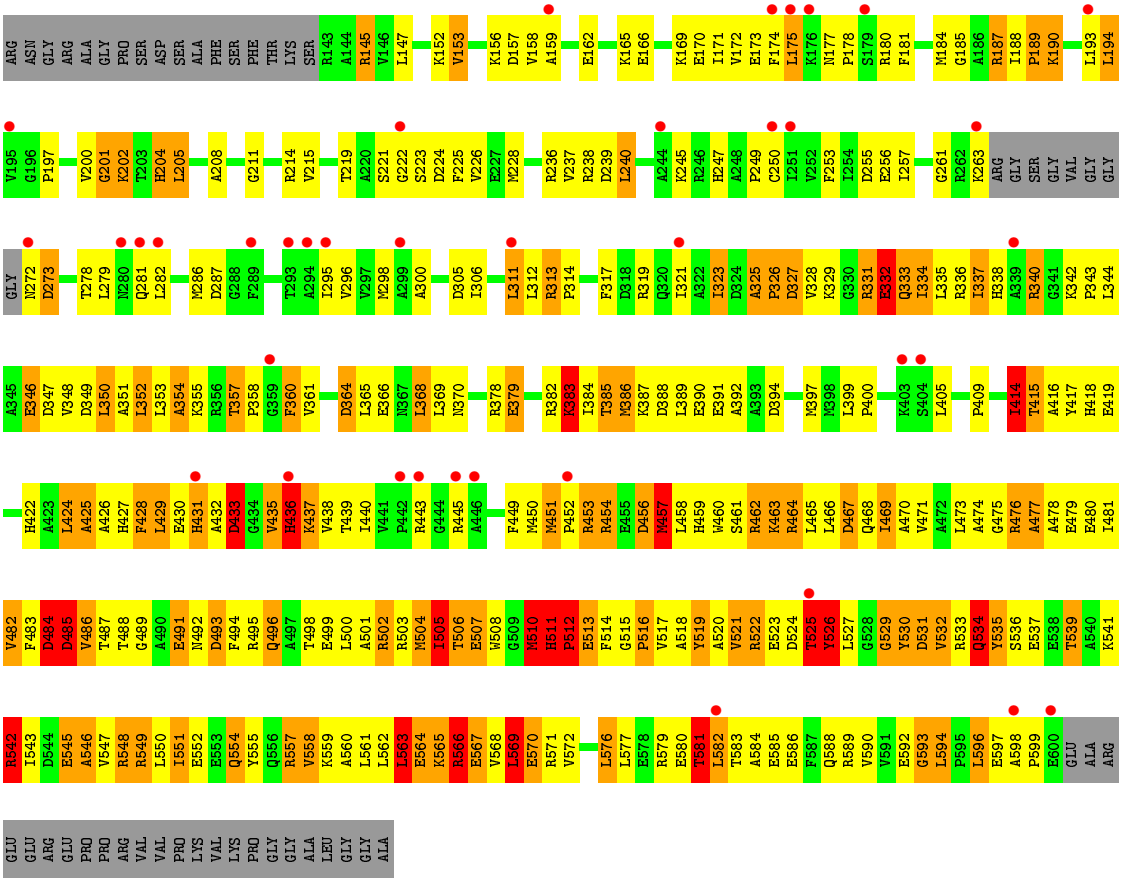




- Molecule 1: FtsH

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	146.15Å 146.15Å 349.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 3.90 73.08 – 3.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-3.90) 97.4 (73.08-3.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.79 (at 3.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.299 , 0.342 0.288 , 0.286	Depositor DCC
R_{free} test set	1960 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	97.6	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , -18.0	EDS
Estimated twinning fraction	0.247 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.27$, $< L^2 > = 0.11$	Xtriage
Outliers	0 of 39237 reflections	Xtriage
F_o,F_c correlation	0.71	EDS
Total number of atoms	21460	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.78	4/3637 (0.1%)	0.96	14/4908 (0.3%)
1	B	0.77	4/3568 (0.1%)	0.98	18/4815 (0.4%)
1	C	0.78	4/3641 (0.1%)	0.97	19/4913 (0.4%)
1	D	0.79	2/3560 (0.1%)	0.99	22/4804 (0.5%)
1	E	0.74	2/3641 (0.1%)	0.95	20/4913 (0.4%)
1	F	0.77	4/3596 (0.1%)	0.97	18/4853 (0.4%)
All	All	0.77	20/21643 (0.1%)	0.97	111/29206 (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	A	0	3
1	B	0	4
1	C	0	3
1	D	0	4
1	E	0	2
1	F	0	6
All	All	0	22

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	549	ARG	NE-CZ	7.12	1.42	1.33
1	C	553	GLU	CD-OE1	6.86	1.33	1.25
1	D	549	ARG	NE-CZ	6.80	1.41	1.33
1	C	537	GLU	CD-OE1	6.61	1.32	1.25
1	E	537	GLU	CD-OE1	6.42	1.32	1.25
1	A	553	GLU	CD-OE1	6.13	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	542	ARG	CB-CG	5.86	1.68	1.52
1	C	542	ARG	CB-CG	5.79	1.68	1.52
1	B	483	PHE	CB-CG	-5.62	1.41	1.51
1	B	502	ARG	NE-CZ	5.56	1.40	1.33
1	A	537	GLU	CD-OE1	5.54	1.31	1.25
1	B	549	ARG	NE-CZ	5.48	1.40	1.33
1	F	534	GLN	CG-CD	5.48	1.63	1.51
1	F	549	ARG	NE-CZ	5.46	1.40	1.33
1	A	483	PHE	CB-CG	-5.34	1.42	1.51
1	F	537	GLU	CD-OE1	5.21	1.31	1.25
1	D	538	GLU	CD-OE2	5.16	1.31	1.25
1	F	549	ARG	CG-CD	5.06	1.64	1.51
1	B	545	GLU	CG-CD	5.05	1.59	1.51
1	C	549	ARG	CG-CD	5.01	1.64	1.51

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	549	ARG	NE-CZ-NH1	11.19	125.89	120.30
1	C	493	ASP	CB-CG-OD2	8.24	125.72	118.30
1	E	493	ASP	CB-CG-OD2	7.17	124.75	118.30
1	F	549	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	C	548	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	493	ASP	CB-CG-OD2	6.59	124.24	118.30
1	F	485	ASP	CB-CG-OD2	6.43	124.09	118.30
1	D	544	ASP	CB-CG-OD2	6.43	124.08	118.30
1	D	411	ASP	CB-CG-OD2	6.39	124.05	118.30
1	A	157	ASP	CB-CG-OD2	6.33	124.00	118.30
1	D	364	ASP	CB-CG-OD2	6.27	123.95	118.30
1	E	157	ASP	CB-CG-OD2	6.27	123.94	118.30
1	B	484	ASP	CB-CG-OD2	6.23	123.90	118.30
1	F	493	ASP	CB-CG-OD2	6.19	123.87	118.30
1	D	549	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	E	524	ASP	CB-CG-OD2	6.18	123.86	118.30
1	D	531	ASP	CB-CG-OD2	6.13	123.82	118.30
1	D	476	ARG	NE-CZ-NH1	-6.11	117.25	120.30
1	B	436	HIS	N-CA-C	6.10	127.47	111.00
1	F	364	ASP	CB-CG-OD2	6.05	123.75	118.30
1	D	239	ASP	CB-CG-OD2	6.04	123.74	118.30
1	B	239	ASP	CB-CG-OD2	6.04	123.73	118.30
1	F	484	ASP	CB-CG-OD2	6.03	123.73	118.30
1	C	157	ASP	CB-CG-OD2	6.02	123.72	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	493	ASP	CB-CG-OD2	5.97	123.68	118.30
1	C	524	ASP	CB-CG-OD2	5.97	123.67	118.30
1	C	327	ASP	CB-CG-OD2	5.96	123.66	118.30
1	D	436	HIS	N-CA-C	5.96	127.09	111.00
1	C	258	ASP	CB-CG-OD2	5.94	123.65	118.30
1	F	436	HIS	N-CA-C	5.93	127.01	111.00
1	E	544	ASP	CB-CG-OD2	5.92	123.63	118.30
1	F	239	ASP	CB-CG-OD2	5.91	123.62	118.30
1	D	305	ASP	CB-CG-OD2	5.91	123.61	118.30
1	F	305	ASP	CB-CG-OD2	5.89	123.60	118.30
1	C	549	ARG	CA-CB-CG	5.86	126.30	113.40
1	B	563	LEU	CA-CB-CG	-5.84	101.87	115.30
1	D	485	ASP	CB-CG-OD2	5.82	123.53	118.30
1	B	467	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	433	ASP	CB-CG-OD2	5.79	123.52	118.30
1	B	364	ASP	CB-CG-OD2	5.79	123.51	118.30
1	C	548	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	D	273	ASP	CB-CG-OD2	5.72	123.45	118.30
1	E	549	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	E	549	ARG	CA-CB-CG	5.70	125.93	113.40
1	E	502	ARG	N-CA-CB	5.67	120.81	110.60
1	A	542	ARG	CA-CB-CG	5.64	125.81	113.40
1	A	510	MET	N-CA-C	-5.64	95.78	111.00
1	F	157	ASP	CB-CG-OD2	5.63	123.37	118.30
1	C	510	MET	N-CA-C	-5.63	95.80	111.00
1	B	502	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	324	ASP	CB-CG-OD2	5.61	123.35	118.30
1	F	462	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	349	ASP	CB-CG-OD2	5.56	123.30	118.30
1	F	273	ASP	CB-CG-OD2	5.53	123.28	118.30
1	D	484	ASP	CB-CG-OD2	5.52	123.27	118.30
1	D	157	ASP	CB-CG-OD2	5.52	123.27	118.30
1	B	549	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	C	509	GLY	N-CA-C	-5.49	99.38	113.10
1	E	273	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	292	ASP	CB-CG-OD2	5.43	123.19	118.30
1	F	550	LEU	CA-CB-CG	5.43	127.80	115.30
1	A	543	ILE	CG1-CB-CG2	-5.42	99.47	111.40
1	F	531	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	157	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	305	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	273	ASP	CB-CG-OD2	5.39	123.15	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	292	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	258	ASP	CB-CG-OD2	5.37	123.13	118.30
1	C	273	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	394	ASP	CB-CG-OD2	5.35	123.12	118.30
1	D	258	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	273	ASP	CB-CG-OD2	5.35	123.11	118.30
1	E	347	ASP	CB-CG-OD2	5.33	123.09	118.30
1	E	542	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	255	ASP	CB-CG-OD2	5.30	123.07	118.30
1	E	364	ASP	CB-CG-OD2	5.29	123.07	118.30
1	E	394	ASP	CB-CG-OD2	5.28	123.05	118.30
1	D	550	LEU	CA-CB-CG	5.27	127.42	115.30
1	E	543	ILE	CB-CA-C	-5.26	101.08	111.60
1	E	292	ASP	CB-CG-OD2	5.25	123.02	118.30
1	F	433	ASP	CB-CG-OD2	5.23	123.01	118.30
1	C	394	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	327	ASP	CB-CG-OD2	5.20	122.98	118.30
1	D	456	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	542	ARG	CA-CB-CG	5.18	124.80	113.40
1	C	500	LEU	CB-CG-CD1	-5.16	102.23	111.00
1	E	305	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	258	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	524	ASP	CB-CG-OD2	5.15	122.94	118.30
1	F	563	LEU	CA-CB-CG	-5.14	103.47	115.30
1	E	349	ASP	CB-CG-OD2	5.14	122.92	118.30
1	C	347	ASP	CB-CG-OD2	5.14	122.92	118.30
1	E	498	THR	OG1-CB-CG2	-5.13	98.20	110.00
1	C	305	ASP	CB-CG-OD2	5.12	122.91	118.30
1	D	493	ASP	CB-CG-OD2	5.12	122.91	118.30
1	F	542	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	E	485	ASP	CB-CG-OD2	5.12	122.90	118.30
1	C	318	ASP	CB-CG-OD2	5.10	122.89	118.30
1	F	349	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	524	ASP	CB-CG-OD2	5.09	122.88	118.30
1	D	563	LEU	CA-CB-CG	-5.08	103.61	115.30
1	B	542	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	F	347	ASP	CB-CG-OD2	5.05	122.84	118.30
1	D	349	ASP	CB-CG-OD2	5.04	122.84	118.30
1	E	258	ASP	CB-CG-OD2	5.04	122.84	118.30
1	C	502	ARG	N-CA-CB	5.03	119.66	110.60
1	A	347	ASP	CB-CG-OD2	5.03	122.83	118.30
1	E	456	ASP	CB-CG-OD2	5.02	122.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	433	ASP	CB-CG-OD2	5.01	122.81	118.30
1	D	548	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	D	347	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	490	ALA	Peptide
1	A	511	HIS	Peptide
1	A	512	PRO	Peptide
1	B	457	MET	Peptide
1	B	505	ILE	Peptide
1	B	510	MET	Peptide
1	B	512	PRO	Peptide
1	C	490	ALA	Peptide
1	C	511	HIS	Peptide
1	C	512	PRO	Peptide
1	D	457	MET	Peptide
1	D	505	ILE	Peptide
1	D	510	MET	Peptide
1	D	512	PRO	Peptide
1	E	490	ALA	Peptide
1	E	511	HIS	Peptide
1	F	457	MET	Peptide
1	F	485	ASP	Peptide
1	F	505	ILE	Peptide
1	F	510	MET	Peptide
1	F	511	HIS	Peptide
1	F	512	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3579	0	3624	251	0
1	B	3511	0	3556	321	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3583	0	3628	252	0
1	D	3503	0	3545	314	0
1	E	3583	0	3628	240	0
1	F	3539	0	3585	318	0
2	A	27	0	12	2	0
2	B	27	0	12	6	0
2	C	27	0	12	1	0
2	D	27	0	12	7	0
2	E	27	0	12	1	0
2	F	27	0	12	4	0
All	All	21460	0	21638	1596	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 37.

All (1596) 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:D:502:ARG:CD	1:D:533:ARG:HH22	1.54	1.20
1:E:510:MET:O	1:E:512:PRO:HD2	1.41	1.17
1:F:502:ARG:CD	1:F:533:ARG:HH22	1.56	1.17
1:C:428:PHE:CD1	1:C:432:ALA:HB1	1.81	1.15
1:E:428:PHE:CD1	1:E:432:ALA:HB1	1.81	1.15
1:A:428:PHE:CD1	1:A:432:ALA:HB1	1.84	1.12
1:D:517:VAL:HG23	1:D:519:TYR:CE1	1.84	1.11
1:B:502:ARG:CD	1:B:533:ARG:HH22	1.66	1.08
1:B:510:MET:O	1:B:512:PRO:HD2	1.53	1.07
1:F:325:ALA:HB3	1:F:326:PRO:HD3	1.36	1.07
1:D:517:VAL:HG21	1:D:519:TYR:CZ	1.89	1.07
1:D:543:ILE:O	1:D:546:ALA:HB3	1.57	1.04
1:A:510:MET:O	1:A:512:PRO:HD2	1.56	1.04
1:D:505:ILE:HG23	1:D:514:PHE:HD1	1.23	1.04
1:D:517:VAL:CG2	1:D:519:TYR:CZ	2.42	1.03
1:D:325:ALA:HB3	1:D:326:PRO:HD3	1.36	1.03
1:B:325:ALA:HB3	1:B:326:PRO:HD3	1.37	1.02
1:F:335:LEU:HB3	1:F:350:LEU:HD22	1.41	1.02
1:D:510:MET:O	1:D:512:PRO:HD2	1.60	1.02
1:B:517:VAL:HG21	1:B:519:TYR:CZ	1.94	1.02
1:F:502:ARG:CD	1:F:533:ARG:NH2	2.23	1.00
1:B:517:VAL:HG23	1:B:519:TYR:CE1	1.95	1.00
1:D:502:ARG:CD	1:D:533:ARG:NH2	2.24	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:LEU:HB3	1:D:350:LEU:HD22	1.40	0.99
1:F:428:PHE:CD1	1:F:432:ALA:HB1	1.97	0.99
1:B:517:VAL:CG2	1:B:519:TYR:CZ	2.45	0.99
1:B:505:ILE:HG23	1:B:514:PHE:HD1	1.26	0.98
1:F:517:VAL:HG21	1:F:519:TYR:CZ	2.00	0.96
1:D:428:PHE:CD1	1:D:432:ALA:HB1	1.99	0.96
1:F:505:ILE:HG23	1:F:514:PHE:HD1	1.29	0.95
1:E:428:PHE:CE1	1:E:432:ALA:HB1	2.01	0.95
1:C:428:PHE:CE1	1:C:432:ALA:HB1	2.01	0.95
1:E:428:PHE:CD1	1:E:432:ALA:CB	2.48	0.95
1:D:502:ARG:HD3	1:D:533:ARG:NH2	1.81	0.95
1:F:517:VAL:HG23	1:F:519:TYR:CE1	2.01	0.95
1:B:428:PHE:CD1	1:B:432:ALA:HB1	2.00	0.95
1:F:502:ARG:CG	1:F:533:ARG:HH22	1.80	0.95
1:C:428:PHE:CD1	1:C:432:ALA:CB	2.50	0.94
1:B:470:ALA:HB2	1:B:554:GLN:HG3	1.48	0.94
1:C:516:PRO:HB2	1:D:494:PHE:CE2	2.01	0.94
1:E:510:MET:C	1:E:512:PRO:HD2	1.88	0.93
1:F:510:MET:O	1:F:512:PRO:HD2	1.68	0.93
1:B:335:LEU:HB3	1:B:350:LEU:HD22	1.48	0.93
1:F:502:ARG:HD3	1:F:533:ARG:NH2	1.84	0.93
1:B:189:PRO:O	1:B:190:LYS:HB2	1.69	0.92
1:E:505:ILE:HG23	1:E:514:PHE:HD1	1.31	0.92
1:F:335:LEU:HD13	1:F:353:LEU:HD23	1.50	0.91
1:F:517:VAL:CG2	1:F:519:TYR:CZ	2.54	0.91
1:F:483:PHE:O	1:F:485:ASP:N	2.03	0.91
1:F:476:ARG:CZ	1:F:487:THR:HG21	2.01	0.91
1:D:435:VAL:HG22	1:D:436:HIS:H	1.36	0.90
1:D:334:ILE:HD11	2:D:4001:ADP:C6	2.05	0.90
1:F:511:HIS:CE1	1:F:516:PRO:HD3	2.06	0.90
1:A:505:ILE:HG23	1:A:514:PHE:HD1	1.36	0.90
1:B:502:ARG:CD	1:B:533:ARG:NH2	2.33	0.90
1:B:511:HIS:CE1	1:B:516:PRO:HD3	2.06	0.90
1:B:483:PHE:O	1:B:485:ASP:N	2.03	0.90
1:A:483:PHE:O	1:A:485:ASP:N	2.03	0.89
1:A:428:PHE:CD1	1:A:432:ALA:CB	2.55	0.89
1:A:428:PHE:CE1	1:A:432:ALA:HB1	2.07	0.89
1:B:542:ARG:HA	1:B:542:ARG:HH11	1.37	0.89
1:E:483:PHE:O	1:E:485:ASP:N	2.04	0.89
1:D:476:ARG:CZ	1:D:487:THR:HG21	2.03	0.89
1:E:516:PRO:HB2	1:F:494:PHE:CE2	2.07	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:PRO:O	1:D:190:LYS:HB2	1.73	0.89
1:B:502:ARG:CG	1:B:533:ARG:HH22	1.86	0.88
1:A:467:ASP:O	1:A:471:VAL:HG23	1.74	0.88
1:D:483:PHE:O	1:D:485:ASP:N	2.05	0.88
1:F:502:ARG:HD3	1:F:533:ARG:HH22	1.38	0.88
1:A:513:GLU:O	1:B:548:ARG:NH2	2.07	0.87
1:F:554:GLN:HE22	1:F:557:ARG:HD3	1.37	0.87
1:D:335:LEU:HD13	1:D:353:LEU:HD23	1.57	0.87
1:B:335:LEU:HD13	1:B:353:LEU:HD23	1.54	0.87
1:B:337:ILE:HG22	1:B:338:HIS:HD2	1.39	0.87
1:A:399:LEU:H	1:A:400:PRO:HD2	1.39	0.87
1:D:502:ARG:CG	1:D:533:ARG:HH22	1.87	0.86
1:F:335:LEU:CD1	1:F:353:LEU:HD23	2.04	0.86
1:F:467:ASP:O	1:F:471:VAL:HG23	1.75	0.86
1:C:505:ILE:HG22	1:C:506:THR:HG23	1.55	0.86
1:D:517:VAL:CG2	1:D:519:TYR:CE1	2.58	0.86
1:D:502:ARG:HD3	1:D:533:ARG:HH22	1.36	0.86
1:F:543:ILE:O	1:F:546:ALA:HB3	1.76	0.85
1:C:548:ARG:HH11	1:C:548:ARG:HG3	1.39	0.85
1:B:476:ARG:NE	1:B:487:THR:HG21	1.92	0.85
1:D:503:ARG:NH1	1:D:522:ARG:HG3	1.92	0.85
1:C:399:LEU:H	1:C:400:PRO:HD2	1.42	0.85
1:B:476:ARG:CZ	1:B:487:THR:HG21	2.07	0.84
1:B:435:VAL:HG22	1:B:436:HIS:H	1.42	0.84
1:B:326:PRO:O	1:B:327:ASP:HB2	1.75	0.84
1:E:399:LEU:H	1:E:400:PRO:HD2	1.42	0.84
1:B:510:MET:C	1:B:512:PRO:HD2	1.98	0.83
1:D:197:PRO:HD2	1:D:200:VAL:HG21	1.57	0.83
1:B:502:ARG:HD3	1:B:533:ARG:NH2	1.93	0.83
1:D:511:HIS:CE1	1:D:516:PRO:HD3	2.14	0.83
1:D:539:THR:O	1:D:543:ILE:HD12	1.78	0.83
1:F:542:ARG:HH11	1:F:542:ARG:HG2	1.44	0.83
1:C:195:VAL:HG21	1:C:304:PRO:HB3	1.61	0.82
1:E:505:ILE:HG22	1:E:506:THR:N	1.92	0.82
1:E:195:VAL:HG21	1:E:304:PRO:HB3	1.61	0.82
1:C:450:MET:HG3	1:C:451:MET:H	1.45	0.82
1:F:470:ALA:HB2	1:F:554:GLN:HG3	1.62	0.81
1:C:520:ALA:HA	1:C:533:ARG:HB2	1.60	0.81
1:E:537:GLU:O	1:E:540:ALA:HB3	1.79	0.81
1:F:337:ILE:HG22	1:F:338:HIS:HD2	1.45	0.81
1:D:335:LEU:CD1	1:D:353:LEU:HD23	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:LYS:HD2	1:B:486:VAL:CG1	2.11	0.81
1:D:337:ILE:HG22	1:D:338:HIS:HD2	1.42	0.81
1:F:458:LEU:HD12	1:F:459:HIS:H	1.45	0.81
1:C:476:ARG:CZ	1:C:487:THR:HG21	2.11	0.81
1:A:537:GLU:O	1:A:540:ALA:HB3	1.81	0.81
1:D:420:ALA:O	1:D:421:GLY:C	2.17	0.81
1:D:505:ILE:HG23	1:D:514:PHE:CD1	2.14	0.81
1:C:330:GLY:O	1:C:334:ILE:HG12	1.81	0.80
1:C:505:ILE:HG23	1:C:514:PHE:HD1	1.46	0.80
1:A:516:PRO:HB2	1:B:494:PHE:CE2	2.17	0.80
1:A:195:VAL:HG21	1:A:304:PRO:HB3	1.64	0.80
1:B:542:ARG:HA	1:B:542:ARG:NH1	1.95	0.80
1:F:435:VAL:HG22	1:F:436:HIS:H	1.44	0.80
1:E:159:ALA:HB3	1:E:334:ILE:HD13	1.64	0.80
1:D:517:VAL:HG21	1:D:519:TYR:OH	1.81	0.79
1:C:159:ALA:HB3	1:C:334:ILE:HD13	1.64	0.79
1:F:422:HIS:O	1:F:425:ALA:HB3	1.83	0.79
1:B:458:LEU:HD12	1:B:459:HIS:H	1.48	0.79
1:E:520:ALA:HA	1:E:533:ARG:HB2	1.63	0.79
1:A:520:ALA:HA	1:A:533:ARG:HB2	1.64	0.79
1:E:511:HIS:CE1	1:E:516:PRO:HD3	2.18	0.79
1:F:189:PRO:O	1:F:190:LYS:HB2	1.83	0.79
1:A:188:ILE:HD13	1:A:189:PRO:HD2	1.65	0.79
1:B:197:PRO:HD2	1:B:200:VAL:HG21	1.64	0.78
1:D:199:GLY:O	1:D:361:VAL:HB	1.83	0.78
1:B:467:ASP:O	1:B:471:VAL:HG23	1.83	0.78
1:B:502:ARG:HD3	1:B:533:ARG:HH22	1.49	0.78
1:D:332:GLU:OE1	1:D:351:ALA:HA	1.83	0.78
1:F:325:ALA:CB	1:F:326:PRO:HD3	2.13	0.78
1:D:510:MET:C	1:D:512:PRO:HD2	2.04	0.78
1:B:463:LYS:HB2	1:C:486:VAL:HG11	1.65	0.78
1:D:542:ARG:HH11	1:D:542:ARG:HG2	1.47	0.78
1:A:483:PHE:C	1:A:485:ASP:H	1.86	0.78
1:B:548:ARG:HG3	1:B:548:ARG:HH11	1.47	0.78
1:F:197:PRO:HD2	1:F:200:VAL:HG21	1.64	0.78
1:C:565:LYS:O	1:C:568:VAL:HG23	1.84	0.78
1:A:505:ILE:HG23	1:A:514:PHE:CD1	2.19	0.78
1:E:365:LEU:O	1:E:368:LEU:HB3	1.84	0.78
1:F:554:GLN:NE2	1:F:557:ARG:HD3	1.99	0.77
1:C:510:MET:O	1:C:512:PRO:HD2	1.83	0.77
1:E:505:ILE:HG23	1:E:514:PHE:CD1	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:332:GLU:OE1	1:F:351:ALA:HA	1.84	0.77
1:F:526:TYR:H	1:F:526:TYR:HD1	1.33	0.77
1:B:543:ILE:O	1:B:546:ALA:HB3	1.84	0.77
1:C:548:ARG:NH1	1:C:548:ARG:HG3	1.98	0.77
1:F:511:HIS:CE1	1:F:516:PRO:CD	2.68	0.77
1:D:470:ALA:HB2	1:D:554:GLN:HG3	1.67	0.77
1:C:483:PHE:O	1:C:485:ASP:N	2.17	0.77
1:B:503:ARG:NH1	1:B:522:ARG:HG3	2.00	0.76
1:A:505:ILE:HG22	1:A:506:THR:N	1.98	0.76
1:D:326:PRO:HB2	1:D:331:ARG:HH12	1.50	0.76
1:F:569:LEU:O	1:F:571:ARG:N	2.18	0.76
1:E:357:THR:HG23	1:E:357:THR:O	1.85	0.76
1:A:510:MET:C	1:A:512:PRO:HD2	2.05	0.76
1:A:450:MET:HG3	1:A:451:MET:H	1.50	0.76
1:E:565:LYS:O	1:E:568:VAL:HG23	1.85	0.76
1:F:514:PHE:HE2	1:F:542:ARG:NE	1.84	0.76
1:B:548:ARG:CG	1:B:548:ARG:HH11	1.97	0.76
1:F:476:ARG:NE	1:F:487:THR:HG21	1.99	0.76
1:E:330:GLY:O	1:E:334:ILE:HG12	1.84	0.76
1:D:326:PRO:CB	1:D:331:ARG:HH12	1.98	0.76
1:C:447:LEU:HA	1:C:496:GLN:NE2	2.01	0.75
1:F:503:ARG:HB3	1:F:508:TRP:CZ3	2.22	0.75
1:A:330:GLY:O	1:A:334:ILE:HG12	1.86	0.75
1:E:450:MET:HG3	1:E:451:MET:H	1.52	0.75
1:B:332:GLU:OE1	1:B:351:ALA:HA	1.86	0.75
1:C:188:ILE:HD13	1:C:189:PRO:HD2	1.68	0.75
1:B:325:ALA:CB	1:B:326:PRO:HD3	2.16	0.75
1:C:502:ARG:O	1:C:506:THR:OG1	2.05	0.75
1:F:548:ARG:HH11	1:F:548:ARG:CG	2.00	0.75
1:B:199:GLY:O	1:B:361:VAL:HB	1.87	0.75
1:B:548:ARG:NH1	1:B:548:ARG:HG3	2.00	0.74
1:D:542:ARG:HA	1:D:542:ARG:HH11	1.51	0.74
1:B:517:VAL:HG23	1:B:519:TYR:CZ	2.20	0.74
1:D:325:ALA:CB	1:D:326:PRO:HD3	2.15	0.74
1:C:473:LEU:HD13	1:C:555:TYR:HB2	1.70	0.74
1:E:463:LYS:HD2	1:F:486:VAL:CG1	2.16	0.74
1:D:428:PHE:CE1	1:D:432:ALA:HB1	2.22	0.74
1:E:505:ILE:HG22	1:E:506:THR:HG23	1.69	0.74
1:F:542:ARG:HH11	1:F:542:ARG:HA	1.51	0.74
1:A:505:ILE:HG22	1:A:506:THR:HG23	1.70	0.74
1:A:516:PRO:HB2	1:B:494:PHE:CD2	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:516:PRO:HB2	1:D:494:PHE:CD2	2.21	0.74
1:B:479:GLU:OE2	1:B:487:THR:HA	1.87	0.74
1:F:428:PHE:CE1	1:F:432:ALA:HB1	2.23	0.74
1:A:447:LEU:HA	1:A:496:GLN:NE2	2.03	0.74
1:B:505:ILE:HG23	1:B:514:PHE:CD1	2.18	0.73
1:B:542:ARG:HH11	1:B:542:ARG:CG	2.01	0.73
1:E:483:PHE:C	1:E:485:ASP:H	1.91	0.73
1:D:542:ARG:HA	1:D:542:ARG:NH1	2.04	0.73
1:B:334:ILE:HD11	2:B:2001:ADP:C6	2.23	0.73
1:A:425:ALA:O	1:A:427:HIS:N	2.20	0.73
1:E:188:ILE:HD13	1:E:189:PRO:HD2	1.71	0.73
1:C:505:ILE:HG22	1:C:506:THR:N	2.02	0.73
1:C:463:LYS:HD2	1:D:486:VAL:CG1	2.19	0.73
1:D:542:ARG:CG	1:D:542:ARG:HH11	2.01	0.73
1:E:548:ARG:HG3	1:E:548:ARG:HH11	1.53	0.73
1:B:428:PHE:CE1	1:B:432:ALA:HB1	2.24	0.73
1:A:565:LYS:O	1:A:568:VAL:HG23	1.89	0.73
1:F:428:PHE:CD1	1:F:428:PHE:N	2.57	0.72
1:C:510:MET:C	1:C:512:PRO:HD2	2.10	0.72
1:E:525:THR:HG22	1:E:526:TYR:H	1.54	0.72
1:A:357:THR:HG23	1:A:357:THR:O	1.88	0.72
1:A:331:ARG:HD3	1:A:357:THR:O	1.90	0.72
1:E:447:LEU:HA	1:E:496:GLN:NE2	2.04	0.72
1:D:171:ILE:CG2	1:D:296:VAL:HG21	2.19	0.72
1:A:554:GLN:HE22	1:A:557:ARG:CZ	2.01	0.72
1:E:467:ASP:O	1:E:471:VAL:HG23	1.89	0.72
1:E:502:ARG:O	1:E:506:THR:OG1	2.07	0.72
1:F:510:MET:C	1:F:512:PRO:HD2	2.09	0.72
1:F:542:ARG:CG	1:F:542:ARG:HH11	2.02	0.72
1:D:526:TYR:H	1:D:526:TYR:HD1	1.36	0.72
1:E:476:ARG:CZ	1:E:487:THR:HG21	2.20	0.72
1:E:331:ARG:HD3	1:E:357:THR:O	1.90	0.72
1:B:159:ALA:HB1	1:B:333:GLN:HB3	1.71	0.72
1:B:542:ARG:HH11	1:B:542:ARG:HG2	1.52	0.71
1:A:406:VAL:HG12	1:A:407:LEU:H	1.54	0.71
1:D:514:PHE:HE2	1:D:542:ARG:NE	1.86	0.71
1:F:502:ARG:HD2	1:F:533:ARG:NH2	2.04	0.71
1:B:515:GLY:O	1:B:517:VAL:N	2.22	0.71
1:D:502:ARG:HD2	1:D:533:ARG:HH22	1.55	0.71
1:F:348:VAL:HG22	1:F:352:LEU:HB3	1.71	0.71
1:C:357:THR:HG23	1:C:357:THR:O	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:ASP:C	1:A:486:VAL:H	1.93	0.71
1:D:503:ARG:HB3	1:D:508:TRP:CZ3	2.25	0.71
1:F:517:VAL:HG21	1:F:519:TYR:OH	1.88	0.71
1:F:548:ARG:HG3	1:F:548:ARG:HH11	1.56	0.71
1:E:513:GLU:O	1:F:548:ARG:NH2	2.24	0.71
1:D:477:ALA:O	1:D:478:ALA:C	2.29	0.71
1:A:494:PHE:HE2	1:F:516:PRO:HB3	1.54	0.71
1:B:451:MET:HB2	1:C:402:LYS:HE2	1.72	0.71
1:E:220:ALA:O	1:E:254:ILE:HA	1.90	0.71
1:B:424:LEU:O	1:B:427:HIS:N	2.20	0.71
1:C:516:PRO:CB	1:D:494:PHE:CE2	2.73	0.71
1:B:282:LEU:O	1:B:286:MET:HG3	1.91	0.70
1:C:480:GLU:HG2	1:C:559:LYS:HD2	1.71	0.70
1:F:517:VAL:CG2	1:F:519:TYR:CE1	2.74	0.70
1:B:335:LEU:CD1	1:B:353:LEU:HD23	2.21	0.70
1:F:503:ARG:NH1	1:F:522:ARG:HG3	2.06	0.70
1:A:511:HIS:CE1	1:A:516:PRO:HD3	2.25	0.70
1:B:526:TYR:H	1:B:526:TYR:HD1	1.37	0.70
1:D:463:LYS:HB2	1:E:486:VAL:HG11	1.73	0.70
1:D:517:VAL:CG2	1:D:519:TYR:OH	2.39	0.70
1:F:325:ALA:HB1	1:F:361:VAL:HG12	1.72	0.70
1:F:424:LEU:HD22	1:F:569:LEU:HD23	1.74	0.70
1:E:425:ALA:O	1:E:427:HIS:N	2.23	0.70
1:F:548:ARG:HG3	1:F:548:ARG:NH1	2.06	0.70
1:A:313:ARG:NH1	1:A:525:THR:O	2.25	0.70
1:A:428:PHE:N	1:A:428:PHE:CD1	2.60	0.69
1:C:537:GLU:O	1:C:540:ALA:HB3	1.92	0.69
1:D:282:LEU:O	1:D:286:MET:HG3	1.92	0.69
1:B:476:ARG:NE	1:B:487:THR:CG2	2.54	0.69
1:A:476:ARG:CZ	1:A:487:THR:HG21	2.22	0.69
1:D:511:HIS:CE1	1:D:516:PRO:CD	2.75	0.69
1:E:516:PRO:CB	1:F:494:PHE:CE2	2.75	0.69
1:B:503:ARG:HB3	1:B:508:TRP:CZ3	2.26	0.69
1:A:378:ARG:NH2	1:F:169:LYS:HB2	2.08	0.69
1:D:505:ILE:CG2	1:D:514:PHE:HD1	2.01	0.69
1:C:428:PHE:CD1	1:C:428:PHE:N	2.58	0.69
1:D:357:THR:OG1	1:D:360:PHE:CD2	2.46	0.69
1:C:505:ILE:HG23	1:C:514:PHE:CD1	2.28	0.69
1:B:348:VAL:HG22	1:B:352:LEU:HB3	1.75	0.68
1:D:334:ILE:CG2	1:D:365:LEU:HD13	2.22	0.68
1:A:463:LYS:HD2	1:B:486:VAL:HG13	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:VAL:HG11	1:F:463:LYS:HB2	1.75	0.68
1:E:548:ARG:HG3	1:E:548:ARG:NH1	2.08	0.68
1:A:463:LYS:HD2	1:B:486:VAL:CG2	2.23	0.68
1:D:337:ILE:HG22	1:D:338:HIS:CD2	2.28	0.68
1:D:500:LEU:O	1:D:503:ARG:N	2.26	0.68
1:D:521:VAL:HG23	1:D:532:VAL:HG12	1.74	0.68
1:C:481:ILE:HG22	1:C:482:VAL:N	2.07	0.68
1:F:369:LEU:HD23	1:F:389:LEU:HD21	1.74	0.68
1:D:348:VAL:HG22	1:D:352:LEU:HB3	1.76	0.68
1:E:516:PRO:HB2	1:F:494:PHE:CD2	2.28	0.68
1:F:473:LEU:C	1:F:475:GLY:H	1.98	0.68
1:F:470:ALA:O	1:F:558:VAL:HG11	1.94	0.68
1:F:517:VAL:HG23	1:F:519:TYR:CZ	2.27	0.67
1:F:481:ILE:HG22	1:F:482:VAL:N	2.09	0.67
1:B:542:ARG:CA	1:B:542:ARG:HH11	2.05	0.67
1:D:479:GLU:OE2	1:D:487:THR:HA	1.94	0.67
1:B:511:HIS:O	1:B:512:PRO:O	2.11	0.67
1:A:525:THR:HG22	1:A:526:TYR:H	1.59	0.67
1:E:583:THR:O	1:E:586:GLU:HB2	1.95	0.67
1:C:548:ARG:CG	1:C:548:ARG:HH11	2.07	0.67
1:D:326:PRO:O	1:D:327:ASP:HB2	1.94	0.67
1:A:305:ASP:OD2	1:A:447:LEU:HD13	1.93	0.67
1:B:174:PHE:HB2	1:B:181:PHE:CE2	2.29	0.67
1:B:428:PHE:CD1	1:B:428:PHE:N	2.63	0.67
1:D:458:LEU:HD12	1:D:459:HIS:H	1.59	0.67
1:C:372:ALA:O	1:C:375:LEU:HB2	1.95	0.67
1:E:469:ILE:HG12	1:E:500:LEU:HD12	1.77	0.67
1:B:513:GLU:O	1:C:548:ARG:NH2	2.28	0.67
1:A:399:LEU:N	1:A:400:PRO:HD2	2.10	0.67
1:E:473:LEU:HD13	1:E:555:TYR:HB2	1.76	0.67
1:D:502:ARG:HD2	1:D:533:ARG:NH2	2.08	0.67
1:E:428:PHE:CG	1:E:432:ALA:CB	2.77	0.67
1:B:511:HIS:CE1	1:B:516:PRO:CD	2.76	0.66
1:D:507:GLU:HG3	1:D:520:ALA:HB3	1.77	0.66
1:F:424:LEU:O	1:F:425:ALA:C	2.31	0.66
1:B:171:ILE:CG2	1:B:296:VAL:HG21	2.25	0.66
1:E:241:PHE:HE2	1:E:252:VAL:HG21	1.60	0.66
1:F:326:PRO:HB2	1:F:331:ARG:HH12	1.59	0.66
1:D:334:ILE:HG21	1:D:365:LEU:CD1	2.26	0.66
1:B:337:ILE:HG22	1:B:338:HIS:CD2	2.27	0.66
1:C:428:PHE:CG	1:C:432:ALA:CB	2.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:501:ALA:O	1:C:504:MET:HB2	1.96	0.66
1:D:399:LEU:H	1:D:400:PRO:HD2	1.60	0.66
1:C:513:GLU:O	1:D:548:ARG:NH2	2.28	0.66
1:A:462:ARG:NH1	1:A:510:MET:HB3	2.10	0.66
1:D:476:ARG:NE	1:D:487:THR:HG21	2.09	0.66
1:C:483:PHE:C	1:C:485:ASP:H	1.99	0.66
1:A:261:GLY:O	1:A:262:ARG:HB2	1.95	0.66
1:F:171:ILE:CG2	1:F:296:VAL:HG21	2.26	0.66
1:D:334:ILE:HD11	2:D:4001:ADP:C5	2.31	0.66
1:C:463:LYS:HD2	1:D:486:VAL:HG13	1.76	0.66
1:E:439:THR:OG1	1:E:581:THR:HG23	1.96	0.66
1:F:542:ARG:NH1	1:F:542:ARG:HA	2.10	0.66
1:B:503:ARG:NH1	1:B:507:GLU:OE1	2.29	0.66
1:C:469:ILE:HG12	1:C:500:LEU:HD12	1.78	0.66
1:C:447:LEU:HA	1:C:496:GLN:HE22	1.60	0.66
1:B:517:VAL:HG21	1:B:519:TYR:OH	1.96	0.65
1:C:406:VAL:HG12	1:C:407:LEU:H	1.61	0.65
1:F:543:ILE:O	1:F:547:VAL:HG23	1.96	0.65
1:E:469:ILE:O	1:E:472:ALA:HB3	1.97	0.65
1:E:399:LEU:N	1:E:400:PRO:HD2	2.09	0.65
1:F:282:LEU:O	1:F:286:MET:HG3	1.96	0.65
1:B:521:VAL:HG23	1:B:532:VAL:HG12	1.78	0.65
1:B:501:ALA:HA	1:B:504:MET:HE2	1.78	0.65
1:C:516:PRO:HB2	1:D:494:PHE:HE2	1.57	0.65
1:A:365:LEU:O	1:A:368:LEU:HB3	1.96	0.65
1:C:220:ALA:O	1:C:254:ILE:HA	1.96	0.65
1:F:334:ILE:CG2	1:F:365:LEU:HD13	2.26	0.65
1:C:241:PHE:HE2	1:C:252:VAL:HG21	1.61	0.65
1:B:511:HIS:C	1:B:512:PRO:O	2.35	0.65
1:E:484:ASP:C	1:E:486:VAL:H	2.00	0.65
1:B:201:GLY:HA2	2:B:2001:ADP:N7	2.11	0.65
1:F:514:PHE:HE2	1:F:542:ARG:CZ	2.08	0.65
1:F:428:PHE:CG	1:F:432:ALA:HB1	2.32	0.65
1:B:473:LEU:HD11	1:B:551:ILE:HG12	1.78	0.65
1:B:353:LEU:O	1:B:357:THR:HG22	1.97	0.65
1:A:450:MET:HG3	1:A:451:MET:N	2.11	0.65
1:D:424:LEU:O	1:D:425:ALA:C	2.36	0.65
1:D:467:ASP:O	1:D:471:VAL:HG23	1.97	0.65
1:F:399:LEU:H	1:F:400:PRO:HD2	1.61	0.65
1:F:476:ARG:NE	1:F:487:THR:CG2	2.59	0.64
1:F:481:ILE:HD11	1:F:559:LYS:HG3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ALA:O	1:A:254:ILE:HA	1.98	0.64
1:D:515:GLY:O	1:D:517:VAL:N	2.30	0.64
1:D:348:VAL:HG12	1:D:350:LEU:H	1.61	0.64
1:A:435:VAL:HG23	1:A:436:HIS:N	2.12	0.64
1:A:592:GLU:O	1:A:594:LEU:HD12	1.98	0.64
1:A:477:ALA:O	1:A:478:ALA:C	2.36	0.64
1:F:334:ILE:HG21	1:F:365:LEU:CD1	2.26	0.64
1:F:505:ILE:HG23	1:F:514:PHE:CD1	2.22	0.64
1:B:516:PRO:O	1:C:494:PHE:CD2	2.51	0.64
1:F:507:GLU:HG3	1:F:520:ALA:HB3	1.80	0.64
1:A:511:HIS:NE2	1:B:552:GLU:OE2	2.22	0.64
1:C:435:VAL:HG23	1:C:436:HIS:N	2.13	0.64
1:D:503:ARG:HH12	1:D:522:ARG:HG3	1.62	0.64
1:E:520:ALA:HA	1:E:533:ARG:CB	2.28	0.64
1:A:465:LEU:O	1:A:469:ILE:HG13	1.98	0.64
1:C:450:MET:HG3	1:C:451:MET:N	2.10	0.64
1:D:171:ILE:HG21	1:D:296:VAL:HG11	1.80	0.64
1:E:463:LYS:HD2	1:F:486:VAL:CG2	2.28	0.64
1:F:334:ILE:HG21	1:F:365:LEU:HD13	1.79	0.64
1:C:583:THR:O	1:C:586:GLU:HB2	1.98	0.64
1:A:583:THR:O	1:A:586:GLU:HB2	1.98	0.64
1:D:428:PHE:N	1:D:428:PHE:CD1	2.63	0.63
1:B:399:LEU:H	1:B:400:PRO:HD2	1.62	0.63
1:B:516:PRO:HB3	1:C:494:PHE:HE2	1.63	0.63
1:E:516:PRO:HB2	1:F:494:PHE:HE2	1.62	0.63
1:F:479:GLU:OE2	1:F:487:THR:HA	1.98	0.63
1:F:500:LEU:O	1:F:503:ARG:N	2.31	0.63
1:D:174:PHE:HB2	1:D:181:PHE:CE2	2.34	0.63
1:E:261:GLY:HA3	1:E:307:LEU:CD1	2.28	0.63
1:D:503:ARG:HH12	1:D:531:ASP:HB3	1.63	0.63
1:F:506:THR:HG22	1:F:507:GLU:HB2	1.78	0.63
1:D:357:THR:OG1	1:D:360:PHE:HD2	1.78	0.63
1:C:525:THR:HG22	1:C:526:TYR:H	1.64	0.63
1:B:539:THR:O	1:B:543:ILE:HD12	1.99	0.63
1:C:461:SER:O	1:C:464:ARG:N	2.31	0.63
1:F:519:TYR:HB3	1:F:535:TYR:HD2	1.63	0.63
1:D:326:PRO:HB3	1:D:331:ARG:NH1	2.14	0.63
1:C:484:ASP:C	1:C:486:VAL:H	2.02	0.63
1:E:480:GLU:HG2	1:E:559:LYS:HD2	1.80	0.63
1:B:565:LYS:HD2	1:B:568:VAL:HG21	1.81	0.63
1:E:428:PHE:N	1:E:428:PHE:CD1	2.65	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:463:LYS:HD2	1:F:486:VAL:HG13	1.80	0.63
1:B:428:PHE:CG	1:B:432:ALA:HB1	2.33	0.62
1:E:372:ALA:O	1:E:375:LEU:HB2	1.99	0.62
1:D:451:MET:HB2	1:E:402:LYS:HE2	1.80	0.62
1:B:543:ILE:O	1:B:547:VAL:HG23	1.98	0.62
1:E:503:ARG:HB3	1:E:508:TRP:CZ3	2.34	0.62
1:C:467:ASP:O	1:C:471:VAL:HG23	2.00	0.62
1:F:539:THR:HA	1:F:542:ARG:HB2	1.80	0.62
1:A:447:LEU:HA	1:A:496:GLN:HE22	1.63	0.62
1:C:200:VAL:HG22	1:C:325:ALA:HB3	1.80	0.62
1:A:494:PHE:CE2	1:F:516:PRO:HB3	2.34	0.62
1:E:501:ALA:O	1:E:505:ILE:HD12	2.00	0.62
1:C:331:ARG:HD3	1:C:357:THR:O	1.99	0.62
1:A:516:PRO:CB	1:B:494:PHE:CE2	2.82	0.62
1:D:476:ARG:NE	1:D:487:THR:CG2	2.62	0.62
1:D:201:GLY:HA2	2:D:4001:ADP:N7	2.15	0.62
1:A:402:LYS:HE2	1:F:451:MET:HB2	1.81	0.62
1:C:261:GLY:O	1:C:262:ARG:HB2	1.98	0.62
1:C:399:LEU:N	1:C:400:PRO:HD2	2.11	0.62
1:E:447:LEU:HA	1:E:496:GLN:HE22	1.63	0.62
1:B:175:LEU:HD11	1:B:250:CYS:O	1.99	0.62
1:B:171:ILE:HG21	1:B:296:VAL:HG11	1.81	0.62
1:E:548:ARG:CG	1:E:548:ARG:HH11	2.13	0.62
1:A:461:SER:O	1:A:464:ARG:N	2.33	0.62
1:B:458:LEU:CB	1:C:405:LEU:HD13	2.29	0.62
1:F:503:ARG:HH12	1:F:531:ASP:HB3	1.64	0.62
1:A:484:ASP:C	1:A:486:VAL:N	2.53	0.61
1:B:171:ILE:HG23	1:B:296:VAL:HG21	1.82	0.61
1:F:174:PHE:HB2	1:F:181:PHE:CE2	2.35	0.61
1:E:435:VAL:HG23	1:E:436:HIS:N	2.14	0.61
1:F:465:LEU:O	1:F:469:ILE:N	2.30	0.61
1:D:326:PRO:CB	1:D:331:ARG:NH1	2.61	0.61
1:D:353:LEU:O	1:D:357:THR:HG22	1.99	0.61
1:A:501:ALA:O	1:A:505:ILE:HD12	1.99	0.61
1:C:520:ALA:HA	1:C:533:ARG:CB	2.29	0.61
1:F:473:LEU:HD11	1:F:551:ILE:HG12	1.81	0.61
1:A:428:PHE:CG	1:A:432:ALA:CB	2.83	0.61
1:D:175:LEU:HD11	1:D:250:CYS:O	2.00	0.61
1:C:488:THR:CG2	1:C:488:THR:O	2.49	0.61
1:D:506:THR:HG22	1:D:507:GLU:HB2	1.81	0.61
1:B:539:THR:HA	1:B:542:ARG:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ILE:HG21	1:B:365:LEU:HD13	1.83	0.61
1:F:569:LEU:C	1:F:571:ARG:H	2.01	0.61
1:D:159:ALA:HB1	1:D:333:GLN:HB3	1.82	0.61
1:E:261:GLY:O	1:E:262:ARG:HB2	2.00	0.61
1:A:502:ARG:O	1:A:506:THR:OG1	2.18	0.61
1:D:554:GLN:NE2	1:D:557:ARG:HD3	2.15	0.61
1:C:503:ARG:HB3	1:C:508:TRP:CZ3	2.36	0.61
1:A:473:LEU:HD13	1:A:555:TYR:HB2	1.81	0.61
1:E:459:HIS:HB2	1:F:488:THR:HB	1.83	0.61
1:B:503:ARG:HH12	1:B:531:ASP:HB3	1.65	0.61
1:D:348:VAL:HG12	1:D:350:LEU:N	2.16	0.61
1:D:369:LEU:HD23	1:D:389:LEU:HD21	1.83	0.61
1:F:539:THR:O	1:F:543:ILE:HD12	2.01	0.61
1:D:346:GLU:HG2	1:D:348:VAL:H	1.64	0.61
1:F:171:ILE:HG21	1:F:296:VAL:HG11	1.81	0.61
1:D:222:GLY:HA2	1:D:225:PHE:HD1	1.66	0.61
1:B:505:ILE:HG22	1:B:506:THR:CA	2.31	0.61
1:F:346:GLU:HG2	1:F:348:VAL:H	1.66	0.61
1:B:326:PRO:O	1:B:327:ASP:CB	2.47	0.61
1:A:241:PHE:HE2	1:A:252:VAL:HG21	1.65	0.61
1:E:450:MET:HG3	1:E:451:MET:N	2.15	0.60
1:F:439:THR:O	1:F:440:ILE:HG13	2.01	0.60
1:D:576:LEU:HG	1:D:582:LEU:HD12	1.83	0.60
1:E:200:VAL:HG22	1:E:325:ALA:HB3	1.82	0.60
1:F:511:HIS:O	1:F:512:PRO:O	2.19	0.60
1:B:334:ILE:HD11	2:B:2001:ADP:C5	2.35	0.60
1:F:565:LYS:O	1:F:567:GLU:N	2.35	0.60
1:D:580:GLU:O	1:D:581:THR:HB	1.99	0.60
1:F:505:ILE:CG2	1:F:514:PHE:HD1	2.10	0.60
1:F:517:VAL:CG2	1:F:519:TYR:OH	2.47	0.60
1:D:428:PHE:CG	1:D:432:ALA:HB1	2.35	0.60
1:D:548:ARG:CG	1:D:548:ARG:HH11	2.14	0.60
1:B:548:ARG:CG	1:B:548:ARG:NH1	2.62	0.60
1:A:192:VAL:HG13	1:A:319:ARG:HB3	1.84	0.60
1:F:473:LEU:C	1:F:475:GLY:N	2.54	0.60
1:A:511:HIS:O	1:A:512:PRO:O	2.19	0.60
1:E:159:ALA:HB1	1:E:333:GLN:HB3	1.83	0.60
1:E:484:ASP:O	1:E:486:VAL:N	2.35	0.60
1:B:481:ILE:HG22	1:B:482:VAL:N	2.15	0.60
1:B:369:LEU:HD23	1:B:389:LEU:HD21	1.84	0.60
1:B:517:VAL:CG2	1:B:519:TYR:OH	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:424:LEU:O	1:D:427:HIS:N	2.29	0.60
1:B:424:LEU:HD22	1:B:569:LEU:HD23	1.83	0.60
1:C:417:TYR:HD2	1:C:569:LEU:HD13	1.66	0.60
1:B:507:GLU:HG3	1:B:520:ALA:HB3	1.83	0.60
1:F:353:LEU:O	1:F:357:THR:HG22	2.02	0.60
1:F:357:THR:OG1	1:F:360:PHE:CD2	2.55	0.60
1:A:501:ALA:HA	1:A:504:MET:HB2	1.84	0.60
1:A:334:ILE:HD12	2:A:1001:ADP:C6	2.37	0.60
1:F:473:LEU:HD11	1:F:551:ILE:CG1	2.32	0.60
1:C:425:ALA:O	1:C:427:HIS:N	2.35	0.60
1:A:197:PRO:HG3	1:A:443:ARG:HB2	1.82	0.60
1:E:406:VAL:HG12	1:E:407:LEU:H	1.65	0.60
1:A:200:VAL:HG22	1:A:325:ALA:HB3	1.84	0.60
1:F:548:ARG:CB	1:F:548:ARG:HH11	2.15	0.59
1:B:189:PRO:O	1:B:190:LYS:CB	2.47	0.59
1:A:413:ARG:HA	1:A:577:LEU:HD11	1.84	0.59
1:D:519:TYR:HB3	1:D:535:TYR:HD2	1.68	0.59
1:A:480:GLU:HG2	1:A:559:LYS:HD2	1.83	0.59
1:B:506:THR:HG22	1:B:507:GLU:HB2	1.84	0.59
1:B:586:GLU:O	1:B:590:VAL:HG23	2.02	0.59
1:C:365:LEU:O	1:C:368:LEU:HB3	2.02	0.59
1:B:502:ARG:HD2	1:B:533:ARG:NH2	2.15	0.59
1:B:519:TYR:HB3	1:B:535:TYR:HD2	1.67	0.59
1:B:470:ALA:O	1:B:558:VAL:HG11	2.02	0.59
1:B:583:THR:H	1:B:586:GLU:HB2	1.67	0.59
1:F:171:ILE:HG23	1:F:296:VAL:HG21	1.85	0.59
1:D:175:LEU:HD12	1:D:249:PRO:HB2	1.85	0.59
1:E:462:ARG:NH1	1:E:510:MET:HB3	2.17	0.59
1:F:580:GLU:O	1:F:581:THR:HB	2.01	0.59
1:B:477:ALA:O	1:B:478:ALA:C	2.39	0.59
1:C:516:PRO:O	1:D:494:PHE:CD2	2.56	0.59
1:B:346:GLU:HG2	1:B:348:VAL:H	1.68	0.59
1:F:417:TYR:CE2	1:F:482:VAL:HG21	2.38	0.59
1:A:499:GLU:HG2	1:A:502:ARG:HH12	1.68	0.59
1:C:541:LYS:HG2	1:C:545:GLU:OE2	2.02	0.59
1:D:502:ARG:O	1:D:506:THR:HB	2.02	0.59
1:D:476:ARG:CZ	1:D:487:THR:CG2	2.79	0.59
1:B:357:THR:OG1	1:B:360:PHE:CD2	2.56	0.59
1:C:514:PHE:CD2	1:C:514:PHE:N	2.69	0.59
1:B:505:ILE:CG2	1:B:514:PHE:HD1	2.06	0.59
1:B:335:LEU:HD21	1:B:365:LEU:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:ILE:HG22	1:A:482:VAL:N	2.18	0.59
1:B:516:PRO:O	1:C:494:PHE:HD2	1.86	0.58
1:D:565:LYS:O	1:D:567:GLU:N	2.34	0.58
1:C:200:VAL:HA	1:C:361:VAL:CG1	2.32	0.58
1:D:539:THR:HA	1:D:542:ARG:HB2	1.85	0.58
1:A:484:ASP:O	1:A:486:VAL:N	2.36	0.58
1:C:598:ALA:HB3	1:C:600:GLU:CD	2.23	0.58
1:A:542:ARG:HA	1:A:542:ARG:HE	1.66	0.58
1:F:337:ILE:HG22	1:F:338:HIS:CD2	2.33	0.58
1:F:201:GLY:HA2	2:F:6001:ADP:N7	2.19	0.58
1:F:174:PHE:O	1:F:178:PRO:HD3	2.04	0.58
1:A:325:ALA:O	1:A:327:ASP:N	2.36	0.58
1:D:334:ILE:HG21	1:D:365:LEU:HD13	1.83	0.58
1:C:501:ALA:HA	1:C:504:MET:HG2	1.85	0.58
1:E:454:ARG:HD3	1:E:503:ARG:NH2	2.17	0.58
1:F:175:LEU:HD12	1:F:249:PRO:HB2	1.86	0.58
1:D:505:ILE:HG22	1:D:506:THR:CA	2.34	0.58
1:D:474:ALA:HB2	1:D:558:VAL:HG11	1.86	0.58
1:E:465:LEU:O	1:E:469:ILE:HG13	2.03	0.58
1:F:424:LEU:O	1:F:427:HIS:N	2.30	0.58
1:F:428:PHE:CD1	1:F:432:ALA:CB	2.83	0.58
1:C:501:ALA:O	1:C:505:ILE:HD12	2.03	0.58
1:A:172:VAL:HG22	1:A:209:VAL:HG13	1.86	0.58
1:E:442:PRO:HD2	1:E:443:ARG:H	1.69	0.58
1:A:503:ARG:HB3	1:A:508:TRP:CZ3	2.38	0.58
1:E:542:ARG:HE	1:E:542:ARG:HA	1.69	0.58
1:A:486:VAL:HG11	1:F:463:LYS:HD2	1.84	0.58
1:D:166:GLU:HA	1:D:169:LYS:HD2	1.85	0.58
1:B:569:LEU:C	1:B:571:ARG:H	2.08	0.57
1:B:473:LEU:HD13	1:B:555:TYR:HB2	1.86	0.57
1:B:222:GLY:HA2	1:B:225:PHE:HD1	1.68	0.57
1:F:222:GLY:HA2	1:F:225:PHE:HD1	1.68	0.57
1:C:463:LYS:HD2	1:D:486:VAL:CG2	2.33	0.57
1:B:565:LYS:O	1:B:567:GLU:N	2.36	0.57
1:C:346:GLU:HB2	1:C:386:MET:SD	2.44	0.57
1:B:331:ARG:HB3	1:B:354:ALA:HB1	1.84	0.57
1:E:461:SER:O	1:E:464:ARG:N	2.36	0.57
1:F:503:ARG:HB3	1:F:508:TRP:CE3	2.39	0.57
1:F:505:ILE:HG22	1:F:506:THR:CA	2.34	0.57
1:B:516:PRO:HB3	1:C:494:PHE:CE2	2.39	0.57
1:F:521:VAL:HG23	1:F:532:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:477:ALA:O	1:E:478:ALA:C	2.42	0.57
1:F:503:ARG:NE	1:F:522:ARG:NH2	2.52	0.57
1:B:554:GLN:HE22	1:B:557:ARG:HD3	1.68	0.57
1:A:465:LEU:HA	1:A:468:GLN:HB2	1.87	0.57
1:D:583:THR:H	1:D:586:GLU:HB2	1.70	0.57
1:E:412:ARG:NH1	1:E:577:LEU:O	2.38	0.57
1:B:417:TYR:CE2	1:B:482:VAL:HG21	2.39	0.57
1:A:202:LYS:HE3	1:A:301:THR:H	1.70	0.57
1:F:511:HIS:C	1:F:512:PRO:O	2.42	0.57
1:A:372:ALA:O	1:A:375:LEU:HB2	2.04	0.57
1:F:311:LEU:O	1:F:317:PHE:HB2	2.05	0.57
1:A:451:MET:HB3	1:A:452:PRO:HD3	1.87	0.57
1:D:473:LEU:HD11	1:D:551:ILE:HG12	1.84	0.57
1:A:462:ARG:HH11	1:A:510:MET:HB3	1.69	0.57
1:E:592:GLU:O	1:E:594:LEU:HD12	2.05	0.57
1:F:503:ARG:NH1	1:F:507:GLU:OE1	2.37	0.57
1:D:158:VAL:HG22	1:D:204:HIS:NE2	2.20	0.57
1:C:459:HIS:HE1	1:D:415:THR:HG23	1.70	0.57
1:F:484:ASP:O	1:F:485:ASP:C	2.43	0.57
1:D:326:PRO:O	1:D:327:ASP:CB	2.52	0.57
1:C:505:ILE:CG2	1:C:506:THR:HG23	2.33	0.57
1:A:309:PRO:HD2	1:A:530:TYR:CD2	2.40	0.57
1:D:379:GLU:HG3	1:D:379:GLU:O	2.04	0.57
1:D:514:PHE:HE2	1:D:542:ARG:CZ	2.18	0.56
1:E:465:LEU:HA	1:E:468:GLN:HB2	1.86	0.56
1:A:454:ARG:HD3	1:A:503:ARG:NH2	2.20	0.56
1:D:311:LEU:O	1:D:317:PHE:HB2	2.04	0.56
1:D:435:VAL:HG22	1:D:436:HIS:N	2.14	0.56
1:B:536:SER:OG	1:C:544:ASP:OD2	2.23	0.56
1:D:543:ILE:O	1:D:547:VAL:HG23	2.05	0.56
1:F:474:ALA:O	1:F:477:ALA:HB3	2.05	0.56
1:F:554:GLN:HE22	1:F:557:ARG:CD	2.13	0.56
1:B:554:GLN:NE2	1:B:557:ARG:HD3	2.21	0.56
1:D:474:ALA:HA	1:D:477:ALA:HB3	1.87	0.56
1:D:564:GLU:O	1:D:564:GLU:HG2	2.04	0.56
1:B:580:GLU:O	1:B:581:THR:HB	2.04	0.56
1:B:311:LEU:O	1:B:317:PHE:HB2	2.06	0.56
1:F:253:PHE:HE2	1:F:255:ASP:HB2	1.70	0.56
1:E:510:MET:O	1:E:512:PRO:CD	2.35	0.56
1:B:502:ARG:HD2	1:B:533:ARG:HH22	1.65	0.56
1:B:474:ALA:HB2	1:B:558:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:551:ILE:O	1:C:552:GLU:C	2.42	0.56
1:C:192:VAL:HG13	1:C:319:ARG:HB3	1.87	0.56
1:B:253:PHE:HE2	1:B:255:ASP:HB2	1.71	0.56
1:E:202:LYS:HE3	1:E:301:THR:H	1.70	0.56
1:C:442:PRO:HD2	1:C:443:ARG:H	1.70	0.56
1:A:548:ARG:HG3	1:A:548:ARG:HH11	1.69	0.56
1:B:514:PHE:HB3	1:B:519:TYR:CE1	2.41	0.56
1:F:331:ARG:HB3	1:F:354:ALA:HB1	1.86	0.56
1:E:517:VAL:HG21	1:E:519:TYR:OH	2.06	0.56
1:B:565:LYS:O	1:B:568:VAL:HG23	2.05	0.56
1:A:494:PHE:HD2	1:F:516:PRO:O	1.88	0.56
1:A:494:PHE:CD2	1:F:516:PRO:O	2.59	0.56
1:B:348:VAL:HG12	1:B:350:LEU:H	1.70	0.56
1:A:514:PHE:CD2	1:A:514:PHE:N	2.71	0.56
1:B:465:LEU:O	1:B:469:ILE:N	2.37	0.56
1:F:532:VAL:CG1	1:F:532:VAL:O	2.53	0.56
1:B:473:LEU:HD11	1:B:551:ILE:CG1	2.35	0.56
1:B:439:THR:O	1:B:440:ILE:HG13	2.05	0.56
1:B:517:VAL:CG2	1:B:519:TYR:CE1	2.69	0.56
1:D:325:ALA:HB1	1:D:361:VAL:HG12	1.88	0.56
1:E:192:VAL:HG13	1:E:319:ARG:HB3	1.88	0.56
1:B:503:ARG:HH12	1:B:522:ARG:HG3	1.70	0.56
1:B:542:ARG:CB	1:B:542:ARG:HH11	2.18	0.56
1:A:511:HIS:C	1:A:512:PRO:O	2.44	0.56
1:E:501:ALA:HA	1:E:504:MET:HB2	1.86	0.56
1:C:477:ALA:O	1:C:478:ALA:C	2.44	0.56
1:B:334:ILE:CG2	1:B:365:LEU:HD13	2.35	0.56
1:E:399:LEU:H	1:E:400:PRO:CD	2.18	0.56
1:E:541:LYS:HG2	1:E:545:GLU:OE2	2.06	0.56
1:B:514:PHE:HE2	1:B:542:ARG:CZ	2.18	0.55
1:B:428:PHE:CD1	1:B:432:ALA:CB	2.83	0.55
1:D:523:GLU:HB2	1:D:530:TYR:O	2.06	0.55
1:C:462:ARG:NH1	1:C:510:MET:HB3	2.21	0.55
1:A:463:LYS:HD2	1:B:486:VAL:HG22	1.88	0.55
1:E:189:PRO:HG3	1:E:319:ARG:HD2	1.87	0.55
1:A:303:ARG:O	1:A:306:ILE:HG12	2.06	0.55
1:F:369:LEU:CD2	1:F:389:LEU:HD21	2.37	0.55
1:D:565:LYS:C	1:D:567:GLU:H	2.08	0.55
1:D:171:ILE:HG23	1:D:296:VAL:HG21	1.88	0.55
1:A:486:VAL:CG1	1:F:463:LYS:HD2	2.37	0.55
1:F:175:LEU:HD11	1:F:250:CYS:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:564:GLU:O	1:F:564:GLU:HG2	2.06	0.55
1:B:334:ILE:HG21	1:B:365:LEU:CD1	2.35	0.55
1:E:505:ILE:CG2	1:E:506:THR:HG23	2.36	0.55
1:F:532:VAL:HG12	1:F:532:VAL:O	2.06	0.55
1:D:592:GLU:O	1:D:594:LEU:HD12	2.06	0.55
1:C:202:LYS:HE3	1:C:301:THR:H	1.71	0.55
1:D:554:GLN:HE22	1:D:557:ARG:NH1	2.04	0.55
1:C:465:LEU:O	1:C:469:ILE:HG13	2.06	0.55
1:E:521:VAL:O	1:E:522:ARG:C	2.45	0.55
1:B:548:ARG:CB	1:B:548:ARG:HH11	2.19	0.55
1:D:169:LYS:HD3	1:E:378:ARG:NH2	2.22	0.55
1:D:331:ARG:HB3	1:D:354:ALA:HB1	1.88	0.55
1:B:458:LEU:HB2	1:C:405:LEU:HD13	1.87	0.55
1:C:479:GLU:O	1:C:480:GLU:C	2.45	0.55
1:B:523:GLU:HB2	1:B:530:TYR:O	2.07	0.55
1:C:513:GLU:OE2	1:C:549:ARG:NH1	2.40	0.55
1:A:262:ARG:NH2	1:A:264:ARG:HE	2.04	0.55
1:C:257:ILE:HG21	1:C:299:ALA:HB1	1.88	0.55
1:F:501:ALA:HA	1:F:504:MET:HE2	1.88	0.55
1:E:476:ARG:O	1:E:477:ALA:C	2.46	0.55
1:C:261:GLY:HA3	1:C:307:LEU:CD1	2.37	0.55
1:F:589:ARG:HD2	1:F:596:LEU:CD1	2.36	0.55
1:D:505:ILE:CG2	1:D:514:PHE:CD1	2.84	0.54
1:B:565:LYS:C	1:B:567:GLU:H	2.10	0.54
1:F:166:GLU:HA	1:F:169:LYS:HD2	1.89	0.54
1:B:175:LEU:HD12	1:B:249:PRO:HB2	1.89	0.54
1:B:464:ARG:O	1:B:468:GLN:N	2.30	0.54
1:B:532:VAL:O	1:B:532:VAL:CG1	2.54	0.54
1:A:377:ALA:HB1	1:F:181:PHE:CE1	2.42	0.54
1:B:500:LEU:O	1:B:503:ARG:N	2.40	0.54
1:B:505:ILE:HG22	1:B:506:THR:N	2.22	0.54
1:A:499:GLU:HG2	1:A:502:ARG:NH1	2.23	0.54
1:C:399:LEU:H	1:C:400:PRO:CD	2.18	0.54
1:C:542:ARG:HA	1:C:542:ARG:HE	1.72	0.54
1:E:513:GLU:OE2	1:E:549:ARG:NH1	2.41	0.54
1:D:428:PHE:CD1	1:D:432:ALA:CB	2.83	0.54
1:F:338:HIS:O	1:F:369:LEU:HD13	2.08	0.54
1:B:424:LEU:O	1:B:425:ALA:C	2.45	0.54
1:E:554:GLN:HE22	1:E:557:ARG:CZ	2.20	0.54
1:F:326:PRO:HB2	1:F:331:ARG:NH1	2.23	0.54
1:F:473:LEU:HD13	1:F:555:TYR:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:LYS:HA	1:D:172:VAL:HB	1.89	0.54
1:C:439:THR:OG1	1:C:581:THR:HG23	2.07	0.54
1:E:261:GLY:HA3	1:E:307:LEU:HD13	1.89	0.54
1:D:253:PHE:HE2	1:D:255:ASP:HB2	1.72	0.54
1:D:470:ALA:O	1:D:558:VAL:HG11	2.08	0.54
1:D:554:GLN:O	1:D:557:ARG:HB3	2.08	0.54
1:A:501:ALA:O	1:A:504:MET:HB2	2.07	0.54
1:A:468:GLN:HA	1:A:468:GLN:NE2	2.21	0.54
1:D:548:ARG:CB	1:D:548:ARG:HH11	2.21	0.54
1:B:514:PHE:HE2	1:B:542:ARG:NE	2.05	0.54
1:C:468:GLN:HA	1:C:468:GLN:NE2	2.22	0.54
1:C:451:MET:HB3	1:C:452:PRO:HD3	1.90	0.54
1:C:484:ASP:C	1:C:486:VAL:N	2.61	0.54
1:B:569:LEU:O	1:B:571:ARG:N	2.31	0.54
1:D:511:HIS:C	1:D:512:PRO:O	2.46	0.54
1:C:484:ASP:O	1:C:486:VAL:N	2.40	0.54
1:A:476:ARG:O	1:A:477:ALA:C	2.45	0.54
1:A:308:ASP:OD1	1:A:530:TYR:HE2	1.91	0.54
1:C:439:THR:HG22	1:C:440:ILE:N	2.22	0.54
1:B:537:GLU:O	1:B:540:ALA:HB3	2.08	0.53
1:E:468:GLN:HA	1:E:468:GLN:NE2	2.23	0.53
1:F:458:LEU:CD1	1:F:459:HIS:H	2.19	0.53
1:A:261:GLY:HA3	1:A:307:LEU:CD1	2.38	0.53
1:B:325:ALA:HB3	1:B:326:PRO:CD	2.25	0.53
1:D:189:PRO:O	1:D:190:LYS:CB	2.49	0.53
1:A:325:ALA:C	1:A:327:ASP:H	2.10	0.53
1:C:465:LEU:HA	1:C:468:GLN:HB2	1.90	0.53
1:F:565:LYS:HD2	1:F:568:VAL:HG21	1.90	0.53
1:A:189:PRO:C	1:A:191:GLY:H	2.11	0.53
1:B:570:GLU:O	1:B:570:GLU:HG2	2.06	0.53
1:F:414:ILE:HA	1:F:483:PHE:CE1	2.43	0.53
1:A:171:ILE:HD11	1:A:189:PRO:HG2	1.91	0.53
1:C:200:VAL:HA	1:C:361:VAL:HG12	1.90	0.53
1:F:153:VAL:O	1:F:211:GLY:HA3	2.08	0.53
1:F:514:PHE:CE2	1:F:542:ARG:CZ	2.91	0.53
1:C:536:SER:O	1:C:537:GLU:C	2.47	0.53
1:D:439:THR:O	1:D:440:ILE:HG13	2.09	0.53
1:D:542:ARG:HH11	1:D:542:ARG:CA	2.18	0.53
1:D:334:ILE:CD1	2:D:4001:ADP:C6	2.86	0.53
1:F:414:ILE:HG13	1:F:483:PHE:CE1	2.44	0.53
1:F:225:PHE:HB3	1:F:278:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:257:ILE:HG21	1:E:299:ALA:HB1	1.90	0.53
1:E:505:ILE:CG2	1:E:514:PHE:CD1	2.91	0.53
1:D:548:ARG:HG3	1:D:548:ARG:NH1	2.23	0.53
1:F:343:PRO:HB2	1:F:383:LYS:HG3	1.91	0.53
1:F:348:VAL:HG12	1:F:350:LEU:H	1.73	0.53
1:E:505:ILE:HG22	1:E:506:THR:CG2	2.39	0.53
1:D:414:ILE:O	1:D:416:ALA:N	2.41	0.53
1:C:505:ILE:HG22	1:C:506:THR:CG2	2.35	0.53
1:C:476:ARG:O	1:C:477:ALA:C	2.47	0.53
1:F:158:VAL:HG22	1:F:204:HIS:NE2	2.24	0.53
1:F:589:ARG:HD2	1:F:596:LEU:HD11	1.89	0.53
1:B:503:ARG:NE	1:B:522:ARG:NH2	2.56	0.53
1:A:439:THR:OG1	1:A:581:THR:HG23	2.08	0.53
1:E:511:HIS:O	1:E:512:PRO:O	2.26	0.53
1:B:507:GLU:HG2	1:B:520:ALA:O	2.09	0.53
1:B:502:ARG:HG2	1:B:533:ARG:HH22	1.69	0.53
1:D:554:GLN:HE22	1:D:557:ARG:HD3	1.74	0.53
1:A:376:ALA:O	1:A:380:GLY:N	2.40	0.53
1:A:548:ARG:NH2	1:F:513:GLU:O	2.41	0.52
1:C:241:PHE:CE2	1:C:252:VAL:HG21	2.43	0.52
1:A:517:VAL:HG13	1:B:551:ILE:HG21	1.92	0.52
1:D:492:ASN:O	1:D:495:ARG:N	2.43	0.52
1:A:576:LEU:O	1:A:577:LEU:C	2.47	0.52
1:D:516:PRO:O	1:E:494:PHE:CD2	2.62	0.52
1:F:201:GLY:O	1:F:205:LEU:HB2	2.09	0.52
1:D:464:ARG:O	1:D:468:GLN:N	2.24	0.52
1:F:399:LEU:N	1:F:400:PRO:HD2	2.24	0.52
1:A:442:PRO:HD2	1:A:443:ARG:H	1.74	0.52
1:E:439:THR:HG22	1:E:440:ILE:N	2.23	0.52
1:E:488:THR:O	1:E:488:THR:CG2	2.57	0.52
1:E:241:PHE:CE2	1:E:252:VAL:HG21	2.42	0.52
1:F:202:LYS:CE	1:F:300:ALA:HB1	2.39	0.52
1:B:538:GLU:O	1:B:540:ALA:N	2.42	0.52
1:F:325:ALA:CB	1:F:326:PRO:CD	2.86	0.52
1:F:523:GLU:HB2	1:F:530:TYR:O	2.10	0.52
1:A:548:ARG:HG3	1:A:548:ARG:NH1	2.23	0.52
1:D:586:GLU:O	1:D:590:VAL:HG23	2.09	0.52
1:B:463:LYS:HD2	1:C:486:VAL:CG1	2.40	0.52
1:C:488:THR:O	1:C:488:THR:HG23	2.10	0.52
1:C:454:ARG:HD3	1:C:503:ARG:NH2	2.24	0.52
1:E:417:TYR:HD2	1:E:569:LEU:HD13	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:476:ARG:O	1:F:477:ALA:C	2.49	0.52
1:F:500:LEU:O	1:F:501:ALA:C	2.46	0.52
1:D:346:GLU:HG3	1:D:386:MET:SD	2.50	0.52
1:F:565:LYS:C	1:F:567:GLU:H	2.10	0.52
1:D:576:LEU:HG	1:D:582:LEU:CD1	2.38	0.52
1:C:592:GLU:O	1:C:594:LEU:HD12	2.09	0.52
1:A:459:HIS:HB2	1:B:488:THR:HB	1.92	0.52
1:E:313:ARG:CB	1:E:314:PRO:HD2	2.39	0.52
1:D:542:ARG:CB	1:D:542:ARG:HH11	2.22	0.52
1:E:498:THR:HA	1:E:551:ILE:HD11	1.92	0.52
1:B:521:VAL:CG1	1:C:495:ARG:HG3	2.40	0.52
1:E:417:TYR:CE2	1:E:482:VAL:HG21	2.45	0.52
1:B:399:LEU:N	1:B:400:PRO:HD2	2.25	0.52
1:A:346:GLU:HB2	1:A:386:MET:SD	2.50	0.52
1:C:376:ALA:HA	1:C:381:ARG:HD3	1.91	0.52
1:B:505:ILE:HG22	1:B:506:THR:CB	2.39	0.51
1:B:335:LEU:HD21	1:B:365:LEU:HD22	1.91	0.51
1:A:399:LEU:H	1:A:400:PRO:CD	2.15	0.51
1:C:514:PHE:HB3	1:C:519:TYR:OH	2.10	0.51
1:A:479:GLU:O	1:A:480:GLU:C	2.47	0.51
1:E:521:VAL:HG12	1:F:495:ARG:HE	1.75	0.51
1:F:571:ARG:HG2	1:F:590:VAL:HG12	1.90	0.51
1:F:586:GLU:O	1:F:590:VAL:HG23	2.10	0.51
1:D:521:VAL:CG1	1:E:495:ARG:HG3	2.40	0.51
1:D:424:LEU:HD22	1:D:569:LEU:HD23	1.91	0.51
1:E:451:MET:HB3	1:E:452:PRO:HD3	1.91	0.51
1:C:463:LYS:HD2	1:D:486:VAL:HG22	1.92	0.51
1:C:397:MET:HE3	1:C:406:VAL:HG11	1.92	0.51
1:B:369:LEU:CD2	1:B:389:LEU:HD21	2.40	0.51
1:B:343:PRO:HB2	1:B:383:LYS:HG3	1.92	0.51
1:D:325:ALA:CB	1:D:326:PRO:CD	2.86	0.51
1:C:511:HIS:O	1:C:512:PRO:O	2.28	0.51
1:B:202:LYS:CE	1:B:300:ALA:HB1	2.40	0.51
1:A:226:VAL:HG21	1:A:259:ALA:O	2.10	0.51
1:C:313:ARG:CB	1:C:314:PRO:HD2	2.40	0.51
1:D:503:ARG:HB3	1:D:508:TRP:CE3	2.45	0.51
1:D:331:ARG:HD2	1:D:357:THR:HG23	1.92	0.51
1:A:159:ALA:HB3	1:A:334:ILE:HD13	1.91	0.51
1:C:598:ALA:HB3	1:C:600:GLU:OE1	2.09	0.51
1:E:376:ALA:HA	1:E:381:ARG:HD3	1.91	0.51
1:E:303:ARG:O	1:E:306:ILE:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:554:GLN:HE22	1:C:557:ARG:CZ	2.23	0.51
1:A:376:ALA:HA	1:A:381:ARG:HD3	1.91	0.51
1:B:572:VAL:O	1:B:576:LEU:HB2	2.11	0.51
1:F:554:GLN:O	1:F:557:ARG:HB3	2.11	0.51
1:D:523:GLU:O	1:D:529:GLY:HA2	2.11	0.51
1:A:162:GLU:C	1:A:164:ALA:H	2.13	0.51
1:F:433:ASP:OD2	1:F:433:ASP:N	2.44	0.51
1:D:503:ARG:NE	1:D:522:ARG:NH2	2.58	0.51
1:B:414:ILE:HA	1:B:483:PHE:CE1	2.46	0.51
1:C:468:GLN:CA	1:C:468:GLN:NE2	2.73	0.51
1:A:189:PRO:HG3	1:A:319:ARG:HD2	1.93	0.51
1:E:484:ASP:C	1:E:486:VAL:N	2.59	0.51
1:F:570:GLU:HG2	1:F:570:GLU:O	2.11	0.51
1:B:531:ASP:O	1:B:531:ASP:OD1	2.28	0.51
1:B:348:VAL:HG12	1:B:350:LEU:N	2.26	0.51
1:A:500:LEU:O	1:A:504:MET:HG2	2.09	0.51
1:D:473:LEU:HD13	1:D:555:TYR:HB2	1.93	0.51
1:F:542:ARG:HG2	1:F:542:ARG:NH1	2.18	0.51
1:B:357:THR:OG1	1:B:360:PHE:HD2	1.94	0.51
1:A:483:PHE:C	1:A:485:ASP:N	2.58	0.51
1:F:502:ARG:O	1:F:506:THR:HB	2.11	0.50
1:B:542:ARG:CA	1:B:542:ARG:NH1	2.67	0.50
1:D:481:ILE:HG22	1:D:482:VAL:N	2.25	0.50
1:C:189:PRO:C	1:C:191:GLY:H	2.14	0.50
1:D:343:PRO:HB2	1:D:383:LYS:HG3	1.92	0.50
1:F:515:GLY:O	1:F:517:VAL:N	2.44	0.50
1:C:462:ARG:HH11	1:C:510:MET:HB3	1.76	0.50
1:C:451:MET:C	1:C:453:ARG:H	2.13	0.50
1:A:374:LEU:HD22	1:F:188:ILE:HD11	1.93	0.50
1:E:463:LYS:HD2	1:F:486:VAL:HG22	1.92	0.50
1:A:435:VAL:HG23	1:A:436:HIS:H	1.76	0.50
1:F:576:LEU:HG	1:F:582:LEU:HD12	1.94	0.50
1:D:503:ARG:CZ	1:D:522:ARG:CZ	2.89	0.50
1:A:548:ARG:CG	1:A:548:ARG:HH11	2.25	0.50
1:F:503:ARG:CZ	1:F:522:ARG:CZ	2.90	0.50
1:A:505:ILE:HG22	1:A:506:THR:CG2	2.41	0.50
1:C:189:PRO:HG3	1:C:319:ARG:HD2	1.93	0.50
1:A:261:GLY:HA3	1:A:307:LEU:HD13	1.92	0.50
1:E:514:PHE:HB3	1:E:519:TYR:OH	2.11	0.50
1:A:426:ALA:HB2	1:A:471:VAL:HG11	1.94	0.50
1:E:189:PRO:C	1:E:191:GLY:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:346:GLU:HB2	1:E:386:MET:SD	2.51	0.50
1:E:148:THR:O	1:E:150:ALA:N	2.42	0.50
1:F:379:GLU:O	1:F:379:GLU:HG3	2.11	0.50
1:F:542:ARG:HH11	1:F:542:ARG:CA	2.21	0.50
1:A:462:ARG:HB2	1:A:510:MET:SD	2.52	0.50
1:E:451:MET:C	1:E:453:ARG:H	2.15	0.50
1:B:527:LEU:HD22	1:B:527:LEU:H	1.76	0.50
1:C:172:VAL:HG22	1:C:209:VAL:HG13	1.94	0.50
1:D:503:ARG:CZ	1:D:522:ARG:NE	2.75	0.50
1:D:334:ILE:HG21	1:D:365:LEU:HD12	1.94	0.50
1:C:511:HIS:C	1:C:512:PRO:O	2.49	0.50
1:B:414:ILE:HG13	1:B:483:PHE:CE1	2.47	0.50
1:D:414:ILE:HG13	1:D:483:PHE:CE1	2.46	0.50
1:C:159:ALA:HB1	1:C:333:GLN:HB3	1.94	0.50
1:F:169:LYS:HA	1:F:172:VAL:HB	1.93	0.50
1:B:532:VAL:HG12	1:B:532:VAL:O	2.10	0.50
1:C:261:GLY:HA3	1:C:307:LEU:HD13	1.93	0.50
1:E:194:LEU:HD12	1:E:323:ILE:HD11	1.93	0.50
1:B:158:VAL:HG22	1:B:204:HIS:NE2	2.26	0.50
1:A:469:ILE:O	1:A:472:ALA:HB3	2.12	0.50
1:F:492:ASN:O	1:F:493:ASP:C	2.47	0.50
1:E:175:LEU:HB2	1:E:213:ALA:HB1	1.92	0.50
1:F:357:THR:OG1	1:F:360:PHE:HD2	1.93	0.50
1:D:465:LEU:O	1:D:469:ILE:N	2.43	0.50
1:C:303:ARG:O	1:C:306:ILE:HG12	2.10	0.50
1:F:592:GLU:O	1:F:594:LEU:HD12	2.11	0.50
1:D:385:THR:H	1:D:388:ASP:HB2	1.76	0.50
1:E:357:THR:O	1:E:357:THR:CG2	2.56	0.50
1:D:399:LEU:N	1:D:400:PRO:HD2	2.24	0.50
1:A:379:GLU:HB2	1:A:381:ARG:HD2	1.94	0.50
1:B:589:ARG:HD2	1:B:596:LEU:CD1	2.42	0.50
1:D:503:ARG:NH1	1:D:507:GLU:OE1	2.44	0.49
1:C:400:PRO:O	1:C:401:ALA:HB2	2.12	0.49
1:E:479:GLU:O	1:E:480:GLU:C	2.49	0.49
1:C:503:ARG:HB3	1:C:508:TRP:CE3	2.47	0.49
1:D:492:ASN:O	1:D:493:ASP:C	2.50	0.49
1:D:369:LEU:CD2	1:D:389:LEU:HD21	2.42	0.49
1:B:576:LEU:HG	1:B:582:LEU:HD12	1.92	0.49
1:A:241:PHE:CE2	1:A:252:VAL:HG21	2.46	0.49
1:C:175:LEU:HB2	1:C:213:ALA:HB1	1.94	0.49
1:B:517:VAL:HG21	1:B:519:TYR:CE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:LEU:HD21	1:D:365:LEU:HD22	1.93	0.49
1:A:502:ARG:HB2	1:A:533:ARG:HH22	1.76	0.49
1:A:521:VAL:O	1:A:522:ARG:C	2.49	0.49
1:F:583:THR:H	1:F:586:GLU:HB2	1.77	0.49
1:B:458:LEU:CD2	1:C:405:LEU:HD22	2.42	0.49
1:A:192:VAL:O	1:A:298:MET:HA	2.12	0.49
1:A:331:ARG:NH2	1:A:580:GLU:OE2	2.46	0.49
1:C:521:VAL:HG12	1:D:495:ARG:HE	1.77	0.49
1:D:225:PHE:HB3	1:D:278:THR:HG21	1.94	0.49
1:D:473:LEU:HD11	1:D:551:ILE:CG1	2.42	0.49
1:E:297:VAL:O	1:E:317:PHE:CE2	2.65	0.49
1:B:458:LEU:HB3	1:C:405:LEU:HD13	1.94	0.49
1:B:465:LEU:O	1:B:469:ILE:HG13	2.11	0.49
1:A:430:GLU:OE1	1:A:431:HIS:NE2	2.46	0.49
1:B:152:LYS:O	1:B:153:VAL:HB	2.11	0.49
1:F:428:PHE:C	1:F:429:LEU:HG	2.33	0.49
1:C:458:LEU:HG	1:C:459:HIS:N	2.27	0.49
1:C:461:SER:HB3	1:C:464:ARG:HG2	1.95	0.49
1:C:502:ARG:HB2	1:C:533:ARG:HH22	1.76	0.49
1:A:536:SER:O	1:A:537:GLU:C	2.51	0.49
1:C:397:MET:O	1:C:406:VAL:HG22	2.12	0.49
1:A:194:LEU:HD12	1:A:323:ILE:HD11	1.95	0.49
1:F:487:THR:HG22	1:F:488:THR:H	1.78	0.49
1:D:420:ALA:O	1:D:423:ALA:N	2.46	0.49
1:C:507:GLU:OE2	1:D:491:GLU:OE2	2.31	0.49
1:E:379:GLU:HB2	1:E:381:ARG:HD2	1.94	0.49
1:D:507:GLU:HG2	1:D:520:ALA:O	2.13	0.49
1:F:476:ARG:CZ	1:F:487:THR:CG2	2.82	0.49
1:B:476:ARG:CD	1:B:487:THR:HG21	2.43	0.49
1:E:201:GLY:O	1:E:204:HIS:HB3	2.11	0.49
1:B:204:HIS:HB2	2:B:2001:ADP:H3'	1.94	0.49
1:E:411:ASP:HA	1:E:414:ILE:HG22	1.95	0.49
1:D:247:HIS:O	1:D:250:CYS:HB3	2.13	0.49
1:D:548:ARG:NH1	1:D:548:ARG:CG	2.75	0.49
1:A:297:VAL:O	1:A:317:PHE:CE2	2.66	0.49
1:C:379:GLU:HB2	1:C:381:ARG:HD2	1.94	0.49
1:B:166:GLU:HA	1:B:169:LYS:HD2	1.93	0.49
1:D:511:HIS:O	1:D:512:PRO:O	2.31	0.49
1:D:542:ARG:NH1	1:D:542:ARG:HG2	2.21	0.49
1:E:462:ARG:HB2	1:E:510:MET:SD	2.53	0.49
1:B:499:GLU:O	1:B:503:ARG:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:ALA:HA	1:A:504:MET:CG	2.43	0.49
1:A:520:ALA:C	1:A:521:VAL:HG22	2.32	0.49
1:C:171:ILE:HD11	1:C:189:PRO:HG2	1.93	0.49
1:C:425:ALA:HB3	1:C:471:VAL:HG13	1.94	0.49
1:B:523:GLU:O	1:B:529:GLY:HA2	2.13	0.49
1:B:592:GLU:O	1:B:594:LEU:HD12	2.12	0.49
1:C:511:HIS:CE1	1:C:516:PRO:HD3	2.48	0.49
1:D:484:ASP:O	1:D:485:ASP:C	2.51	0.49
1:A:458:LEU:HG	1:A:459:HIS:N	2.26	0.49
1:D:510:MET:C	1:D:512:PRO:CD	2.79	0.48
1:E:462:ARG:HH11	1:E:510:MET:HB3	1.78	0.48
1:F:188:ILE:HD13	1:F:189:PRO:HD2	1.95	0.48
1:C:498:THR:HA	1:C:551:ILE:HD11	1.95	0.48
1:A:309:PRO:HD2	1:A:530:TYR:CE2	2.48	0.48
1:A:551:ILE:O	1:A:552:GLU:C	2.51	0.48
1:F:431:HIS:ND1	1:F:431:HIS:N	2.61	0.48
1:B:492:ASN:O	1:B:493:ASP:C	2.51	0.48
1:B:476:ARG:CZ	1:B:487:THR:CG2	2.87	0.48
1:B:464:ARG:H	1:B:464:ARG:HG2	1.50	0.48
1:D:169:LYS:HD3	1:E:378:ARG:HH21	1.77	0.48
1:C:148:THR:O	1:C:150:ALA:N	2.41	0.48
1:A:279:LEU:C	1:A:281:GLN:H	2.15	0.48
1:B:503:ARG:HB3	1:B:508:TRP:CE3	2.48	0.48
1:D:199:GLY:HA3	1:D:363:ALA:HB3	1.95	0.48
1:A:408:SER:O	1:A:411:ASP:N	2.43	0.48
1:A:425:ALA:O	1:A:426:ALA:C	2.51	0.48
1:B:435:VAL:HG22	1:B:436:HIS:N	2.19	0.48
1:D:597:GLU:O	1:D:599:PRO:HD3	2.13	0.48
1:B:474:ALA:HA	1:B:477:ALA:HB3	1.96	0.48
1:E:414:ILE:HG23	1:E:415:THR:N	2.28	0.48
1:B:169:LYS:HA	1:B:172:VAL:HB	1.95	0.48
1:D:499:GLU:O	1:D:503:ARG:HB2	2.12	0.48
1:B:325:ALA:CB	1:B:326:PRO:CD	2.87	0.48
1:D:414:ILE:HA	1:D:483:PHE:CE1	2.49	0.48
1:E:477:ALA:O	1:E:480:GLU:HB3	2.14	0.48
1:A:325:ALA:N	1:A:326:PRO:HD3	2.28	0.48
1:E:587:PHE:CE2	1:E:591:VAL:HG21	2.49	0.48
1:C:162:GLU:C	1:C:164:ALA:H	2.17	0.48
1:E:468:GLN:CA	1:E:468:GLN:NE2	2.75	0.48
1:B:424:LEU:HD21	1:B:568:VAL:HB	1.96	0.48
1:C:481:ILE:HG12	1:C:563:LEU:HD22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ARG:HH21	1:A:264:ARG:HG3	1.77	0.48
1:D:450:MET:HA	1:D:453:ARG:HB2	1.96	0.48
1:D:531:ASP:O	1:D:531:ASP:OD1	2.32	0.48
1:D:476:ARG:O	1:D:477:ALA:C	2.52	0.48
1:C:476:ARG:CZ	1:C:487:THR:CG2	2.88	0.48
1:F:565:LYS:O	1:F:568:VAL:HG23	2.14	0.48
1:E:440:ILE:HD11	1:E:576:LEU:HD22	1.94	0.48
1:C:262:ARG:HH21	1:C:264:ARG:HG3	1.77	0.48
1:E:376:ALA:O	1:E:380:GLY:N	2.44	0.48
1:A:501:ALA:HA	1:A:504:MET:HG2	1.95	0.48
1:A:520:ALA:HA	1:A:533:ARG:CB	2.38	0.48
1:F:498:THR:HG23	1:F:547:VAL:HG11	1.95	0.48
1:C:496:GLN:O	1:C:500:LEU:HB2	2.14	0.48
1:E:171:ILE:HD11	1:E:189:PRO:HG2	1.95	0.48
1:A:357:THR:CG2	1:A:357:THR:O	2.59	0.48
1:A:257:ILE:HG21	1:A:299:ALA:HB1	1.96	0.48
1:D:382:ARG:O	1:D:383:LYS:HB2	2.12	0.48
1:A:175:LEU:HB2	1:A:213:ALA:HB1	1.96	0.48
1:C:430:GLU:OE1	1:C:431:HIS:NE2	2.47	0.48
1:B:542:ARG:NH1	1:B:542:ARG:HG2	2.25	0.48
1:D:204:HIS:HB2	2:D:4001:ADP:H3'	1.95	0.48
1:A:378:ARG:HG3	1:F:170:GLU:OE2	2.13	0.48
1:D:465:LEU:O	1:D:469:ILE:HG13	2.14	0.48
1:C:516:PRO:O	1:D:494:PHE:HD2	1.95	0.47
1:C:516:PRO:CB	1:D:494:PHE:HE2	2.21	0.47
1:B:202:LYS:N	2:B:2001:ADP:O1A	2.47	0.47
1:A:505:ILE:CG2	1:A:514:PHE:CD1	2.95	0.47
1:E:414:ILE:HA	1:E:483:PHE:CE1	2.49	0.47
1:D:464:ARG:H	1:D:464:ARG:HG2	1.39	0.47
1:A:306:ILE:CD1	1:F:525:THR:HB	2.44	0.47
1:B:422:HIS:O	1:B:425:ALA:HB3	2.14	0.47
1:D:548:ARG:HG3	1:D:548:ARG:HH11	1.76	0.47
1:B:564:GLU:O	1:B:564:GLU:HG2	2.13	0.47
1:D:326:PRO:HB2	1:D:331:ARG:NH1	2.23	0.47
1:D:417:TYR:CE2	1:D:482:VAL:HG21	2.50	0.47
1:E:569:LEU:O	1:E:570:GLU:C	2.52	0.47
1:E:511:HIS:C	1:E:512:PRO:O	2.53	0.47
1:A:414:ILE:HG23	1:A:415:THR:N	2.30	0.47
1:D:481:ILE:HD11	1:D:559:LYS:HG3	1.97	0.47
1:B:458:LEU:CD1	1:B:459:HIS:H	2.24	0.47
1:C:411:ASP:HA	1:C:414:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:VAL:HG23	1:B:364:ASP:H	1.79	0.47
1:A:495:ARG:O	1:A:496:GLN:C	2.53	0.47
1:B:203:THR:HG23	1:B:253:PHE:CZ	2.49	0.47
1:B:530:TYR:N	1:B:530:TYR:CD1	2.82	0.47
1:E:226:VAL:HG21	1:E:259:ALA:O	2.14	0.47
1:E:516:PRO:CB	1:F:494:PHE:HE2	2.23	0.47
1:F:361:VAL:HG23	1:F:364:ASP:H	1.79	0.47
1:E:501:ALA:O	1:E:504:MET:HB2	2.15	0.47
1:D:464:ARG:O	1:D:467:ASP:N	2.47	0.47
1:C:226:VAL:HG21	1:C:259:ALA:O	2.15	0.47
1:A:370:ASN:HD21	1:F:187:ARG:HB3	1.79	0.47
1:A:495:ARG:NE	1:F:521:VAL:HG11	2.30	0.47
1:F:334:ILE:HD11	2:F:6001:ADP:C6	2.49	0.47
1:A:430:GLU:O	1:A:431:HIS:HB2	2.15	0.47
1:B:184:MET:SD	1:C:342:LYS:CE	3.03	0.47
1:E:491:GLU:O	1:E:494:PHE:N	2.46	0.47
1:B:538:GLU:O	1:B:541:LYS:N	2.48	0.47
1:D:361:VAL:HG23	1:D:364:ASP:H	1.79	0.47
1:C:461:SER:O	1:C:462:ARG:C	2.52	0.47
1:D:476:ARG:HG3	1:D:477:ALA:N	2.30	0.47
1:A:505:ILE:CG2	1:A:506:THR:HG23	2.41	0.47
1:F:569:LEU:C	1:F:571:ARG:N	2.67	0.47
1:B:468:GLN:HA	1:B:471:VAL:HG23	1.97	0.47
1:C:536:SER:O	1:C:538:GLU:N	2.48	0.47
1:F:171:ILE:O	1:F:175:LEU:HB2	2.14	0.47
1:F:204:HIS:HB2	2:F:6001:ADP:H3'	1.96	0.47
1:F:439:THR:HG22	1:F:440:ILE:N	2.30	0.47
1:E:359:GLY:O	1:E:360:PHE:HB2	2.14	0.47
1:C:348:VAL:HB	1:C:386:MET:SD	2.55	0.47
1:B:153:VAL:O	1:B:211:GLY:HA3	2.15	0.47
1:B:592:GLU:O	1:B:593:GLY:C	2.53	0.47
1:F:456:ASP:O	1:F:457:MET:SD	2.72	0.47
1:B:379:GLU:HG3	1:B:379:GLU:O	2.13	0.47
1:E:433:ASP:N	1:E:433:ASP:OD2	2.47	0.47
1:B:476:ARG:O	1:B:479:GLU:N	2.48	0.47
1:C:325:ALA:O	1:C:327:ASP:N	2.46	0.47
1:F:545:GLU:O	1:F:548:ARG:N	2.47	0.47
1:A:428:PHE:CG	1:A:432:ALA:HB1	2.42	0.47
1:B:538:GLU:C	1:B:540:ALA:N	2.67	0.47
1:C:501:ALA:HA	1:C:504:MET:HB2	1.97	0.47
1:E:400:PRO:O	1:E:401:ALA:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:LEU:HD21	1:B:251:ILE:HG13	1.97	0.47
1:C:435:VAL:HG23	1:C:436:HIS:H	1.79	0.47
1:F:222:GLY:HA2	1:F:225:PHE:CD1	2.50	0.47
1:A:148:THR:O	1:A:150:ALA:N	2.41	0.47
1:B:252:VAL:HG21	1:B:295:ILE:HD11	1.97	0.47
1:E:551:ILE:O	1:E:552:GLU:C	2.53	0.47
1:D:476:ARG:CZ	1:D:494:PHE:HZ	2.28	0.47
1:C:514:PHE:HB3	1:C:519:TYR:CZ	2.50	0.47
1:F:389:LEU:O	1:F:392:ALA:HB3	2.15	0.47
1:A:495:ARG:HG3	1:F:521:VAL:CG1	2.45	0.47
1:D:465:LEU:HA	1:D:468:GLN:HB2	1.97	0.47
1:B:481:ILE:HD11	1:B:559:LYS:HG3	1.97	0.47
1:B:420:ALA:O	1:B:421:GLY:C	2.53	0.47
1:D:589:ARG:HD2	1:D:596:LEU:CD1	2.44	0.47
1:C:349:ASP:C	1:C:351:ALA:H	2.18	0.47
1:C:279:LEU:C	1:C:281:GLN:H	2.18	0.47
1:D:171:ILE:O	1:D:175:LEU:HB2	2.15	0.46
1:A:313:ARG:CB	1:A:314:PRO:HD2	2.44	0.46
1:B:247:HIS:O	1:B:250:CYS:HB3	2.15	0.46
1:C:149:GLU:O	1:C:150:ALA:HB2	2.15	0.46
1:E:162:GLU:C	1:E:164:ALA:H	2.19	0.46
1:B:538:GLU:O	1:B:539:THR:C	2.53	0.46
1:F:331:ARG:HD2	1:F:357:THR:HG23	1.97	0.46
1:A:449:PHE:HB2	1:A:468:GLN:NE2	2.30	0.46
1:D:222:GLY:HA2	1:D:225:PHE:CD1	2.48	0.46
1:E:279:LEU:C	1:E:281:GLN:H	2.18	0.46
1:D:202:LYS:CE	1:D:300:ALA:HB1	2.45	0.46
1:F:511:HIS:NE2	1:F:516:PRO:HD2	2.30	0.46
1:A:159:ALA:HB1	1:A:333:GLN:HB3	1.96	0.46
1:E:325:ALA:N	1:E:326:PRO:CD	2.78	0.46
1:D:428:PHE:C	1:D:429:LEU:HG	2.34	0.46
1:F:511:HIS:CE1	1:F:516:PRO:HD2	2.50	0.46
1:B:171:ILE:O	1:B:175:LEU:HB2	2.16	0.46
1:C:325:ALA:C	1:C:327:ASP:H	2.19	0.46
1:D:542:ARG:NH1	1:D:542:ARG:CA	2.75	0.46
1:F:477:ALA:O	1:F:478:ALA:C	2.54	0.46
1:F:542:ARG:CG	1:F:542:ARG:NH1	2.71	0.46
1:D:491:GLU:O	1:D:492:ASN:C	2.54	0.46
1:E:205:LEU:O	1:E:209:VAL:HG23	2.16	0.46
1:B:201:GLY:O	1:B:205:LEU:HB2	2.16	0.46
1:E:449:PHE:HB2	1:E:468:GLN:NE2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ILE:HA	1:A:483:PHE:CE1	2.50	0.46
1:A:513:GLU:O	1:B:548:ARG:CZ	2.64	0.46
1:B:174:PHE:O	1:B:178:PRO:HD3	2.16	0.46
1:A:342:LYS:NZ	1:F:184:MET:HB3	2.30	0.46
1:B:453:ARG:HD2	1:B:453:ARG:HA	1.71	0.46
1:C:424:LEU:HD12	1:C:572:VAL:HG21	1.97	0.46
1:D:513:GLU:O	1:E:548:ARG:NH2	2.48	0.46
1:F:348:VAL:HG12	1:F:350:LEU:N	2.31	0.46
1:A:451:MET:C	1:A:453:ARG:H	2.17	0.46
1:A:400:PRO:O	1:A:401:ALA:HB2	2.16	0.46
1:B:225:PHE:HB3	1:B:278:THR:HG21	1.96	0.46
1:B:439:THR:HA	1:B:581:THR:OG1	2.15	0.46
1:D:454:ARG:NH2	1:D:530:TYR:OH	2.49	0.46
1:B:184:MET:HB3	1:C:342:LYS:NZ	2.30	0.46
1:E:172:VAL:HG22	1:E:209:VAL:HG13	1.98	0.46
1:D:152:LYS:O	1:D:153:VAL:HB	2.16	0.46
1:D:514:PHE:CE2	1:D:542:ARG:CZ	2.98	0.46
1:D:516:PRO:HB2	1:E:551:ILE:CG2	2.45	0.46
1:F:464:ARG:HG2	1:F:464:ARG:H	1.40	0.46
1:F:503:ARG:HH12	1:F:522:ARG:HG3	1.78	0.46
1:F:514:PHE:CE2	1:F:542:ARG:NE	2.74	0.46
1:E:399:LEU:N	1:E:400:PRO:CD	2.78	0.46
1:A:525:THR:HG22	1:A:526:TYR:N	2.30	0.46
1:F:473:LEU:O	1:F:475:GLY:N	2.48	0.46
1:C:503:ARG:CZ	1:C:522:ARG:HH11	2.29	0.46
1:F:524:ASP:HB3	1:F:525:THR:H	1.37	0.46
1:A:349:ASP:C	1:A:351:ALA:H	2.19	0.46
1:D:431:HIS:N	1:D:431:HIS:ND1	2.64	0.46
1:E:510:MET:C	1:E:512:PRO:CD	2.72	0.46
1:F:557:ARG:O	1:F:560:ALA:HB3	2.15	0.46
1:C:462:ARG:HH12	1:C:511:HIS:H	1.64	0.46
1:A:503:ARG:HB3	1:A:508:TRP:CE3	2.51	0.46
1:A:414:ILE:O	1:A:416:ALA:N	2.49	0.46
1:E:536:SER:O	1:E:539:THR:N	2.49	0.46
1:F:458:LEU:HG	1:F:459:HIS:N	2.31	0.46
1:D:571:ARG:HG2	1:D:590:VAL:HG12	1.98	0.46
1:D:521:VAL:HG11	1:E:495:ARG:NE	2.31	0.46
1:E:576:LEU:HD23	1:E:576:LEU:HA	1.82	0.46
1:B:454:ARG:NH2	1:B:530:TYR:OH	2.48	0.46
1:B:385:THR:H	1:B:388:ASP:HB2	1.81	0.46
1:D:433:ASP:N	1:D:433:ASP:OD2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:503:ARG:NH2	1:F:522:ARG:CZ	2.79	0.46
1:C:428:PHE:N	1:C:428:PHE:HD1	2.11	0.46
1:F:414:ILE:O	1:F:417:TYR:N	2.47	0.46
1:A:463:LYS:CD	1:B:486:VAL:CG2	2.94	0.46
1:A:305:ASP:OD1	1:A:447:LEU:HD22	2.16	0.46
1:E:262:ARG:HH21	1:E:264:ARG:HG3	1.81	0.46
1:E:481:ILE:HG22	1:E:482:VAL:N	2.31	0.46
1:C:194:LEU:HD12	1:C:323:ILE:HD11	1.98	0.46
1:F:585:GLU:HG2	1:F:588:GLN:OE1	2.15	0.46
1:E:338:HIS:CE1	2:E:5001:ADP:N3	2.84	0.46
1:F:476:ARG:CZ	1:F:494:PHE:HZ	2.29	0.45
1:C:491:GLU:O	1:C:494:PHE:N	2.49	0.45
1:C:462:ARG:HB2	1:C:510:MET:SD	2.56	0.45
1:F:563:LEU:HA	1:F:566:ARG:HB3	1.98	0.45
1:B:464:ARG:O	1:B:467:ASP:N	2.47	0.45
1:B:174:PHE:HD1	1:B:181:PHE:CD2	2.34	0.45
1:F:334:ILE:HG21	1:F:365:LEU:HD12	1.98	0.45
1:B:476:ARG:O	1:B:477:ALA:C	2.54	0.45
1:A:374:LEU:HD11	1:F:187:ARG:O	2.15	0.45
1:A:325:ALA:N	1:A:326:PRO:CD	2.79	0.45
1:B:206:ALA:CB	1:B:298:MET:HG2	2.46	0.45
1:D:505:ILE:HG22	1:D:506:THR:CB	2.47	0.45
1:F:505:ILE:HG22	1:F:506:THR:N	2.31	0.45
1:E:414:ILE:HG23	1:E:415:THR:H	1.81	0.45
1:E:536:SER:O	1:E:537:GLU:C	2.55	0.45
1:B:426:ALA:HB2	1:B:471:VAL:HG11	1.98	0.45
1:C:414:ILE:HA	1:C:483:PHE:CE1	2.50	0.45
1:C:473:LEU:HD11	1:C:551:ILE:HG23	1.98	0.45
1:D:526:TYR:HB2	1:D:527:LEU:HD22	1.98	0.45
1:C:423:ALA:HA	1:C:436:HIS:HE1	1.81	0.45
1:B:222:GLY:HA2	1:B:225:PHE:CD1	2.50	0.45
1:B:439:THR:HG22	1:B:440:ILE:N	2.32	0.45
1:B:596:LEU:HD12	1:B:596:LEU:HA	1.79	0.45
1:D:153:VAL:O	1:D:211:GLY:HA3	2.16	0.45
1:D:512:PRO:C	1:D:514:PHE:H	2.20	0.45
1:B:326:PRO:HB2	1:B:327:ASP:H	1.54	0.45
1:F:435:VAL:HG22	1:F:436:HIS:N	2.23	0.45
1:D:458:LEU:HD22	1:E:405:LEU:HB3	1.97	0.45
1:C:325:ALA:N	1:C:326:PRO:CD	2.79	0.45
1:F:576:LEU:HG	1:F:582:LEU:CD1	2.46	0.45
1:A:587:PHE:CE2	1:A:591:VAL:HG21	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:504:MET:HE2	1:D:504:MET:HB3	1.43	0.45
1:F:326:PRO:HB3	1:F:360:PHE:O	2.17	0.45
1:B:334:ILE:CD1	2:B:2001:ADP:C6	2.97	0.45
1:C:469:ILE:O	1:C:469:ILE:HG22	2.16	0.45
1:F:159:ALA:HB2	1:F:337:ILE:HD13	1.98	0.45
1:F:597:GLU:O	1:F:599:PRO:HD3	2.17	0.45
1:A:423:ALA:HA	1:A:436:HIS:HE1	1.82	0.45
1:E:521:VAL:CG1	1:F:495:ARG:HE	2.29	0.45
1:A:322:ALA:C	1:A:323:ILE:HG13	2.37	0.45
1:E:349:ASP:C	1:E:351:ALA:H	2.19	0.45
1:D:524:ASP:HB3	1:D:525:THR:H	1.35	0.45
1:D:513:GLU:O	1:D:514:PHE:HD2	1.99	0.45
1:A:399:LEU:N	1:A:400:PRO:CD	2.78	0.45
1:C:563:LEU:HD13	1:C:563:LEU:HA	1.60	0.45
1:C:326:PRO:HB3	1:C:360:PHE:O	2.16	0.45
1:D:439:THR:HA	1:D:581:THR:OG1	2.16	0.45
1:A:152:LYS:O	1:A:153:VAL:HB	2.16	0.45
1:E:342:LYS:HA	1:E:343:PRO:HD3	1.77	0.45
1:A:201:GLY:O	1:A:204:HIS:HB3	2.16	0.45
1:F:542:ARG:HH11	1:F:542:ARG:CB	2.30	0.45
1:B:194:LEU:HD13	1:B:323:ILE:HD11	1.98	0.45
1:D:414:ILE:O	1:D:417:TYR:N	2.49	0.45
1:B:187:ARG:O	1:C:374:LEU:HD11	2.17	0.45
1:D:387:LYS:H	1:D:387:LYS:HG3	1.59	0.45
1:B:585:GLU:HG2	1:B:588:GLN:OE1	2.17	0.45
1:D:504:MET:HG2	1:D:510:MET:HG3	1.99	0.45
1:F:503:ARG:HE	1:F:522:ARG:NH2	2.14	0.45
1:F:503:ARG:CB	1:F:508:TRP:CZ3	2.99	0.45
1:A:501:ALA:HA	1:A:504:MET:CB	2.46	0.45
1:B:458:LEU:HD23	1:C:405:LEU:HD22	1.99	0.45
1:F:527:LEU:HD22	1:F:527:LEU:H	1.82	0.45
1:D:526:TYR:N	1:D:526:TYR:CD1	2.81	0.45
1:B:521:VAL:HG11	1:C:495:ARG:NE	2.31	0.45
1:E:503:ARG:CZ	1:E:522:ARG:HH11	2.30	0.45
1:C:413:ARG:HA	1:C:577:LEU:HD11	1.98	0.45
1:C:412:ARG:NH1	1:C:577:LEU:O	2.50	0.45
1:E:309:PRO:HD2	1:E:530:TYR:HE2	1.82	0.45
1:B:503:ARG:CZ	1:B:522:ARG:CZ	2.95	0.45
1:A:411:ASP:HA	1:A:414:ILE:HG22	1.99	0.45
1:B:417:TYR:CG	1:B:482:VAL:HG11	2.51	0.45
1:D:530:TYR:N	1:D:530:TYR:CD1	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:LEU:HG	1:B:582:LEU:CD1	2.47	0.45
1:C:587:PHE:CE2	1:C:591:VAL:HG21	2.52	0.45
1:C:244:ALA:HB1	1:C:295:ILE:HD11	1.99	0.45
1:C:201:GLY:O	1:C:204:HIS:HB3	2.16	0.45
1:B:331:ARG:HD2	1:B:357:THR:HG23	1.99	0.44
1:E:325:ALA:O	1:E:327:ASP:N	2.51	0.44
1:F:236:ARG:O	1:F:240:LEU:HB3	2.17	0.44
1:B:524:ASP:HB3	1:B:525:THR:H	1.34	0.44
1:A:563:LEU:HA	1:A:563:LEU:HD13	1.67	0.44
1:C:570:GLU:O	1:C:574:GLU:HG2	2.18	0.44
1:C:399:LEU:N	1:C:400:PRO:CD	2.79	0.44
1:A:476:ARG:O	1:A:479:GLU:N	2.51	0.44
1:E:435:VAL:HG23	1:E:436:HIS:H	1.80	0.44
1:B:318:ASP:O	1:B:319:ARG:HB2	2.17	0.44
1:F:554:GLN:NE2	1:F:557:ARG:CD	2.77	0.44
1:F:465:LEU:HA	1:F:468:GLN:HB2	2.00	0.44
1:A:554:GLN:NE2	1:A:557:ARG:CZ	2.75	0.44
1:C:499:GLU:HG2	1:C:502:ARG:NH1	2.32	0.44
1:B:448:GLY:HA2	1:B:451:MET:CE	2.47	0.44
1:F:247:HIS:O	1:F:250:CYS:HB3	2.17	0.44
1:F:492:ASN:O	1:F:495:ARG:N	2.51	0.44
1:C:440:ILE:HD11	1:C:576:LEU:HD22	1.99	0.44
1:C:430:GLU:O	1:C:431:HIS:HB2	2.17	0.44
1:D:393:ALA:O	1:D:395:ARG:N	2.51	0.44
1:C:253:PHE:HA	1:C:298:MET:O	2.17	0.44
1:F:503:ARG:CZ	1:F:522:ARG:NE	2.80	0.44
1:C:305:ASP:OD2	1:C:447:LEU:HD13	2.18	0.44
1:B:420:ALA:O	1:B:423:ALA:N	2.51	0.44
1:B:236:ARG:O	1:B:240:LEU:HB3	2.17	0.44
2:D:4001:ADP:O1A	2:D:4001:ADP:O2B	2.35	0.44
1:E:499:GLU:HG2	1:E:502:ARG:NH1	2.32	0.44
1:A:412:ARG:NH1	1:A:577:LEU:O	2.50	0.44
1:F:523:GLU:O	1:F:529:GLY:HA2	2.18	0.44
1:F:385:THR:H	1:F:388:ASP:HB2	1.81	0.44
1:A:273:ASP:HA	1:A:276:GLU:HB3	1.99	0.44
1:E:563:LEU:HD13	1:E:563:LEU:HA	1.74	0.44
1:B:476:ARG:CZ	1:B:494:PHE:HZ	2.31	0.44
1:E:313:ARG:HG2	1:E:314:PRO:HD2	2.00	0.44
1:F:340:ARG:HG2	1:F:340:ARG:H	1.59	0.44
1:E:178:PRO:HB2	1:E:182:HIS:NE2	2.33	0.44
1:C:400:PRO:O	1:C:401:ALA:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:424:LEU:HD21	1:F:568:VAL:HB	1.99	0.44
1:E:362:GLY:HA2	1:E:365:LEU:HB2	2.00	0.44
1:C:260:VAL:O	1:C:279:LEU:HB2	2.18	0.44
1:B:456:ASP:O	1:B:457:MET:HB2	2.18	0.44
1:D:511:HIS:NE2	1:D:516:PRO:HD2	2.33	0.44
1:F:545:GLU:O	1:F:546:ALA:C	2.56	0.44
1:E:505:ILE:HG22	1:E:506:THR:CA	2.47	0.44
1:D:416:ALA:HB2	1:D:577:LEU:HD23	1.98	0.44
1:C:467:ASP:OD1	1:C:557:ARG:NH2	2.47	0.44
1:D:389:LEU:O	1:D:392:ALA:HB3	2.18	0.44
1:B:589:ARG:HD2	1:B:596:LEU:HD11	1.99	0.44
1:B:492:ASN:O	1:B:495:ARG:N	2.51	0.44
1:D:547:VAL:HG12	1:D:547:VAL:O	2.16	0.44
1:B:502:ARG:O	1:B:506:THR:HB	2.18	0.44
1:D:487:THR:C	1:D:488:THR:HG23	2.37	0.44
1:C:536:SER:O	1:C:539:THR:N	2.51	0.44
1:F:473:LEU:HD23	1:F:473:LEU:HA	1.67	0.44
1:D:439:THR:HG22	1:D:440:ILE:N	2.33	0.44
1:A:149:GLU:O	1:A:150:ALA:HB2	2.18	0.44
1:C:255:ASP:C	1:C:256:GLU:HG3	2.38	0.44
1:E:428:PHE:CD1	1:E:432:ALA:HB3	2.47	0.43
1:F:417:TYR:CG	1:F:482:VAL:HG11	2.53	0.43
1:C:501:ALA:HA	1:C:504:MET:CG	2.48	0.43
1:A:463:LYS:CD	1:B:486:VAL:HG22	2.48	0.43
1:D:171:ILE:HG22	1:D:296:VAL:HG21	1.97	0.43
1:E:507:GLU:OE2	1:F:491:GLU:OE2	2.37	0.43
1:D:252:VAL:HG21	1:D:295:ILE:HD11	1.99	0.43
1:A:562:LEU:HD23	1:A:562:LEU:HA	1.89	0.43
1:E:514:PHE:N	1:E:514:PHE:CD2	2.83	0.43
1:A:468:GLN:CA	1:A:468:GLN:NE2	2.74	0.43
1:A:503:ARG:CZ	1:A:522:ARG:HH11	2.31	0.43
1:E:331:ARG:NH2	1:E:580:GLU:OE2	2.50	0.43
1:E:426:ALA:HB2	1:E:471:VAL:HG11	2.00	0.43
1:E:262:ARG:NH2	1:E:264:ARG:HE	2.16	0.43
1:A:218:ILE:HB	1:A:252:VAL:HA	2.00	0.43
1:E:325:ALA:N	1:E:326:PRO:HD3	2.32	0.43
1:B:439:THR:HG22	1:B:440:ILE:H	1.82	0.43
1:B:529:GLY:C	1:B:530:TYR:CD1	2.91	0.43
1:F:454:ARG:NH2	1:F:530:TYR:OH	2.51	0.43
1:E:584:ALA:O	1:E:587:PHE:HB3	2.18	0.43
1:A:342:LYS:HA	1:A:343:PRO:HD3	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:VAL:O	1:D:213:ALA:N	2.49	0.43
1:B:340:ARG:H	1:B:340:ARG:HG2	1.60	0.43
1:F:483:PHE:C	1:F:485:ASP:N	2.71	0.43
1:A:554:GLN:NE2	1:A:557:ARG:NE	2.66	0.43
1:C:476:ARG:HD3	1:C:476:ARG:HA	1.68	0.43
1:F:563:LEU:C	1:F:565:LYS:H	2.20	0.43
1:B:463:LYS:CB	1:C:486:VAL:HG11	2.42	0.43
1:B:571:ARG:HG2	1:B:590:VAL:HG12	2.01	0.43
1:A:311:LEU:O	1:A:317:PHE:HB2	2.17	0.43
1:D:580:GLU:O	1:D:581:THR:CB	2.65	0.43
1:B:187:ARG:HB3	1:C:370:ASN:HD21	1.82	0.43
1:D:258:ASP:CG	1:D:301:THR:HG1	2.22	0.43
1:A:425:ALA:C	1:A:427:HIS:N	2.70	0.43
1:D:563:LEU:C	1:D:565:LYS:H	2.22	0.43
1:B:463:LYS:HD2	1:C:486:VAL:HG11	1.99	0.43
1:F:414:ILE:O	1:F:415:THR:C	2.56	0.43
1:D:424:LEU:HD21	1:D:568:VAL:HB	2.00	0.43
1:D:422:HIS:O	1:D:425:ALA:HB3	2.18	0.43
1:D:174:PHE:O	1:D:178:PRO:HD3	2.19	0.43
1:E:503:ARG:HB3	1:E:508:TRP:CE3	2.52	0.43
1:A:428:PHE:N	1:A:428:PHE:HD1	2.14	0.43
1:B:513:GLU:O	1:B:514:PHE:HD2	2.02	0.43
1:F:526:TYR:HB2	1:F:527:LEU:HD22	2.00	0.43
1:C:376:ALA:O	1:C:380:GLY:N	2.47	0.43
1:E:543:ILE:HD13	1:E:543:ILE:HG21	1.69	0.43
1:B:597:GLU:O	1:B:599:PRO:HD3	2.18	0.43
1:E:511:HIS:CE1	1:E:516:PRO:CD	2.97	0.43
1:B:545:GLU:O	1:B:546:ALA:C	2.56	0.43
1:E:400:PRO:O	1:E:401:ALA:CB	2.67	0.43
1:C:325:ALA:N	1:C:326:PRO:HD3	2.34	0.43
1:B:439:THR:C	1:B:440:ILE:HG13	2.38	0.43
1:C:178:PRO:HB2	1:C:182:HIS:NE2	2.34	0.43
1:F:313:ARG:HG3	1:F:314:PRO:HD2	2.00	0.43
1:B:431:HIS:N	1:B:431:HIS:ND1	2.67	0.43
1:A:511:HIS:HE1	1:A:516:PRO:HD3	1.80	0.43
1:E:502:ARG:HB2	1:E:533:ARG:HH22	1.84	0.43
1:E:517:VAL:HG23	1:E:519:TYR:CE1	2.53	0.43
1:D:417:TYR:HA	1:D:573:ALA:HB2	2.01	0.43
1:D:420:ALA:O	1:D:422:HIS:N	2.50	0.43
1:B:563:LEU:C	1:B:565:LYS:H	2.22	0.43
1:C:262:ARG:NH2	1:C:264:ARG:HE	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:439:THR:C	1:D:440:ILE:HG13	2.39	0.43
1:C:442:PRO:CD	1:C:443:ARG:H	2.32	0.43
1:C:152:LYS:O	1:C:153:VAL:HB	2.18	0.43
1:C:273:ASP:HA	1:C:276:GLU:HB3	2.00	0.43
1:E:273:ASP:HA	1:E:276:GLU:HB3	2.01	0.43
1:F:414:ILE:O	1:F:416:ALA:N	2.52	0.43
1:D:527:LEU:H	1:D:527:LEU:HD22	1.83	0.43
1:B:209:VAL:O	1:B:213:ALA:N	2.52	0.43
1:B:194:LEU:HB2	1:B:300:ALA:CB	2.49	0.43
1:A:469:ILE:HG12	1:A:500:LEU:HD12	2.01	0.43
1:A:467:ASP:OD1	1:A:557:ARG:NH2	2.41	0.43
1:C:499:GLU:HG2	1:C:502:ARG:HH12	1.83	0.43
1:C:313:ARG:HG2	1:C:314:PRO:HD2	2.01	0.43
1:F:592:GLU:O	1:F:593:GLY:C	2.57	0.43
1:D:585:GLU:O	1:D:588:GLN:HB2	2.18	0.43
1:D:562:LEU:HD23	1:D:562:LEU:HA	1.91	0.43
1:D:503:ARG:NH2	1:D:522:ARG:CZ	2.82	0.42
1:E:491:GLU:O	1:E:492:ASN:C	2.56	0.42
1:D:411:ASP:O	1:D:414:ILE:HB	2.19	0.42
1:A:513:GLU:OE2	1:A:549:ARG:NH1	2.52	0.42
1:F:188:ILE:CD1	1:F:189:PRO:HD2	2.49	0.42
1:D:332:GLU:O	1:D:333:GLN:C	2.57	0.42
1:B:332:GLU:HB3	1:B:333:GLN:H	1.67	0.42
1:D:342:LYS:HB3	1:D:343:PRO:CD	2.49	0.42
1:B:453:ARG:NH1	1:B:456:ASP:OD2	2.52	0.42
1:E:543:ILE:HG22	1:E:543:ILE:O	2.18	0.42
1:E:466:LEU:HA	1:E:466:LEU:HD23	1.84	0.42
1:F:513:GLU:O	1:F:514:PHE:HD2	2.02	0.42
1:E:514:PHE:HB3	1:E:519:TYR:CZ	2.54	0.42
1:D:328:VAL:CG2	1:D:580:GLU:HB2	2.49	0.42
1:E:488:THR:O	1:E:488:THR:HG23	2.18	0.42
1:B:511:HIS:O	1:B:512:PRO:C	2.57	0.42
1:F:326:PRO:HB2	1:F:327:ASP:H	1.74	0.42
1:C:483:PHE:C	1:C:485:ASP:N	2.69	0.42
1:A:406:VAL:HG12	1:A:407:LEU:N	2.27	0.42
1:C:357:THR:CG2	1:C:357:THR:O	2.58	0.42
1:A:576:LEU:HD23	1:A:576:LEU:HA	1.64	0.42
1:D:592:GLU:O	1:D:593:GLY:C	2.57	0.42
1:A:178:PRO:HB2	1:A:182:HIS:NE2	2.34	0.42
1:F:507:GLU:HG2	1:F:520:ALA:O	2.19	0.42
1:B:510:MET:C	1:B:512:PRO:CD	2.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:LEU:HD13	1:D:323:ILE:HD11	2.02	0.42
1:D:202:LYS:N	2:D:4001:ADP:O1A	2.52	0.42
1:A:491:GLU:O	1:A:494:PHE:N	2.51	0.42
1:A:474:ALA:O	1:A:477:ALA:HB3	2.18	0.42
1:C:359:GLY:O	1:C:360:PHE:HB2	2.19	0.42
1:C:307:LEU:HD12	1:C:311:LEU:HD13	2.01	0.42
1:C:576:LEU:HA	1:C:576:LEU:HD23	1.69	0.42
1:E:386:MET:HG3	1:E:389:LEU:HD12	2.02	0.42
1:F:450:MET:HA	1:F:453:ARG:HB2	2.00	0.42
1:C:543:ILE:HD13	1:C:543:ILE:HG21	1.57	0.42
1:D:516:PRO:HB2	1:E:551:ILE:HG21	2.01	0.42
1:F:505:ILE:HG22	1:F:506:THR:CB	2.50	0.42
1:F:526:TYR:N	1:F:526:TYR:CD1	2.79	0.42
1:E:503:ARG:HD3	1:E:507:GLU:OE1	2.18	0.42
1:B:417:TYR:OH	1:B:570:GLU:HG3	2.20	0.42
1:E:194:LEU:H	1:E:194:LEU:HD23	1.84	0.42
1:A:598:ALA:HA	1:A:599:PRO:HD3	1.76	0.42
1:A:199:GLY:HA2	2:A:1001:ADP:PA	2.60	0.42
1:E:413:ARG:HA	1:E:577:LEU:HD11	2.01	0.42
1:E:439:THR:HG1	1:E:581:THR:HG23	1.84	0.42
1:B:382:ARG:HA	1:B:382:ARG:HD3	1.97	0.42
1:E:149:GLU:O	1:E:150:ALA:HB2	2.18	0.42
1:E:598:ALA:HA	1:E:599:PRO:HD3	1.79	0.42
1:F:514:PHE:CD2	1:F:514:PHE:N	2.87	0.42
1:B:504:MET:HA	1:B:508:TRP:HE3	1.84	0.42
1:E:499:GLU:HG2	1:E:502:ARG:HH12	1.84	0.42
1:D:175:LEU:HD12	1:D:175:LEU:HA	1.85	0.42
1:D:463:LYS:HD2	1:E:486:VAL:CG1	2.50	0.42
1:D:532:VAL:CG1	1:D:532:VAL:O	2.63	0.42
1:B:306:ILE:H	1:B:306:ILE:HG13	1.74	0.42
1:D:570:GLU:HG2	1:D:570:GLU:O	2.20	0.42
1:D:504:MET:N	1:D:508:TRP:HE3	2.18	0.42
1:F:477:ALA:HB1	1:F:562:LEU:HD12	2.02	0.42
1:B:500:LEU:HD23	1:B:500:LEU:HA	1.90	0.42
1:C:459:HIS:HB2	1:D:488:THR:HB	2.02	0.42
1:F:415:THR:O	1:F:419:GLU:N	2.50	0.42
1:C:447:LEU:HD23	1:C:496:GLN:OE1	2.20	0.42
1:F:189:PRO:O	1:F:190:LYS:CB	2.59	0.42
1:A:479:GLU:OE1	1:A:488:THR:HG22	2.20	0.42
1:F:439:THR:C	1:F:440:ILE:HG13	2.39	0.42
1:F:530:TYR:CD1	1:F:530:TYR:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:592:GLU:O	1:B:594:LEU:N	2.53	0.42
1:F:469:ILE:HD11	1:F:501:ALA:H	1.85	0.42
1:F:338:HIS:CE1	1:F:366:GLU:HB2	2.54	0.42
1:F:332:GLU:HB3	1:F:333:GLN:H	1.69	0.42
1:F:439:THR:HG22	1:F:440:ILE:H	1.85	0.42
1:B:450:MET:HA	1:B:453:ARG:HB2	2.02	0.42
1:F:145:ARG:NH2	1:F:219:THR:HG21	2.34	0.42
1:F:194:LEU:HD13	1:F:323:ILE:HD11	2.00	0.42
1:F:474:ALA:HB2	1:F:558:VAL:HG11	2.02	0.42
1:C:491:GLU:O	1:C:492:ASN:C	2.58	0.42
1:A:461:SER:O	1:A:462:ARG:C	2.58	0.42
1:A:554:GLN:HE22	1:A:557:ARG:NE	2.17	0.42
1:F:426:ALA:HB2	1:F:471:VAL:HG11	2.01	0.42
1:E:525:THR:HG22	1:E:526:TYR:N	2.28	0.42
1:C:331:ARG:NH2	1:C:580:GLU:OE2	2.52	0.42
1:E:303:ARG:HH22	1:E:495:ARG:HH22	1.68	0.42
1:F:152:LYS:O	1:F:153:VAL:HB	2.19	0.42
1:A:584:ALA:O	1:A:587:PHE:HB3	2.20	0.42
1:D:313:ARG:HG3	1:D:314:PRO:HD2	2.02	0.42
1:D:326:PRO:HB2	1:D:327:ASP:H	1.44	0.41
1:D:569:LEU:C	1:D:571:ARG:H	2.21	0.41
1:B:563:LEU:HA	1:B:566:ARG:HB3	2.02	0.41
1:E:576:LEU:O	1:E:577:LEU:C	2.58	0.41
1:A:417:TYR:HD2	1:A:569:LEU:HD13	1.84	0.41
1:A:309:PRO:HD2	1:A:530:TYR:HD2	1.85	0.41
1:A:244:ALA:HB1	1:A:295:ILE:HD11	2.01	0.41
1:B:526:TYR:HB2	1:B:527:LEU:HD22	2.01	0.41
1:A:252:VAL:HB	1:A:297:VAL:HG13	2.02	0.41
1:E:326:PRO:HB3	1:E:360:PHE:O	2.20	0.41
1:E:481:ILE:O	1:E:482:VAL:C	2.59	0.41
1:F:449:PHE:HZ	1:F:496:GLN:HG2	1.85	0.41
1:E:511:HIS:HE1	1:E:516:PRO:HD3	1.80	0.41
1:F:506:THR:CG2	1:F:507:GLU:HB2	2.50	0.41
1:A:428:PHE:HB2	1:A:429:LEU:H	1.70	0.41
1:D:194:LEU:HB2	1:D:300:ALA:CB	2.50	0.41
1:D:576:LEU:O	1:D:580:GLU:N	2.46	0.41
1:C:576:LEU:O	1:C:577:LEU:C	2.57	0.41
1:A:544:ASP:O	1:A:545:GLU:C	2.58	0.41
1:F:506:THR:HG23	1:F:520:ALA:HB3	2.01	0.41
1:E:536:SER:O	1:E:538:GLU:N	2.54	0.41
1:F:569:LEU:HD23	1:F:569:LEU:HA	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:552:GLU:O	1:F:555:TYR:N	2.51	0.41
1:C:525:THR:HG22	1:C:526:TYR:N	2.33	0.41
1:A:205:LEU:O	1:A:209:VAL:HG23	2.21	0.41
1:B:261:GLY:HA2	1:B:279:LEU:HD13	2.02	0.41
1:B:387:LYS:HG3	1:B:387:LYS:H	1.56	0.41
1:D:500:LEU:HD23	1:D:500:LEU:HA	1.88	0.41
1:D:504:MET:HA	1:D:508:TRP:HE3	1.86	0.41
1:F:531:ASP:O	1:F:531:ASP:OD1	2.38	0.41
1:A:491:GLU:O	1:A:492:ASN:C	2.58	0.41
1:A:449:PHE:O	1:A:450:MET:HB3	2.20	0.41
1:D:410:ARG:O	1:D:414:ILE:HD12	2.21	0.41
1:D:565:LYS:HD2	1:D:568:VAL:HG21	2.00	0.41
1:B:469:ILE:O	1:B:472:ALA:HB3	2.20	0.41
1:F:202:LYS:N	2:F:6001:ADP:O1A	2.53	0.41
1:A:417:TYR:CE2	1:A:482:VAL:HG21	2.55	0.41
1:A:439:THR:HG22	1:A:440:ILE:N	2.35	0.41
1:F:572:VAL:O	1:F:576:LEU:HB2	2.20	0.41
1:C:342:LYS:HA	1:C:343:PRO:HD3	1.77	0.41
1:B:313:ARG:HG3	1:B:314:PRO:HD2	2.02	0.41
1:E:255:ASP:C	1:E:256:GLU:HG3	2.41	0.41
1:D:540:ALA:HA	1:D:543:ILE:HD12	2.01	0.41
1:E:491:GLU:O	1:E:493:ASP:N	2.53	0.41
1:F:514:PHE:HB3	1:F:519:TYR:CE1	2.55	0.41
1:B:503:ARG:CZ	1:B:522:ARG:NE	2.84	0.41
1:B:335:LEU:CD2	1:B:365:LEU:HB3	2.50	0.41
1:D:188:ILE:HD13	1:D:189:PRO:HD2	2.03	0.41
1:C:521:VAL:CG1	1:D:495:ARG:HE	2.32	0.41
1:A:308:ASP:CG	1:A:530:TYR:HE2	2.23	0.41
1:E:175:LEU:HD12	1:E:249:PRO:HB2	2.02	0.41
1:C:221:SER:OG	1:C:255:ASP:HB3	2.21	0.41
1:D:498:THR:HG23	1:D:547:VAL:HG11	2.03	0.41
1:E:500:LEU:O	1:E:504:MET:HG2	2.20	0.41
1:E:189:PRO:O	1:E:190:LYS:HB2	2.21	0.41
1:C:584:ALA:O	1:C:587:PHE:HB3	2.20	0.41
1:E:197:PRO:CB	1:E:198:PRO:CD	2.99	0.41
1:F:261:GLY:HA2	1:F:279:LEU:HD13	2.02	0.41
1:B:511:HIS:NE2	1:B:516:PRO:HD2	2.35	0.41
1:F:326:PRO:CB	1:F:331:ARG:NH1	2.84	0.41
1:E:501:ALA:HA	1:E:504:MET:CG	2.51	0.41
1:A:400:PRO:O	1:A:401:ALA:CB	2.69	0.41
1:C:447:LEU:HA	1:C:496:GLN:CD	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:532:VAL:HG12	1:D:532:VAL:O	2.21	0.41
1:B:175:LEU:HA	1:B:175:LEU:HD12	1.84	0.41
1:B:382:ARG:O	1:B:383:LYS:HB2	2.21	0.41
1:A:587:PHE:O	1:A:588:GLN:C	2.59	0.41
1:C:338:HIS:CE1	2:C:3001:ADP:N3	2.89	0.41
1:F:474:ALA:HA	1:F:477:ALA:CB	2.50	0.41
1:F:539:THR:O	1:F:542:ARG:HB2	2.20	0.41
1:F:499:GLU:O	1:F:503:ARG:HB2	2.21	0.41
1:D:348:VAL:HG21	1:D:386:MET:CE	2.51	0.41
1:B:205:LEU:HA	1:B:208:ALA:HB3	2.03	0.41
1:E:414:ILE:O	1:E:415:THR:C	2.59	0.41
1:C:517:VAL:HG23	1:C:519:TYR:CE1	2.56	0.41
1:B:458:LEU:HG	1:B:459:HIS:N	2.35	0.41
1:B:160:GLY:H	1:B:333:GLN:CD	2.24	0.41
1:B:171:ILE:HG22	1:B:175:LEU:HD22	2.03	0.41
1:C:397:MET:HG2	1:C:406:VAL:CG1	2.51	0.41
1:F:202:LYS:HD2	1:F:300:ALA:HB1	2.02	0.41
1:C:521:VAL:O	1:C:522:ARG:C	2.60	0.41
1:E:325:ALA:C	1:E:327:ASP:H	2.24	0.41
1:B:389:LEU:O	1:B:392:ALA:HB3	2.20	0.41
1:C:598:ALA:HA	1:C:599:PRO:HD3	1.79	0.41
1:C:205:LEU:O	1:C:209:VAL:HG23	2.21	0.41
1:D:384:ILE:HG22	1:D:388:ASP:HB3	2.03	0.41
1:B:184:MET:SD	1:C:342:LYS:HE3	2.61	0.41
1:D:589:ARG:HD2	1:D:596:LEU:HD11	2.03	0.41
1:C:207:ARG:HG2	1:C:217:PHE:CE2	2.56	0.41
1:B:393:ALA:O	1:B:397:MET:HB2	2.21	0.41
1:F:386:MET:HE3	1:F:390:GLU:HG3	2.01	0.41
1:F:466:LEU:HD13	1:F:466:LEU:HA	1.88	0.41
1:E:461:SER:O	1:E:462:ARG:C	2.58	0.41
1:D:201:GLY:O	1:D:205:LEU:HB2	2.20	0.41
1:A:501:ALA:CA	1:A:504:MET:HB2	2.51	0.41
1:F:458:LEU:CG	1:F:459:HIS:N	2.84	0.41
1:A:488:THR:CG2	1:A:488:THR:O	2.69	0.41
1:D:458:LEU:CB	1:E:405:LEU:HD13	2.51	0.41
1:D:453:ARG:HA	1:D:453:ARG:HD2	1.72	0.41
1:E:286:MET:HA	1:E:289:PHE:CE1	2.56	0.41
1:B:501:ALA:O	1:B:505:ILE:HD12	2.21	0.40
1:B:554:GLN:O	1:B:557:ARG:HB3	2.21	0.40
1:D:362:GLY:O	1:D:365:LEU:HB2	2.21	0.40
1:B:334:ILE:CG2	1:B:335:LEU:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:GLU:C	1:A:540:ALA:N	2.75	0.40
1:B:465:LEU:HA	1:B:468:GLN:HB2	2.03	0.40
1:A:313:ARG:HG2	1:A:314:PRO:HD2	2.03	0.40
1:F:171:ILE:HG22	1:F:175:LEU:HD22	2.02	0.40
1:D:469:ILE:O	1:D:472:ALA:HB3	2.21	0.40
1:E:311:LEU:HD23	1:E:317:PHE:CD1	2.56	0.40
1:D:453:ARG:NH1	1:D:456:ASP:OD2	2.54	0.40
1:C:322:ALA:C	1:C:323:ILE:HG13	2.40	0.40
1:C:470:ALA:C	1:C:472:ALA:N	2.73	0.40
1:F:360:PHE:HD1	1:F:360:PHE:HA	1.73	0.40
1:D:422:HIS:O	1:D:423:ALA:C	2.56	0.40
1:E:159:ALA:HB2	1:E:337:ILE:HD13	2.04	0.40
1:E:425:ALA:O	1:E:426:ALA:C	2.59	0.40
1:F:205:LEU:HA	1:F:208:ALA:HB3	2.03	0.40
1:E:544:ASP:O	1:E:545:GLU:C	2.59	0.40
1:F:456:ASP:O	1:F:457:MET:HB2	2.22	0.40
1:F:193:LEU:HG	1:F:194:LEU:N	2.36	0.40
1:C:562:LEU:HA	1:C:562:LEU:HD23	1.84	0.40
1:D:514:PHE:CE2	1:D:542:ARG:NE	2.77	0.40
1:E:458:LEU:HG	1:E:459:HIS:N	2.34	0.40
1:B:194:LEU:HB2	1:B:300:ALA:HB2	2.03	0.40
1:B:451:MET:HG3	1:B:452:PRO:HD3	2.03	0.40
1:A:303:ARG:HB3	1:A:306:ILE:HG12	2.03	0.40
1:A:257:ILE:C	1:A:259:ALA:N	2.74	0.40
1:D:505:ILE:HG22	1:D:506:THR:N	2.34	0.40
1:F:474:ALA:HA	1:F:477:ALA:HB3	2.04	0.40
1:F:505:ILE:CG2	1:F:514:PHE:CD1	2.96	0.40
1:F:518:ALA:C	1:F:520:ALA:H	2.25	0.40
1:B:514:PHE:CE2	1:B:542:ARG:CZ	3.01	0.40
1:E:465:LEU:HB2	1:E:504:MET:CE	2.52	0.40
1:E:501:ALA:HA	1:E:504:MET:CB	2.51	0.40
1:A:454:ARG:HD2	1:A:522:ARG:CZ	2.51	0.40
1:D:416:ALA:CB	1:D:577:LEU:HD23	2.52	0.40
1:C:465:LEU:HB2	1:C:504:MET:CE	2.52	0.40
1:C:502:ARG:HB2	1:C:533:ARG:NH2	2.37	0.40
1:A:424:LEU:HD11	1:A:568:VAL:HB	2.03	0.40
1:D:463:LYS:HD2	1:E:486:VAL:HG11	2.04	0.40
1:C:466:LEU:HD23	1:C:466:LEU:HA	1.80	0.40
1:C:466:LEU:HD22	1:C:554:GLN:OE1	2.22	0.40
1:A:190:LYS:O	1:A:297:VAL:HG23	2.21	0.40
1:A:312:LEU:HA	1:A:317:PHE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:GLU:O	1:B:492:ASN:C	2.58	0.40
1:B:525:THR:O	1:B:528:GLY:O	2.40	0.40
1:E:210:ALA:HA	1:E:251:ILE:HD12	2.04	0.40
1:D:466:LEU:HD22	1:D:466:LEU:HA	1.86	0.40
1:F:464:ARG:O	1:F:465:LEU:C	2.60	0.40
1:D:487:THR:HG22	1:D:488:THR:H	1.87	0.40
1:E:501:ALA:HA	1:E:504:MET:HG2	2.02	0.40
1:F:368:LEU:HD12	1:F:392:ALA:C	2.42	0.40
1:E:328:VAL:HA	1:E:331:ARG:CZ	2.51	0.40
1:F:451:MET:CB	1:F:452:PRO:HD3	2.51	0.40
1:F:439:THR:HA	1:F:581:THR:OG1	2.22	0.40
1:A:386:MET:HG3	1:A:389:LEU:HD12	2.03	0.40
1:D:382:ARG:HD3	1:D:382:ARG:HA	2.01	0.40
1:D:236:ARG:O	1:D:240:LEU:HB3	2.21	0.40
1:A:543:ILE:O	1:A:543:ILE:HG22	2.21	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	456/499 (91%)	311 (68%)	102 (22%)	43 (9%)	1	15
1	B	442/499 (89%)	320 (72%)	79 (18%)	43 (10%)	1	14
1	C	456/499 (91%)	319 (70%)	100 (22%)	37 (8%)	1	18
1	D	441/499 (88%)	314 (71%)	80 (18%)	47 (11%)	0	11
1	E	456/499 (91%)	320 (70%)	98 (22%)	38 (8%)	1	18
1	F	446/499 (89%)	315 (71%)	83 (19%)	48 (11%)	0	11
All	All	2697/2994 (90%)	1899 (70%)	542 (20%)	256 (10%)	1	15

All (256) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	ALA
1	A	401	ALA
1	A	442	PRO
1	A	457	MET
1	A	477	ALA
1	A	484	ASP
1	A	511	HIS
1	A	512	PRO
1	B	189	PRO
1	B	202	LYS
1	B	327	ASP
1	B	435	VAL
1	B	437	LYS
1	B	477	ALA
1	B	484	ASP
1	B	511	HIS
1	B	512	PRO
1	B	513	GLU
1	B	516	PRO
1	B	526	TYR
1	B	546	ALA
1	B	566	ARG
1	B	593	GLY
1	C	150	ALA
1	C	401	ALA
1	C	442	PRO
1	C	457	MET
1	C	477	ALA
1	C	484	ASP
1	C	511	HIS
1	C	512	PRO
1	D	189	PRO
1	D	202	LYS
1	D	327	ASP
1	D	383	LYS
1	D	430	GLU
1	D	435	VAL
1	D	437	LYS
1	D	477	ALA
1	D	484	ASP
1	D	511	HIS
1	D	512	PRO
1	D	513	GLU

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Mol	Chain	Res	Type
1	D	516	PRO
1	D	526	TYR
1	D	546	ALA
1	E	150	ALA
1	E	401	ALA
1	E	442	PRO
1	E	457	MET
1	E	477	ALA
1	E	484	ASP
1	E	511	HIS
1	E	512	PRO
1	F	189	PRO
1	F	202	LYS
1	F	326	PRO
1	F	425	ALA
1	F	430	GLU
1	F	435	VAL
1	F	437	LYS
1	F	477	ALA
1	F	484	ASP
1	F	511	HIS
1	F	512	PRO
1	F	513	GLU
1	F	516	PRO
1	F	526	TYR
1	F	546	ALA
1	F	593	GLY
1	A	258	ASP
1	A	360	PHE
1	A	426	ALA
1	A	445	ARG
1	A	448	GLY
1	A	450	MET
1	A	476	ARG
1	A	481	ILE
1	A	593	GLY
1	B	185	GLY
1	B	190	LYS
1	B	332	GLU
1	B	358	PRO
1	B	383	LYS
1	B	430	GLU

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Mol	Chain	Res	Type
1	B	545	GLU
1	B	581	THR
1	C	258	ASP
1	C	262	ARG
1	C	426	ALA
1	C	446	ALA
1	C	448	GLY
1	C	450	MET
1	C	489	GLY
1	C	593	GLY
1	D	185	GLY
1	D	190	LYS
1	D	326	PRO
1	D	332	GLU
1	D	358	PRO
1	D	425	ALA
1	D	581	THR
1	D	593	GLY
1	D	598	ALA
1	E	258	ASP
1	E	360	PHE
1	E	426	ALA
1	E	445	ARG
1	E	448	GLY
1	E	450	MET
1	E	478	ALA
1	E	593	GLY
1	F	185	GLY
1	F	190	LYS
1	F	327	ASP
1	F	358	PRO
1	F	383	LYS
1	F	519	TYR
1	F	566	ARG
1	F	570	GLU
1	F	581	THR
1	A	262	ARG
1	A	478	ALA
1	A	492	ASN
1	B	228	MET
1	B	325	ALA
1	B	326	PRO

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Mol	Chain	Res	Type
1	B	409	PRO
1	B	425	ALA
1	B	476	ARG
1	B	584	ALA
1	B	598	ALA
1	C	317	PHE
1	C	327	ASP
1	C	360	PHE
1	C	478	ALA
1	C	481	ILE
1	C	521	VAL
1	D	228	MET
1	D	347	ASP
1	D	354	ALA
1	D	394	ASP
1	D	409	PRO
1	D	476	ARG
1	D	566	ARG
1	D	570	GLU
1	E	262	ARG
1	E	317	PHE
1	E	327	ASP
1	E	446	ALA
1	E	481	ILE
1	F	228	MET
1	F	325	ALA
1	F	332	GLU
1	F	354	ALA
1	F	489	GLY
1	F	534	GLN
1	F	569	LEU
1	F	598	ALA
1	A	149	GLU
1	A	317	PHE
1	A	342	LYS
1	A	399	LEU
1	A	446	ALA
1	A	504	MET
1	B	153	VAL
1	B	201	GLY
1	B	204	HIS
1	B	214	ARG

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Mol	Chain	Res	Type
1	B	525	THR
1	B	539	THR
1	B	570	GLU
1	C	342	LYS
1	C	437	LYS
1	C	452	PRO
1	C	537	GLU
1	D	153	VAL
1	D	201	GLY
1	D	204	HIS
1	D	214	ARG
1	D	295	ILE
1	D	325	ALA
1	D	489	GLY
1	D	534	GLN
1	D	539	THR
1	D	584	ALA
1	E	342	LYS
1	E	430	GLU
1	E	492	ASN
1	F	153	VAL
1	F	201	GLY
1	F	204	HIS
1	F	409	PRO
1	F	424	LEU
1	F	460	TRP
1	F	476	ARG
1	F	584	ALA
1	A	153	VAL
1	A	189	PRO
1	A	326	PRO
1	A	437	LYS
1	A	452	PRO
1	A	493	ASP
1	A	516	PRO
1	A	576	LEU
1	B	569	LEU
1	C	149	GLU
1	C	153	VAL
1	C	189	PRO
1	C	326	PRO
1	C	399	LEU

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Mol	Chain	Res	Type
1	C	476	ARG
1	D	333	GLN
1	D	525	THR
1	E	149	GLU
1	E	153	VAL
1	E	189	PRO
1	E	326	PRO
1	E	399	LEU
1	E	437	LYS
1	E	452	PRO
1	E	476	ARG
1	F	214	ARG
1	F	295	ILE
1	F	545	GLU
1	F	564	GLU
1	A	409	PRO
1	A	430	GLU
1	A	459	HIS
1	A	521	VAL
1	B	354	ALA
1	C	445	ARG
1	C	516	PRO
1	D	500	LEU
1	D	549	ARG
1	E	460	TRP
1	F	525	THR
1	B	295	ILE
1	C	400	PRO
1	E	358	PRO
1	E	400	PRO
1	A	358	PRO
1	A	400	PRO
1	C	358	PRO
1	F	414	ILE
1	A	489	GLY
1	B	489	GLY
1	B	529	GLY
1	D	529	GLY
1	E	516	PRO
1	F	529	GLY
1	A	197	PRO
1	A	435	VAL

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Mol	Chain	Res	Type
1	C	309	PRO
1	E	489	GLY
1	E	521	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	365/397 (92%)	234 (64%)	131 (36%)	0 1
1	B	361/397 (91%)	228 (63%)	133 (37%)	0 1
1	C	366/397 (92%)	232 (63%)	134 (37%)	0 1
1	D	360/397 (91%)	226 (63%)	134 (37%)	0 1
1	E	366/397 (92%)	230 (63%)	136 (37%)	0 1
1	F	363/397 (91%)	228 (63%)	135 (37%)	0 1
All	All	2181/2382 (92%)	1378 (63%)	803 (37%)	0 1

All (803) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	VAL
1	A	147	LEU
1	A	148	THR
1	A	152	LYS
1	A	154	THR
1	A	156	LYS
1	A	162	GLU
1	A	167	GLU
1	A	168	LEU
1	A	171	ILE
1	A	175	LEU
1	A	180	ARG
1	A	188	ILE
1	A	205	LEU
1	A	214	ARG

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Mol	Chain	Res	Type
1	A	215	VAL
1	A	219	THR
1	A	221	SER
1	A	227	GLU
1	A	236	ARG
1	A	239	ASP
1	A	240	LEU
1	A	243	THR
1	A	250	CYS
1	A	256	GLU
1	A	260	VAL
1	A	262	ARG
1	A	263	LYS
1	A	264	ARG
1	A	292	ASP
1	A	295	ILE
1	A	305	ASP
1	A	311	LEU
1	A	312	LEU
1	A	319	ARG
1	A	320	GLN
1	A	323	ILE
1	A	336	ARG
1	A	337	ILE
1	A	342	LYS
1	A	344	LEU
1	A	347	ASP
1	A	348	VAL
1	A	352	LEU
1	A	355	LYS
1	A	356	ARG
1	A	360	PHE
1	A	361	VAL
1	A	368	LEU
1	A	378	ARG
1	A	381	ARG
1	A	384	ILE
1	A	385	THR
1	A	386	MET
1	A	387	LYS
1	A	394	ASP
1	A	395	ARG

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Mol	Chain	Res	Type
1	A	397	MET
1	A	406	VAL
1	A	407	LEU
1	A	408	SER
1	A	410	ARG
1	A	413	ARG
1	A	414	ILE
1	A	424	LEU
1	A	428	PHE
1	A	433	ASP
1	A	436	HIS
1	A	437	LYS
1	A	443	ARG
1	A	445	ARG
1	A	450	MET
1	A	451	MET
1	A	454	ARG
1	A	455	GLU
1	A	457	MET
1	A	459	HIS
1	A	460	TRP
1	A	461	SER
1	A	462	ARG
1	A	468	GLN
1	A	480	GLU
1	A	483	PHE
1	A	484	ASP
1	A	485	ASP
1	A	486	VAL
1	A	491	GLU
1	A	492	ASN
1	A	495	ARG
1	A	496	GLN
1	A	499	GLU
1	A	500	LEU
1	A	502	ARG
1	A	503	ARG
1	A	505	ILE
1	A	511	HIS
1	A	512	PRO
1	A	514	PHE
1	A	517	VAL

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Mol	Chain	Res	Type
1	A	519	TYR
1	A	521	VAL
1	A	524	ASP
1	A	526	TYR
1	A	530	TYR
1	A	532	VAL
1	A	533	ARG
1	A	535	TYR
1	A	537	GLU
1	A	539	THR
1	A	542	ARG
1	A	548	ARG
1	A	549	ARG
1	A	550	LEU
1	A	551	ILE
1	A	558	VAL
1	A	561	LEU
1	A	563	LEU
1	A	564	GLU
1	A	568	VAL
1	A	569	LEU
1	A	570	GLU
1	A	571	ARG
1	A	577	LEU
1	A	580	GLU
1	A	582	LEU
1	A	586	GLU
1	A	589	ARG
1	A	592	GLU
1	A	594	LEU
1	A	596	LEU
1	A	597	GLU
1	B	148	THR
1	B	156	LYS
1	B	162	GLU
1	B	165	LYS
1	B	173	GLU
1	B	175	LEU
1	B	177	ASN
1	B	180	ARG
1	B	187	ARG
1	B	194	LEU

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Mol	Chain	Res	Type
1	B	205	LEU
1	B	215	VAL
1	B	221	SER
1	B	223	SER
1	B	224	ASP
1	B	226	VAL
1	B	237	VAL
1	B	238	ARG
1	B	240	LEU
1	B	245	LYS
1	B	256	GLU
1	B	257	ILE
1	B	263	LYS
1	B	272	ASN
1	B	273	ASP
1	B	281	GLN
1	B	287	ASP
1	B	298	MET
1	B	306	ILE
1	B	311	LEU
1	B	312	LEU
1	B	313	ARG
1	B	319	ARG
1	B	321	ILE
1	B	323	ILE
1	B	328	VAL
1	B	329	LYS
1	B	331	ARG
1	B	332	GLU
1	B	333	GLN
1	B	334	ILE
1	B	336	ARG
1	B	337	ILE
1	B	340	ARG
1	B	342	LYS
1	B	344	LEU
1	B	346	GLU
1	B	350	LEU
1	B	352	LEU
1	B	355	LYS
1	B	357	THR
1	B	360	PHE

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Mol	Chain	Res	Type
1	B	368	LEU
1	B	370	ASN
1	B	378	ARG
1	B	379	GLU
1	B	382	ARG
1	B	383	LYS
1	B	384	ILE
1	B	385	THR
1	B	386	MET
1	B	387	LYS
1	B	391	GLU
1	B	394	ASP
1	B	397	MET
1	B	405	LEU
1	B	414	ILE
1	B	415	THR
1	B	418	HIS
1	B	428	PHE
1	B	429	LEU
1	B	431	HIS
1	B	433	ASP
1	B	436	HIS
1	B	437	LYS
1	B	438	VAL
1	B	443	ARG
1	B	445	ARG
1	B	451	MET
1	B	453	ARG
1	B	454	ARG
1	B	456	ASP
1	B	457	MET
1	B	461	SER
1	B	462	ARG
1	B	463	LYS
1	B	464	ARG
1	B	467	ASP
1	B	469	ILE
1	B	480	GLU
1	B	482	VAL
1	B	485	ASP
1	B	486	VAL
1	B	496	GLN

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Mol	Chain	Res	Type
1	B	502	ARG
1	B	503	ARG
1	B	504	MET
1	B	505	ILE
1	B	506	THR
1	B	507	GLU
1	B	510	MET
1	B	511	HIS
1	B	521	VAL
1	B	522	ARG
1	B	525	THR
1	B	526	TYR
1	B	530	TYR
1	B	532	VAL
1	B	534	GLN
1	B	535	TYR
1	B	536	SER
1	B	539	THR
1	B	541	LYS
1	B	542	ARG
1	B	548	ARG
1	B	549	ARG
1	B	550	LEU
1	B	551	ILE
1	B	554	GLN
1	B	558	VAL
1	B	561	LEU
1	B	563	LEU
1	B	565	LYS
1	B	566	ARG
1	B	567	GLU
1	B	569	LEU
1	B	576	LEU
1	B	577	LEU
1	B	579	ARG
1	B	581	THR
1	B	582	LEU
1	B	594	LEU
1	B	596	LEU
1	C	146	VAL
1	C	147	LEU
1	C	148	THR

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Mol	Chain	Res	Type
1	C	152	LYS
1	C	154	THR
1	C	156	LYS
1	C	162	GLU
1	C	167	GLU
1	C	171	ILE
1	C	175	LEU
1	C	180	ARG
1	C	188	ILE
1	C	194	LEU
1	C	205	LEU
1	C	214	ARG
1	C	215	VAL
1	C	219	THR
1	C	221	SER
1	C	227	GLU
1	C	236	ARG
1	C	239	ASP
1	C	240	LEU
1	C	243	THR
1	C	250	CYS
1	C	252	VAL
1	C	256	GLU
1	C	260	VAL
1	C	262	ARG
1	C	263	LYS
1	C	264	ARG
1	C	292	ASP
1	C	295	ILE
1	C	305	ASP
1	C	307	LEU
1	C	311	LEU
1	C	312	LEU
1	C	319	ARG
1	C	320	GLN
1	C	323	ILE
1	C	334	ILE
1	C	336	ARG
1	C	337	ILE
1	C	342	LYS
1	C	344	LEU
1	C	347	ASP

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Mol	Chain	Res	Type
1	C	348	VAL
1	C	352	LEU
1	C	355	LYS
1	C	356	ARG
1	C	360	PHE
1	C	361	VAL
1	C	368	LEU
1	C	378	ARG
1	C	381	ARG
1	C	384	ILE
1	C	385	THR
1	C	386	MET
1	C	387	LYS
1	C	394	ASP
1	C	395	ARG
1	C	397	MET
1	C	406	VAL
1	C	407	LEU
1	C	408	SER
1	C	410	ARG
1	C	413	ARG
1	C	414	ILE
1	C	424	LEU
1	C	428	PHE
1	C	433	ASP
1	C	435	VAL
1	C	436	HIS
1	C	437	LYS
1	C	443	ARG
1	C	445	ARG
1	C	450	MET
1	C	451	MET
1	C	454	ARG
1	C	455	GLU
1	C	457	MET
1	C	459	HIS
1	C	461	SER
1	C	462	ARG
1	C	468	GLN
1	C	480	GLU
1	C	483	PHE
1	C	484	ASP

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Mol	Chain	Res	Type
1	C	485	ASP
1	C	486	VAL
1	C	491	GLU
1	C	492	ASN
1	C	495	ARG
1	C	496	GLN
1	C	499	GLU
1	C	500	LEU
1	C	502	ARG
1	C	503	ARG
1	C	504	MET
1	C	505	ILE
1	C	506	THR
1	C	511	HIS
1	C	512	PRO
1	C	514	PHE
1	C	517	VAL
1	C	519	TYR
1	C	521	VAL
1	C	524	ASP
1	C	526	TYR
1	C	530	TYR
1	C	532	VAL
1	C	533	ARG
1	C	535	TYR
1	C	537	GLU
1	C	539	THR
1	C	542	ARG
1	C	548	ARG
1	C	549	ARG
1	C	550	LEU
1	C	558	VAL
1	C	561	LEU
1	C	563	LEU
1	C	564	GLU
1	C	568	VAL
1	C	569	LEU
1	C	576	LEU
1	C	577	LEU
1	C	580	GLU
1	C	582	LEU
1	C	586	GLU

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Mol	Chain	Res	Type
1	C	589	ARG
1	C	592	GLU
1	C	594	LEU
1	C	596	LEU
1	C	597	GLU
1	D	156	LYS
1	D	162	GLU
1	D	165	LYS
1	D	173	GLU
1	D	175	LEU
1	D	177	ASN
1	D	180	ARG
1	D	187	ARG
1	D	194	LEU
1	D	205	LEU
1	D	215	VAL
1	D	221	SER
1	D	223	SER
1	D	224	ASP
1	D	226	VAL
1	D	237	VAL
1	D	238	ARG
1	D	240	LEU
1	D	245	LYS
1	D	256	GLU
1	D	257	ILE
1	D	263	LYS
1	D	272	ASN
1	D	273	ASP
1	D	281	GLN
1	D	286	MET
1	D	287	ASP
1	D	298	MET
1	D	306	ILE
1	D	311	LEU
1	D	312	LEU
1	D	313	ARG
1	D	319	ARG
1	D	321	ILE
1	D	323	ILE
1	D	328	VAL
1	D	329	LYS

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Mol	Chain	Res	Type
1	D	332	GLU
1	D	333	GLN
1	D	334	ILE
1	D	336	ARG
1	D	337	ILE
1	D	340	ARG
1	D	342	LYS
1	D	344	LEU
1	D	346	GLU
1	D	350	LEU
1	D	352	LEU
1	D	355	LYS
1	D	357	THR
1	D	360	PHE
1	D	368	LEU
1	D	370	ASN
1	D	378	ARG
1	D	379	GLU
1	D	382	ARG
1	D	383	LYS
1	D	384	ILE
1	D	385	THR
1	D	386	MET
1	D	387	LYS
1	D	391	GLU
1	D	394	ASP
1	D	397	MET
1	D	405	LEU
1	D	414	ILE
1	D	415	THR
1	D	418	HIS
1	D	428	PHE
1	D	429	LEU
1	D	431	HIS
1	D	433	ASP
1	D	436	HIS
1	D	437	LYS
1	D	438	VAL
1	D	443	ARG
1	D	445	ARG
1	D	451	MET
1	D	453	ARG

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Mol	Chain	Res	Type
1	D	454	ARG
1	D	456	ASP
1	D	457	MET
1	D	461	SER
1	D	462	ARG
1	D	463	LYS
1	D	464	ARG
1	D	467	ASP
1	D	469	ILE
1	D	479	GLU
1	D	480	GLU
1	D	482	VAL
1	D	485	ASP
1	D	486	VAL
1	D	496	GLN
1	D	502	ARG
1	D	503	ARG
1	D	504	MET
1	D	505	ILE
1	D	506	THR
1	D	507	GLU
1	D	510	MET
1	D	511	HIS
1	D	512	PRO
1	D	513	GLU
1	D	517	VAL
1	D	521	VAL
1	D	522	ARG
1	D	525	THR
1	D	526	TYR
1	D	530	TYR
1	D	532	VAL
1	D	534	GLN
1	D	535	TYR
1	D	536	SER
1	D	539	THR
1	D	542	ARG
1	D	548	ARG
1	D	549	ARG
1	D	551	ILE
1	D	554	GLN
1	D	557	ARG

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Mol	Chain	Res	Type
1	D	558	VAL
1	D	561	LEU
1	D	563	LEU
1	D	565	LYS
1	D	566	ARG
1	D	567	GLU
1	D	569	LEU
1	D	576	LEU
1	D	577	LEU
1	D	579	ARG
1	D	581	THR
1	D	594	LEU
1	D	596	LEU
1	E	146	VAL
1	E	147	LEU
1	E	148	THR
1	E	152	LYS
1	E	154	THR
1	E	156	LYS
1	E	162	GLU
1	E	167	GLU
1	E	171	ILE
1	E	175	LEU
1	E	180	ARG
1	E	188	ILE
1	E	200	VAL
1	E	205	LEU
1	E	214	ARG
1	E	215	VAL
1	E	219	THR
1	E	221	SER
1	E	227	GLU
1	E	236	ARG
1	E	239	ASP
1	E	240	LEU
1	E	243	THR
1	E	250	CYS
1	E	252	VAL
1	E	256	GLU
1	E	260	VAL
1	E	262	ARG
1	E	263	LYS

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Mol	Chain	Res	Type
1	E	264	ARG
1	E	292	ASP
1	E	295	ILE
1	E	301	THR
1	E	305	ASP
1	E	307	LEU
1	E	311	LEU
1	E	312	LEU
1	E	319	ARG
1	E	320	GLN
1	E	323	ILE
1	E	334	ILE
1	E	336	ARG
1	E	337	ILE
1	E	342	LYS
1	E	344	LEU
1	E	347	ASP
1	E	348	VAL
1	E	352	LEU
1	E	355	LYS
1	E	356	ARG
1	E	360	PHE
1	E	361	VAL
1	E	368	LEU
1	E	378	ARG
1	E	381	ARG
1	E	384	ILE
1	E	385	THR
1	E	386	MET
1	E	387	LYS
1	E	394	ASP
1	E	395	ARG
1	E	397	MET
1	E	406	VAL
1	E	407	LEU
1	E	408	SER
1	E	410	ARG
1	E	413	ARG
1	E	414	ILE
1	E	424	LEU
1	E	428	PHE
1	E	433	ASP

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Mol	Chain	Res	Type
1	E	435	VAL
1	E	436	HIS
1	E	437	LYS
1	E	443	ARG
1	E	445	ARG
1	E	450	MET
1	E	451	MET
1	E	454	ARG
1	E	455	GLU
1	E	457	MET
1	E	459	HIS
1	E	460	TRP
1	E	461	SER
1	E	462	ARG
1	E	468	GLN
1	E	480	GLU
1	E	483	PHE
1	E	484	ASP
1	E	485	ASP
1	E	486	VAL
1	E	492	ASN
1	E	495	ARG
1	E	499	GLU
1	E	500	LEU
1	E	502	ARG
1	E	503	ARG
1	E	505	ILE
1	E	510	MET
1	E	511	HIS
1	E	512	PRO
1	E	514	PHE
1	E	517	VAL
1	E	519	TYR
1	E	521	VAL
1	E	523	GLU
1	E	524	ASP
1	E	526	TYR
1	E	530	TYR
1	E	532	VAL
1	E	533	ARG
1	E	535	TYR
1	E	537	GLU

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Mol	Chain	Res	Type
1	E	539	THR
1	E	542	ARG
1	E	548	ARG
1	E	549	ARG
1	E	550	LEU
1	E	558	VAL
1	E	561	LEU
1	E	563	LEU
1	E	564	GLU
1	E	568	VAL
1	E	569	LEU
1	E	570	GLU
1	E	571	ARG
1	E	576	LEU
1	E	577	LEU
1	E	580	GLU
1	E	582	LEU
1	E	586	GLU
1	E	589	ARG
1	E	592	GLU
1	E	594	LEU
1	E	596	LEU
1	E	597	GLU
1	F	145	ARG
1	F	147	LEU
1	F	156	LYS
1	F	162	GLU
1	F	165	LYS
1	F	173	GLU
1	F	175	LEU
1	F	177	ASN
1	F	180	ARG
1	F	187	ARG
1	F	194	LEU
1	F	205	LEU
1	F	215	VAL
1	F	221	SER
1	F	223	SER
1	F	224	ASP
1	F	226	VAL
1	F	237	VAL
1	F	238	ARG

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Mol	Chain	Res	Type
1	F	240	LEU
1	F	245	LYS
1	F	256	GLU
1	F	257	ILE
1	F	263	LYS
1	F	272	ASN
1	F	273	ASP
1	F	281	GLN
1	F	287	ASP
1	F	298	MET
1	F	306	ILE
1	F	311	LEU
1	F	312	LEU
1	F	313	ARG
1	F	319	ARG
1	F	321	ILE
1	F	323	ILE
1	F	328	VAL
1	F	329	LYS
1	F	331	ARG
1	F	332	GLU
1	F	333	GLN
1	F	334	ILE
1	F	336	ARG
1	F	337	ILE
1	F	340	ARG
1	F	342	LYS
1	F	344	LEU
1	F	346	GLU
1	F	350	LEU
1	F	352	LEU
1	F	355	LYS
1	F	357	THR
1	F	360	PHE
1	F	368	LEU
1	F	370	ASN
1	F	378	ARG
1	F	379	GLU
1	F	382	ARG
1	F	383	LYS
1	F	384	ILE
1	F	385	THR

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Mol	Chain	Res	Type
1	F	386	MET
1	F	387	LYS
1	F	391	GLU
1	F	394	ASP
1	F	397	MET
1	F	405	LEU
1	F	414	ILE
1	F	415	THR
1	F	418	HIS
1	F	428	PHE
1	F	429	LEU
1	F	431	HIS
1	F	433	ASP
1	F	436	HIS
1	F	437	LYS
1	F	438	VAL
1	F	443	ARG
1	F	445	ARG
1	F	451	MET
1	F	453	ARG
1	F	454	ARG
1	F	456	ASP
1	F	457	MET
1	F	461	SER
1	F	462	ARG
1	F	463	LYS
1	F	464	ARG
1	F	467	ASP
1	F	469	ILE
1	F	480	GLU
1	F	482	VAL
1	F	485	ASP
1	F	486	VAL
1	F	491	GLU
1	F	496	GLN
1	F	502	ARG
1	F	504	MET
1	F	505	ILE
1	F	506	THR
1	F	507	GLU
1	F	510	MET
1	F	511	HIS

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Mol	Chain	Res	Type
1	F	512	PRO
1	F	521	VAL
1	F	522	ARG
1	F	525	THR
1	F	526	TYR
1	F	530	TYR
1	F	532	VAL
1	F	534	GLN
1	F	535	TYR
1	F	536	SER
1	F	539	THR
1	F	541	LYS
1	F	542	ARG
1	F	548	ARG
1	F	549	ARG
1	F	551	ILE
1	F	554	GLN
1	F	557	ARG
1	F	558	VAL
1	F	561	LEU
1	F	563	LEU
1	F	565	LYS
1	F	566	ARG
1	F	567	GLU
1	F	569	LEU
1	F	576	LEU
1	F	577	LEU
1	F	579	ARG
1	F	581	THR
1	F	582	LEU
1	F	594	LEU
1	F	596	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	HIS
1	A	370	ASN
1	A	459	HIS
1	A	468	GLN
1	A	554	GLN
1	A	556	GLN

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Mol	Chain	Res	Type
1	B	338	HIS
1	B	554	GLN
1	C	247	HIS
1	C	338	HIS
1	C	370	ASN
1	C	468	GLN
1	C	554	GLN
1	C	556	GLN
1	D	338	HIS
1	D	554	GLN
1	E	247	HIS
1	E	338	HIS
1	E	468	GLN
1	E	554	GLN
1	F	338	HIS
1	F	554	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

6 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	$\#\|Z\|>2$
2	ADP	A	1001	-	22,29,29	1.15	2 (9%)	27,45,45	2.31	3 (11%)
2	ADP	B	2001	-	22,29,29	1.16	2 (9%)	27,45,45	2.52	4 (14%)
2	ADP	C	3001	-	22,29,29	1.11	2 (9%)	27,45,45	2.47	3 (11%)
2	ADP	D	4001	-	22,29,29	1.13	2 (9%)	27,45,45	2.51	4 (14%)
2	ADP	E	5001	-	22,29,29	1.14	2 (9%)	27,45,45	2.44	3 (11%)
2	ADP	F	6001	-	22,29,29	1.14	2 (9%)	27,45,45	2.46	3 (11%)

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
2	ADP	A	1001	-	-	0/12/32/32	0/3/3/3
2	ADP	B	2001	-	-	0/12/32/32	0/3/3/3
2	ADP	C	3001	-	-	0/12/32/32	0/3/3/3
2	ADP	D	4001	-	-	0/12/32/32	0/3/3/3
2	ADP	E	5001	-	-	0/12/32/32	0/3/3/3
2	ADP	F	6001	-	-	0/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4001	ADP	C2-N1	2.14	1.38	1.33
2	C	3001	ADP	C2-N1	2.37	1.38	1.33
2	E	5001	ADP	C2-N1	2.44	1.38	1.33
2	A	1001	ADP	C2-N1	2.46	1.38	1.33
2	F	6001	ADP	C2-N1	2.50	1.38	1.33
2	B	2001	ADP	C2-N1	2.57	1.38	1.33
2	D	4001	ADP	C2-N3	3.66	1.38	1.32
2	B	2001	ADP	C2-N3	3.71	1.38	1.32
2	C	3001	ADP	C2-N3	3.72	1.38	1.32
2	F	6001	ADP	C2-N3	3.79	1.38	1.32
2	E	5001	ADP	C2-N3	3.81	1.38	1.32
2	A	1001	ADP	C2-N3	3.82	1.38	1.32

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2001	ADP	N3-C2-N1	-11.47	120.11	128.89
2	C	3001	ADP	N3-C2-N1	-11.06	120.43	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	6001	ADP	N3-C2-N1	-10.99	120.48	128.89
2	E	5001	ADP	N3-C2-N1	-10.90	120.55	128.89
2	D	4001	ADP	N3-C2-N1	-10.82	120.61	128.89
2	A	1001	ADP	N3-C2-N1	-9.74	121.44	128.89
2	A	1001	ADP	PA-O3A-PB	-4.72	116.83	132.67
2	E	5001	ADP	PA-O3A-PB	-4.70	116.91	132.67
2	D	4001	ADP	C2'-C1'-N9	-4.62	107.24	114.29
2	C	3001	ADP	PA-O3A-PB	-4.59	117.29	132.67
2	F	6001	ADP	C2'-C1'-N9	-4.26	107.78	114.29
2	B	2001	ADP	C2'-C1'-N9	-3.85	108.40	114.29
2	D	4001	ADP	PA-O3A-PB	-3.64	120.46	132.67
2	F	6001	ADP	PA-O3A-PB	-3.56	120.73	132.67
2	B	2001	ADP	PA-O3A-PB	-3.36	121.40	132.67
2	D	4001	ADP	C4-C5-N7	-2.70	107.00	109.48
2	A	1001	ADP	C4-C5-N7	-2.64	107.05	109.48
2	B	2001	ADP	C4-C5-N7	-2.20	107.46	109.48
2	C	3001	ADP	C4-C5-N7	-2.18	107.47	109.48
2	E	5001	ADP	C4-C5-N7	-2.12	107.53	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	ADP	2	0
2	B	2001	ADP	6	0
2	C	3001	ADP	1	0
2	D	4001	ADP	7	0
2	E	5001	ADP	1	0
2	F	6001	ADP	4	0

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	458/499 (91%)	0.56	38 (8%) 14 9	2, 19, 55, 80	0
1	B	446/499 (89%)	0.60	47 (10%) 8 6	2, 19, 50, 97	0
1	C	458/499 (91%)	0.70	49 (10%) 8 6	2, 20, 57, 84	0
1	D	445/499 (89%)	0.55	35 (7%) 15 10	2, 18, 50, 97	0
1	E	458/499 (91%)	0.61	41 (8%) 12 8	2, 21, 55, 82	0
1	F	450/499 (90%)	0.64	38 (8%) 14 9	2, 19, 51, 94	0
All	All	2715/2994 (90%)	0.61	248 (9%) 11 8	2, 19, 54, 97	0

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	271	GLY	7.5
1	A	144	ALA	7.4
1	C	403	LYS	6.8
1	F	272	ASN	6.6
1	A	292	ASP	5.7
1	E	269	GLY	5.6
1	A	443	ARG	5.2
1	F	431	HIS	5.1
1	E	149	GLU	5.1
1	A	429	LEU	4.9
1	B	446	ALA	4.9
1	A	430	GLU	4.8
1	E	402	LYS	4.8
1	F	176	LYS	4.8
1	C	402	LYS	4.7
1	C	186	ALA	4.7
1	E	526	TYR	4.4
1	E	446	ALA	4.4
1	D	448	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	145	ARG	4.3
1	D	221	SER	4.3
1	A	143	ARG	4.2
1	D	222	GLY	4.2
1	C	405	LEU	4.1
1	C	272	ASN	4.1
1	A	527	LEU	4.1
1	D	295	ILE	4.1
1	E	349	ASP	4.0
1	A	269	GLY	4.0
1	B	370	ASN	4.0
1	B	340	ARG	3.9
1	D	223	SER	3.9
1	B	402	LYS	3.9
1	F	359	GLY	3.9
1	B	598	ALA	3.9
1	F	525	THR	3.8
1	A	250	CYS	3.8
1	D	225	PHE	3.6
1	C	299	ALA	3.6
1	A	403	LYS	3.6
1	E	533	ARG	3.6
1	F	446	ALA	3.6
1	F	443	ARG	3.6
1	D	443	ARG	3.6
1	E	324	ASP	3.5
1	B	341	GLY	3.5
1	F	311	LEU	3.5
1	D	299	ALA	3.5
1	A	528	GLY	3.5
1	C	241	PHE	3.5
1	C	250	CYS	3.4
1	D	349	ASP	3.4
1	A	273	ASP	3.4
1	A	390	GLU	3.4
1	A	431	HIS	3.4
1	F	250	CYS	3.3
1	C	373	ALA	3.3
1	B	148	THR	3.3
1	B	597	GLU	3.3
1	D	174	PHE	3.3
1	D	250	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	296	VAL	3.3
1	F	251	ILE	3.3
1	C	212	GLU	3.2
1	E	369	LEU	3.2
1	C	430	GLU	3.2
1	E	401	ALA	3.2
1	E	404	SER	3.2
1	C	404	SER	3.2
1	E	282	LEU	3.2
1	F	175	LEU	3.1
1	A	291	LYS	3.1
1	A	270	GLY	3.1
1	D	298	MET	3.1
1	E	367	ASN	3.1
1	A	187	ARG	3.1
1	A	272	ASN	3.1
1	D	170	GLU	3.1
1	E	452	PRO	3.0
1	C	239	ASP	3.0
1	B	447	LEU	3.0
1	F	159	ALA	3.0
1	D	324	ASP	3.0
1	B	448	GLY	3.0
1	B	225	PHE	3.0
1	B	324	ASP	3.0
1	D	442	PRO	3.0
1	F	445	ARG	3.0
1	E	325	ALA	2.9
1	F	403	LYS	2.9
1	E	270	GLY	2.9
1	B	445	ARG	2.9
1	B	462	ARG	2.9
1	A	290	GLU	2.9
1	C	273	ASP	2.9
1	D	228	MET	2.9
1	D	527	LEU	2.9
1	F	582	LEU	2.9
1	C	159	ALA	2.9
1	B	371	GLU	2.8
1	B	452	PRO	2.8
1	F	294	ALA	2.8
1	A	599	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	272	ASN	2.8
1	C	371	GLU	2.8
1	E	443	ARG	2.8
1	C	262	ARG	2.7
1	F	436	HIS	2.7
1	E	527	LEU	2.7
1	B	526	TYR	2.7
1	E	248	ALA	2.7
1	B	315	GLY	2.7
1	B	429	LEU	2.7
1	D	280	ASN	2.7
1	E	370	ASN	2.7
1	F	263	LYS	2.7
1	B	157	ASP	2.7
1	B	387	LYS	2.6
1	F	222	GLY	2.6
1	F	339	ALA	2.6
1	E	371	GLU	2.6
1	B	226	VAL	2.6
1	F	452	PRO	2.6
1	C	243	THR	2.6
1	C	270	GLY	2.6
1	C	158	VAL	2.6
1	A	600	GLU	2.5
1	A	159	ALA	2.5
1	B	425	ALA	2.5
1	D	431	HIS	2.5
1	E	374	LEU	2.5
1	C	242	GLU	2.5
1	B	311	LEU	2.5
1	A	511	HIS	2.5
1	C	431	HIS	2.5
1	D	274	GLU	2.5
1	D	175	LEU	2.5
1	F	321	ILE	2.5
1	A	439	THR	2.5
1	A	468	GLN	2.5
1	F	293	THR	2.4
1	D	256	GLU	2.4
1	E	278	THR	2.4
1	C	240	LEU	2.4
1	D	171	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	451	MET	2.4
1	B	366	GLU	2.4
1	C	266	SER	2.4
1	E	326	PRO	2.4
1	A	254	ILE	2.4
1	C	396	VAL	2.4
1	D	227	GLU	2.4
1	E	294	ALA	2.4
1	E	348	VAL	2.4
1	A	436	HIS	2.4
1	D	344	LEU	2.4
1	B	347	ASP	2.4
1	A	244	ALA	2.4
1	E	264	ARG	2.4
1	C	388	ASP	2.4
1	A	216	PRO	2.3
1	B	382	ARG	2.3
1	C	395	ARG	2.3
1	C	594	LEU	2.3
1	C	599	PRO	2.3
1	F	442	PRO	2.3
1	C	230	VAL	2.3
1	E	268	VAL	2.3
1	F	280	ASN	2.3
1	E	368	LEU	2.3
1	E	445	ARG	2.3
1	E	409	PRO	2.3
1	F	193	LEU	2.3
1	D	272	ASN	2.3
1	A	455	GLU	2.3
1	C	452	PRO	2.3
1	E	161	ALA	2.3
1	C	323	ILE	2.3
1	F	281	GLN	2.3
1	B	222	GLY	2.3
1	A	453	ARG	2.3
1	F	174	PHE	2.3
1	F	179	SER	2.3
1	B	224	ASP	2.3
1	B	376	ALA	2.3
1	D	172	VAL	2.3
1	D	177	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	597	GLU	2.3
1	E	147	LEU	2.2
1	C	229	PHE	2.2
1	C	237	VAL	2.2
1	F	600	GLU	2.2
1	C	355	LYS	2.2
1	E	373	ALA	2.2
1	B	323	ILE	2.2
1	E	148	THR	2.2
1	B	188	ILE	2.2
1	B	289	PHE	2.2
1	C	265	GLY	2.2
1	B	388	ASP	2.2
1	B	165	LYS	2.2
1	F	282	LEU	2.2
1	C	187	ARG	2.1
1	D	445	ARG	2.1
1	F	244	ALA	2.1
1	F	598	ALA	2.1
1	C	595	PRO	2.1
1	C	291	LYS	2.1
1	C	290	GLU	2.1
1	C	391	GLU	2.1
1	B	246	ARG	2.1
1	F	404	SER	2.1
1	F	295	ILE	2.1
1	B	261	GLY	2.1
1	B	205	LEU	2.1
1	C	387	LYS	2.1
1	E	290	GLU	2.1
1	D	220	ALA	2.1
1	D	224	ASP	2.1
1	B	360	PHE	2.1
1	A	487	THR	2.1
1	C	406	VAL	2.1
1	A	271	GLY	2.1
1	E	163	GLU	2.1
1	F	299	ALA	2.1
1	C	336	ARG	2.1
1	B	314	PRO	2.1
1	E	311	LEU	2.1
1	C	448	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	383	LYS	2.1
1	A	449	PHE	2.1
1	D	373	ALA	2.1
1	B	250	CYS	2.1
1	B	435	VAL	2.1
1	A	249	PRO	2.0
1	E	347	ASP	2.0
1	C	543	ILE	2.0
1	B	292	ASP	2.0
1	B	527	LEU	2.0
1	D	511	HIS	2.0
1	C	314	PRO	2.0
1	B	499	GLU	2.0
1	F	289	PHE	2.0
1	C	449	PHE	2.0
1	F	195	VAL	2.0
1	D	168	LEU	2.0
1	E	335	LEU	2.0
1	B	219	THR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ADP	A	1001	27/27	0.88	0.26	-0.39	14,15,17,18	0
2	ADP	C	3001	27/27	0.86	0.27	-0.64	18,18,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ADP	D	4001	27/27	0.92	0.25	-0.84	2,2,8,8	0
2	ADP	E	5001	27/27	0.85	0.27	-1.01	14,17,18,18	0
2	ADP	F	6001	27/27	0.88	0.22	-1.04	11,15,15,18	0
2	ADP	B	2001	27/27	0.85	0.21	-1.08	5,9,13,13	0

6.5 Other polymers (i)

There are no such residues in this entry.