



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:05 AM UTC

PDB ID : 2DHR / pdb_00002dhr
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

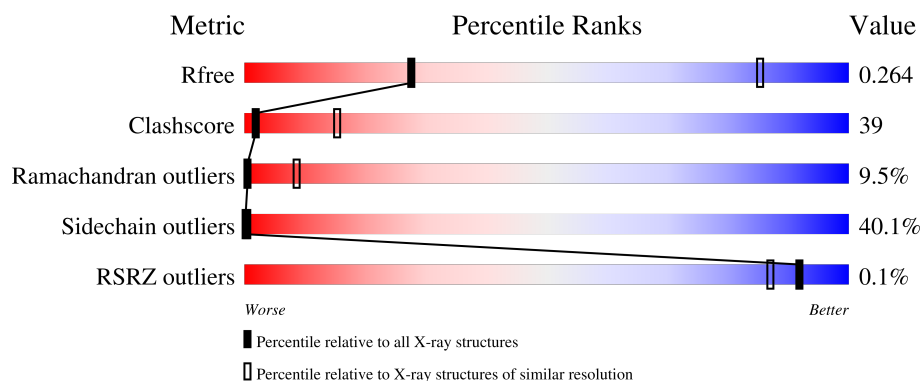
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	499	
1	B	499	
1	C	499	
1	D	499	
1	E	499	

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Mol	Chain	Length	Quality of chain
1	F	499	28%37%19%5%10%

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 mutation	UNP Q9LCZ4
B	399	LEU	GLY	engineered mutation	UNP Q9LCZ4
C	399	LEU	GLY	engineered mutation	UNP Q9LCZ4
D	399	LEU	GLY	engineered mutation	UNP Q9LCZ4
E	399	LEU	GLY	engineered mutation	UNP Q9LCZ4
F	399	LEU	GLY	engineered mutation	UNP Q9LCZ4

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

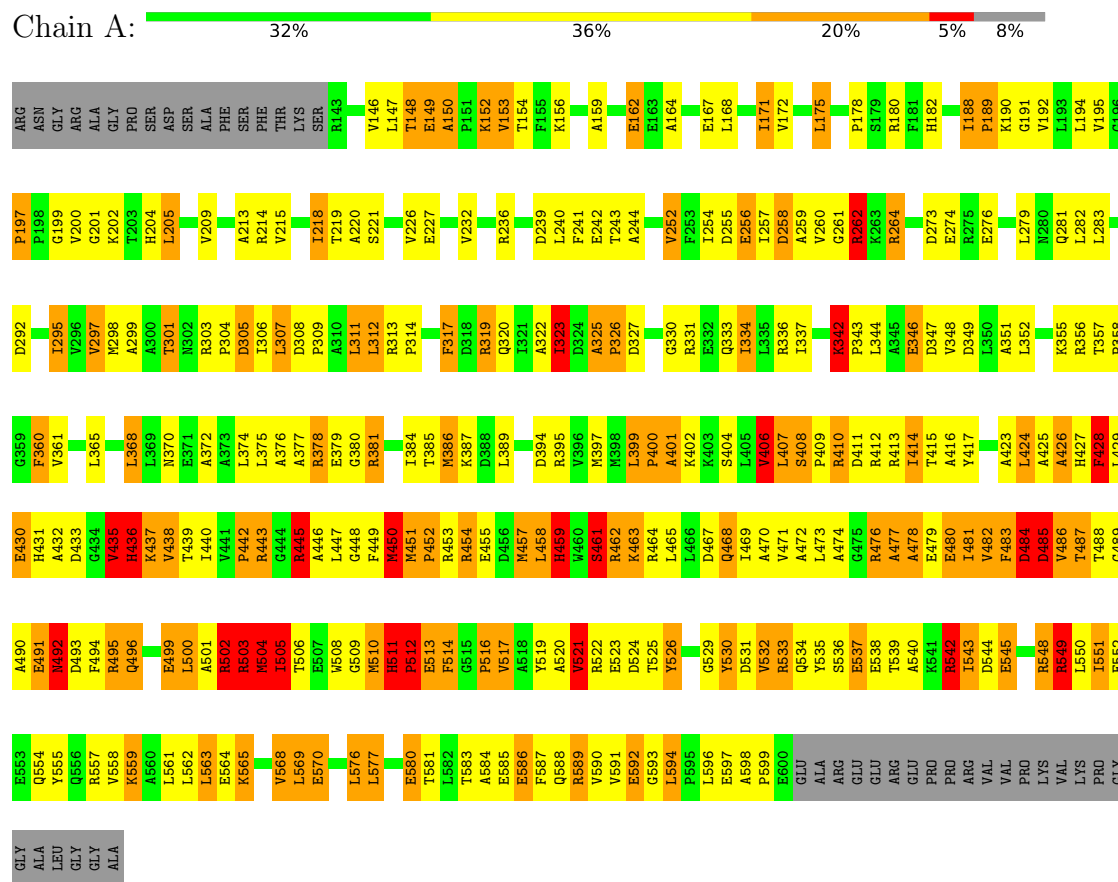


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

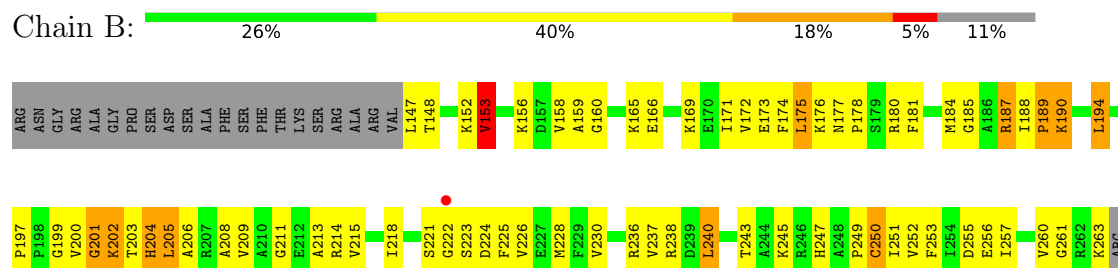
3 Residue-property plots

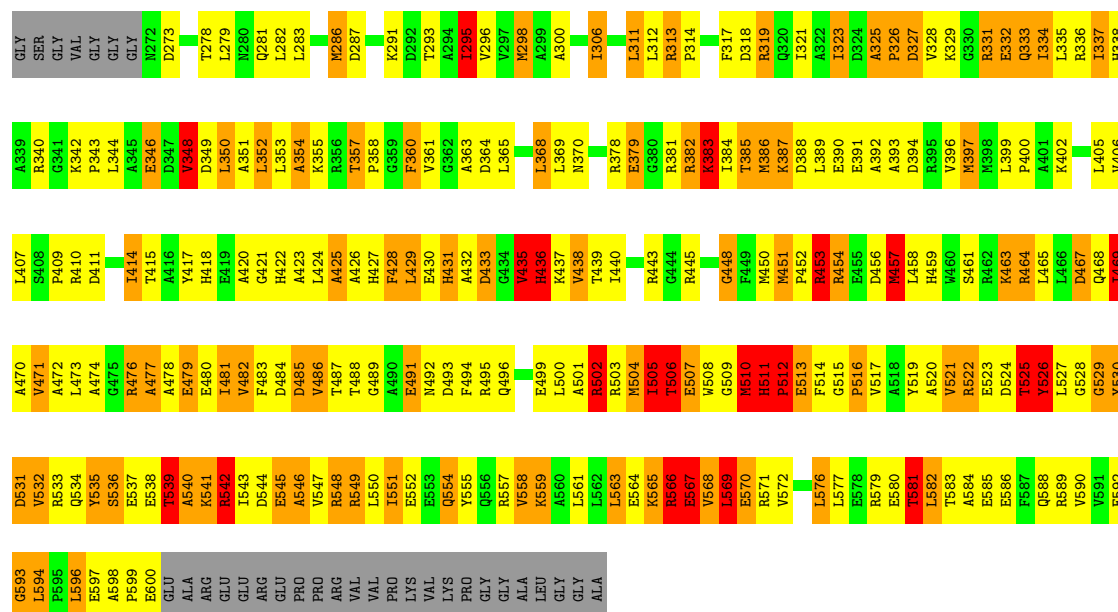
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: FtsH



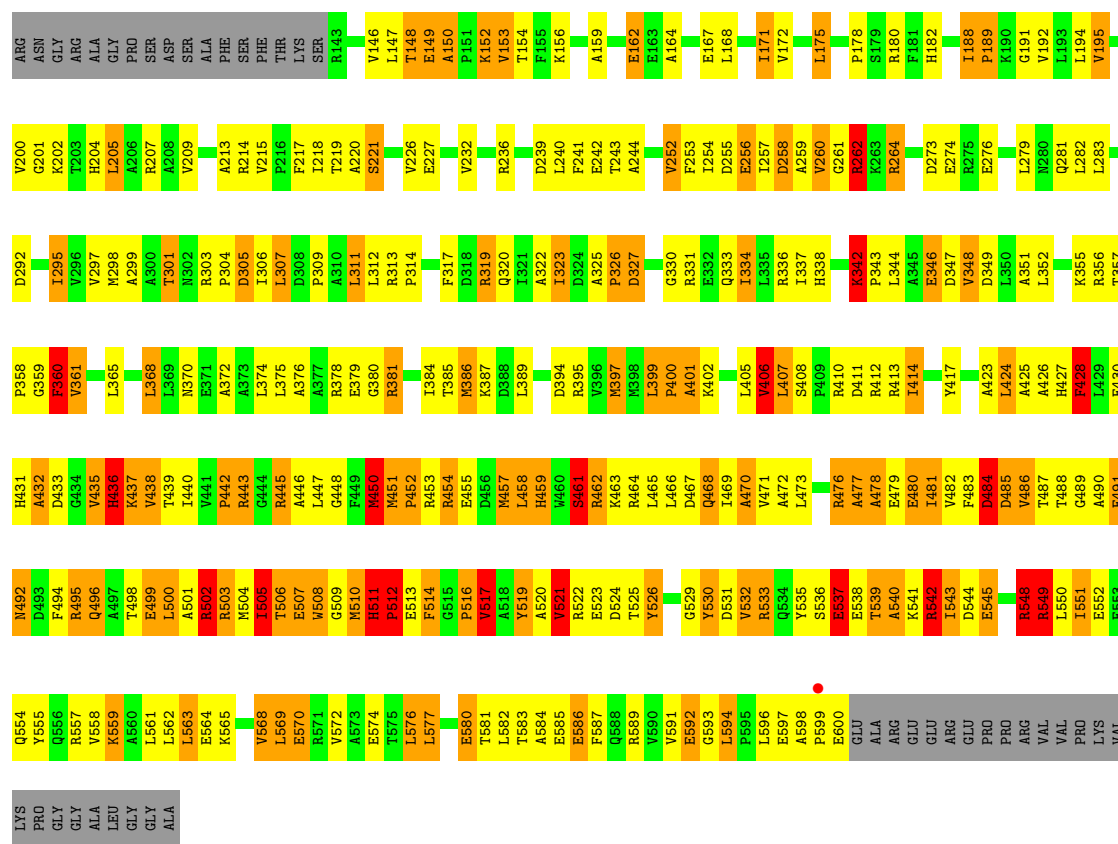
• Molecule 1: FtsH





• Molecule 1: FtsH

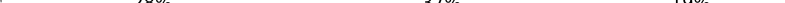
Chain C: 32% 36% 20% 8%

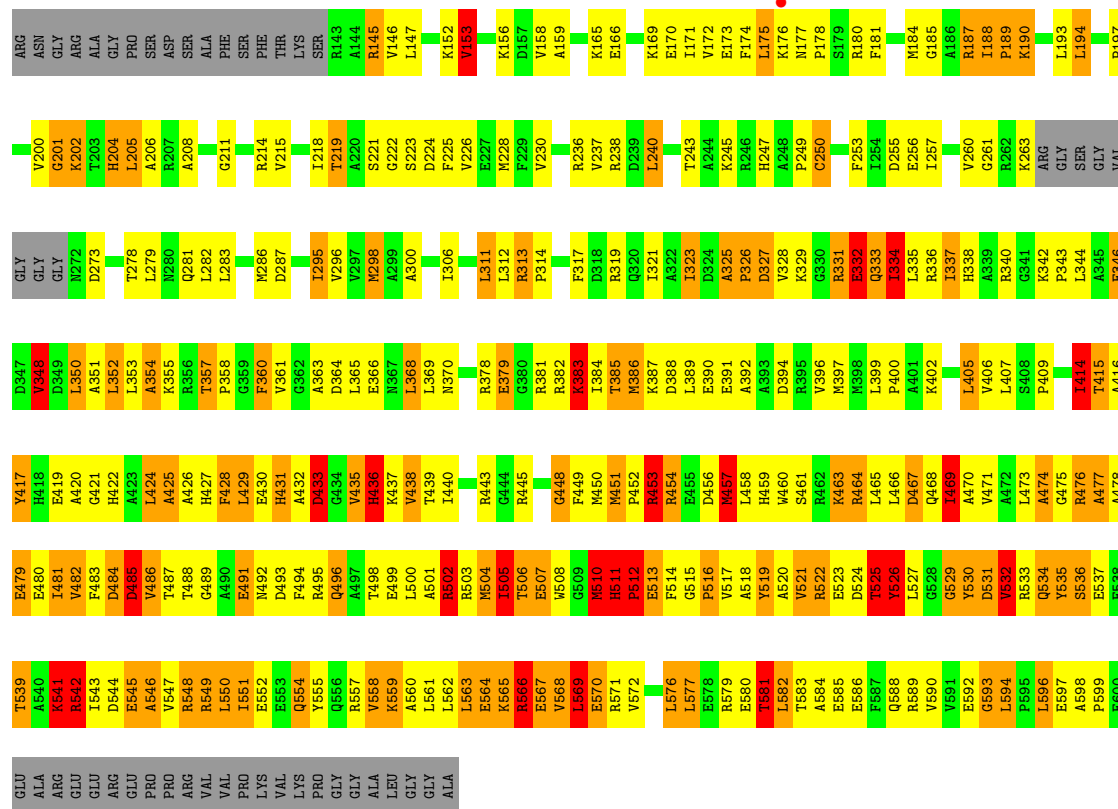


• Molecule 1: FtsH

Chain D: 28% 37% 19% 5% 11%



Chain F: 



4 Data and refinement statistics

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 15.00 – 3.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-3.90) 97.4 (15.00-3.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.64 (at 3.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.299 , 0.342 (Not available) , 0.264	Depositor DCC
R_{free} test set	1960 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	98.2	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 287.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.27$, $\langle L^2 \rangle = 0.11$	Xtriage
Estimated twinning fraction	0.240 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	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 1.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.98	12/3637 (0.3%)	1.19	21/4908 (0.4%)
1	B	0.95	7/3568 (0.2%)	1.20	14/4815 (0.3%)
1	C	0.96	9/3641 (0.2%)	1.20	20/4913 (0.4%)
1	D	0.97	5/3560 (0.1%)	1.20	17/4804 (0.4%)
1	E	0.92	7/3641 (0.2%)	1.18	16/4913 (0.3%)
1	F	0.96	6/3596 (0.2%)	1.20	17/4853 (0.4%)
All	All	0.96	46/21643 (0.2%)	1.20	105/29206 (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 (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	549	ARG	NE-CZ	8.42	1.42	1.33
1	D	549	ARG	NE-CZ	8.03	1.41	1.33
1	C	505	ILE	CA-CB	-8.02	1.44	1.54
1	E	505	ILE	CA-CB	-7.46	1.44	1.54
1	E	532	VAL	CA-CB	7.30	1.64	1.54
1	A	532	VAL	CA-CB	6.96	1.64	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	406	VAL	CA-C	6.74	1.59	1.52
1	A	487	THR	CA-CB	-6.65	1.44	1.53
1	C	540	ALA	CA-CB	-6.62	1.42	1.53
1	B	502	ARG	NE-CZ	6.57	1.40	1.33
1	B	549	ARG	NE-CZ	6.47	1.40	1.33
1	F	549	ARG	NE-CZ	6.46	1.40	1.33
1	F	433	ASP	CA-C	6.23	1.59	1.52
1	C	428	PHE	CA-C	6.23	1.61	1.52
1	A	504	MET	SD-CE	-6.00	1.64	1.79
1	A	428	PHE	CA-C	5.89	1.60	1.52
1	F	542	ARG	NE-CZ	5.82	1.39	1.33
1	B	469	ILE	CA-CB	-5.82	1.47	1.54
1	F	469	ILE	CA-CB	-5.80	1.47	1.54
1	C	532	VAL	CA-CB	5.72	1.62	1.54
1	C	470	ALA	CA-C	-5.65	1.45	1.52
1	D	474	ALA	N-CA	5.63	1.53	1.46
1	B	435	VAL	CA-C	5.62	1.59	1.52
1	A	502	ARG	NE-CZ	5.59	1.39	1.33
1	B	542	ARG	NE-CZ	5.56	1.39	1.33
1	A	510	MET	CA-C	-5.46	1.46	1.52
1	C	432	ALA	CA-CB	-5.37	1.44	1.53
1	A	505	ILE	CA-CB	-5.32	1.47	1.54
1	A	542	ARG	CB-CG	5.31	1.68	1.52
1	D	433	ASP	CA-C	5.29	1.58	1.52
1	D	542	ARG	NE-CZ	5.25	1.38	1.33
1	C	542	ARG	CB-CG	5.25	1.68	1.52
1	E	428	PHE	CA-C	5.19	1.59	1.52
1	C	510	MET	SD-CE	-5.18	1.66	1.79
1	F	436	HIS	CA-C	5.18	1.59	1.52
1	E	546	ALA	CA-CB	-5.17	1.45	1.53
1	A	542	ARG	CA-CB	5.16	1.61	1.53
1	B	540	ALA	CA-CB	-5.09	1.45	1.53
1	C	549	ARG	NE-CZ	5.09	1.38	1.33
1	E	432	ALA	CA-CB	-5.09	1.45	1.53
1	E	504	MET	SD-CE	-5.09	1.66	1.79
1	A	435	VAL	CA-CB	5.07	1.61	1.54
1	B	544	ASP	CA-CB	-5.05	1.45	1.53
1	D	437	LYS	N-CA	5.02	1.52	1.46
1	F	502	ARG	NE-CZ	5.01	1.38	1.33
1	A	470	ALA	CA-CB	-5.00	1.45	1.53

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	436	HIS	N-CA-C	12.59	127.47	108.46
1	F	436	HIS	N-CA-C	12.28	127.01	108.46
1	F	541	LYS	N-CA-C	-9.22	101.18	111.14
1	A	406	VAL	N-CA-C	8.70	119.14	108.53
1	B	559	LYS	N-CA-C	-8.50	101.97	111.07
1	E	543	ILE	CB-CA-C	-8.19	101.08	112.14
1	D	467	ASP	N-CA-C	-8.05	100.45	112.04
1	A	543	ILE	CB-CA-C	-7.72	101.72	112.14
1	C	510	MET	N-CA-C	-7.67	95.80	108.76
1	A	510	MET	N-CA-C	-7.66	95.78	108.34
1	D	436	HIS	N-CA-C	7.65	127.09	110.80
1	F	433	ASP	N-CA-C	7.42	120.63	107.80
1	B	502	ARG	N-CA-C	-7.41	103.20	111.28
1	F	467	ASP	N-CA-C	-7.40	102.16	112.45
1	A	485	ASP	N-CA-C	-7.28	104.86	113.38
1	D	502	ARG	N-CA-C	-7.24	103.39	111.28
1	E	406	VAL	N-CA-C	7.18	117.29	108.53
1	D	531	ASP	N-CA-C	7.08	120.21	108.96
1	B	438	VAL	N-CA-C	6.91	119.39	108.89
1	F	405	LEU	N-CA-C	6.87	119.43	110.43
1	E	502	ARG	N-CA-CB	6.82	120.81	110.30
1	C	543	ILE	CB-CA-C	-6.78	102.86	112.22
1	F	417	TYR	N-CA-C	-6.77	103.98	111.36
1	D	433	ASP	N-CA-C	6.76	119.49	107.80
1	D	420	ALA	N-CA-C	-6.74	102.55	111.24
1	B	448	GLY	N-CA-C	6.70	120.77	112.73
1	B	531	ASP	N-CA-C	6.65	119.57	108.73
1	C	507	GLU	N-CA-C	-6.64	103.22	112.45
1	F	474	ALA	N-CA-C	-6.63	104.92	112.87
1	C	531	ASP	N-CA-C	6.55	120.18	109.76
1	D	559	LYS	N-CA-C	-6.50	104.11	111.07
1	C	406	VAL	N-CA-C	6.50	116.46	108.53
1	F	559	LYS	N-CA-C	-6.48	104.14	111.07
1	D	541	LYS	N-CA-C	-6.45	104.17	111.14
1	D	438	VAL	N-CA-C	6.44	119.19	109.20
1	E	531	ASP	N-CA-C	6.31	119.43	109.96
1	A	436	HIS	N-CA-C	6.26	124.13	110.80
1	C	436	HIS	N-CA-C	6.21	124.03	110.80
1	D	448	GLY	N-CA-C	6.18	120.15	112.73
1	A	487	THR	N-CA-C	6.14	118.73	108.73
1	B	567	GLU	N-CA-C	-6.11	106.43	114.31
1	C	549	ARG	CA-CB-CG	6.10	126.30	114.10
1	E	436	HIS	N-CA-C	6.07	123.73	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	438	VAL	N-CA-C	6.04	117.00	108.36
1	F	448	GLY	N-CA-C	6.01	119.94	112.73
1	A	323	ILE	N-CA-C	5.95	117.23	107.24
1	A	483	PHE	N-CA-C	5.95	118.38	110.53
1	A	503	ARG	N-CA-C	-5.93	103.78	111.02
1	D	506	THR	N-CA-CB	-5.92	101.95	110.65
1	E	549	ARG	CA-CB-CG	5.92	125.93	114.10
1	B	467	ASP	N-CA-C	-5.91	103.53	112.04
1	A	463	LYS	N-CA-C	-5.89	104.77	111.07
1	B	506	THR	N-CA-CB	-5.88	102.76	110.88
1	A	542	ARG	CA-CB-CG	5.86	125.81	114.10
1	E	535	TYR	N-CA-C	-5.85	98.33	110.80
1	B	348	VAL	N-CA-C	5.84	117.77	111.58
1	A	502	ARG	N-CA-CB	5.83	119.28	110.30
1	C	346	GLU	N-CA-C	5.82	117.41	110.19
1	C	509	GLY	N-CA-C	-5.82	99.38	113.18
1	B	457	MET	N-CA-C	5.81	123.17	110.80
1	B	433	ASP	N-CA-C	5.79	117.82	107.80
1	E	346	GLU	N-CA-C	5.72	117.28	110.19
1	C	502	ARG	N-CA-CB	5.68	119.66	110.40
1	C	517	VAL	CB-CA-C	-5.65	103.47	111.38
1	D	348	VAL	N-CA-C	5.60	117.52	111.58
1	C	438	VAL	N-CA-C	5.59	116.36	108.36
1	A	549	ARG	N-CA-CB	5.56	119.17	109.72
1	E	498	THR	OG1-CB-CG2	-5.55	98.20	109.30
1	C	542	ARG	N-CA-C	-5.51	104.50	111.11
1	A	531	ASP	N-CA-C	5.50	118.50	109.76
1	A	461	SER	N-CA-C	5.49	117.44	108.55
1	E	542	ARG	N-CA-C	-5.45	104.37	111.02
1	F	438	VAL	N-CA-C	5.43	117.62	109.20
1	F	531	ASP	N-CA-C	5.43	117.58	108.73
1	E	534	GLN	N-CA-C	5.41	117.21	108.34
1	A	404	SER	N-CA-C	5.39	118.05	109.96
1	A	325	ALA	N-CA-C	5.38	121.71	109.81
1	C	542	ARG	CA-CB-CG	5.35	124.80	114.10
1	D	508	TRP	N-CA-C	-5.34	103.64	110.53
1	F	348	VAL	N-CA-C	5.33	117.24	111.58
1	D	457	MET	N-CA-C	5.33	122.16	110.80
1	F	457	MET	N-CA-C	5.28	122.05	110.80
1	A	346	GLU	N-CA-C	5.27	116.72	110.19
1	C	508	TRP	N-CA-C	-5.26	102.96	110.59
1	E	549	ARG	N-CA-CB	5.26	117.81	109.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	405	LEU	N-CA-C	5.25	117.64	110.55
1	E	461	SER	N-CA-C	5.25	117.05	108.55
1	C	502	ARG	N-CA-C	-5.23	106.40	112.89
1	B	453	ARG	N-CA-C	-5.23	107.56	114.04
1	C	461	SER	N-CA-C	5.21	117.85	108.48
1	C	549	ARG	N-CA-CB	5.19	117.71	109.82
1	F	334	ILE	N-CA-C	5.19	115.96	110.72
1	D	516	PRO	N-CA-C	5.16	123.09	112.47
1	A	509	GLY	N-CA-C	-5.15	100.97	113.18
1	F	250	CYS	N-CA-C	5.15	114.64	107.73
1	D	453	ARG	N-CA-C	-5.13	107.67	114.04
1	B	250	CYS	N-CA-C	5.11	114.98	108.24
1	C	505	ILE	N-CA-CB	-5.08	103.20	110.52
1	C	548	ARG	N-CA-C	-5.06	105.45	110.97
1	F	532	VAL	CB-CA-C	-5.06	104.58	111.15
1	A	438	VAL	CB-CA-C	-5.05	103.86	110.98
1	E	542	ARG	CA-CB-CG	5.05	124.20	114.10
1	A	549	ARG	CA-CB-CG	5.04	124.19	114.10
1	E	404	SER	N-CA-C	5.02	117.58	110.10
1	F	453	ARG	N-CA-C	-5.02	107.82	114.04

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

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Mol	Chain	Res	Type	Group
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

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	269	0
1	B	3511	0	3556	341	0
1	C	3583	0	3628	264	0
1	D	3503	0	3545	337	0
1	E	3583	0	3628	253	0
1	F	3539	0	3585	334	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	1698	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 39.

All (1698) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:510:MET:O	1:A:512:PRO:HD2	1.56	1.04
1:D:543:ILE:O	1:D:546:ALA:HB3	1.57	1.04
1:D:505:ILE:HG23	1:D:514:PHE:HD1	1.23	1.04
1:D:325:ALA:HB3	1:D:326:PRO:HD3	1.36	1.03
1:D:517:VAL:CG2	1:D:519:TYR:CZ	2.42	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:B:517:VAL:HG21	1:B:519:TYR:CZ	1.94	1.02
1:D:510:MET:O	1:D:512:PRO:HD2	1.60	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:335:LEU:HB3	1:D:350:LEU:HD22	1.40	0.99
1:D:502:ARG:CD	1:D:533:ARG:NH2	2.24	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:E:510:MET:C	1:E:512:PRO:HD2	1.88	0.98
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:B:428:PHE:CD1	1:B:432:ALA:HB1	2.00	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:505:ILE:HG23	1:A:514:PHE:HD1	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: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
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:B:510:MET:C	1:B:512:PRO:HD2	1.98	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:B:335:LEU:HD13	1:B:353:LEU:HD23	1.54	0.87
1:D:335:LEU:HD13	1:D:353:LEU:HD23	1.57	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:D:420:ALA:O	1:D:421:GLY:C	2.17	0.85
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:C:399:LEU:H	1:C:400:PRO:HD2	1.42	0.85
1:D:503:ARG:NH1	1:D:522:ARG:HG3	1.92	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:VAL:HG22	1:B:436:HIS:H	1.42	0.84
1:B:476:ARG:CZ	1:B:487:THR:HG21	2.07	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: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:HG2	1:F:542:ARG:HH11	1.44	0.83
1:D:510:MET:C	1:D:512:PRO:HD2	2.04	0.83
1:A:483:PHE:C	1:A:485:ASP:H	1.86	0.82
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:C:520:ALA:HA	1:C:533:ARG:HB2	1.60	0.81
1:F:470:ALA:HB2	1:F:554:GLN:HG3	1.62	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:A:463:LYS:HD2	1:B:486:VAL:CG1	2.11	0.81
1:D:335:LEU:CD1	1:D:353:LEU:HD23	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:A:510:MET:C	1:A:512:PRO:HD2	2.05	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: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:195:VAL:HG21	1:A:304:PRO:HB3	1.64	0.80
1:A:516:PRO:HB2	1:B:494:PHE:CE2	2.17	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:C:159:ALA:HB3	1:C:334:ILE:HD13	1.64	0.79
1:D:517:VAL:HG21	1:D:519:TYR:OH	1.81	0.79
1:B:448:GLY:HA2	1:B:451:MET:HE2	1.63	0.79
1:B:458:LEU:HD12	1:B:459:HIS:H	1.48	0.79
1:F:422:HIS:O	1:F:425:ALA:HB3	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:511:HIS:CE1	1:E:516:PRO:HD3	2.18	0.79
1:A:188:ILE:HD13	1:A:189:PRO:HD2	1.65	0.79
1:F:189:PRO:O	1:F:190:LYS:HB2	1.83	0.79
1:B:197:PRO:HD2	1:B:200:VAL:HG21	1.64	0.78
1:B:467:ASP:O	1:B:471:VAL:HG23	1.83	0.78
1:D:199:GLY:O	1:D:361:VAL:HB	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:E:483:PHE:C	1:E:485:ASP:H	1.91	0.78
1:F:325:ALA:CB	1:F:326:PRO:HD3	2.13	0.78
1:B:463:LYS:HB2	1:C:486:VAL:HG11	1.65	0.78
1:D:542:ARG:HG2	1:D:542:ARG:HH11	1.47	0.78
1:B:548:ARG:HH11	1:B:548:ARG:HG3	1.47	0.78
1:C:565:LYS:O	1:C:568:VAL:HG23	1.84	0.78
1:F:197:PRO:HD2	1:F:200:VAL:HG21	1.64	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:448:GLY:HA2	1:F:451:MET:HE2	1.66	0.78
1:F:554:GLN:NE2	1:F:557:ARG:HD3	1.99	0.77
1:C:510:MET:C	1:C:512:PRO:HD2	2.10	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
1:F:332:GLU:OE1	1:F:351:ALA:HA	1.84	0.77
1:F:510:MET:C	1:F:512:PRO:HD2	2.09	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:HG3	1:C:548:ARG:NH1	1.98	0.77
1:F:511:HIS:CE1	1:F:516:PRO:CD	2.68	0.77
1:C:483:PHE:O	1:C:485:ASP:N	2.17	0.77
1:D:470:ALA:HB2	1:D:554:GLN:HG3	1.67	0.77
1:A:505:ILE:HG22	1:A:506:THR:N	1.98	0.76
1:B:503:ARG:NH1	1:B:522:ARG:HG3	2.00	0.76
1:D:448:GLY:HA2	1:D:451:MET:HE2	1.65	0.76
1:D:326:PRO:HB2	1:D:331:ARG:HH12	1.50	0.76
1:E:357:THR:HG23	1:E:357:THR:O	1.85	0.76
1:F:569:LEU:O	1:F:571:ARG:N	2.18	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:HH11	1:B:548:ARG:CG	1.97	0.76
1:E:330:GLY:O	1:E:334:ILE:HG12	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:476:ARG:NE	1:F:487:THR:HG21	1.99	0.76
1:D:326:PRO:CB	1:D:331:ARG:HH12	1.98	0.76
1:D:477:ALA:O	1:D:478:ALA:C	2.29	0.76
1:C:447:LEU:HA	1:C:496:GLN:NE2	2.01	0.75
1:A:484:ASP:C	1:A:486:VAL:H	1.93	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:F:503:ARG:HB3	1:F:508:TRP:CZ3	2.22	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:HG3	1:B:548:ARG:NH1	2.00	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:D:542:ARG:HH11	1:D:542:ARG:HA	1.51	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:A:505:ILE:HG22	1:A:506:THR:HG23	1.70	0.74
1:F:542:ARG:HH11	1:F:542:ARG:HA	1.51	0.74
1:A:516:PRO:HB2	1:B:494:PHE:CD2	2.23	0.74
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:A:447:LEU:HA	1:A:496:GLN:NE2	2.03	0.74
1:F:428:PHE:CE1	1:F:432:ALA:HB1	2.23	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:A:425:ALA:O	1:A:427:HIS:N	2.20	0.73
1:B:334:ILE:HD11	2:B:2001:ADP:C6	2.23	0.73
1:D:542:ARG:HA	1:D:542:ARG:NH1	2.04	0.73
1:E:188:ILE:HD13	1:E:189:PRO:HD2	1.71	0.73
1:C:463:LYS:HD2	1:D:486:VAL:CG1	2.19	0.73
1:C:505:ILE:HG22	1:C:506:THR:N	2.02	0.73
1:D:542:ARG:HH11	1:D:542:ARG:CG	2.01	0.73
1:B:428:PHE:CE1	1:B:432:ALA:HB1	2.24	0.73
1:E:548:ARG:HH11	1:E:548:ARG:HG3	1.53	0.73
1:A:565:LYS:O	1:A:568:VAL:HG23	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:THR:HG23	1:A:357:THR:O	1.88	0.72
1:E:525:THR:HG22	1:E:526:TYR:H	1.54	0.72
1:F:428:PHE:CD1	1:F:428:PHE:N	2.57	0.72
1:A:331:ARG:HD3	1:A:357:THR:O	1.90	0.72
1:D:171:ILE:CG2	1:D:296:VAL:HG21	2.19	0.72
1:E:447:LEU:HA	1:E:496:GLN:NE2	2.04	0.72
1:F:473:LEU:C	1:F:475:GLY:H	1.98	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:D:526:TYR:HD1	1:D:526:TYR:H	1.36	0.72
1:F:542:ARG:HH11	1:F:542:ARG:CG	2.02	0.72
1:E:476:ARG:CZ	1:E:487:THR:HG21	2.20	0.72
1:B:159:ALA:HB1	1:B:333:GLN:HB3	1.71	0.72
1:E:331:ARG:HD3	1:E:357:THR:O	1.90	0.72
1:A:406:VAL:HG12	1:A:407:LEU:H	1.54	0.71
1:B:542:ARG:HH11	1:B:542:ARG:HG2	1.52	0.71
1:B:515:GLY:O	1:B:517:VAL:N	2.22	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: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
1:A:494:PHE:HE2	1:F:516:PRO:HB3	1.54	0.71
1:D:503:ARG:HB3	1:D:508:TRP:CZ3	2.25	0.71
1:E:513:GLU:O	1:F:548:ARG:NH2	2.24	0.71
1:F:517:VAL:HG21	1:F:519:TYR:OH	1.88	0.71
1:F:548:ARG:HH11	1:F:548:ARG:HG3	1.56	0.71
1:B:424:LEU:O	1:B:427:HIS:N	2.20	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:C:516:PRO:CB	1:D:494:PHE:CE2	2.73	0.71
1:C:483:PHE:C	1:C:485:ASP:H	1.99	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:B:335:LEU:CD1	1:B:353:LEU:HD23	2.21	0.70
1:F:517:VAL:CG2	1:F:519:TYR:CE1	2.74	0.70
1:A:511:HIS:CE1	1:A:516:PRO:HD3	2.25	0.70
1:B:526:TYR:HD1	1:B:526:TYR:H	1.37	0.70
1:F:424:LEU:O	1:F:425:ALA:C	2.31	0.70
1:F:503:ARG:NH1	1:F:522:ARG:HG3	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:511:HIS:C	1:B:512:PRO:O	2.35	0.70
1:E:484:ASP:C	1:E:486:VAL:H	2.00	0.70
1:A:428:PHE:CD1	1:A:428:PHE:N	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:A:476:ARG:CZ	1:A:487:THR:HG21	2.22	0.69
1:B:476:ARG:NE	1:B:487:THR:CG2	2.54	0.69
1:D:424:LEU:O	1:D:425:ALA:C	2.36	0.69
1:A:378:ARG:NH2	1:F:169:LYS:HB2	2.08	0.69
1:A:477:ALA:O	1:A:478:ALA:C	2.36	0.69
1:B:503:ARG:HB3	1:B:508:TRP:CZ3	2.26	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:C:428:PHE:CD1	1:C:428:PHE:N	2.58	0.69
1:C:505:ILE:HG23	1:C:514:PHE:CD1	2.28	0.69
1:D:357:THR:OG1	1:D:360:PHE:CD2	2.46	0.69
1:D:505:ILE:CG2	1:D:514:PHE:HD1	2.01	0.69
1:B:348:VAL:HG22	1:B:352:LEU:HB3	1.75	0.68
1:D:348:VAL:HG21	1:D:386:MET:HE2	1.74	0.68
1:A:463:LYS:HD2	1:B:486:VAL:HG13	1.74	0.68
1:A:486:VAL:HG11	1:F:463:LYS:HB2	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:CG2	2.23	0.68
1:D:337:ILE:HG22	1:D:338:HIS:CD2	2.28	0.68
1:E:548:ARG:HG3	1:E:548:ARG:NH1	2.08	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:470:ALA:O	1:F:558:VAL:HG11	1.94	0.68
1:C:484:ASP:C	1:C:486:VAL:H	2.02	0.67
1:F:481:ILE:HG22	1:F:482:VAL:N	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:517:VAL:HG23	1:F:519:TYR:CZ	2.27	0.67
1:B:542:ARG:HH11	1:B:542:ARG:CA	2.05	0.67
1:D:479:GLU:OE2	1:D:487:THR:HA	1.94	0.67
1:A:525:THR:HG22	1:A:526:TYR:H	1.59	0.67
1:B:511:HIS:O	1:B:512:PRO:O	2.11	0.67
1:E:583:THR:O	1:E:586:GLU:HB2	1.95	0.67
1:A:305:ASP:OD2	1:A:447:LEU:HD13	1.93	0.67
1:C:548:ARG:HH11	1:C:548:ARG:CG	2.07	0.67
1:D:326:PRO:O	1:D:327:ASP:HB2	1.94	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:C:372:ALA:O	1:C:375:LEU:HB2	1.95	0.67
1:D:458:LEU:HD12	1:D:459:HIS:H	1.59	0.67
1:E:469:ILE:HG12	1:E:500:LEU:HD12	1.77	0.67
1:A:399:LEU:N	1:A:400:PRO:HD2	2.10	0.67
1:B:513:GLU:O	1:C:548:ARG:NH2	2.28	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:B:171:ILE:CG2	1:B:296:VAL:HG21	2.25	0.66
1:D:507:GLU:HG3	1:D:520:ALA:HB3	1.77	0.66
1:E:241:PHE:HE2	1:E:252:VAL:HG21	1.60	0.66
1:A:484:ASP:C	1:A:486:VAL:N	2.53	0.66
1:D:334:ILE:HG21	1:D:365:LEU:CD1	2.26	0.66
1:F:326:PRO:HB2	1:F:331:ARG:HH12	1.59	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
1:C:501:ALA:O	1:C:504:MET:HB2	1.96	0.66
1:C:513:GLU:O	1:D:548:ARG:NH2	2.28	0.66
1:D:399:LEU:H	1:D:400:PRO:HD2	1.60	0.66
1:A:261:GLY:O	1:A:262:ARG:HB2	1.95	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:F:171:ILE:CG2	1:F:296:VAL:HG21	2.26	0.66
1:F:569:LEU:C	1:F:571:ARG:H	2.01	0.66
1:C:463:LYS:HD2	1:D:486:VAL:HG13	1.76	0.66
1:D:334:ILE:HD11	2:D:4001:ADP:C5	2.31	0.66
1:E:439:THR:OG1	1:E:581:THR:HG23	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:501:ALA:HA	1:D:504:MET:HE2	1.78	0.66
1:F:542:ARG:HA	1:F:542:ARG:NH1	2.10	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:B:521:VAL:HG23	1:B:532:VAL:HG12	1.78	0.65
1:E:399:LEU:N	1:E:400:PRO:HD2	2.09	0.65
1:E:469:ILE:O	1:E:472:ALA:HB3	1.97	0.65
1:F:282:LEU:O	1:F:286:MET:HG3	1.96	0.65
1:F:543:ILE:O	1:F:547:VAL:HG23	1.96	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:C:516:PRO:HB2	1:D:494:PHE:HE2	1.57	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:201:GLY:HA2	2:B:2001:ADP:N7	2.11	0.65
1:B:473:LEU:HD11	1:B:551:ILE:HG12	1.78	0.65
1:F:428:PHE:CG	1:F:432:ALA:HB1	2.32	0.65
1:F:473:LEU:C	1:F:475:GLY:N	2.54	0.65
1:F:514:PHE:HE2	1:F:542:ARG:CZ	2.08	0.65
1:A:450:MET:HG3	1:A:451:MET:N	2.11	0.65
1:B:353:LEU:O	1:B:357:THR:HG22	1.97	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:206:ALA:HA	1:F:298:MET:HE2	1.79	0.64
1:A:220:ALA:O	1:A:254:ILE:HA	1.98	0.64
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
1:D:515:GLY:O	1:D:517:VAL:N	2.30	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:C:598:ALA:HB3	1:C:600:GLU:CD	2.23	0.64
1:D:348:VAL:HG12	1:D:350:LEU:H	1.61	0.64
1:F:334:ILE:HG21	1:F:365:LEU:CD1	2.26	0.64
1:B:206:ALA:HA	1:B:298:MET:HE2	1.79	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: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:F:507:GLU:HG3	1:F:520:ALA:HB3	1.80	0.64
1:A:465:LEU:O	1:A:469:ILE:HG13	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:ILE:HG21	1:D:296:VAL:HG11	1.80	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:583:THR:O	1:A:586:GLU:HB2	1.98	0.64
1:B:477:ALA:O	1:B:478:ALA:C	2.39	0.64
1:C:583:THR:O	1:C:586:GLU:HB2	1.98	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:B:399:LEU:H	1:B:400:PRO:HD2	1.62	0.63
1:D:428:PHE:CD1	1:D:428:PHE:N	2.63	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:348:VAL:HG21	1:F:386:MET:HE2	1.79	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:C:525:THR:HG22	1:C:526:TYR:H	1.64	0.63
1:D:357:THR:OG1	1:D:360:PHE:HD2	1.78	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: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:B:565:LYS:HD2	1:B:568:VAL:HG21	1.81	0.63
1:D:326:PRO:HB3	1:D:331:ARG:NH1	2.14	0.63
1:E:480:GLU:HG2	1:E:559:LYS:HD2	1.80	0.63
1:B:348:VAL:HG21	1:B:386:MET:HE2	1.80	0.63
1:E:428:PHE:CD1	1:E:428:PHE:N	2.65	0.63
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:D:451:MET:HB2	1:E:402:LYS:HE2	1.80	0.62
1:E:372:ALA:O	1:E:375:LEU:HB2	1.99	0.62
1:B:543:ILE:O	1:B:547:VAL:HG23	1.98	0.62
1:C:467:ASP:O	1:C:471:VAL:HG23	2.00	0.62
1:E:503:ARG:HB3	1:E:508:TRP:CZ3	2.34	0.62
1:A:447:LEU:HA	1:A:496:GLN:HE22	1.63	0.62
1:B:569:LEU:C	1:B:571:ARG:H	2.08	0.62
1:C:200:VAL:HG22	1:C:325:ALA:HB3	1.80	0.62
1:F:539:THR:HA	1:F:542:ARG:HB2	1.80	0.62
1:A:494:PHE:CE2	1:F:516:PRO:HB3	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:ARG:HD3	1:C:357:THR:O	1.99	0.62
1:E:501:ALA:O	1:E:505:ILE:HD12	2.00	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: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:D:201:GLY:HA2	2:D:4001:ADP:N7	2.15	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:E:477:ALA:O	1:E:478:ALA:C	2.42	0.62
1:B:171:ILE:HG21	1:B:296:VAL:HG11	1.81	0.62
1:B:175:LEU:HD11	1:B:250:CYS:O	1.99	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:C:450:MET:HG3	1:C:451:MET:N	2.10	0.62
1:E:548:ARG:HH11	1:E:548:ARG:CG	2.13	0.62
1:F:511:HIS:C	1:F:512:PRO:O	2.42	0.62
1:F:503:ARG:HH12	1:F:531:ASP:HB3	1.64	0.62
1:B:171:ILE:HG23	1:B:296:VAL:HG21	1.82	0.61
1:E:435:VAL:HG23	1:E:436:HIS:N	2.14	0.61
1:F:174:PHE:HB2	1:F:181:PHE:CE2	2.35	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: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:F:465:LEU:O	1:F:469:ILE:N	2.30	0.61
1:F:473:LEU:HD11	1:F:551:ILE:HG12	1.81	0.61
1:F:484:ASP:O	1:F:485:ASP:C	2.43	0.61
1:A:428:PHE:CG	1:A:432:ALA:CB	2.83	0.61
1:C:488:THR:CG2	1:C:488:THR:O	2.49	0.61
1:D:175:LEU:HD11	1:D:250:CYS:O	2.00	0.61
1:B:334:ILE:HG21	1:B:365:LEU:HD13	1.83	0.61
1:B:539:THR:HA	1:B:542:ARG:HB2	1.81	0.61
1:D:159:ALA:HB1	1:D:333:GLN:HB3	1.82	0.61
1:D:506:THR:HG22	1:D:507:GLU:HB2	1.81	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:A:473:LEU:HD13	1:A:555:TYR:HB2	1.81	0.61
1:C:503:ARG:HB3	1:C:508:TRP:CZ3	2.36	0.61
1:D:554:GLN:NE2	1:D:557:ARG:HD3	2.15	0.61
1:D:565:LYS:C	1:D:567:GLU:H	2.08	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:ARG:HH12	1:B:531:ASP:HB3	1.65	0.61
1:C:551:ILE:O	1:C:552:GLU:C	2.42	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:E:459:HIS:HB2	1:F:488:THR:HB	1.83	0.61
1:D:222:GLY:HA2	1:D:225:PHE:HD1	1.66	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:F:539:THR:O	1:F:543:ILE:HD12	2.01	0.61
1:A:241:PHE:HE2	1:A:252:VAL:HG21	1.65	0.61
1:B:326:PRO:O	1:B:327:ASP:CB	2.47	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: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:A:511:HIS:C	1:A:512:PRO:O	2.44	0.60
1:B:334:ILE:HD11	2:B:2001:ADP:C5	2.35	0.60
1:C:477:ALA:O	1:C:478:ALA:C	2.44	0.60
1:D:580:GLU:O	1:D:581:THR:HB	1.99	0.60
1:F:511:HIS:O	1:F:512:PRO:O	2.19	0.60
1:F:565:LYS:O	1:F:567:GLU:N	2.35	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: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:A:192:VAL:HG13	1:A:319:ARG:HB3	1.84	0.60
1:B:548:ARG:CG	1:B:548:ARG:NH1	2.62	0.60
1:A:511:HIS:O	1:A:512:PRO:O	2.19	0.60
1:B:369:LEU:HD23	1:B:389:LEU:HD21	1.84	0.60
1:B:481:ILE:HG22	1:B:482:VAL:N	2.15	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:517:VAL:CG2	1:B:519:TYR:OH	2.49	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:D:424:LEU:O	1:D:427:HIS:N	2.29	0.60
1:A:334:ILE:HD12	2:A:1001:ADP:C6	2.37	0.60
1:A:501:ALA:HA	1:A:504:MET:HB2	1.84	0.60
1:B:507:GLU:HG3	1:B:520:ALA:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:521:VAL:O	1:E:522:ARG:C	2.45	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:F:473:LEU:HD11	1:F:551:ILE:CG1	2.32	0.60
1:A:197:PRO:HG3	1:A:443:ARG:HB2	1.82	0.60
1:A:200:VAL:HG22	1:A:325:ALA:HB3	1.84	0.60
1:C:425:ALA:O	1:C:427:HIS:N	2.35	0.60
1:E:406:VAL:HG12	1:E:407:LEU:H	1.65	0.60
1:B:189:PRO:O	1:B:190:LYS:CB	2.47	0.59
1:B:501:ALA:HA	1:B:504:MET:HE2	1.83	0.59
1:F:548:ARG:HH11	1:F:548:ARG:CB	2.15	0.59
1:A:413:ARG:HA	1:A:577:LEU:HD11	1.84	0.59
1:C:479:GLU:O	1:C:480:GLU:C	2.45	0.59
1:A:480:GLU:HG2	1:A:559:LYS:HD2	1.83	0.59
1:D:519:TYR:HB3	1:D:535:TYR:HD2	1.68	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:E:476:ARG:O	1:E:477:ALA:C	2.46	0.59
1:B:470:ALA:O	1:B:558:VAL:HG11	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:565:LYS:C	1:B:567:GLU:H	2.10	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:B:424:LEU:O	1:B:425:ALA:C	2.45	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:A:499:GLU:HG2	1:A:502:ARG:HH12	1.68	0.59
1:B:346:GLU:HG2	1:B:348:VAL:H	1.68	0.59
1:C:516:PRO:O	1:D:494:PHE:CD2	2.56	0.59
1:C:541:LYS:HG2	1:C:545:GLU:OE2	2.02	0.59
1:F:417:TYR:CE2	1:F:482:VAL:HG21	2.38	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:D:476:ARG:CZ	1:D:487:THR:CG2	2.79	0.59
1:D:502:ARG:O	1:D:506:THR:HB	2.02	0.59
1:A:481:ILE:HG22	1:A:482:VAL:N	2.18	0.59
1:B:335:LEU:HD21	1:B:365:LEU:HB3	1.85	0.59
1:B:505:ILE:CG2	1:B:514:PHE:HD1	2.06	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:PRO:O	1:C:494:PHE:HD2	1.86	0.58
1:C:200:VAL:HA	1:C:361:VAL:CG1	2.32	0.58
1:D:565:LYS:O	1:D:567:GLU:N	2.34	0.58
1:A:484:ASP:O	1:A:486:VAL:N	2.36	0.58
1:A:542:ARG:HA	1:A:542:ARG:HE	1.66	0.58
1:D:539:THR:HA	1:D:542:ARG:HB2	1.85	0.58
1:A:325:ALA:O	1:A:327:ASP:N	2.36	0.58
1:A:476:ARG:O	1:A:477:ALA:C	2.45	0.58
1:D:511:HIS:C	1:D:512:PRO:O	2.46	0.58
1:F:174:PHE:O	1:F:178:PRO:HD3	2.04	0.58
1:F:201:GLY:HA2	2:F:6001:ADP:N7	2.19	0.58
1:F:337:ILE:HG22	1:F:338:HIS:CD2	2.33	0.58
1:C:501:ALA:HA	1:C:504:MET:HG2	1.85	0.58
1:D:334:ILE:HG21	1:D:365:LEU:HD13	1.83	0.58
1:E:454:ARG:HD3	1:E:503:ARG:NH2	2.17	0.58
1:A:325:ALA:C	1:A:327:ASP:H	2.10	0.58
1:F:175:LEU:HD12	1:F:249:PRO:HB2	1.86	0.58
1:A:189:PRO:C	1:A:191:GLY:H	2.11	0.58
1:D:474:ALA:HB2	1:D:558:VAL:HG11	1.86	0.58
1:D:505:ILE:HG22	1:D:506:THR:CA	2.34	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:A:172:VAL:HG22	1:A:209:VAL:HG13	1.86	0.58
1:C:501:ALA:O	1:C:505:ILE:HD12	2.03	0.58
1:E:442:PRO:HD2	1:E:443:ARG:H	1.69	0.58
1:F:428:PHE:CD1	1:F:432:ALA:CB	2.83	0.58
1:A:503:ARG:HB3	1:A:508:TRP:CZ3	2.38	0.58
1:C:536:SER:O	1:C:537:GLU:C	2.47	0.58
1:E:542:ARG:HA	1:E:542:ARG:HE	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:222:GLY:HA2	1:B:225:PHE:HD1	1.68	0.57
1:B:473:LEU:HD13	1:B:555:TYR:HB2	1.86	0.57
1:F:222:GLY:HA2	1:F:225:PHE:HD1	1.68	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:C:463:LYS:HD2	1:D:486:VAL:CG2	2.33	0.57
1:C:476:ARG:O	1:C:477:ALA:C	2.47	0.57
1:B:331:ARG:HB3	1:B:354:ALA:HB1	1.84	0.57
1:B:516:PRO:HB3	1:C:494:PHE:CE2	2.39	0.57
1:E:461:SER:O	1:E:464:ARG:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:521:VAL:HG23	1:F:532:VAL:HG12	1.86	0.57
1:A:202:LYS:HE3	1:A:301:THR:H	1.70	0.57
1:A:465:LEU:HA	1:A:468:GLN:HB2	1.87	0.57
1:B:417:TYR:CE2	1:B:482:VAL:HG21	2.39	0.57
1:B:554:GLN:HE22	1:B:557:ARG:HD3	1.68	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:F:503:ARG:NE	1:F:522:ARG:NH2	2.52	0.57
1:A:372:ALA:O	1:A:375:LEU:HB2	2.04	0.57
1:A:576:LEU:O	1:A:577:LEU:C	2.47	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:B:386:MET:HE3	1:B:390:GLU:HG3	1.85	0.57
1:D:473:LEU:HD11	1:D:551:ILE:HG12	1.84	0.57
1:F:386:MET:HE3	1:F:390:GLU:HG3	1.85	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:C:459:HIS:HE1	1:D:415:THR:HG23	1.70	0.57
1:D:158:VAL:HG22	1:D:204:HIS:NE2	2.20	0.57
1:F:503:ARG:NH1	1:F:507:GLU:OE1	2.37	0.57
1:A:309:PRO:HD2	1:A:530:TYR:CD2	2.40	0.57
1:C:505:ILE:CG2	1:C:506:THR:HG23	2.33	0.57
1:D:326:PRO:O	1:D:327:ASP:CB	2.52	0.57
1:D:379:GLU:HG3	1:D:379:GLU:O	2.04	0.57
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: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:E:510:MET:C	1:E:512:PRO:CD	2.72	0.56
1:B:536:SER:OG	1:C:544:ASP:OD2	2.23	0.56
1:D:435:VAL:HG22	1:D:436:HIS:N	2.14	0.56
1:F:476:ARG:O	1:F:477:ALA:C	2.49	0.56
1:F:500:LEU:O	1:F:501:ALA:C	2.46	0.56
1:F:565:LYS:C	1:F:567:GLU:H	2.10	0.56
1:B:311:LEU:O	1:B:317:PHE:HB2	2.06	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:543:ILE:O	1:D:547:VAL:HG23	2.05	0.56
1:D:564:GLU:O	1:D:564:GLU:HG2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:253:PHE:HE2	1:F:255:ASP:HB2	1.70	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:A:479:GLU:O	1:A:480:GLU:C	2.47	0.56
1:B:474:ALA:HB2	1:B:558:VAL:HG11	1.87	0.56
1:B:502:ARG:HD2	1:B:533:ARG:HH22	1.65	0.56
1:E:510:MET:O	1:E:512:PRO:CD	2.35	0.56
1:B:253:PHE:HE2	1:B:255:ASP:HB2	1.71	0.56
1:C:192:VAL:HG13	1:C:319:ARG:HB3	1.87	0.56
1:C:442:PRO:HD2	1:C:443:ARG:H	1.70	0.56
1:E:202:LYS:HE3	1:E:301:THR:H	1.70	0.56
1:A:548:ARG:HH11	1:A:548:ARG:HG3	1.69	0.56
1:B:514:PHE:HB3	1:B:519:TYR:CE1	2.41	0.56
1:B:565:LYS:O	1:B:568:VAL:HG23	2.05	0.56
1:E:517:VAL:HG21	1:E:519:TYR:OH	2.06	0.56
1:F:331:ARG:HB3	1:F:354:ALA:HB1	1.86	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:A:514:PHE:CD2	1:A:514:PHE:N	2.71	0.56
1:B:348:VAL:HG12	1:B:350:LEU:H	1.70	0.56
1:B:439:THR:O	1:B:440:ILE:HG13	2.05	0.56
1:B:465:LEU:O	1:B:469:ILE:N	2.37	0.56
1:B:473:LEU:HD11	1:B:551:ILE:CG1	2.35	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:HH11	1:B:542:ARG:CB	2.18	0.56
1:E:501:ALA:HA	1:E:504:MET:HB2	1.86	0.56
1:A:162:GLU:C	1:A:164:ALA:H	2.13	0.56
1:B:334:ILE:CG2	1:B:365:LEU:HD13	2.35	0.56
1:B:580:GLU:O	1:B:581:THR:HB	2.04	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:428:PHE:CD1	1:B:432:ALA:CB	2.83	0.55
1:B:514:PHE:HE2	1:B:542:ARG:CZ	2.18	0.55
1:D:523:GLU:HB2	1:D:530:TYR:O	2.06	0.55
1:A:303:ARG:O	1:A:306:ILE:HG12	2.06	0.55
1:A:463:LYS:HD2	1:B:486:VAL:HG22	1.88	0.55
1:C:462:ARG:NH1	1:C:510:MET:HB3	2.21	0.55
1:E:189:PRO:HG3	1:E:319:ARG:HD2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:VAL:CG1	1:F:463:LYS:HD2	2.37	0.55
1:C:189:PRO:C	1:C:191:GLY:H	2.14	0.55
1:D:171:ILE:HG23	1:D:296:VAL:HG21	1.88	0.55
1:F:175:LEU:HD11	1:F:250:CYS:O	2.06	0.55
1:F:369:LEU:CD2	1:F:389:LEU:HD21	2.37	0.55
1:F:564:GLU:HG2	1:F:564:GLU:O	2.06	0.55
1:B:334:ILE:HG21	1:B:365:LEU:CD1	2.35	0.55
1:C:202:LYS:HE3	1:C:301:THR:H	1.71	0.55
1:D:592:GLU:O	1:D:594:LEU:HD12	2.06	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:C:451:MET:C	1:C:453:ARG:H	2.13	0.55
1:C:465:LEU:O	1:C:469:ILE:HG13	2.06	0.55
1:D:554:GLN:HE22	1:D:557:ARG:NH1	2.04	0.55
1:B:548:ARG:HH11	1:B:548:ARG:CB	2.19	0.55
1:D:169:LYS:HD3	1:E:378:ARG:NH2	2.22	0.55
1:B:458:LEU:HB2	1:C:405:LEU:HD13	1.87	0.55
1:B:523:GLU:HB2	1:B:530:TYR:O	2.07	0.55
1:D:331:ARG:HB3	1:D:354:ALA:HB1	1.88	0.55
1:E:189:PRO:C	1:E:191:GLY:H	2.15	0.55
1:E:451:MET:C	1:E:453:ARG:H	2.15	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:C:511:HIS:C	1:C:512:PRO:O	2.49	0.55
1:C:513:GLU:OE2	1:C:549:ARG:NH1	2.40	0.55
1:C:261:GLY:HA3	1:C:307:LEU:CD1	2.37	0.55
1:F:492:ASN:O	1:F:493:ASP:C	2.47	0.55
1:F:589:ARG:HD2	1:F:596:LEU:CD1	2.36	0.55
1:B:175:LEU:HD12	1:B:249:PRO:HB2	1.89	0.54
1:D:505:ILE:CG2	1:D:514:PHE:CD1	2.84	0.54
1:F:166:GLU:HA	1:F:169:LYS:HD2	1.89	0.54
1:A:377:ALA:HB1	1:F:181:PHE:CE1	2.42	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:D:492:ASN:O	1:D:493:ASP:C	2.50	0.54
1:D:504:MET:HE1	1:D:550:LEU:HD11	1.89	0.54
1:A:499:GLU:HG2	1:A:502:ARG:NH1	2.23	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:479:GLU:O	1:E:480:GLU:C	2.49	0.54
1:D:428:PHE:CD1	1:D:432:ALA:CB	2.83	0.54
1:E:513:GLU:OE2	1:E:549:ARG:NH1	2.41	0.54
1:E:554:GLN:HE22	1:E:557:ARG:CZ	2.20	0.54
1:F:338:HIS:O	1:F:369:LEU:HD13	2.08	0.54
1:A:521:VAL:O	1:A:522:ARG:C	2.49	0.54
1:C:439:THR:OG1	1:C:581:THR:HG23	2.07	0.54
1:D:169:LYS:HA	1:D:172:VAL:HB	1.89	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
1:D:253:PHE:HE2	1:D:255:ASP:HB2	1.72	0.54
1:E:261:GLY:HA3	1:E:307:LEU:HD13	1.89	0.54
1:A:501:ALA:O	1:A:504:MET:HB2	2.07	0.54
1:A:536:SER:O	1:A:537:GLU:C	2.51	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:F:428:PHE:C	1:F:429:LEU:HG	2.33	0.54
1:A:468:GLN:HA	1:A:468:GLN:NE2	2.21	0.54
1:D:548:ARG:HH11	1:D:548:ARG:CB	2.21	0.54
1:B:514:PHE:HE2	1:B:542:ARG:NE	2.05	0.54
1:B:569:LEU:O	1:B:571:ARG:N	2.31	0.54
1:C:397:MET:HE3	1:C:406:VAL:HG11	1.89	0.54
1:C:451:MET:HB3	1:C:452:PRO:HD3	1.90	0.54
1:C:468:GLN:NE2	1:C:468:GLN:HA	2.22	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:C:484:ASP:O	1:C:486:VAL:N	2.40	0.54
1:D:206:ALA:HA	1:D:298:MET:HE2	1.88	0.54
1:A:261:GLY:HA3	1:A:307:LEU:CD1	2.38	0.53
1:B:537:GLU:O	1:B:540:ALA:HB3	2.08	0.53
1:E:468:GLN:NE2	1:E:468:GLN:HA	2.23	0.53
1:F:458:LEU:CD1	1:F:459:HIS:H	2.19	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:D:484:ASP:O	1:D:485:ASP:C	2.51	0.53
1:A:279:LEU:C	1:A:281:GLN:H	2.15	0.53
1:A:520:ALA:C	1:A:521:VAL:HG22	2.32	0.53
1:A:551:ILE:O	1:A:552:GLU:C	2.51	0.53
1:B:492:ASN:O	1:B:493:ASP:C	2.51	0.53
1:B:570:GLU:HG2	1:B:570:GLU:O	2.06	0.53
1:C:465:LEU:HA	1:C:468:GLN:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:565:LYS:HD2	1:F:568:VAL:HG21	1.90	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:414:ILE:HA	1:F:483:PHE:CE1	2.43	0.53
1:A:425:ALA:O	1:A:426:ALA:C	2.51	0.53
1:D:439:THR:O	1:D:440:ILE:HG13	2.09	0.53
1:D:510:MET:C	1:D:512:PRO:CD	2.79	0.53
1:F:514:PHE:CE2	1:F:542:ARG:CZ	2.91	0.53
1:D:334:ILE:CD1	2:D:4001:ADP:C6	2.86	0.53
1:D:542:ARG:HH11	1:D:542:ARG:CA	2.18	0.53
1:E:257:ILE:HG21	1:E:299:ALA:HB1	1.90	0.53
1:E:484:ASP:C	1:E:486:VAL:N	2.59	0.53
1:F:225:PHE:HB3	1:F:278:THR:HG21	1.90	0.53
1:F:414:ILE:HG13	1:F:483:PHE:CE1	2.44	0.53
1:C:162:GLU:C	1:C:164:ALA:H	2.17	0.53
1:D:548:ARG:HG3	1:D:548:ARG:NH1	2.23	0.53
1:E:505:ILE:CG2	1:E:514:PHE:CD1	2.91	0.53
1:F:343:PRO:HB2	1:F:383:LYS:HG3	1.91	0.53
1:C:505:ILE:HG22	1:C:506:THR:CG2	2.35	0.53
1:D:386:MET:HE3	1:D:390:GLU:HG3	1.91	0.53
1:D:414:ILE:O	1:D:416:ALA:N	2.41	0.53
1:E:505:ILE:HG22	1:E:506:THR:CG2	2.39	0.53
1:F:158:VAL:HG22	1:F:204:HIS:NE2	2.24	0.53
1:F:348:VAL:HG12	1:F:350:LEU:H	1.73	0.53
1:F:589:ARG:HD2	1:F:596:LEU:HD11	1.89	0.53
1:A:439:THR:OG1	1:A:581:THR:HG23	2.08	0.53
1:B:503:ARG:NE	1:B:522:ARG:NH2	2.56	0.53
1:D:476:ARG:O	1:D:477:ALA:C	2.52	0.53
1:A:376:ALA:O	1:A:380:GLY:N	2.40	0.53
1:B:502:ARG:HG2	1:B:533:ARG:HH22	1.69	0.53
1:B:507:GLU:HG2	1:B:520:ALA:O	2.09	0.53
1:D:554:GLN:HE22	1:D:557:ARG:HD3	1.74	0.53
1:E:511:HIS:O	1:E:512:PRO:O	2.26	0.53
1:A:517:VAL:HG13	1:B:551:ILE:HG21	1.92	0.52
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:C:484:ASP:C	1:C:486:VAL:N	2.61	0.52
1:D:492:ASN:O	1:D:495:ARG:N	2.43	0.52
1:A:442:PRO:HD2	1:A:443:ARG:H	1.74	0.52
1:D:464:ARG:O	1:D:468:GLN:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:399:LEU:N	1:F:400:PRO:HD2	2.24	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:E:569:LEU:O	1:E:570:GLU:C	2.52	0.52
1:F:202:LYS:CE	1:F:300:ALA:HB1	2.39	0.52
1:A:495:ARG:O	1:A:496:GLN:C	2.53	0.52
1:B:538:GLU:O	1:B:540:ALA:N	2.42	0.52
1:C:465:LEU:HB2	1:C:504:MET:HE1	1.91	0.52
1:E:511:HIS:C	1:E:512:PRO:O	2.53	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:B:463:LYS:HD2	1:C:486:VAL:CG1	2.40	0.52
1:C:454:ARG:HD3	1:C:503:ARG:NH2	2.24	0.52
1:C:488:THR:O	1:C:488:THR:HG23	2.10	0.52
1:D:586:GLU:O	1:D:590:VAL:HG23	2.09	0.52
1:E:417:TYR:HD2	1:E:569:LEU:HD13	1.74	0.52
1:A:459:HIS:HB2	1:B:488:THR:HB	1.92	0.52
1:C:592:GLU:O	1:C:594:LEU:HD12	2.09	0.52
1:D:346:GLU:HG3	1:D:386:MET:SD	2.50	0.52
1:D:576:LEU:HG	1:D:582:LEU:CD1	2.38	0.52
1:E:313:ARG:CB	1:E:314:PRO:HD2	2.39	0.52
1:B:521:VAL:CG1	1:C:495:ARG:HG3	2.40	0.52
1:B:592:GLU:O	1:B:593:GLY:C	2.53	0.52
1:C:461:SER:O	1:C:462:ARG:C	2.52	0.52
1:D:542:ARG:HH11	1:D:542:ARG:CB	2.22	0.52
1:E:417:TYR:CE2	1:E:482:VAL:HG21	2.45	0.52
1:E:498:THR:HA	1:E:551:ILE:HD11	1.92	0.52
1:A:346:GLU:HB2	1:A:386:MET:SD	2.50	0.52
1:B:399:LEU:N	1:B:400:PRO:HD2	2.25	0.52
1:C:376:ALA:HA	1:C:381:ARG:HD3	1.91	0.52
1:A:399:LEU:H	1:A:400:PRO:CD	2.15	0.51
1:B:335:LEU:HD21	1:B:365:LEU:HD22	1.91	0.51
1:B:505:ILE:HG22	1:B:506:THR:CB	2.39	0.51
1:C:514:PHE:HB3	1:C:519:TYR:OH	2.10	0.51
1:E:521:VAL:HG12	1:F:495:ARG:HE	1.75	0.51
1:B:538:GLU:C	1:B:540:ALA:N	2.67	0.51
1:C:279:LEU:C	1:C:281:GLN:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:521:VAL:CG1	1:E:495:ARG:HG3	2.40	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:B:343:PRO:HB2	1:B:383:LYS:HG3	1.92	0.51
1:B:369:LEU:CD2	1:B:389:LEU:HD21	2.40	0.51
1:B:420:ALA:O	1:B:421:GLY:C	2.53	0.51
1:C:349:ASP:C	1:C:351:ALA:H	2.18	0.51
1:C:463:LYS:HD2	1:D:486:VAL:HG22	1.92	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:E:551:ILE:O	1:E:552:GLU:C	2.53	0.51
1:A:226:VAL:HG21	1:A:259:ALA:O	2.10	0.51
1:B:202:LYS:CE	1:B:300:ALA:HB1	2.40	0.51
1:C:313:ARG:CB	1:C:314:PRO:HD2	2.40	0.51
1:C:511:HIS:O	1:C:512:PRO:O	2.28	0.51
1:D:325:ALA:CB	1:D:326:PRO:CD	2.86	0.51
1:E:162:GLU:C	1:E:164:ALA:H	2.19	0.51
1:A:159:ALA:HB3	1:A:334:ILE:HD13	1.91	0.51
1:B:538:GLU:O	1:B:539:THR:C	2.53	0.51
1:C:598:ALA:HB3	1:C:600:GLU:OE1	2.09	0.51
1:D:331:ARG:HD2	1:D:357:THR:HG23	1.92	0.51
1:D:503:ARG:HB3	1:D:508:TRP:CE3	2.45	0.51
1:E:376:ALA:HA	1:E:381:ARG:HD3	1.91	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:C:554:GLN:HE22	1:C:557:ARG:CZ	2.23	0.51
1:E:279:LEU:C	1:E:281:GLN:H	2.18	0.51
1:E:303:ARG:O	1:E:306:ILE:HG12	2.11	0.51
1:C:325:ALA:C	1:C:327:ASP:H	2.19	0.51
1:D:523:GLU:O	1:D:529:GLY:HA2	2.11	0.51
1:F:433:ASP:OD2	1:F:433:ASP:N	2.44	0.51
1:F:554:GLN:O	1:F:557:ARG:HB3	2.11	0.51
1:A:189:PRO:HG3	1:A:319:ARG:HD2	1.93	0.51
1:B:414:ILE:HA	1:B:483:PHE:CE1	2.46	0.51
1:D:428:PHE:C	1:D:429:LEU:HG	2.34	0.51
1:D:491:GLU:O	1:D:492:ASN:C	2.54	0.51
1:D:503:ARG:NE	1:D:522:ARG:NH2	2.58	0.51
1:F:477:ALA:O	1:F:478:ALA:C	2.54	0.51
1:A:500:LEU:O	1:A:504:MET:HG2	2.09	0.51
1:B:348:VAL:HG12	1:B:350:LEU:N	2.26	0.51
1:B:531:ASP:OD1	1:B:531:ASP:O	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:473:LEU:HD13	1:D:555:TYR:HB2	1.93	0.51
1:A:349:ASP:C	1:A:351:ALA:H	2.19	0.51
1:B:357:THR:OG1	1:B:360:PHE:HD2	1.94	0.51
1:F:542:ARG:HG2	1:F:542:ARG:NH1	2.18	0.51
1:A:451:MET:C	1:A:453:ARG:H	2.17	0.50
1:B:542:ARG:NH1	1:B:542:ARG:CA	2.67	0.50
1:D:343:PRO:HB2	1:D:383:LYS:HG3	1.92	0.50
1:D:481:ILE:HG22	1:D:482:VAL:N	2.25	0.50
1:F:502:ARG:O	1:F:506:THR:HB	2.11	0.50
1:A:374:LEU:HD22	1:F:188:ILE:HD11	1.93	0.50
1:A:435:VAL:HG23	1:A:436:HIS:H	1.76	0.50
1:C:462:ARG:HH11	1:C:510:MET:HB3	1.76	0.50
1:E:463:LYS:HD2	1:F:486:VAL:HG22	1.92	0.50
1:F:515:GLY:O	1:F:517:VAL:N	2.44	0.50
1:F:576:LEU:HG	1:F:582:LEU:HD12	1.94	0.50
1:A:261:GLY:HA3	1:A:307:LEU:HD13	1.92	0.50
1:A:505:ILE:HG22	1:A:506:THR:CG2	2.41	0.50
1:A:548:ARG:HH11	1:A:548:ARG:CG	2.25	0.50
1:C:189:PRO:HG3	1:C:319:ARG:HD2	1.93	0.50
1:D:503:ARG:CZ	1:D:522:ARG:CZ	2.89	0.50
1:F:503:ARG:CZ	1:F:522:ARG:CZ	2.90	0.50
1:A:426:ALA:HB2	1:A:471:VAL:HG11	1.94	0.50
1:E:148:THR:O	1:E:150:ALA:N	2.42	0.50
1:E:346:GLU:HB2	1:E:386:MET:SD	2.51	0.50
1:E:514:PHE:HB3	1:E:519:TYR:OH	2.11	0.50
1:F:379:GLU:O	1:F:379:GLU:HG3	2.11	0.50
1:A:462:ARG:HB2	1:A:510:MET:SD	2.52	0.50
1:B:476:ARG:O	1:B:477:ALA:C	2.54	0.50
1:B:527:LEU:H	1:B:527:LEU:HD22	1.76	0.50
1:C:172:VAL:HG22	1:C:209:VAL:HG13	1.94	0.50
1:F:532:VAL:O	1:F:532:VAL:CG1	2.53	0.50
1:F:542:ARG:HH11	1:F:542:ARG:CA	2.21	0.50
1:B:414:ILE:HG13	1:B:483:PHE:CE1	2.47	0.50
1:B:532:VAL:HG12	1:B:532:VAL:O	2.10	0.50
1:C:159:ALA:HB1	1:C:333:GLN:HB3	1.94	0.50
1:C:261:GLY:HA3	1:C:307:LEU:HD13	1.93	0.50
1:D:334:ILE:HG21	1:D:365:LEU:HD12	1.94	0.50
1:D:414:ILE:HG13	1:D:483:PHE:CE1	2.46	0.50
1:D:503:ARG:CZ	1:D:522:ARG:NE	2.75	0.50
1:E:194:LEU:HD12	1:E:323:ILE:HD11	1.93	0.50
1:E:536:SER:O	1:E:537:GLU:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:169:LYS:HA	1:F:172:VAL:HB	1.93	0.50
1:A:469:ILE:O	1:A:472:ALA:HB3	2.12	0.50
1:B:158:VAL:HG22	1:B:204:HIS:NE2	2.26	0.50
1:D:512:PRO:C	1:D:514:PHE:H	2.20	0.50
1:E:175:LEU:HB2	1:E:213:ALA:HB1	1.92	0.50
1:C:303:ARG:O	1:C:306:ILE:HG12	2.10	0.50
1:C:346:GLU:HB3	1:C:386:MET:HE1	1.93	0.50
1:D:385:THR:H	1:D:388:ASP:HB2	1.76	0.50
1:D:465:LEU:O	1:D:469:ILE:N	2.43	0.50
1:F:357:THR:OG1	1:F:360:PHE:HD2	1.93	0.50
1:F:592:GLU:O	1:F:594:LEU:HD12	2.11	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:399:LEU:N	1:D:400:PRO:HD2	2.24	0.50
1:E:357:THR:O	1:E:357:THR:CG2	2.56	0.50
1:A:322:ALA:C	1:A:323:ILE:HG13	2.37	0.49
1:B:576:LEU:HG	1:B:582:LEU:HD12	1.92	0.49
1:C:400:PRO:O	1:C:401:ALA:HB2	2.12	0.49
1:C:503:ARG:HB3	1:C:508:TRP:CE3	2.47	0.49
1:D:369:LEU:CD2	1:D:389:LEU:HD21	2.42	0.49
1:D:503:ARG:NH1	1:D:507:GLU:OE1	2.44	0.49
1:E:349:ASP:C	1:E:351:ALA:H	2.19	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:F:570:GLU:O	1:F:570:GLU:HG2	2.11	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:A:502:ARG:HB2	1:A:533:ARG:HH22	1.76	0.49
1:B:458:LEU:CD2	1:C:405:LEU:HD22	2.42	0.49
1:B:517:VAL:HG21	1:B:519:TYR:CE2	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:335:LEU:HD21	1:D:365:LEU:HD22	1.93	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:F:583:THR:H	1:F:586:GLU:HB2	1.77	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: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:194:LEU:HD12	1:A:323:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:MET:O	1:C:406:VAL:HG22	2.12	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:C:507:GLU:OE2	1:D:491:GLU:OE2	2.31	0.49
1:D:420:ALA:O	1:D:423:ALA:N	2.46	0.49
1:E:379:GLU:HB2	1:E:381:ARG:HD2	1.94	0.49
1:F:487:THR:HG22	1:F:488:THR:H	1.78	0.49
1:B:476:ARG:CD	1:B:487:THR:HG21	2.43	0.49
1:D:507:GLU:HG2	1:D:520:ALA:O	2.13	0.49
1:E:201:GLY:O	1:E:204:HIS:HB3	2.11	0.49
1:F:476:ARG:CZ	1:F:487:THR:CG2	2.82	0.49
1:A:297:VAL:O	1:A:317:PHE:CE2	2.66	0.49
1:B:166:GLU:HA	1:B:169:LYS:HD2	1.93	0.49
1:B:204:HIS:HB2	2:B:2001:ADP:H3'	1.94	0.49
1:C:379:GLU:HB2	1:C:381:ARG:HD2	1.94	0.49
1:D:247:HIS:O	1:D:250:CYS:HB3	2.13	0.49
1:D:548:ARG:CG	1:D:548:ARG:NH1	2.75	0.49
1:E:411:ASP:HA	1:E:414:ILE:HG22	1.95	0.49
1:A:501:ALA:HA	1:A:504:MET:CG	2.43	0.49
1:B:499:GLU:O	1:B:503:ARG:HB2	2.13	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:171:ILE:HD11	1:C:189:PRO:HG2	1.93	0.49
1:C:255:ASP:C	1:C:256:GLU:HG3	2.38	0.49
1:C:425:ALA:HB3	1:C:471:VAL:HG13	1.94	0.49
1:D:511:HIS:O	1:D:512:PRO:O	2.31	0.49
1:D:542:ARG:HG2	1:D:542:ARG:NH1	2.21	0.49
1:E:462:ARG:HB2	1:E:510:MET:SD	2.53	0.49
1:A:458:LEU:HG	1:A:459:HIS:N	2.26	0.49
1:C:511:HIS:CE1	1:C:516:PRO:HD3	2.48	0.49
1:A:309:PRO:HD2	1:A:530:TYR:CE2	2.48	0.48
1:C:498:THR:HA	1:C:551:ILE:HD11	1.95	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:F:431:HIS:ND1	1:F:431:HIS:N	2.61	0.48
1:F:501:ALA:HA	1:F:504:MET:HE2	1.95	0.48
1:B:464:ARG:H	1:B:464:ARG:HG2	1.50	0.48
1:B:476:ARG:CZ	1:B:487:THR:CG2	2.87	0.48
1:C:148:THR:O	1:C:150:ALA:N	2.41	0.48
1:D:169:LYS:HD3	1:E:378:ARG:HH21	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:SER:O	1:A:411:ASP:N	2.43	0.48
1:B:435:VAL:HG22	1:B:436:HIS:N	2.19	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:D:487:THR:C	1:D:488:THR:HG23	2.37	0.48
1:D:597:GLU:O	1:D:599:PRO:HD3	2.13	0.48
1:B:169:LYS:HA	1:B:172:VAL:HB	1.95	0.48
1:B:474:ALA:HA	1:B:477:ALA:HB3	1.96	0.48
1:C:468:GLN:NE2	1:C:468:GLN:CA	2.73	0.48
1:E:414:ILE:HG23	1:E:415:THR:N	2.28	0.48
1:A:325:ALA:N	1:A:326:PRO:HD3	2.28	0.48
1:B:325:ALA:CB	1:B:326:PRO:CD	2.87	0.48
1:B:529:GLY:C	1:B:530:TYR:CD1	2.91	0.48
1:D:414:ILE:HA	1:D:483:PHE:CE1	2.49	0.48
1:D:499:GLU:O	1:D:503:ARG:HB2	2.12	0.48
1:E:477:ALA:O	1:E:480:GLU:HB3	2.14	0.48
1:E:587:PHE:CE2	1:E:591:VAL:HG21	2.49	0.48
1:A:262:ARG:HH21	1:A:264:ARG:HG3	1.77	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
1:D:450:MET:HA	1:D:453:ARG:HB2	1.96	0.48
1:E:468:GLN:NE2	1:E:468:GLN:CA	2.75	0.48
1:F:483:PHE:C	1:F:485:ASP:N	2.71	0.48
1:F:563:LEU:C	1:F:565:LYS:H	2.20	0.48
1:A:425:ALA:C	1:A:427:HIS:N	2.70	0.48
1:C:262:ARG:HH21	1:C:264:ARG:HG3	1.77	0.48
1:C:476:ARG:CZ	1:C:487:THR:CG2	2.88	0.48
1:D:531:ASP:O	1:D:531:ASP:OD1	2.32	0.48
1:E:376:ALA:O	1:E:380:GLY:N	2.44	0.48
1:E:440:ILE:HD11	1:E:576:LEU:HD22	1.94	0.48
1:F:565:LYS:O	1:F:568:VAL:HG23	2.14	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:D:563:LEU:C	1:D:565:LYS:H	2.22	0.48
1:F:414:ILE:O	1:F:415:THR:C	2.56	0.48
1:F:545:GLU:O	1:F:546:ALA:C	2.56	0.48
1:A:175:LEU:HB2	1:A:213:ALA:HB1	1.96	0.48
1:A:257:ILE:HG21	1:A:299:ALA:HB1	1.96	0.48
1:A:357:THR:O	1:A:357:THR:CG2	2.59	0.48
1:C:430:GLU:OE1	1:C:431:HIS:NE2	2.47	0.48
1:C:496:GLN:O	1:C:500:LEU:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:ILE:HD11	1:E:189:PRO:HG2	1.95	0.48
1:F:498:THR:HG23	1:F:547:VAL:HG11	1.95	0.48
1:A:378:ARG:HG3	1:F:170:GLU:OE2	2.13	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:D:465:LEU:O	1:D:469:ILE:HG13	2.14	0.48
1:F:439:THR:C	1:F:440:ILE:HG13	2.39	0.48
1:A:306:ILE:CD1	1:F:525:THR:HB	2.44	0.47
1:A:505:ILE:CG2	1:A:514:PHE:CD1	2.95	0.47
1:B:202:LYS:N	2:B:2001:ADP:O1A	2.47	0.47
1:B:439:THR:C	1:B:440:ILE:HG13	2.38	0.47
1:C:516:PRO:CB	1:D:494:PHE:HE2	2.21	0.47
1:C:516:PRO:O	1:D:494:PHE:HD2	1.95	0.47
1:D:382:ARG:O	1:D:383:LYS:HB2	2.12	0.47
1:D:464:ARG:H	1:D:464:ARG:HG2	1.39	0.47
1:E:414:ILE:HA	1:E:483:PHE:CE1	2.49	0.47
1:B:422:HIS:O	1:B:425:ALA:HB3	2.14	0.47
1:B:563:LEU:C	1:B:565:LYS:H	2.22	0.47
1:D:548:ARG:HH11	1:D:548:ARG:HG3	1.76	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:F:592:GLU:O	1:F:593:GLY:C	2.57	0.47
1:A:414:ILE:HG23	1:A:415:THR:N	2.30	0.47
1:B:203:THR:HG23	1:B:253:PHE:CZ	2.49	0.47
1:B:361:VAL:HG23	1:B:364:ASP:H	1.79	0.47
1:B:458:LEU:CD1	1:B:459:HIS:H	2.24	0.47
1:B:530:TYR:CD1	1:B:530:TYR:N	2.82	0.47
1:C:411:ASP:HA	1:C:414:ILE:HG22	1.96	0.47
1:D:481:ILE:HD11	1:D:559:LYS:HG3	1.97	0.47
1:E:226:VAL:HG21	1:E:259:ALA:O	2.14	0.47
1:E:491:GLU:O	1:E:492:ASN:C	2.56	0.47
1:B:545:GLU:O	1:B:546:ALA:C	2.56	0.47
1:C:226:VAL:HG21	1:C:259:ALA:O	2.15	0.47
1:D:464:ARG:O	1:D:467:ASP:N	2.47	0.47
1:E:501:ALA:O	1:E:504:MET:HB2	2.15	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:A:370:ASN:HD21	1:F:187:ARG:HB3	1.79	0.47
1:A:430:GLU:O	1:A:431:HIS:HB2	2.15	0.47
1:A:495:ARG:NE	1:F:521:VAL:HG11	2.30	0.47
1:B:184:MET:SD	1:C:342:LYS:CE	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:HIS:O	1:B:512:PRO:C	2.57	0.47
1:B:564:GLU:O	1:B:564:GLU:HG2	2.13	0.47
1:D:592:GLU:O	1:D:593:GLY:C	2.57	0.47
1:F:334:ILE:HD11	2:F:6001:ADP:C6	2.49	0.47
1:A:346:GLU:HB3	1:A:386:MET:HE1	1.97	0.47
1:A:505:ILE:CG2	1:A:506:THR:HG23	2.41	0.47
1:B:153:VAL:O	1:B:211:GLY:HA3	2.15	0.47
1:B:379:GLU:HG3	1:B:379:GLU:O	2.13	0.47
1:B:468:GLN:HA	1:B:471:VAL:HG23	1.97	0.47
1:B:538:GLU:O	1:B:541:LYS:N	2.48	0.47
1:C:348:VAL:HB	1:C:386:MET:SD	2.55	0.47
1:C:536:SER:O	1:C:538:GLU:N	2.48	0.47
1:D:361:VAL:HG23	1:D:364:ASP:H	1.79	0.47
1:D:476:ARG:HG3	1:D:477:ALA:N	2.30	0.47
1:E:359:GLY:O	1:E:360:PHE:HB2	2.14	0.47
1:E:433:ASP:OD2	1:E:433:ASP:N	2.47	0.47
1:E:491:GLU:O	1:E:494:PHE:N	2.46	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:F:456:ASP:O	1:F:457:MET:SD	2.72	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:A:148:THR:O	1:A:150:ALA:N	2.41	0.47
1:A:428:PHE:CG	1:A:432:ALA:HB1	2.42	0.47
1:B:175:LEU:HD21	1:B:251:ILE:HG13	1.97	0.47
1:B:252:VAL:HG21	1:B:295:ILE:HD11	1.97	0.47
1:C:435:VAL:HG23	1:C:436:HIS:H	1.79	0.47
1:C:501:ALA:HA	1:C:504:MET:HB2	1.97	0.47
1:D:332:GLU:O	1:D:333:GLN:C	2.57	0.47
1:D:439:THR:C	1:D:440:ILE:HG13	2.39	0.47
1:E:400:PRO:O	1:E:401:ALA:HB2	2.14	0.47
1:F:222:GLY:HA2	1:F:225:PHE:CD1	2.50	0.47
1:F:545:GLU:O	1:F:548:ARG:N	2.47	0.47
1:A:495:ARG:HG3	1:F:521:VAL:CG1	2.45	0.47
1:B:481:ILE:HD11	1:B:559:LYS:HG3	1.97	0.47
1:C:514:PHE:HB3	1:C:519:TYR:CZ	2.50	0.47
1:D:465:LEU:HA	1:D:468:GLN:HB2	1.97	0.47
1:D:476:ARG:CZ	1:D:494:PHE:HZ	2.28	0.47
1:D:589:ARG:HD2	1:D:596:LEU:CD1	2.44	0.47
1:F:389:LEU:O	1:F:392:ALA:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:171:ILE:O	1:D:175:LEU:HB2	2.15	0.46
1:A:449:PHE:HB2	1:A:468:GLN:NE2	2.30	0.46
1:A:461:SER:O	1:A:462:ARG:C	2.58	0.46
1:B:510:MET:C	1:B:512:PRO:CD	2.80	0.46
1:C:491:GLU:O	1:C:492:ASN:C	2.58	0.46
1:D:222:GLY:HA2	1:D:225:PHE:CD1	2.48	0.46
1:D:569:LEU:C	1:D:571:ARG:H	2.21	0.46
1:F:331:ARG:HD2	1:F:357:THR:HG23	1.97	0.46
1:A:159:ALA:HB1	1:A:333:GLN:HB3	1.96	0.46
1:D:202:LYS:CE	1:D:300:ALA:HB1	2.45	0.46
1:E:325:ALA:N	1:E:326:PRO:CD	2.78	0.46
1:E:576:LEU:O	1:E:577:LEU:C	2.58	0.46
1:F:511:HIS:NE2	1:F:516:PRO:HD2	2.30	0.46
1:B:171:ILE:O	1:B:175:LEU:HB2	2.16	0.46
1:E:481:ILE:O	1:E:482:VAL:C	2.59	0.46
1:F:511:HIS:CE1	1:F:516:PRO:HD2	2.50	0.46
1:A:308:ASP:CG	1:A:530:TYR:HE2	2.23	0.46
1:A:544:ASP:O	1:A:545:GLU:C	2.58	0.46
1:C:576:LEU:O	1:C:577:LEU:C	2.57	0.46
1:D:542:ARG:NH1	1:D:542:ARG:CA	2.75	0.46
1:E:205:LEU:O	1:E:209:VAL:HG23	2.16	0.46
1:F:542:ARG:CG	1:F:542:ARG:NH1	2.71	0.46
1:A:342:LYS:NZ	1:F:184:MET:HB3	2.30	0.46
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:B:201:GLY:O	1:B:205:LEU:HB2	2.16	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:E:449:PHE:HB2	1:E:468:GLN:NE2	2.29	0.46
1:A:400:PRO:O	1:A:401:ALA:HB2	2.16	0.46
1:A:491:GLU:O	1:A:492:ASN:C	2.58	0.46
1:B:184:MET:HB3	1:C:342:LYS:NZ	2.30	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:152:LYS:O	1:D:153:VAL:HB	2.16	0.46
1:D:454:ARG:NH2	1:D:530:TYR:OH	2.49	0.46
1:D:513:GLU:O	1:E:548:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:VAL:HG22	1:E:209:VAL:HG13	1.98	0.46
1:E:386:MET:HE2	1:E:389:LEU:CD1	2.45	0.46
1:F:348:VAL:HG12	1:F:350:LEU:N	2.31	0.46
1:A:525:THR:HG22	1:A:526:TYR:N	2.30	0.46
1:C:503:ARG:CZ	1:C:522:ARG:HH11	2.29	0.46
1:D:431:HIS:N	1:D:431:HIS:ND1	2.64	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:E:399:LEU:N	1:E:400:PRO:CD	2.78	0.46
1:F:464:ARG:H	1:F:464:ARG:HG2	1.40	0.46
1:F:473:LEU:O	1:F:475:GLY:N	2.48	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:F:524:ASP:HB3	1:F:525:THR:H	1.37	0.46
1:A:414:ILE:O	1:A:416:ALA:N	2.49	0.46
1:A:503:ARG:HB3	1:A:508:TRP:CE3	2.51	0.46
1:B:353:LEU:HD13	1:B:386:MET:HE1	1.98	0.46
1:B:385:THR:H	1:B:388:ASP:HB2	1.81	0.46
1:B:454:ARG:NH2	1:B:530:TYR:OH	2.48	0.46
1:C:462:ARG:HH12	1:C:511:HIS:H	1.64	0.46
1:D:433:ASP:OD2	1:D:433:ASP:N	2.48	0.46
1:D:521:VAL:HG11	1:E:495:ARG:NE	2.31	0.46
1:D:571:ARG:HG2	1:D:590:VAL:HG12	1.98	0.46
1:E:536:SER:O	1:E:539:THR:N	2.49	0.46
1:E:576:LEU:HD23	1:E:576:LEU:HA	1.82	0.46
1:F:557:ARG:O	1:F:560:ALA:HB3	2.15	0.46
1:A:305:ASP:OD1	1:A:447:LEU:HD22	2.16	0.46
1:A:463:LYS:CD	1:B:486:VAL:CG2	2.94	0.46
1:A:587:PHE:O	1:A:588:GLN:C	2.59	0.46
1:C:194:LEU:HD12	1:C:323:ILE:HD11	1.98	0.46
1:C:428:PHE:N	1:C:428:PHE:HD1	2.11	0.46
1:C:447:LEU:HA	1:C:496:GLN:CD	2.40	0.46
1:E:262:ARG:HH21	1:E:264:ARG:HG3	1.81	0.46
1:E:338:HIS:CE1	2:E:5001:ADP:N3	2.84	0.46
1:E:481:ILE:HG22	1:E:482:VAL:N	2.31	0.46
1:F:414:ILE:O	1:F:417:TYR:N	2.47	0.46
1:F:458:LEU:HG	1:F:459:HIS:N	2.31	0.46
1:F:503:ARG:NH2	1:F:522:ARG:CZ	2.79	0.46
1:F:585:GLU:HG2	1:F:588:GLN:OE1	2.15	0.46
1:B:160:GLY:H	1:B:333:GLN:CD	2.24	0.45
1:B:174:PHE:HD1	1:B:181:PHE:CD2	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:ARG:O	1:B:467:ASP:N	2.47	0.45
1:C:462:ARG:HB2	1:C:510:MET:SD	2.56	0.45
1:C:491:GLU:O	1:C:494:PHE:N	2.49	0.45
1:E:325:ALA:C	1:E:327:ASP:H	2.24	0.45
1:F:334:ILE:HG21	1:F:365:LEU:HD12	1.98	0.45
1:F:476:ARG:CZ	1:F:494:PHE:HZ	2.29	0.45
1:F:563:LEU:HA	1:F:566:ARG:HB3	1.98	0.45
1:A:162:GLU:C	1:A:164:ALA:N	2.74	0.45
1:A:325:ALA:N	1:A:326:PRO:CD	2.79	0.45
1:A:374:LEU:HD11	1:F:187:ARG:O	2.15	0.45
1:B:206:ALA:CB	1:B:298:MET:HG2	2.46	0.45
1:C:521:VAL:O	1:C:522:ARG:C	2.60	0.45
1:E:414:ILE:O	1:E:415:THR:C	2.59	0.45
1:A:538:GLU:C	1:A:540:ALA:N	2.75	0.45
1:B:222:GLY:HA2	1:B:225:PHE:CD1	2.50	0.45
1:B:426:ALA:HB2	1:B:471:VAL:HG11	1.98	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:C:414:ILE:HA	1:C:483:PHE:CE1	2.50	0.45
1:C:423:ALA:HA	1:C:436:HIS:HE1	1.81	0.45
1:C:473:LEU:HD11	1:C:551:ILE:HG23	1.98	0.45
1:D:153:VAL:O	1:D:211:GLY:HA3	2.16	0.45
1:D:483:PHE:C	1:D:485:ASP:N	2.74	0.45
1:D:505:ILE:HG22	1:D:506:THR:CB	2.47	0.45
1:D:526:TYR:HB2	1:D:527:LEU:HD22	1.98	0.45
1:E:414:ILE:HG23	1:E:415:THR:H	1.81	0.45
1:E:461:SER:O	1:E:462:ARG:C	2.58	0.45
1:A:587:PHE:CE2	1:A:591:VAL:HG21	2.52	0.45
1:B:326:PRO:HB2	1:B:327:ASP:H	1.54	0.45
1:B:569:LEU:C	1:B:571:ARG:N	2.74	0.45
1:C:325:ALA:N	1:C:326:PRO:CD	2.79	0.45
1:D:458:LEU:HD22	1:E:405:LEU:HB3	1.97	0.45
1:F:435:VAL:HG22	1:F:436:HIS:N	2.23	0.45
1:F:576:LEU:HG	1:F:582:LEU:CD1	2.46	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:D:422:HIS:O	1:D:423:ALA:C	2.56	0.45
1:E:425:ALA:O	1:E:426:ALA:C	2.59	0.45
1:E:544:ASP:O	1:E:545:GLU:C	2.59	0.45
1:F:159:ALA:HB2	1:F:337:ILE:HD13	1.98	0.45
1:F:326:PRO:HB3	1:F:360:PHE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:597:GLU:O	1:F:599:PRO:HD3	2.17	0.45
1:A:257:ILE:C	1:A:259:ALA:N	2.74	0.45
1:A:423:ALA:HA	1:A:436:HIS:HE1	1.82	0.45
1:D:524:ASP:HB3	1:D:525:THR:H	1.35	0.45
1:E:521:VAL:CG1	1:F:495:ARG:HE	2.29	0.45
1:A:152:LYS:O	1:A:153:VAL:HB	2.16	0.45
1:A:201:GLY:O	1:A:204:HIS:HB3	2.16	0.45
1:A:399:LEU:N	1:A:400:PRO:CD	2.78	0.45
1:B:491:GLU:O	1:B:492:ASN:C	2.58	0.45
1:C:326:PRO:HB3	1:C:360:PHE:O	2.16	0.45
1:C:563:LEU:HA	1:C:563:LEU:HD13	1.60	0.45
1:D:439:THR:HA	1:D:581:THR:OG1	2.16	0.45
1:D:513:GLU:O	1:D:514:PHE:HD2	1.99	0.45
1:E:342:LYS:HA	1:E:343:PRO:HD3	1.77	0.45
1:E:346:GLU:HB3	1:E:386:MET:HE1	1.98	0.45
1:F:474:ALA:C	1:F:477:ALA:HB3	2.41	0.45
1:F:518:ALA:C	1:F:520:ALA:H	2.25	0.45
1:B:187:ARG:O	1:C:374:LEU:HD11	2.17	0.45
1:B:194:LEU:HD13	1:B:323:ILE:HD11	1.98	0.45
1:B:585:GLU:HG2	1:B:588:GLN:OE1	2.17	0.45
1:D:387:LYS:H	1:D:387:LYS:HG3	1.59	0.45
1:D:414:ILE:O	1:D:417:TYR:N	2.49	0.45
1:E:450:MET:HE3	1:E:450:MET:HB2	1.80	0.45
1:F:464:ARG:O	1:F:465:LEU:C	2.60	0.45
1:F:542:ARG:HH11	1:F:542:ARG:CB	2.30	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:B:521:VAL:HG11	1:C:495:ARG:NE	2.31	0.45
1:C:412:ARG:NH1	1:C:577:LEU:O	2.50	0.45
1:C:413:ARG:HA	1:C:577:LEU:HD11	1.98	0.45
1:C:569:LEU:O	1:C:570:GLU:C	2.59	0.45
1:D:504:MET:HG2	1:D:510:MET:HG3	1.99	0.45
1:D:526:TYR:CD1	1:D:526:TYR:N	2.81	0.45
1:E:309:PRO:HD2	1:E:530:TYR:HE2	1.82	0.45
1:E:503:ARG:CZ	1:E:522:ARG:HH11	2.30	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:F:527:LEU:HD22	1:F:527:LEU:H	1.82	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:B:428:PHE:C	1:B:429:LEU:HG	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:ARG:CZ	1:B:522:ARG:CZ	2.95	0.45
1:B:576:LEU:HG	1:B:582:LEU:CD1	2.47	0.45
1:C:201:GLY:O	1:C:204:HIS:HB3	2.16	0.45
1:C:244:ALA:HB1	1:C:295:ILE:HD11	1.99	0.45
1:C:587:PHE:CE2	1:C:591:VAL:HG21	2.52	0.45
1:D:386:MET:C	1:D:388:ASP:H	2.25	0.45
1:D:530:TYR:N	1:D:530:TYR:CD1	2.85	0.45
1:A:255:ASP:C	1:A:256:GLU:HG3	2.42	0.44
1:A:563:LEU:HD13	1:A:563:LEU:HA	1.67	0.44
1:B:331:ARG:HD2	1:B:357:THR:HG23	1.99	0.44
1:B:524:ASP:HB3	1:B:525:THR:H	1.34	0.44
1:C:322:ALA:C	1:C:323:ILE:HG13	2.40	0.44
1:C:470:ALA:C	1:C:472:ALA:N	2.73	0.44
1:C:570:GLU:O	1:C:574:GLU:HG2	2.18	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:A:476:ARG:O	1:A:479:GLU:N	2.51	0.44
1:C:399:LEU:N	1:C:400:PRO:CD	2.79	0.44
1:E:255:ASP:C	1:E:256:GLU:HG3	2.41	0.44
1:E:432:ALA:C	1:E:433:ASP:CG	2.85	0.44
1:E:435:VAL:HG23	1:E:436:HIS:H	1.80	0.44
1:A:447:LEU:HA	1:A:496:GLN:CD	2.41	0.44
1:A:554:GLN:NE2	1:A:557:ARG:CZ	2.75	0.44
1:B:500:LEU:O	1:B:501:ALA:C	2.60	0.44
1:C:253:PHE:HA	1:C:298:MET:O	2.17	0.44
1:C:430:GLU:O	1:C:431:HIS:HB2	2.17	0.44
1:C:440:ILE:HD11	1:C:576:LEU:HD22	1.99	0.44
1:C:499:GLU:HG2	1:C:502:ARG:NH1	2.32	0.44
1:D:393:ALA:O	1:D:395:ARG:N	2.51	0.44
1:F:247:HIS:O	1:F:250:CYS:HB3	2.17	0.44
1:F:465:LEU:HA	1:F:468:GLN:HB2	2.00	0.44
1:F:492:ASN:O	1:F:495:ARG:N	2.51	0.44
1:F:554:GLN:NE2	1:F:557:ARG:CD	2.77	0.44
1:B:236:ARG:O	1:B:240:LEU:HB3	2.17	0.44
1:B:420:ALA:O	1:B:423:ALA:N	2.51	0.44
1:C:305:ASP:OD2	1:C:447:LEU:HD13	2.18	0.44
1:D:529:GLY:C	1:D:530:TYR:CD1	2.96	0.44
1:F:503:ARG:CZ	1:F:522:ARG:NE	2.80	0.44
1:A:273:ASP:HA	1:A:276:GLU:HB3	1.99	0.44
1:A:412:ARG:NH1	1:A:577:LEU:O	2.50	0.44
1:B:318:ASP:O	1:B:319:ARG:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4001:ADP:O2B	2:D:4001:ADP:O1A	2.35	0.44
1:E:499:GLU:HG2	1:E:502:ARG:NH1	2.32	0.44
1:E:563:LEU:HD13	1:E:563:LEU:HA	1.74	0.44
1:F:385:THR:H	1:F:388:ASP:HB2	1.81	0.44
1:F:523:GLU:O	1:F:529:GLY:HA2	2.18	0.44
1:B:476:ARG:CZ	1:B:494:PHE:HZ	2.31	0.44
1:E:178:PRO:HB2	1:E:182:HIS:NE2	2.33	0.44
1:E:313:ARG:HG2	1:E:314:PRO:HD2	2.00	0.44
1:F:340:ARG:H	1:F:340:ARG:HG2	1.59	0.44
1:F:491:GLU:O	1:F:492:ASN:C	2.60	0.44
1:A:569:LEU:O	1:A:570:GLU:C	2.60	0.44
1:C:260:VAL:O	1:C:279:LEU:HB2	2.18	0.44
1:C:386:MET:HE2	1:C:389:LEU:CD1	2.47	0.44
1:C:400:PRO:O	1:C:401:ALA:CB	2.65	0.44
1:D:512:PRO:C	1:D:514:PHE:N	2.76	0.44
1:D:545:GLU:O	1:D:546:ALA:C	2.60	0.44
1:E:362:GLY:HA2	1:E:365:LEU:HB2	2.00	0.44
1:E:538:GLU:C	1:E:540:ALA:N	2.75	0.44
1:F:368:LEU:HD12	1:F:392:ALA:C	2.42	0.44
1:F:424:LEU:HD21	1:F:568:VAL:HB	1.99	0.44
1:A:257:ILE:C	1:A:259:ALA:H	2.26	0.44
1:A:533:ARG:C	1:A:534:GLN:CD	2.86	0.44
1:B:492:ASN:O	1:B:495:ARG:N	2.51	0.44
1:B:589:ARG:HD2	1:B:596:LEU:HD11	1.99	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:D:416:ALA:HB2	1:D:577:LEU:HD23	1.98	0.44
1:D:511:HIS:NE2	1:D:516:PRO:HD2	2.33	0.44
1:E:505:ILE:HG22	1:E:506:THR:CA	2.47	0.44
1:A:149:GLU:O	1:A:150:ALA:HB2	2.18	0.44
1:B:502:ARG:O	1:B:506:THR:HB	2.18	0.44
1:C:536:SER:O	1:C:539:THR:N	2.51	0.44
1:D:291:LYS:C	1:D:293:THR:H	2.26	0.44
1:D:439:THR:HG22	1:D:440:ILE:N	2.33	0.44
1:D:487:THR:C	1:D:488:THR:CG2	2.91	0.44
1:D:547:VAL:O	1:D:547:VAL:HG12	2.16	0.44
1:D:572:VAL:O	1:D:573:ALA:C	2.61	0.44
1:F:473:LEU:HD23	1:F:473:LEU:HA	1.67	0.44
1:F:536:SER:O	1:F:537:GLU:C	2.61	0.44
1:A:463:LYS:CD	1:B:486:VAL:HG22	2.48	0.43
1:A:562:LEU:HD23	1:A:562:LEU:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:ASP:O	1:B:457:MET:HB2	2.18	0.43
1:B:483:PHE:C	1:B:485:ASP:H	2.14	0.43
1:C:501:ALA:HA	1:C:504:MET:CG	2.48	0.43
1:D:171:ILE:HG22	1:D:296:VAL:HG21	1.97	0.43
1:D:252:VAL:HG21	1:D:295:ILE:HD11	1.99	0.43
1:E:428:PHE:CD1	1:E:432:ALA:HB3	2.47	0.43
1:E:507:GLU:OE2	1:F:491:GLU:OE2	2.37	0.43
1:F:417:TYR:CG	1:F:482:VAL:HG11	2.53	0.43
1:A:218:ILE:HB	1:A:252:VAL:HA	2.00	0.43
1:A:342:LYS:HA	1:A:343:PRO:HD3	1.77	0.43
1:A:468:GLN:NE2	1:A:468:GLN:CA	2.74	0.43
1:A:503:ARG:CZ	1:A:522:ARG:HH11	2.31	0.43
1:A:529:GLY:C	1:A:530:TYR:CG	2.96	0.43
1:B:340:ARG:H	1:B:340:ARG:HG2	1.60	0.43
1:B:410:ARG:O	1:B:411:ASP:C	2.61	0.43
1:B:439:THR:HG22	1:B:440:ILE:H	1.82	0.43
1:D:209:VAL:O	1:D:213:ALA:N	2.49	0.43
1:E:262:ARG:NH2	1:E:264:ARG:HE	2.16	0.43
1:E:325:ALA:N	1:E:326:PRO:HD3	2.32	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:503:ARG:O	1:E:504:MET:C	2.60	0.43
1:E:514:PHE:N	1:E:514:PHE:CD2	2.83	0.43
1:E:584:ALA:O	1:E:587:PHE:HB3	2.18	0.43
1:F:454:ARG:NH2	1:F:530:TYR:OH	2.51	0.43
1:A:311:LEU:O	1:A:317:PHE:HB2	2.17	0.43
1:A:483:PHE:C	1:A:485:ASP:N	2.58	0.43
1:A:554:GLN:NE2	1:A:557:ARG:NE	2.66	0.43
1:B:187:ARG:HB3	1:C:370:ASN:HD21	1.82	0.43
1:B:463:LYS:CB	1:C:486:VAL:HG11	2.42	0.43
1:B:509:GLY:C	1:B:510:MET:HG2	2.43	0.43
1:B:571:ARG:HG2	1:B:590:VAL:HG12	2.01	0.43
1:C:476:ARG:HD3	1:C:476:ARG:HA	1.68	0.43
1:D:580:GLU:O	1:D:581:THR:CB	2.65	0.43
1:E:425:ALA:C	1:E:427:HIS:N	2.75	0.43
1:A:473:LEU:O	1:A:474:ALA:C	2.62	0.43
1:A:589:ARG:O	1:A:590:VAL:C	2.60	0.43
1:B:463:LYS:HD2	1:C:486:VAL:HG11	1.99	0.43
1:D:414:ILE:O	1:D:415:THR:C	2.60	0.43
1:D:174:PHE:O	1:D:178:PRO:HD3	2.19	0.43
1:D:422:HIS:O	1:D:425:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:424:LEU:HD21	1:D:568:VAL:HB	2.00	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:B:597:GLU:O	1:B:599:PRO:HD3	2.18	0.43
1:C:376:ALA:O	1:C:380:GLY:N	2.47	0.43
1:D:500:LEU:O	1:D:501:ALA:C	2.60	0.43
1:E:543:ILE:HD13	1:E:543:ILE:HG21	1.69	0.43
1:F:526:TYR:HB2	1:F:527:LEU:HD22	2.00	0.43
1:B:431:HIS:ND1	1:B:431:HIS:N	2.67	0.43
1:C:178:PRO:HB2	1:C:182:HIS:NE2	2.34	0.43
1:C:325:ALA:N	1:C:326:PRO:HD3	2.34	0.43
1:E:400:PRO:O	1:E:401:ALA:CB	2.67	0.43
1:E:511:HIS:CE1	1:E:516:PRO:CD	2.97	0.43
1:F:313:ARG:HG3	1:F:314:PRO:HD2	2.00	0.43
1:F:544:ASP:O	1:F:545:GLU:C	2.61	0.43
1:A:256:GLU:C	1:A:258:ASP:N	2.76	0.43
1:A:511:HIS:HE1	1:A:516:PRO:HD3	1.80	0.43
1:C:152:LYS:O	1:C:153:VAL:HB	2.18	0.43
1:C:262:ARG:NH2	1:C:264:ARG:HE	2.16	0.43
1:C:273:ASP:HA	1:C:276:GLU:HB3	2.00	0.43
1:C:442:PRO:CD	1:C:443:ARG:H	2.32	0.43
1:C:520:ALA:C	1:C:521:VAL:HG22	2.44	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:E:273:ASP:HA	1:E:276:GLU:HB3	2.01	0.43
1:E:447:LEU:HA	1:E:496:GLN:CD	2.43	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:B:209:VAL:O	1:B:213:ALA:N	2.52	0.43
1:D:527:LEU:HD22	1:D:527:LEU:H	1.83	0.43
1:F:414:ILE:O	1:F:416:ALA:N	2.52	0.43
1:A:467:ASP:OD1	1:A:557:ARG:NH2	2.41	0.43
1:A:469:ILE:HG12	1:A:500:LEU:HD12	2.01	0.43
1:B:194:LEU:HB2	1:B:300:ALA:CB	2.49	0.43
1:C:313:ARG:HG2	1:C:314:PRO:HD2	2.01	0.43
1:C:499:GLU:HG2	1:C:502:ARG:HH12	1.83	0.43
1:D:562:LEU:HD23	1:D:562:LEU:HA	1.91	0.43
1:D:585:GLU:O	1:D:588:GLN:HB2	2.18	0.43
1:F:569:LEU:C	1:F:571:ARG:N	2.67	0.43
1:A:513:GLU:OE2	1:A:549:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:GLU:HB3	1:B:333:GLN:H	1.67	0.42
1:B:453:ARG:NH1	1:B:456:ASP:OD2	2.52	0.42
1:C:162:GLU:C	1:C:164:ALA:N	2.77	0.42
1:D:342:LYS:HB3	1:D:343:PRO:CD	2.49	0.42
1:D:411:ASP:O	1:D:414:ILE:HB	2.19	0.42
1:D:503:ARG:NH2	1:D:522:ARG:CZ	2.82	0.42
1:D:565:LYS:C	1:D:567:GLU:N	2.77	0.42
1:E:466:LEU:HA	1:E:466:LEU:HD23	1.84	0.42
1:E:543:ILE:O	1:E:543:ILE:HG22	2.18	0.42
1:F:188:ILE:CD1	1:F:189:PRO:HD2	2.49	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:E:514:PHE:HB3	1:E:519:TYR:CZ	2.54	0.42
1:E:538:GLU:C	1:E:540:ALA:H	2.28	0.42
1:F:513:GLU:O	1:F:514:PHE:HD2	2.02	0.42
1:A:178:PRO:HB2	1:A:182:HIS:NE2	2.34	0.42
1:A:406:VAL:HG12	1:A:407:LEU:N	2.27	0.42
1:A:576:LEU:HD23	1:A:576:LEU:HA	1.64	0.42
1:C:357:THR:O	1:C:357:THR:CG2	2.58	0.42
1:C:450:MET:HE3	1:C:450:MET:HB2	1.78	0.42
1:F:326:PRO:HB2	1:F:327:ASP:H	1.74	0.42
1:A:474:ALA:O	1:A:477:ALA:HB3	2.18	0.42
1:A:491:GLU:O	1:A:494:PHE:N	2.51	0.42
1:C:307:LEU:HD12	1:C:311:LEU:HD13	2.01	0.42
1:C:359:GLY:O	1:C:360:PHE:HB2	2.19	0.42
1:C:543:ILE:HD13	1:C:543:ILE:HG21	1.57	0.42
1:C:576:LEU:HD23	1:C:576:LEU:HA	1.69	0.42
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: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:F:507:GLU:HG2	1:F:520:ALA:O	2.19	0.42
1:F:541:LYS:O	1:F:542:ARG:C	2.62	0.42
1:A:598:ALA:HA	1:A:599:PRO:HD3	1.76	0.42
1:B:363:ALA:C	1:B:365:LEU:H	2.27	0.42
1:B:417:TYR:OH	1:B:570:GLU:HG3	2.20	0.42
1:D:516:PRO:HB2	1:E:551:ILE:HG21	2.01	0.42
1:E:194:LEU:HD23	1:E:194:LEU:H	1.84	0.42
1:E:503:ARG:HD3	1:E:507:GLU:OE1	2.18	0.42
1:F:505:ILE:HG22	1:F:506:THR:CB	2.50	0.42
1:F:526:TYR:CD1	1:F:526:TYR:N	2.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:GLY:HA2	2:A:1001:ADP:PA	2.60	0.42
1:B:382:ARG:HD3	1:B:382:ARG:HA	1.97	0.42
1:C:529:GLY:C	1:C:530:TYR:CG	2.97	0.42
1:D:408:SER:C	1:D:410:ARG:N	2.78	0.42
1:E:149:GLU:O	1:E:150:ALA:HB2	2.18	0.42
1:E:413:ARG:HA	1:E:577:LEU:HD11	2.01	0.42
1:E:598:ALA:HA	1:E:599:PRO:HD3	1.79	0.42
1:F:363:ALA:C	1:F:365:LEU:H	2.28	0.42
1:B:306:ILE:H	1:B:306:ILE:HG13	1.74	0.42
1:B:504:MET:HA	1:B:508:TRP:HE3	1.84	0.42
1:C:425:ALA:C	1:C:427:HIS:N	2.78	0.42
1:C:538:GLU:C	1:C:540:ALA:N	2.77	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:O	1:D:532:VAL:CG1	2.63	0.42
1:D:570:GLU:O	1:D:570:GLU:HG2	2.20	0.42
1:E:499:GLU:HG2	1:E:502:ARG:HH12	1.84	0.42
1:F:514:PHE:CD2	1:F:514:PHE:N	2.87	0.42
1:A:479:GLU:OE1	1:A:488:THR:HG22	2.20	0.42
1:B:291:LYS:C	1:B:293:THR:H	2.28	0.42
1:B:483:PHE:C	1:B:485:ASP:N	2.72	0.42
1:B:500:LEU:HD23	1:B:500:LEU:HA	1.90	0.42
1:B:592:GLU:O	1:B:594:LEU:N	2.53	0.42
1:C:447:LEU:HD23	1:C:496:GLN:OE1	2.20	0.42
1:C:459:HIS:HB2	1:D:488:THR:HB	2.02	0.42
1:D:504:MET:N	1:D:508:TRP:HE3	2.18	0.42
1:F:189:PRO:O	1:F:190:LYS:CB	2.59	0.42
1:F:415:THR:O	1:F:419:GLU:N	2.50	0.42
1:F:477:ALA:HB1	1:F:562:LEU:HD12	2.02	0.42
1:F:530:TYR:N	1:F:530:TYR:CD1	2.87	0.42
1:B:386:MET:C	1:B:388:ASP:H	2.27	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:332:GLU:HB3	1:F:333:GLN:H	1.69	0.42
1:F:338:HIS:CE1	1:F:366:GLU:HB2	2.54	0.42
1:F:439:THR:HG22	1:F:440:ILE:H	1.85	0.42
1:F:469:ILE:HD11	1:F:501:ALA:H	1.85	0.42
1:A:502:ARG:O	1:A:503:ARG:C	2.61	0.42
1:A:554:GLN:HE22	1:A:557:ARG:NE	2.17	0.42
1:A:584:ALA:O	1:A:587:PHE:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:ARG:NH2	1:C:580:GLU:OE2	2.52	0.42
1:D:313:ARG:HG3	1:D:314:PRO:HD2	2.02	0.42
1:D:548:ARG:O	1:D:549:ARG:C	2.63	0.42
1:E:303:ARG:HH22	1:E:495:ARG:HH22	1.68	0.42
1:E:525:THR:HG22	1:E:526:TYR:N	2.28	0.42
1:F:152:LYS:O	1:F:153:VAL:HB	2.19	0.42
1:F:426:ALA:HB2	1:F:471:VAL:HG11	2.01	0.42
1:F:474:ALA:HB2	1:F:558:VAL:HG11	2.02	0.42
1:F:529:GLY:C	1:F:530:TYR:CD1	2.98	0.42
1:A:244:ALA:HB1	1:A:295:ILE:HD11	2.01	0.41
1:A:309:PRO:HD2	1:A:530:TYR:HD2	1.85	0.41
1:A:386:MET:HE2	1:A:389:LEU:CD1	2.50	0.41
1:A:417:TYR:HD2	1:A:569:LEU:HD13	1.84	0.41
1:B:425:ALA:C	1:B:427:HIS:H	2.28	0.41
1:B:563:LEU:HA	1:B:566:ARG:HB3	2.02	0.41
1:D:326:PRO:HB2	1:D:327:ASP:H	1.44	0.41
1:F:505:ILE:HG22	1:F:506:THR:N	2.31	0.41
1:A:252:VAL:HB	1:A:297:VAL:HG13	2.02	0.41
1:B:526:TYR:HB2	1:B:527:LEU:HD22	2.01	0.41
1:D:587:PHE:O	1:D:588:GLN:C	2.63	0.41
1:E:326:PRO:HB3	1:E:360:PHE:O	2.20	0.41
1:E:465:LEU:HB2	1:E:504:MET:HE1	2.02	0.41
1:F:449:PHE:HZ	1:F:496:GLN:HG2	1.85	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:E:483:PHE:C	1:E:485:ASP:N	2.60	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: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:286:MET:HE2	1:B:286:MET:HB3	2.00	0.41
1:B:387:LYS:H	1:B:387:LYS:HG3	1.56	0.41
1:C:256:GLU:C	1:C:258:ASP:N	2.78	0.41
1:C:525:THR:HG22	1:C:526:TYR:N	2.33	0.41
1:E:536:SER:O	1:E:538:GLU:N	2.54	0.41
1:F:506:THR:HG23	1:F:520:ALA:HB3	2.01	0.41
1:F:552:GLU:O	1:F:555:TYR:N	2.51	0.41
1:F:569:LEU:HD23	1:F:569:LEU:HA	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:PHE:O	1:A:450:MET:HB3	2.20	0.41
1:B:313:ARG:HG3	1:B:314:PRO:HD2	2.02	0.41
1:B:469:ILE:O	1:B:472:ALA:HB3	2.20	0.41
1:C:342:LYS:HA	1:C:343:PRO:HD3	1.77	0.41
1:D:410:ARG:O	1:D:414:ILE:HD12	2.21	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:D:565:LYS:HD2	1:D:568:VAL:HG21	2.00	0.41
1:F:202:LYS:N	2:F:6001:ADP:O1A	2.53	0.41
1:F:420:ALA:O	1:F:421:GLY:C	2.64	0.41
1:F:531:ASP:OD1	1:F:531:ASP:O	2.38	0.41
1:F:572:VAL:O	1:F:576:LEU:HB2	2.20	0.41
1:A:408:SER:C	1:A:410:ARG:N	2.78	0.41
1:B:335:LEU:CD2	1:B:365:LEU:HB3	2.50	0.41
1:B:503:ARG:CZ	1:B:522:ARG:NE	2.84	0.41
1:C:221:SER:OG	1:C:255:ASP:HB3	2.21	0.41
1:C:521:VAL:CG1	1:D:495:ARG:HE	2.32	0.41
1:D:188:ILE:HD13	1:D:189:PRO:HD2	2.03	0.41
1:D:540:ALA:HA	1:D:543:ILE:HD12	2.01	0.41
1:E:175:LEU:HD12	1:E:249:PRO:HB2	2.02	0.41
1:E:491:GLU:O	1:E:493:ASP:N	2.53	0.41
1:F:386:MET:C	1:F:388:ASP:H	2.28	0.41
1:F:514:PHE:HB3	1:F:519:TYR:CE1	2.55	0.41
1:C:584:ALA:O	1:C:587:PHE:HB3	2.20	0.41
1:D:425:ALA:C	1:D:427:HIS:H	2.28	0.41
1:D:498:THR:HG23	1:D:547:VAL:HG11	2.03	0.41
1:E:189:PRO:O	1:E:190:LYS:HB2	2.21	0.41
1:E:197:PRO:CB	1:E:198:PRO:CD	2.99	0.41
1:E:500:LEU:O	1:E:504:MET:HG2	2.20	0.41
1:F:261:GLY:HA2	1:F:279:LEU:HD13	2.02	0.41
1:A:400:PRO:O	1:A:401:ALA:CB	2.69	0.41
1:B:175:LEU:HD12	1:B:175:LEU:HA	1.84	0.41
1:B:382:ARG:O	1:B:383:LYS:HB2	2.21	0.41
1:B:511:HIS:NE2	1:B:516:PRO:HD2	2.35	0.41
1:C:338:HIS:CE1	2:C:3001:ADP:N3	2.89	0.41
1:D:532:VAL:HG12	1:D:532:VAL:O	2.21	0.41
1:E:322:ALA:C	1:E:323:ILE:HG13	2.46	0.41
1:E:501:ALA:HA	1:E:504:MET:CG	2.51	0.41
1:F:326:PRO:CB	1:F:331:ARG:NH1	2.84	0.41
1:A:414:ILE:C	1:A:416:ALA:N	2.79	0.41
1:B:171:ILE:HG22	1:B:175:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:MET:SD	1:C:342:LYS:HE3	2.61	0.41
1:B:205:LEU:HA	1:B:208:ALA:HB3	2.03	0.41
1:B:349:ASP:C	1:B:351:ALA:H	2.28	0.41
1:B:389:LEU:O	1:B:392:ALA:HB3	2.20	0.41
1:B:393:ALA:O	1:B:397:MET:HB2	2.21	0.41
1:B:458:LEU:HG	1:B:459:HIS:N	2.35	0.41
1:B:464:ARG:O	1:B:465:LEU:C	2.64	0.41
1:C:205:LEU:O	1:C:209:VAL:HG23	2.21	0.41
1:C:207:ARG:HG2	1:C:217:PHE:CE2	2.56	0.41
1:C:397:MET:HG2	1:C:406:VAL:CG1	2.51	0.41
1:C:517:VAL:HG23	1:C:519:TYR:CE1	2.56	0.41
1:C:598:ALA:HA	1:C:599:PRO:HD3	1.79	0.41
1:D:384:ILE:HG22	1:D:388:ASP:HB3	2.03	0.41
1:D:589:ARG:HD2	1:D:596:LEU:HD11	2.03	0.41
1:F:202:LYS:HD2	1:F:300:ALA:HB1	2.02	0.41
1:F:466:LEU:HA	1:F:466:LEU:HD13	1.88	0.41
1:F:474:ALA:HA	1:F:477:ALA:CB	2.50	0.41
1:F:499:GLU:O	1:F:503:ARG:HB2	2.21	0.41
1:F:539:THR:O	1:F:542:ARG:HB2	2.20	0.41
1:A:488:THR:O	1:A:488:THR:CG2	2.69	0.41
1:A:501:ALA:CA	1:A:504:MET:HB2	2.51	0.41
1:B:599:PRO:O	1:B:600:GLU:C	2.64	0.41
1:C:538:GLU:C	1:C:540:ALA:H	2.29	0.41
1:D:201:GLY:O	1:D:205:LEU:HB2	2.20	0.41
1:D:453:ARG:HA	1:D:453:ARG:HD2	1.72	0.41
1:D:458:LEU:CB	1:E:405:LEU:HD13	2.51	0.41
1:E:286:MET:HA	1:E:289:PHE:CE1	2.56	0.41
1:F:458:LEU:CG	1:F:459:HIS:N	2.84	0.41
1:A:313:ARG:HG2	1:A:314:PRO:HD2	2.03	0.40
1:B:465:LEU:HA	1:B:468:GLN:HB2	2.03	0.40
1:B:501:ALA:O	1:B:505:ILE:HD12	2.21	0.40
1:B:551:ILE:O	1:B:552:GLU:C	2.63	0.40
1:B:554:GLN:O	1:B:557:ARG:HB3	2.21	0.40
1:C:257:ILE:C	1:C:259:ALA:N	2.79	0.40
1:D:286:MET:C	1:D:288:GLY:H	2.30	0.40
1:D:362:GLY:O	1:D:365:LEU:HB2	2.21	0.40
1:D:453:ARG:NH1	1:D:456:ASP:OD2	2.54	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:F:171:ILE:HG22	1:F:175:LEU:HD22	2.02	0.40
1:A:445:ARG:C	1:A:447:LEU:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ARG:O	1:A:504:MET:C	2.63	0.40
1:C:562:LEU:HD23	1:C:562:LEU:HA	1.84	0.40
1:E:159:ALA:HB2	1:E:337:ILE:HD13	2.04	0.40
1:F:193:LEU:HG	1:F:194:LEU:N	2.36	0.40
1:F:205:LEU:HA	1:F:208:ALA:HB3	2.03	0.40
1:F:360:PHE:HD1	1:F:360:PHE:HA	1.73	0.40
1:F:511:HIS:O	1:F:512:PRO:C	2.64	0.40
1:F:513:GLU:C	1:F:514:PHE:CD2	2.99	0.40
1:A:303:ARG:HB3	1:A:306:ILE:HG12	2.03	0.40
1:A:425:ALA:C	1:A:427:HIS:H	2.30	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:D:353:LEU:HD13	1:D:386:MET:HE1	2.04	0.40
1:D:509:GLY:C	1:D:510:MET:HG2	2.46	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: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
1:A:424:LEU:HD11	1:A:568:VAL:HB	2.03	0.40
1:A:454:ARG:HD2	1:A:522:ARG:CZ	2.51	0.40
1:B:368:LEU:HD12	1:B:392:ALA:C	2.46	0.40
1:B:514:PHE:CE2	1:B:542:ARG:CZ	3.01	0.40
1:B:525:THR:O	1:B:528:GLY:O	2.40	0.40
1:C:465:LEU:HB2	1:C:504:MET:CE	2.52	0.40
1:C:466:LEU:HA	1:C:466:LEU:HD23	1.80	0.40
1:C:466:LEU:HD22	1:C:554:GLN:OE1	2.22	0.40
1:C:502:ARG:HB2	1:C:533:ARG:NH2	2.37	0.40
1:D:416:ALA:CB	1:D:577:LEU:HD23	2.52	0.40
1:D:463:LYS:HD2	1:E:486:VAL:HG11	2.04	0.40
1:D:466:LEU:HA	1:D:466:LEU:HD22	1.86	0.40
1:D:505:ILE:HG22	1:D:506:THR:N	2.34	0.40
1:E:210:ALA:HA	1:E:251:ILE:HD12	2.04	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:E:529:GLY:C	1:E:530:TYR:CG	2.99	0.40
1:F:474:ALA:HA	1:F:477:ALA:HB3	2.04	0.40
1:F:504:MET:HE1	1:F:550:LEU:HD11	2.03	0.40
1:F:505:ILE:CG2	1:F:514:PHE:CD1	2.96	0.40
1:F:576:LEU:O	1:F:577:LEU:C	2.65	0.40
1:A:386:MET:HG3	1:A:389:LEU:HD12	2.03	0.40
1:A:543:ILE:O	1:A:543:ILE:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:ILE:O	1:D:189:PRO:C	2.64	0.40
1:D:236:ARG:O	1:D:240:LEU:HB3	2.21	0.40
1:D:349:ASP:C	1:D:351:ALA:H	2.29	0.40
1:D:382:ARG:HD3	1:D:382:ARG:HA	2.01	0.40
1:D:487:THR:HG22	1:D:488:THR:H	1.87	0.40
1:E:162:GLU:C	1:E:164:ALA:N	2.79	0.40
1:E:328:VAL:HA	1:E:331:ARG:CZ	2.51	0.40
1:E:501:ALA:HA	1:E:504:MET:HG2	2.02	0.40
1:F:439:THR:HA	1:F:581:THR:OG1	2.22	0.40
1:F:451:MET:CB	1:F:452:PRO:HD3	2.51	0.40
1:F:456:ASP:O	1:F:457:MET:HB2	2.22	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%)	0	9
1	B	442/499 (89%)	320 (72%)	79 (18%)	43 (10%)	0	8
1	C	456/499 (91%)	319 (70%)	100 (22%)	37 (8%)	1	11
1	D	441/499 (88%)	314 (71%)	80 (18%)	47 (11%)	0	6
1	E	456/499 (91%)	320 (70%)	98 (22%)	38 (8%)	0	10
1	F	446/499 (89%)	315 (71%)	83 (19%)	48 (11%)	0	6
All	All	2697/2994 (90%)	1899 (70%)	542 (20%)	256 (10%)	0	8

All (256) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	ALA

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Mol	Chain	Res	Type
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

Continued on next page...

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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 ⓘ

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%)	220 (60%)	145 (40%)	0	0
1	B	361/397 (91%)	215 (60%)	146 (40%)	0	0
1	C	366/397 (92%)	220 (60%)	146 (40%)	0	0
1	D	360/397 (91%)	216 (60%)	144 (40%)	0	0
1	E	366/397 (92%)	219 (60%)	147 (40%)	0	0
1	F	363/397 (91%)	216 (60%)	147 (40%)	0	0
All	All	2181/2382 (92%)	1306 (60%)	875 (40%)	0	0

All (875) 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	218	ILE
1	A	219	THR
1	A	221	SER
1	A	227	GLU
1	A	232	VAL
1	A	236	ARG
1	A	239	ASP
1	A	240	LEU
1	A	242	GLU
1	A	243	THR
1	A	252	VAL
1	A	256	GLU
1	A	260	VAL
1	A	262	ARG
1	A	264	ARG
1	A	274	GLU
1	A	282	LEU
1	A	283	LEU
1	A	292	ASP
1	A	295	ILE
1	A	297	VAL
1	A	301	THR
1	A	305	ASP
1	A	307	LEU
1	A	311	LEU
1	A	312	LEU
1	A	319	ARG
1	A	320	GLN
1	A	323	ILE
1	A	334	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

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Mol	Chain	Res	Type
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
1	A	397	MET
1	A	406	VAL
1	A	407	LEU
1	A	408	SER
1	A	410	ARG
1	A	414	ILE
1	A	424	LEU
1	A	428	PHE
1	A	433	ASP
1	A	435	VAL
1	A	436	HIS
1	A	437	LYS
1	A	438	VAL
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	458	LEU
1	A	459	HIS
1	A	461	SER
1	A	462	ARG
1	A	468	GLN
1	A	480	GLU
1	A	482	VAL
1	A	484	ASP
1	A	485	ASP
1	A	486	VAL
1	A	491	GLU
1	A	492	ASN
1	A	495	ARG

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Mol	Chain	Res	Type
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	513	GLU
1	A	514	PHE
1	A	517	VAL
1	A	519	TYR
1	A	521	VAL
1	A	523	GLU
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	545	GLU
1	A	548	ARG
1	A	549	ARG
1	A	550	LEU
1	A	551	ILE
1	A	558	VAL
1	A	559	LYS
1	A	561	LEU
1	A	563	LEU
1	A	564	GLU
1	A	565	LYS
1	A	568	VAL
1	A	569	LEU
1	A	570	GLU
1	A	577	LEU
1	A	580	GLU
1	A	585	GLU
1	A	586	GLU
1	A	589	ARG

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Mol	Chain	Res	Type
1	A	592	GLU
1	A	594	LEU
1	A	596	LEU
1	A	597	GLU
1	B	147	LEU
1	B	148	THR
1	B	153	VAL
1	B	156	LYS
1	B	165	LYS
1	B	173	GLU
1	B	175	LEU
1	B	176	LYS
1	B	177	ASN
1	B	180	ARG
1	B	187	ARG
1	B	188	ILE
1	B	194	LEU
1	B	205	LEU
1	B	215	VAL
1	B	218	ILE
1	B	221	SER
1	B	223	SER
1	B	224	ASP
1	B	226	VAL
1	B	230	VAL
1	B	237	VAL
1	B	238	ARG
1	B	240	LEU
1	B	243	THR
1	B	245	LYS
1	B	256	GLU
1	B	257	ILE
1	B	260	VAL
1	B	263	LYS
1	B	273	ASP
1	B	281	GLN
1	B	283	LEU
1	B	286	MET
1	B	287	ASP
1	B	295	ILE
1	B	298	MET
1	B	306	ILE

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Mol	Chain	Res	Type
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	333	GLN
1	B	334	ILE
1	B	336	ARG
1	B	337	ILE
1	B	342	LYS
1	B	344	LEU
1	B	346	GLU
1	B	348	VAL
1	B	350	LEU
1	B	352	LEU
1	B	355	LYS
1	B	357	THR
1	B	360	PHE
1	B	368	LEU
1	B	370	ASN
1	B	378	ARG
1	B	379	GLU
1	B	381	ARG
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	396	VAL
1	B	397	MET
1	B	402	LYS
1	B	405	LEU
1	B	406	VAL
1	B	407	LEU
1	B	414	ILE

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Mol	Chain	Res	Type
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	438	VAL
1	B	443	ARG
1	B	445	ARG
1	B	451	MET
1	B	453	ARG
1	B	454	ARG
1	B	457	MET
1	B	461	SER
1	B	463	LYS
1	B	464	ARG
1	B	469	ILE
1	B	471	VAL
1	B	479	GLU
1	B	480	GLU
1	B	481	ILE
1	B	482	VAL
1	B	485	ASP
1	B	486	VAL
1	B	491	GLU
1	B	496	GLN
1	B	502	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

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Mol	Chain	Res	Type
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	568	VAL
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
1	C	152	LYS
1	C	154	THR
1	C	156	LYS
1	C	162	GLU
1	C	167	GLU
1	C	168	LEU
1	C	171	ILE
1	C	175	LEU
1	C	180	ARG
1	C	188	ILE
1	C	195	VAL
1	C	205	LEU
1	C	214	ARG
1	C	215	VAL
1	C	218	ILE

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Mol	Chain	Res	Type
1	C	219	THR
1	C	221	SER
1	C	227	GLU
1	C	232	VAL
1	C	236	ARG
1	C	239	ASP
1	C	240	LEU
1	C	242	GLU
1	C	243	THR
1	C	252	VAL
1	C	256	GLU
1	C	260	VAL
1	C	262	ARG
1	C	264	ARG
1	C	274	GLU
1	C	282	LEU
1	C	283	LEU
1	C	292	ASP
1	C	295	ILE
1	C	297	VAL
1	C	301	THR
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
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

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Mol	Chain	Res	Type
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	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	438	VAL
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	458	LEU
1	C	459	HIS
1	C	461	SER
1	C	462	ARG
1	C	468	GLN
1	C	480	GLU
1	C	484	ASP
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

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Mol	Chain	Res	Type
1	C	502	ARG
1	C	503	ARG
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	523	GLU
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	545	GLU
1	C	548	ARG
1	C	549	ARG
1	C	550	LEU
1	C	551	ILE
1	C	558	VAL
1	C	559	LYS
1	C	561	LEU
1	C	563	LEU
1	C	564	GLU
1	C	568	VAL
1	C	569	LEU
1	C	570	GLU
1	C	576	LEU
1	C	577	LEU
1	C	580	GLU
1	C	582	LEU
1	C	585	GLU
1	C	586	GLU
1	C	589	ARG
1	C	592	GLU
1	C	594	LEU

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Mol	Chain	Res	Type
1	C	596	LEU
1	C	597	GLU
1	D	153	VAL
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	188	ILE
1	D	194	LEU
1	D	205	LEU
1	D	215	VAL
1	D	218	ILE
1	D	221	SER
1	D	224	ASP
1	D	226	VAL
1	D	230	VAL
1	D	237	VAL
1	D	238	ARG
1	D	240	LEU
1	D	243	THR
1	D	245	LYS
1	D	256	GLU
1	D	257	ILE
1	D	260	VAL
1	D	263	LYS
1	D	273	ASP
1	D	281	GLN
1	D	283	LEU
1	D	286	MET
1	D	287	ASP
1	D	295	ILE
1	D	298	MET
1	D	306	ILE
1	D	311	LEU
1	D	312	LEU
1	D	313	ARG
1	D	321	ILE
1	D	323	ILE

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Mol	Chain	Res	Type
1	D	328	VAL
1	D	329	LYS
1	D	331	ARG
1	D	332	GLU
1	D	333	GLN
1	D	334	ILE
1	D	336	ARG
1	D	337	ILE
1	D	342	LYS
1	D	344	LEU
1	D	346	GLU
1	D	348	VAL
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	381	ARG
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	396	VAL
1	D	397	MET
1	D	402	LYS
1	D	405	LEU
1	D	406	VAL
1	D	407	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

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Mol	Chain	Res	Type
1	D	433	ASP
1	D	436	HIS
1	D	438	VAL
1	D	443	ARG
1	D	445	ARG
1	D	451	MET
1	D	453	ARG
1	D	454	ARG
1	D	456	ASP
1	D	457	MET
1	D	461	SER
1	D	463	LYS
1	D	464	ARG
1	D	469	ILE
1	D	479	GLU
1	D	480	GLU
1	D	481	ILE
1	D	482	VAL
1	D	485	ASP
1	D	486	VAL
1	D	491	GLU
1	D	496	GLN
1	D	502	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

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Mol	Chain	Res	Type
1	D	541	LYS
1	D	542	ARG
1	D	548	ARG
1	D	549	ARG
1	D	551	ILE
1	D	554	GLN
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	568	VAL
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	168	LEU
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	218	ILE
1	E	219	THR
1	E	221	SER
1	E	227	GLU
1	E	232	VAL

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Mol	Chain	Res	Type
1	E	236	ARG
1	E	239	ASP
1	E	240	LEU
1	E	242	GLU
1	E	243	THR
1	E	252	VAL
1	E	256	GLU
1	E	260	VAL
1	E	262	ARG
1	E	264	ARG
1	E	274	GLU
1	E	282	LEU
1	E	283	LEU
1	E	292	ASP
1	E	295	ILE
1	E	297	VAL
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

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Mol	Chain	Res	Type
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	414	ILE
1	E	424	LEU
1	E	428	PHE
1	E	433	ASP
1	E	435	VAL
1	E	436	HIS
1	E	437	LYS
1	E	438	VAL
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	458	LEU
1	E	459	HIS
1	E	461	SER
1	E	462	ARG
1	E	468	GLN
1	E	480	GLU
1	E	482	VAL
1	E	484	ASP
1	E	485	ASP
1	E	486	VAL
1	E	491	GLU
1	E	492	ASN
1	E	495	ARG
1	E	496	GLN
1	E	499	GLU
1	E	500	LEU
1	E	502	ARG
1	E	503	ARG
1	E	505	ILE

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Mol	Chain	Res	Type
1	E	506	THR
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
1	E	539	THR
1	E	541	LYS
1	E	542	ARG
1	E	545	GLU
1	E	548	ARG
1	E	549	ARG
1	E	550	LEU
1	E	551	ILE
1	E	558	VAL
1	E	559	LYS
1	E	561	LEU
1	E	563	LEU
1	E	564	GLU
1	E	565	LYS
1	E	568	VAL
1	E	569	LEU
1	E	570	GLU
1	E	577	LEU
1	E	580	GLU
1	E	585	GLU
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

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Mol	Chain	Res	Type
1	F	146	VAL
1	F	147	LEU
1	F	153	VAL
1	F	156	LYS
1	F	165	LYS
1	F	173	GLU
1	F	175	LEU
1	F	176	LYS
1	F	177	ASN
1	F	180	ARG
1	F	187	ARG
1	F	188	ILE
1	F	194	LEU
1	F	205	LEU
1	F	215	VAL
1	F	218	ILE
1	F	219	THR
1	F	221	SER
1	F	223	SER
1	F	224	ASP
1	F	226	VAL
1	F	230	VAL
1	F	237	VAL
1	F	238	ARG
1	F	240	LEU
1	F	243	THR
1	F	245	LYS
1	F	256	GLU
1	F	257	ILE
1	F	260	VAL
1	F	263	LYS
1	F	273	ASP
1	F	281	GLN
1	F	283	LEU
1	F	287	ASP
1	F	295	ILE
1	F	298	MET
1	F	306	ILE
1	F	311	LEU
1	F	312	LEU
1	F	313	ARG
1	F	319	ARG

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Mol	Chain	Res	Type
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	342	LYS
1	F	344	LEU
1	F	346	GLU
1	F	348	VAL
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	381	ARG
1	F	382	ARG
1	F	383	LYS
1	F	384	ILE
1	F	385	THR
1	F	386	MET
1	F	387	LYS
1	F	391	GLU
1	F	394	ASP
1	F	396	VAL
1	F	397	MET
1	F	402	LYS
1	F	405	LEU
1	F	406	VAL
1	F	407	LEU
1	F	414	ILE
1	F	415	THR
1	F	428	PHE
1	F	429	LEU

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Mol	Chain	Res	Type
1	F	431	HIS
1	F	433	ASP
1	F	436	HIS
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	457	MET
1	F	461	SER
1	F	463	LYS
1	F	464	ARG
1	F	469	ILE
1	F	479	GLU
1	F	480	GLU
1	F	481	ILE
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
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

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Mol	Chain	Res	Type
1	F	548	ARG
1	F	549	ARG
1	F	550	LEU
1	F	551	ILE
1	F	554	GLN
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	568	VAL
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	ASN
1	A	247	HIS
1	A	370	ASN
1	A	418	HIS
1	A	468	GLN
1	A	554	GLN
1	A	556	GLN
1	B	338	HIS
1	B	427	HIS
1	B	554	GLN
1	C	177	ASN
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

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Mol	Chain	Res	Type
1	D	554	GLN
1	E	177	ASN
1	E	247	HIS
1	E	277	GLN
1	E	338	HIS
1	E	427	HIS
1	E	468	GLN
1	E	554	GLN
1	E	588	GLN
1	F	247	HIS
1	F	320	GLN
1	F	338	HIS
1	F	496	GLN
1	F	554	GLN
1	F	556	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	28,29,29	1.09	4 (14%)	43,45,45	1.89	8 (18%)
2	ADP	E	5001	-	28,29,29	1.05	3 (10%)	43,45,45	1.91	10 (23%)
2	ADP	C	3001	-	28,29,29	1.06	3 (10%)	43,45,45	1.92	11 (25%)
2	ADP	B	2001	-	28,29,29	1.11	3 (10%)	43,45,45	1.90	8 (18%)
2	ADP	D	4001	-	28,29,29	1.10	3 (10%)	43,45,45	2.00	10 (23%)
2	ADP	F	6001	-	28,29,29	1.08	3 (10%)	43,45,45	1.87	9 (20%)

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	-	-	4/16/32/32	0/3/3/3
2	ADP	E	5001	-	-	2/16/32/32	0/3/3/3
2	ADP	C	3001	-	-	2/16/32/32	0/3/3/3
2	ADP	B	2001	-	-	6/16/32/32	0/3/3/3
2	ADP	D	4001	-	-	6/16/32/32	0/3/3/3
2	ADP	F	6001	-	-	6/16/32/32	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4001	ADP	C5-N7	-2.88	1.33	1.39
2	A	1001	ADP	C2-N3	2.82	1.38	1.33
2	E	5001	ADP	C2-N3	2.81	1.38	1.33
2	F	6001	ADP	C2-N3	2.79	1.38	1.33
2	B	2001	ADP	C2-N1	2.73	1.38	1.33
2	C	3001	ADP	C2-N3	2.72	1.38	1.33
2	B	2001	ADP	C2-N3	2.71	1.38	1.33
2	D	4001	ADP	C2-N3	2.66	1.38	1.33
2	F	6001	ADP	C2-N1	2.65	1.38	1.33
2	A	1001	ADP	C2-N1	2.61	1.38	1.33
2	E	5001	ADP	C2-N1	2.59	1.38	1.33
2	C	3001	ADP	C2-N1	2.52	1.38	1.33
2	F	6001	ADP	C5-N7	-2.38	1.34	1.39
2	B	2001	ADP	C5-N7	-2.34	1.34	1.39
2	D	4001	ADP	C2-N1	2.27	1.38	1.33
2	C	3001	ADP	C5-N7	-2.19	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5001	ADP	C5-N7	-2.19	1.35	1.39
2	A	1001	ADP	C5-N7	-2.14	1.35	1.39
2	A	1001	ADP	C8-N7	2.02	1.35	1.31

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4001	ADP	C5-C4-N3	-6.11	118.30	126.72
2	A	1001	ADP	C5-C4-N3	-5.61	118.99	126.72
2	B	2001	ADP	N3-C2-N1	-5.59	120.11	128.58
2	C	3001	ADP	N3-C2-N1	-5.39	120.43	128.58
2	C	3001	ADP	C5-C4-N3	-5.38	119.31	126.72
2	F	6001	ADP	N3-C2-N1	-5.35	120.48	128.58
2	E	5001	ADP	N3-C2-N1	-5.31	120.55	128.58
2	D	4001	ADP	N3-C2-N1	-5.27	120.61	128.58
2	E	5001	ADP	C5-C4-N3	-5.23	119.52	126.72
2	F	6001	ADP	C5-C4-N3	-5.21	119.54	126.72
2	B	2001	ADP	C5-C4-N3	-5.15	119.62	126.72
2	A	1001	ADP	N3-C2-N1	-4.72	121.44	128.58
2	B	2001	ADP	N9-C8-N7	-4.06	108.17	113.94
2	B	2001	ADP	C5-N7-C8	3.92	109.61	103.45
2	D	4001	ADP	C2-N3-C4	3.92	121.40	111.83
2	F	6001	ADP	N9-C8-N7	-3.87	108.44	113.94
2	E	5001	ADP	N9-C8-N7	-3.85	108.47	113.94
2	D	4001	ADP	C5-N7-C8	3.77	109.37	103.45
2	E	5001	ADP	C5-N7-C8	3.73	109.32	103.45
2	D	4001	ADP	N3-C4-N9	3.70	133.47	127.17
2	A	1001	ADP	C5-N7-C8	3.69	109.25	103.45
2	C	3001	ADP	C5-N7-C8	3.66	109.20	103.45
2	D	4001	ADP	N9-C8-N7	-3.63	108.78	113.94
2	F	6001	ADP	N3-C4-N9	3.62	133.33	127.17
2	C	3001	ADP	C2-N3-C4	3.61	120.64	111.83
2	F	6001	ADP	C5-N7-C8	3.60	109.11	103.45
2	B	2001	ADP	C2-N3-C4	3.60	120.62	111.83
2	F	6001	ADP	C2-N3-C4	3.59	120.60	111.83
2	E	5001	ADP	N3-C4-N9	3.58	133.26	127.17
2	C	3001	ADP	N9-C8-N7	-3.58	108.86	113.94
2	B	2001	ADP	N3-C4-N9	3.57	133.24	127.17
2	A	1001	ADP	N3-C4-N9	3.56	133.23	127.17
2	C	3001	ADP	N3-C4-N9	3.56	133.22	127.17
2	E	5001	ADP	C2-N3-C4	3.50	120.39	111.83
2	A	1001	ADP	C2-N3-C4	3.41	120.16	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	ADP	N9-C8-N7	-3.41	109.10	113.94
2	D	4001	ADP	C4-C5-N7	-3.13	107.00	110.58
2	A	1001	ADP	C4-C5-N7	-3.09	107.05	110.58
2	D	4001	ADP	C6-C5-C4	2.99	121.25	117.18
2	A	1001	ADP	C6-C5-C4	2.93	121.18	117.18
2	B	2001	ADP	C4-C5-N7	-2.73	107.46	110.58
2	C	3001	ADP	C4-C5-N7	-2.72	107.47	110.58
2	E	5001	ADP	C6-C5-C4	2.68	120.83	117.18
2	E	5001	ADP	C4-C5-N7	-2.67	107.53	110.58
2	C	3001	ADP	C6-C5-C4	2.66	120.81	117.18
2	F	6001	ADP	C4-C5-N7	-2.47	107.75	110.58
2	D	4001	ADP	C2'-C1'-N9	-2.44	107.24	113.30
2	F	6001	ADP	C6-C5-C4	2.42	120.48	117.18
2	B	2001	ADP	C6-C5-C4	2.39	120.45	117.18
2	E	5001	ADP	C5-C6-N6	-2.23	117.77	123.29
2	F	6001	ADP	C2'-C1'-N9	-2.22	107.78	113.30
2	D	4001	ADP	C5-C4-N9	2.22	108.23	105.81
2	C	3001	ADP	C3'-C2'-C1'	2.14	105.50	101.46
2	E	5001	ADP	C3'-C2'-C1'	2.01	105.26	101.46
2	C	3001	ADP	O2A-PA-O3A	2.00	112.69	107.27
2	C	3001	ADP	C5-C6-N6	-2.00	118.33	123.29

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	ADP	O4'-C4'-C5'-O5'
2	B	2001	ADP	PA-O3A-PB-O2B
2	B	2001	ADP	PA-O3A-PB-O3B
2	B	2001	ADP	O4'-C4'-C5'-O5'
2	C	3001	ADP	O4'-C4'-C5'-O5'
2	C	3001	ADP	C3'-C4'-C5'-O5'
2	D	4001	ADP	PA-O3A-PB-O2B
2	D	4001	ADP	PA-O3A-PB-O3B
2	D	4001	ADP	O4'-C4'-C5'-O5'
2	E	5001	ADP	O4'-C4'-C5'-O5'
2	E	5001	ADP	C3'-C4'-C5'-O5'
2	F	6001	ADP	PA-O3A-PB-O2B
2	F	6001	ADP	PA-O3A-PB-O3B
2	F	6001	ADP	O4'-C4'-C5'-O5'
2	A	1001	ADP	C3'-C4'-C5'-O5'
2	B	2001	ADP	C3'-C4'-C5'-O5'

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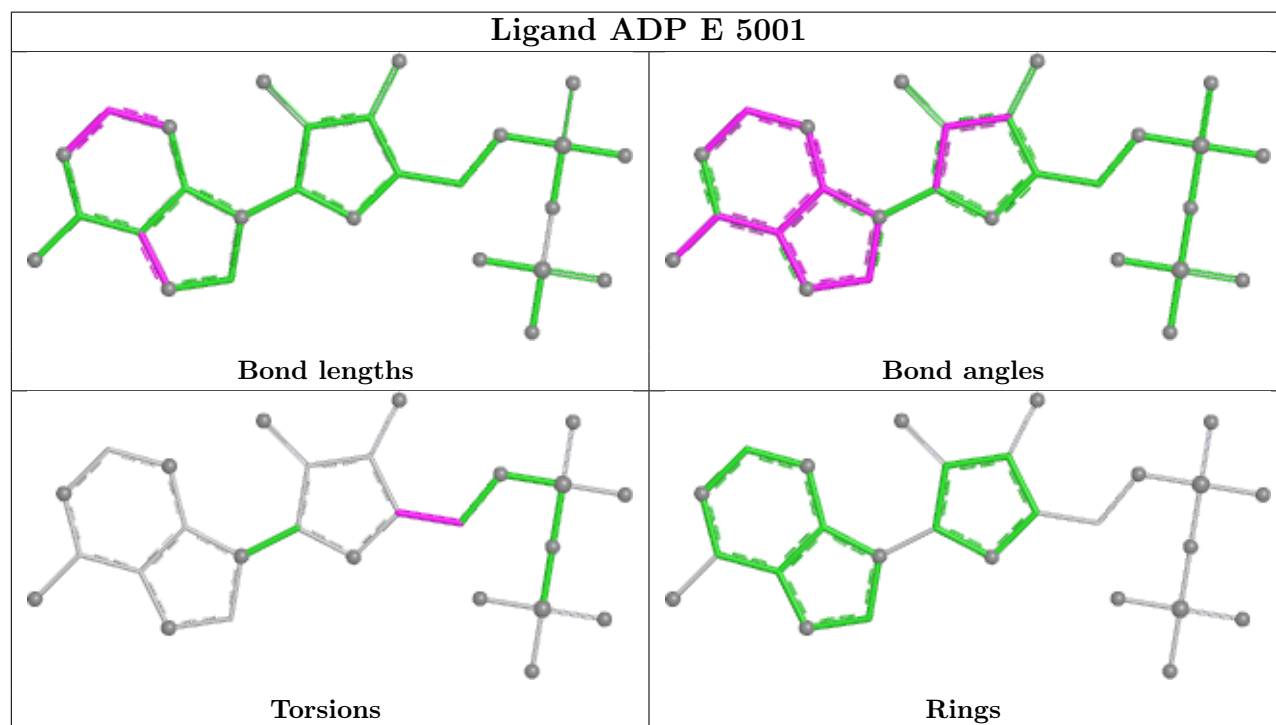
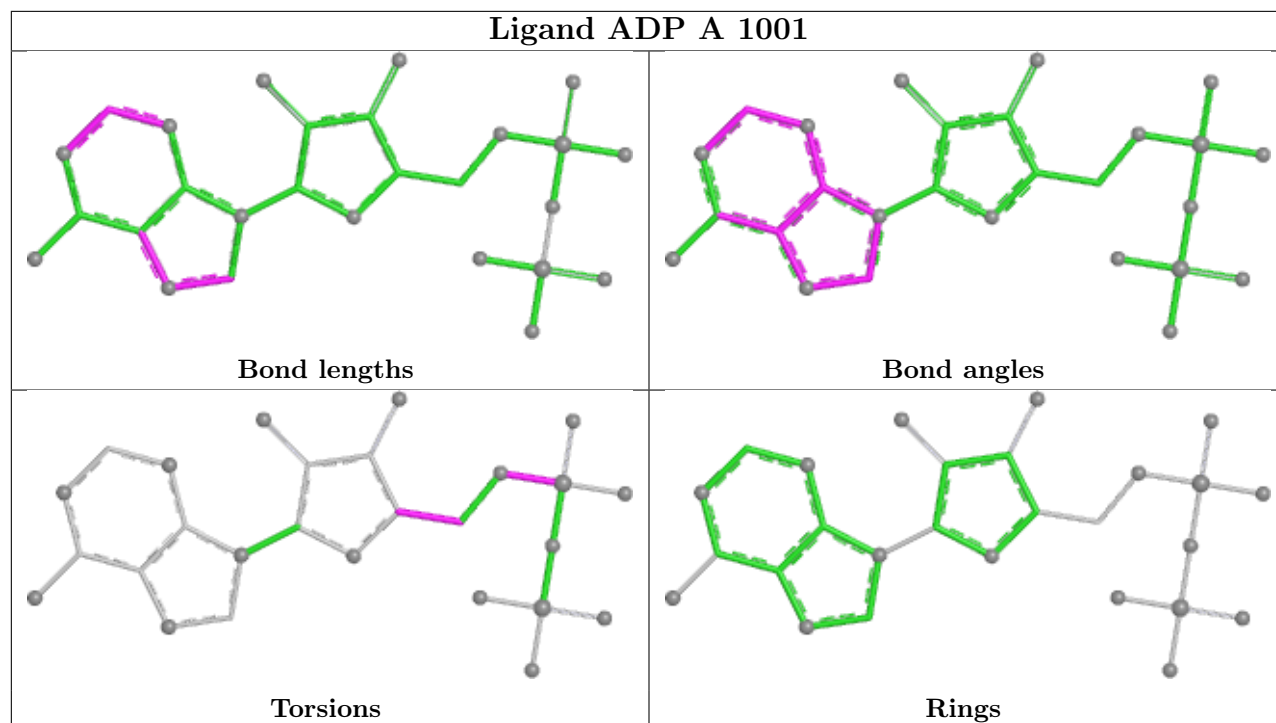
Mol	Chain	Res	Type	Atoms
2	D	4001	ADP	C3'-C4'-C5'-O5'
2	F	6001	ADP	C3'-C4'-C5'-O5'
2	B	2001	ADP	PB-O3A-PA-O1A
2	D	4001	ADP	PB-O3A-PA-O1A
2	F	6001	ADP	PB-O3A-PA-O1A
2	A	1001	ADP	C5'-O5'-PA-O1A
2	A	1001	ADP	C5'-O5'-PA-O3A
2	B	2001	ADP	PB-O3A-PA-O2A
2	D	4001	ADP	PB-O3A-PA-O2A
2	F	6001	ADP	PB-O3A-PA-O2A

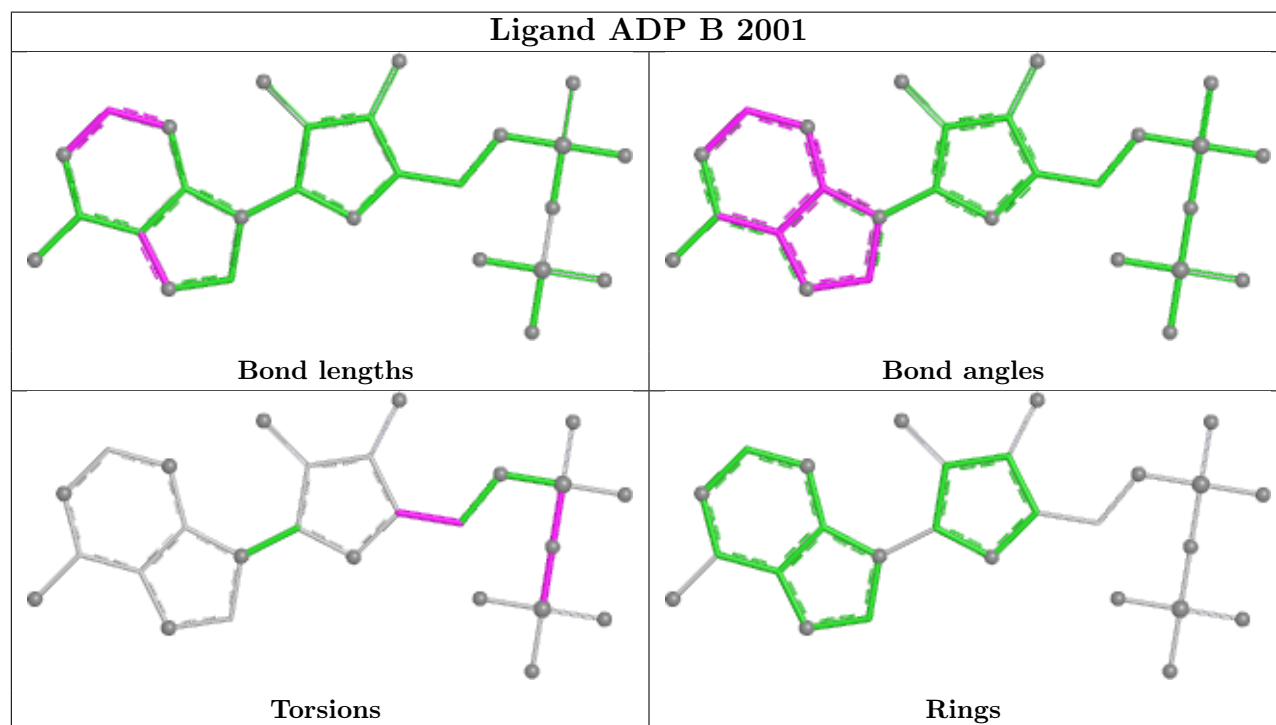
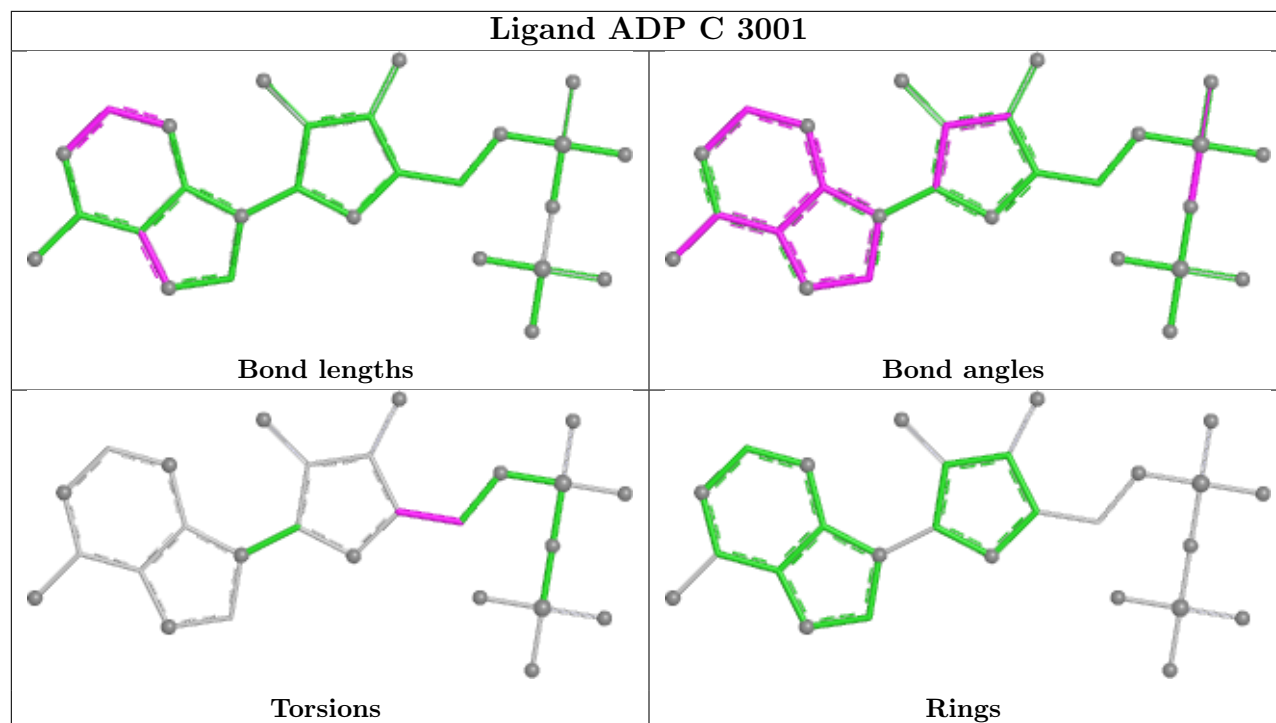
There are no ring outliers.

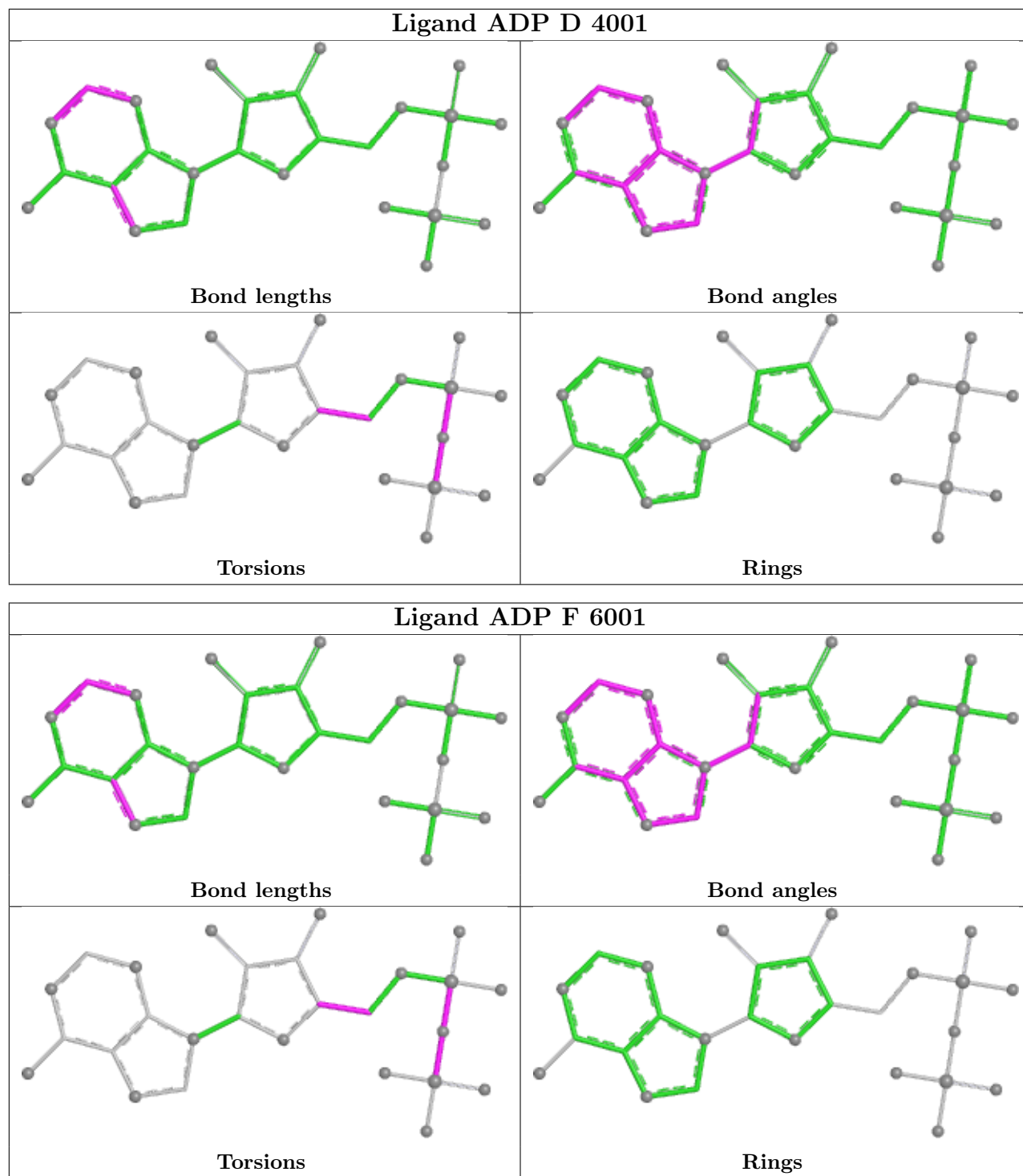
6 monomers are involved in 21 short contacts:

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

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







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	458/499 (91%)	-0.95	0 100 100	2, 19, 55, 80	0
1	B	446/499 (89%)	-0.93	1 (0%) 91 81	2, 19, 50, 97	0
1	C	458/499 (91%)	-0.89	1 (0%) 91 81	2, 20, 57, 84	0
1	D	445/499 (89%)	-0.90	0 100 100	2, 18, 50, 97	0
1	E	458/499 (91%)	-0.88	0 100 100	2, 21, 55, 82	0
1	F	450/499 (90%)	-0.87	1 (0%) 91 81	2, 19, 51, 94	0
All	All	2715/2994 (90%)	-0.90	3 (0%) 92 87	2, 19, 54, 97	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	176	LYS	2.6
1	C	599	PRO	2.5
1	B	222	GLY	2.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

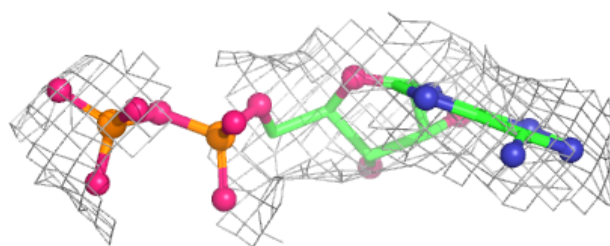
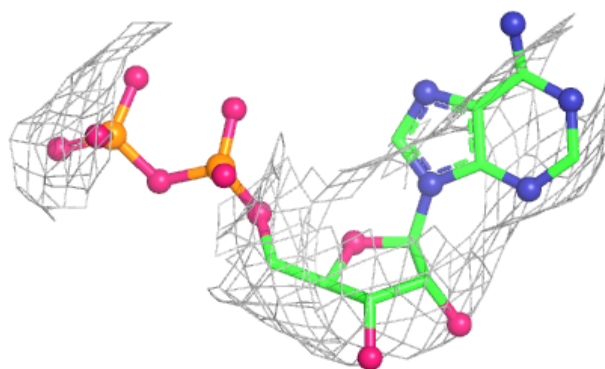
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	A	1001	27/27	0.99	0.04	14,15,17,18	0
2	ADP	B	2001	27/27	0.99	0.03	5,9,13,13	0
2	ADP	C	3001	27/27	0.99	0.05	18,18,19,19	0
2	ADP	D	4001	27/27	0.99	0.04	2,2,8,8	0
2	ADP	E	5001	27/27	0.99	0.03	14,17,18,18	0
2	ADP	F	6001	27/27	0.99	0.04	11,15,15,18	0

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

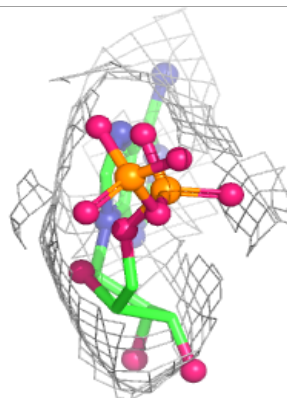
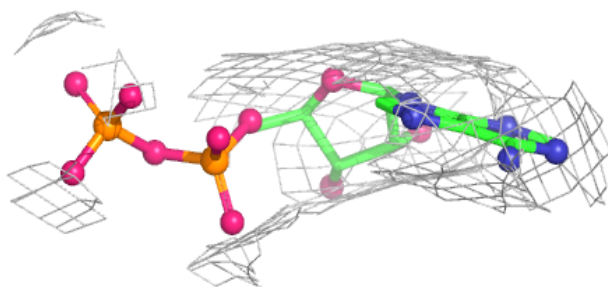
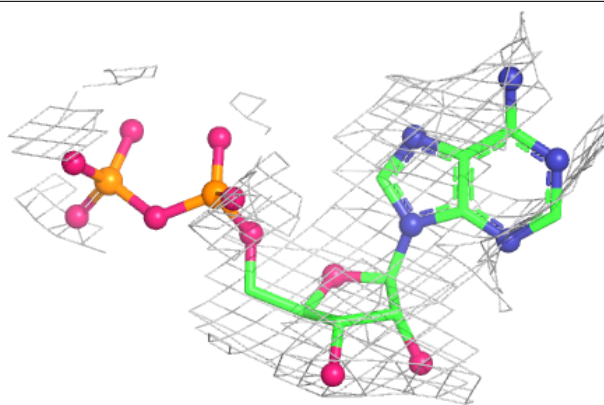
Electron density around ADP A 1001:

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

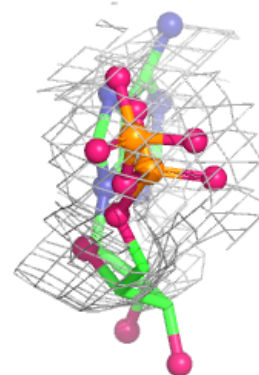
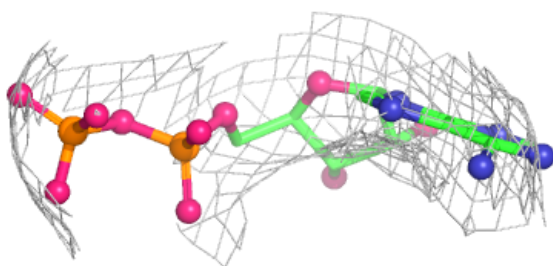
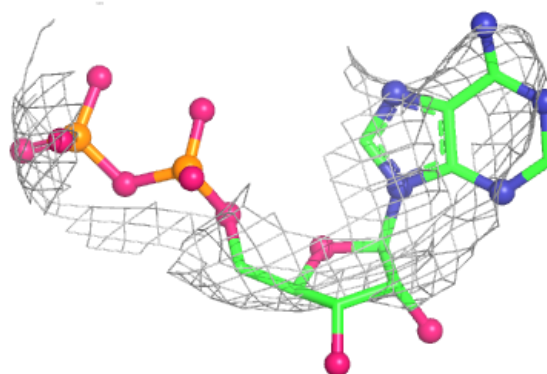


Electron density around ADP B 2001:

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

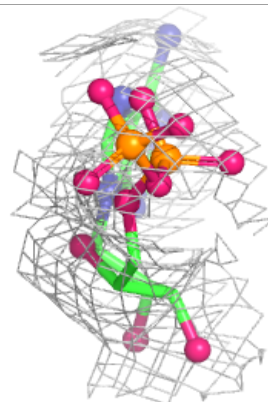
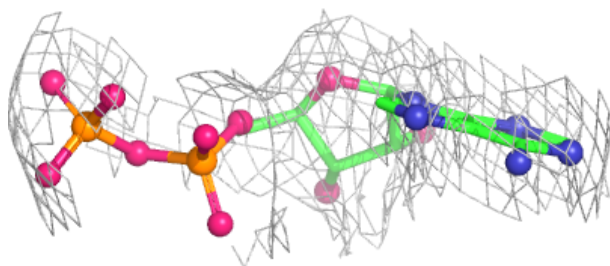
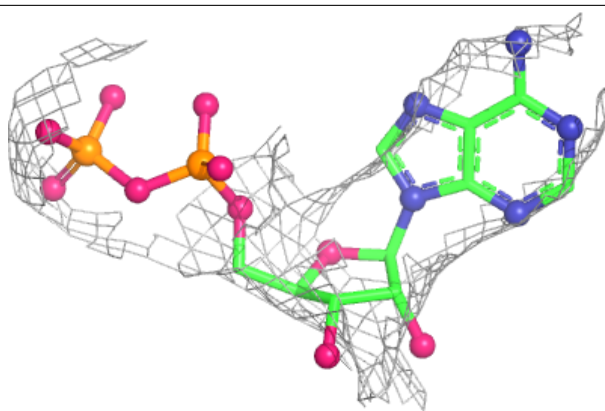
**Electron density around ADP C 3001:**

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

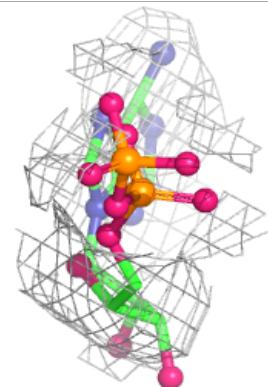
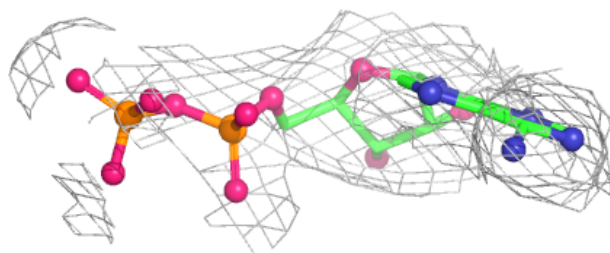
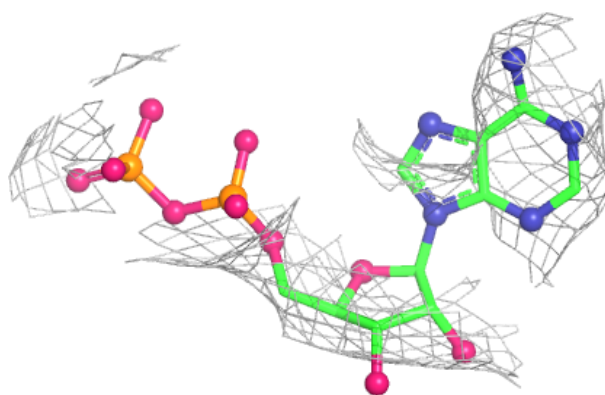


Electron density around ADP D 4001:

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

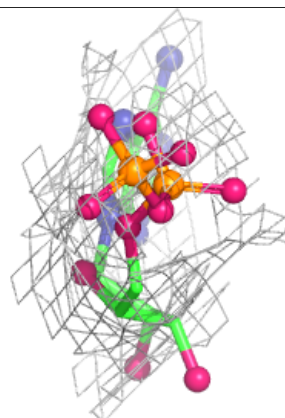
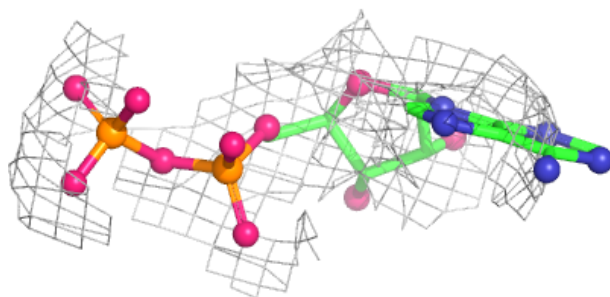
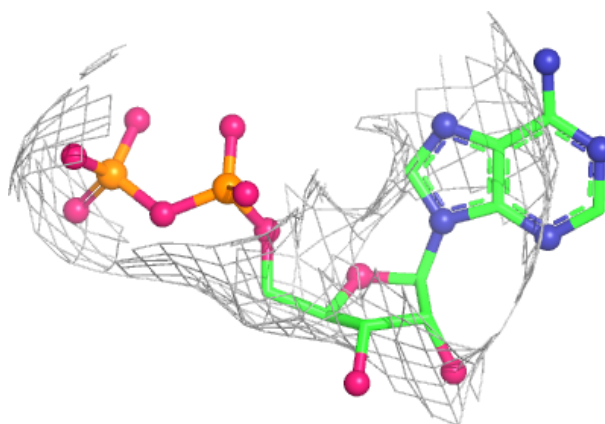
**Electron density around ADP E 5001:**

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



Electron density around ADP F 6001:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.