



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:42 PM UTC

PDB ID : 3B60 / pdb_00003b60
Title : Crystal Structure of MsbA from Salmonella typhimurium with AMPPNP, higher resolution form
Authors : Ward, A.; Reyes, C.L.; Yu, J.; Roth, C.B.; Chang, G.
Deposited on : 2007-10-26
Resolution : 3.70 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

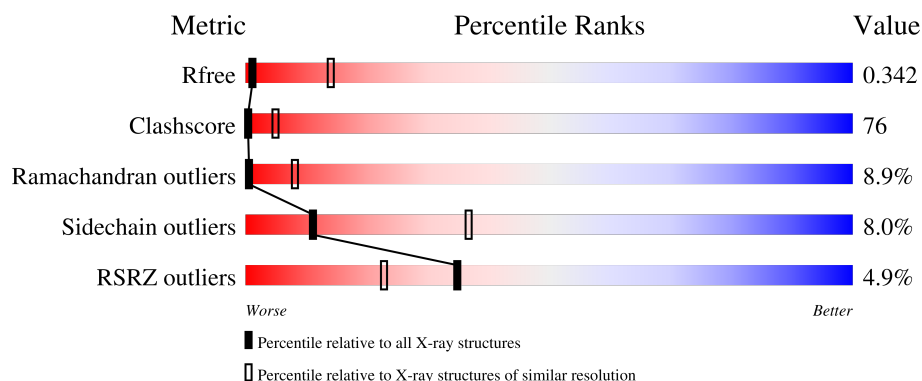
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	582	6% 23% 59% 15% ..
1	B	582	5% 23% 59% 13% ..
1	C	582	5% 23% 60% 13% ..
1	D	582	4% 23% 59% 14% ..

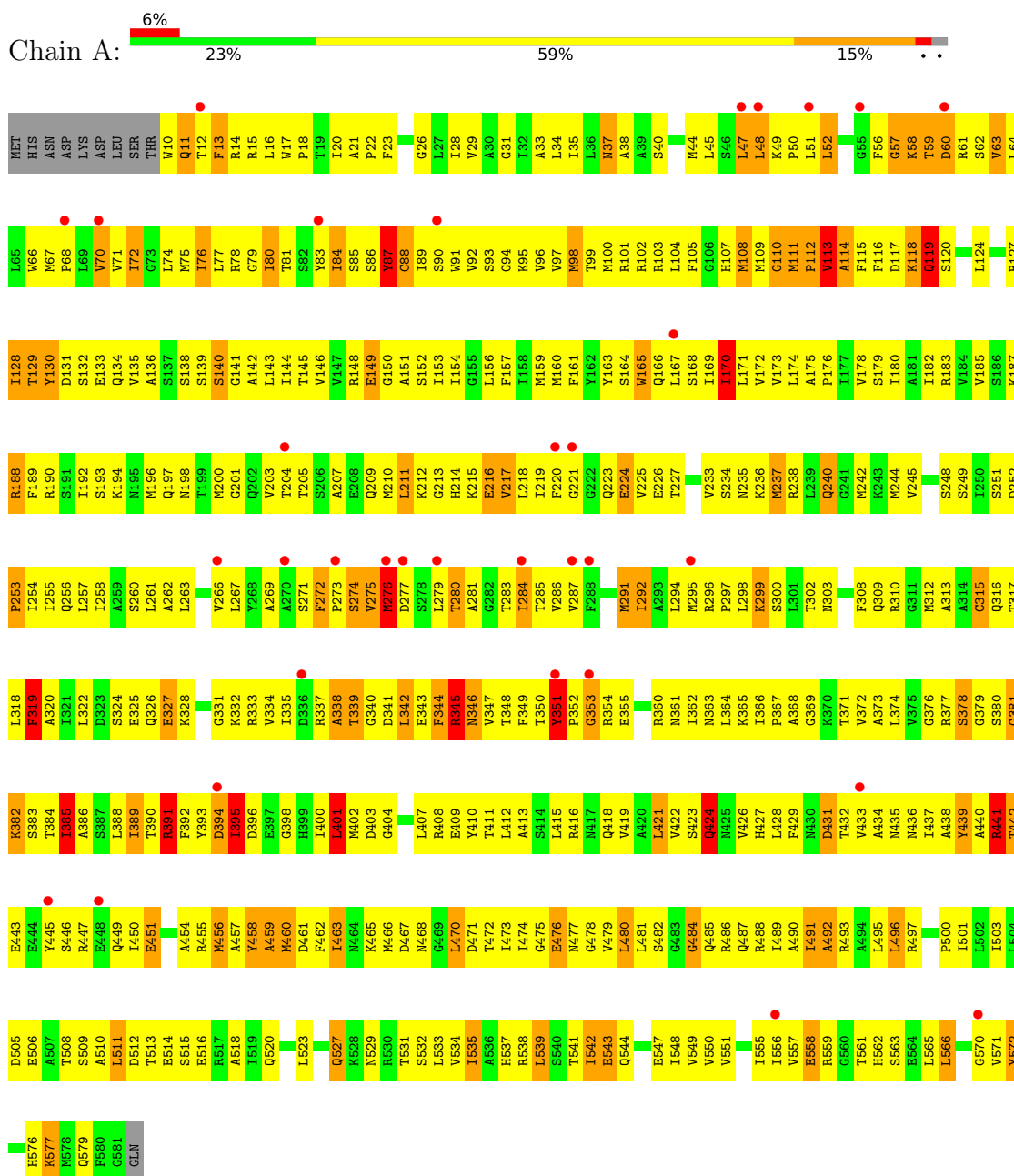
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

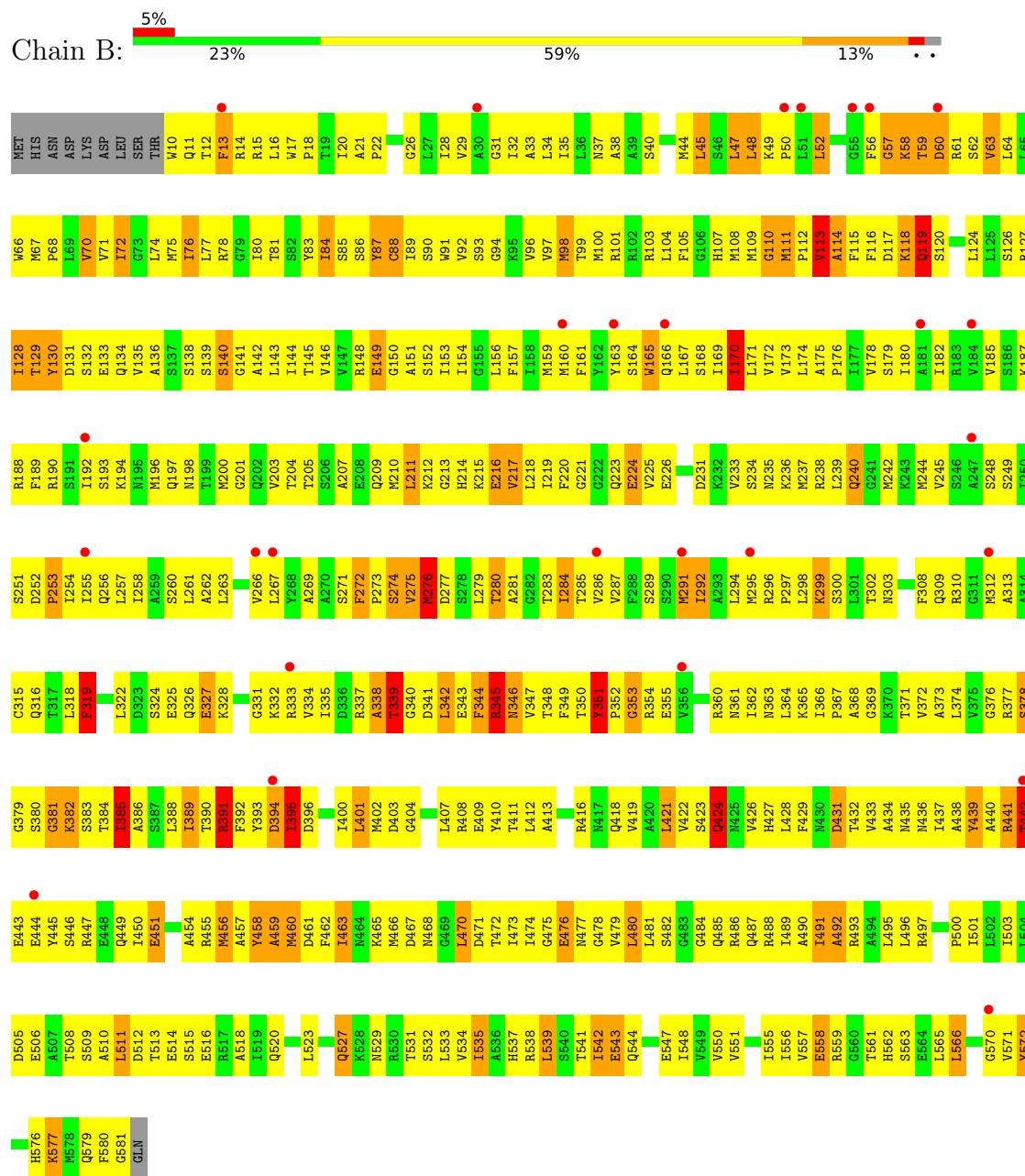
3 Residue-property plots

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.

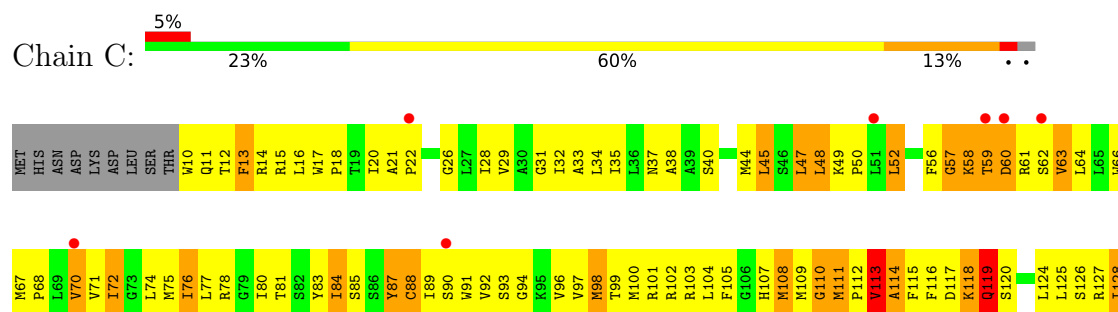
- Molecule 1: Lipid A export ATP-binding/permease protein msbA

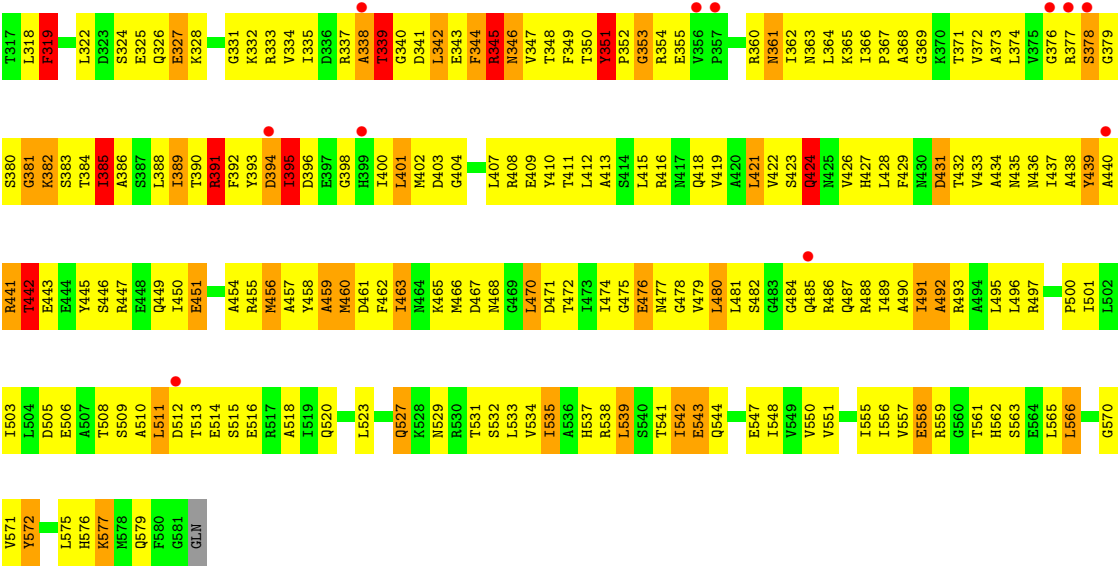


● Molecule 1: Lipid A export ATP-binding/permease protein msbA



● Molecule 1: Lipid A export ATP-binding/permease protein msbA





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	249.64Å 119.90Å 168.80Å 90.00° 120.61° 90.00°	Depositor
Resolution (Å)	20.00 – 3.70 20.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	87.7 (20.00-3.70) 87.1 (20.00-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 3.71Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.307 , 0.343 0.309 , 0.342	Depositor DCC
R_{free} test set	2019 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	118.5	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 104.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	17844	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: ANP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.60	1/4497 (0.0%)	1.14	38/6076 (0.6%)
1	B	0.42	0/4497	1.06	34/6076 (0.6%)
1	C	0.42	0/4497	1.06	34/6076 (0.6%)
1	D	0.43	0/4497	1.06	34/6076 (0.6%)
All	All	0.48	1/17988 (0.0%)	1.08	140/24304 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	ALA	C-N	6.05	1.42	1.33

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	441	ARG	CA-C-N	16.45	152.96	121.54
1	A	441	ARG	C-N-CA	16.45	152.96	121.54
1	A	319	PHE	N-CA-C	-12.45	97.75	111.07
1	D	319	PHE	N-CA-C	-11.94	98.29	111.07
1	C	319	PHE	N-CA-C	-11.93	98.31	111.07
1	B	319	PHE	N-CA-C	-11.89	98.35	111.07
1	D	441	ARG	CA-C-N	10.22	141.07	121.54
1	D	441	ARG	C-N-CA	10.22	141.07	121.54
1	C	441	ARG	CA-C-N	10.19	141.01	121.54
1	C	441	ARG	C-N-CA	10.19	141.01	121.54
1	B	441	ARG	CA-C-N	10.18	140.97	121.54
1	B	441	ARG	C-N-CA	10.18	140.97	121.54
1	A	338	ALA	CA-C-N	-9.85	102.73	121.54
1	A	338	ALA	C-N-CA	-9.85	102.73	121.54
1	C	170	ILE	N-CA-C	-8.81	104.76	111.90
1	B	170	ILE	N-CA-C	-8.77	104.79	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	170	ILE	N-CA-C	-8.76	104.81	111.90
1	A	170	ILE	N-CA-C	-8.48	105.03	111.90
1	A	395	ILE	N-CA-C	8.14	126.28	109.34
1	A	130	TYR	N-CA-C	7.97	119.75	111.14
1	C	130	TYR	N-CA-C	7.91	119.68	111.14
1	B	130	TYR	N-CA-C	7.85	119.62	111.14
1	D	130	TYR	N-CA-C	7.83	119.60	111.14
1	B	395	ILE	N-CA-C	7.68	125.31	109.34
1	C	300	SER	N-CA-C	-7.68	103.76	113.43
1	A	300	SER	N-CA-C	-7.67	103.76	113.43
1	C	395	ILE	N-CA-C	7.67	125.29	109.34
1	D	395	ILE	N-CA-C	7.66	125.27	109.34
1	B	300	SER	N-CA-C	-7.64	103.81	113.43
1	D	300	SER	N-CA-C	-7.63	103.81	113.43
1	A	463	ILE	N-CA-C	-7.39	103.33	110.42
1	B	463	ILE	N-CA-C	-7.15	103.56	110.42
1	C	463	ILE	N-CA-C	-7.07	103.63	110.42
1	D	463	ILE	N-CA-C	-7.04	103.67	110.42
1	B	338	ALA	N-CA-C	6.72	123.81	112.99
1	D	338	ALA	N-CA-C	6.70	123.77	112.99
1	C	338	ALA	N-CA-C	6.69	123.76	112.99
1	A	338	ALA	CA-C-O	-6.35	111.86	118.65
1	D	351	TYR	CA-C-N	-6.00	112.34	119.84
1	D	351	TYR	C-N-CA	-6.00	112.34	119.84
1	C	351	TYR	CA-C-N	-5.97	112.37	119.84
1	C	351	TYR	C-N-CA	-5.97	112.37	119.84
1	B	351	TYR	CA-C-N	-5.97	112.38	119.84
1	B	351	TYR	C-N-CA	-5.97	112.38	119.84
1	A	491	ILE	N-CA-C	-5.96	104.70	110.72
1	A	345	ARG	N-CA-C	5.89	119.08	109.59
1	A	421	LEU	N-CA-C	5.86	118.31	109.23
1	C	572	TYR	N-CA-C	-5.84	104.55	111.03
1	B	572	TYR	N-CA-C	-5.82	104.57	111.03
1	D	572	TYR	N-CA-C	-5.81	104.58	111.03
1	A	572	TYR	N-CA-C	-5.80	104.59	111.03
1	A	110	GLY	N-CA-C	-5.79	105.68	115.34
1	A	240	GLN	N-CA-C	-5.78	104.90	111.14
1	D	149	GLU	N-CA-C	-5.74	105.54	112.54
1	B	442	THR	N-CA-CB	5.73	120.18	110.49
1	C	442	THR	N-CA-CB	5.72	120.17	110.49
1	D	48	LEU	N-CA-C	5.71	117.30	111.14
1	C	149	GLU	N-CA-C	-5.70	105.58	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	48	LEU	N-CA-C	5.70	117.29	111.14
1	B	149	GLU	N-CA-C	-5.69	105.60	112.54
1	D	442	THR	N-CA-CB	5.69	120.10	110.49
1	B	110	GLY	N-CA-C	-5.68	105.85	115.34
1	D	13	PHE	N-CA-C	-5.68	104.29	111.11
1	C	13	PHE	N-CA-C	-5.68	104.30	111.11
1	C	48	LEU	N-CA-C	5.68	117.27	111.14
1	B	13	PHE	N-CA-C	-5.68	104.30	111.11
1	D	110	GLY	N-CA-C	-5.67	105.87	115.34
1	A	351	TYR	CA-C-N	-5.66	112.76	119.84
1	A	351	TYR	C-N-CA	-5.66	112.76	119.84
1	C	110	GLY	N-CA-C	-5.66	105.88	115.34
1	A	353	GLY	N-CA-C	5.63	126.53	113.18
1	D	345	ARG	N-CA-C	5.62	118.89	109.95
1	A	13	PHE	N-CA-C	-5.60	104.39	111.11
1	A	149	GLU	N-CA-C	-5.58	105.73	112.54
1	B	345	ARG	N-CA-C	5.58	118.83	109.95
1	C	345	ARG	N-CA-C	5.58	118.83	109.95
1	B	353	GLY	N-CA-C	5.55	126.33	113.18
1	D	353	GLY	N-CA-C	5.53	126.29	113.18
1	D	511	LEU	N-CA-C	5.53	118.45	109.06
1	B	511	LEU	N-CA-C	5.52	118.45	109.06
1	B	113	VAL	N-CA-C	5.52	120.82	109.34
1	B	577	LYS	N-CA-C	-5.52	103.11	111.56
1	A	84	ILE	N-CA-C	-5.52	105.73	111.58
1	C	353	GLY	N-CA-C	5.52	126.26	113.18
1	C	577	LYS	N-CA-C	-5.51	103.12	111.56
1	C	113	VAL	N-CA-C	5.51	120.80	109.34
1	D	113	VAL	N-CA-C	5.51	120.80	109.34
1	C	511	LEU	N-CA-C	5.51	118.42	109.06
1	A	48	LEU	N-CA-C	5.50	117.08	111.14
1	A	511	LEU	N-CA-C	5.50	118.41	109.06
1	D	577	LYS	N-CA-C	-5.50	103.15	111.56
1	D	84	ILE	N-CA-C	-5.49	105.76	111.58
1	B	240	GLN	N-CA-C	-5.48	105.22	111.14
1	C	240	GLN	N-CA-C	-5.47	105.23	111.14
1	A	577	LYS	N-CA-C	-5.47	103.20	111.56
1	D	240	GLN	N-CA-C	-5.46	105.25	111.14
1	B	84	ILE	N-CA-C	-5.44	105.81	111.58
1	C	84	ILE	N-CA-C	-5.44	105.82	111.58
1	B	274	SER	N-CA-C	-5.43	105.39	112.23
1	D	274	SER	N-CA-C	-5.43	105.39	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	451	GLU	N-CA-C	-5.42	104.40	111.02
1	C	274	SER	N-CA-C	-5.42	105.40	112.23
1	C	421	LEU	N-CA-C	5.41	117.62	109.23
1	D	421	LEU	N-CA-C	5.40	117.61	109.23
1	C	491	ILE	N-CA-C	-5.38	105.28	110.72
1	B	421	LEU	N-CA-C	5.38	117.56	109.23
1	B	491	ILE	N-CA-C	-5.37	105.30	110.72
1	D	491	ILE	N-CA-C	-5.36	105.30	110.72
1	A	276	MET	N-CA-C	-5.30	99.51	110.80
1	C	70	VAL	N-CA-C	-5.30	105.68	110.82
1	D	70	VAL	N-CA-C	-5.30	105.68	110.82
1	A	484	GLY	N-CA-C	-5.29	106.37	112.50
1	D	45	LEU	N-CA-C	-5.27	105.59	112.23
1	B	70	VAL	N-CA-C	-5.26	105.71	110.82
1	B	45	LEU	N-CA-C	-5.26	105.61	112.23
1	A	274	SER	N-CA-C	-5.25	105.61	112.23
1	A	113	VAL	N-CA-C	5.25	120.25	109.34
1	C	45	LEU	N-CA-C	-5.24	105.63	112.23
1	A	391	ARG	N-CA-C	5.22	121.92	110.80
1	A	119	GLN	N-CA-C	5.21	118.20	110.48
1	A	401	LEU	N-CA-C	5.21	117.57	108.76
1	C	391	ARG	N-CA-C	5.21	121.89	110.80
1	D	391	ARG	N-CA-C	5.20	121.88	110.80
1	B	451	GLU	N-CA-C	-5.20	104.68	111.02
1	B	391	ARG	N-CA-C	5.18	121.83	110.80
1	C	451	GLU	N-CA-C	-5.16	104.72	111.02
1	D	119	GLN	N-CA-C	5.16	118.11	110.48
1	A	338	ALA	N-CA-C	5.15	121.99	113.50
1	B	119	GLN	N-CA-C	5.15	118.10	110.48
1	C	119	GLN	N-CA-C	5.13	118.07	110.48
1	A	385	ILE	N-CA-C	-5.13	105.39	110.62
1	C	276	MET	N-CA-C	-5.12	99.89	110.80
1	D	451	GLU	N-CA-C	-5.11	104.78	111.02
1	B	276	MET	N-CA-C	-5.11	99.92	110.80
1	D	276	MET	N-CA-C	-5.10	99.93	110.80
1	A	188	ARG	N-CA-C	-5.06	107.06	113.18
1	D	385	ILE	N-CA-C	-5.05	105.47	110.62
1	C	385	ILE	N-CA-C	-5.03	105.48	110.62
1	B	385	ILE	N-CA-C	-5.01	105.51	110.62
1	A	70	VAL	N-CA-C	-5.00	105.97	110.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4430	0	4555	752	0
1	B	4430	0	4556	727	0
1	C	4430	0	4556	756	0
1	D	4430	0	4556	749	0
2	A	31	0	13	5	0
2	B	31	0	13	6	0
2	C	31	0	13	3	0
2	D	31	0	13	5	0
All	All	17844	0	18275	2728	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 76.

All (2728) 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:A:221:GLY:HA3	1:B:441:ARG:CD	1.57	1.35
1:A:221:GLY:CA	1:B:441:ARG:HD3	1.67	1.22
1:C:11:GLN:HG2	1:C:12:THR:H	1.10	1.17
1:C:281:ALA:HB2	1:D:56:PHE:HB3	1.24	1.17
1:C:441:ARG:CD	1:D:221:GLY:HA3	1.75	1.16
1:C:441:ARG:HD3	1:D:221:GLY:CA	1.77	1.15
1:A:441:ARG:HD3	1:B:221:GLY:HA3	1.17	1.14
1:D:11:GLN:HG2	1:D:12:THR:H	1.10	1.13
1:A:11:GLN:N	1:A:14:ARG:HB3	1.62	1.12
1:C:56:PHE:HB3	1:D:281:ALA:HB2	1.26	1.12
1:B:338:ALA:HB3	1:B:500:PRO:HG2	1.12	1.11
1:A:338:ALA:O	1:A:339:THR:C	1.92	1.11
1:B:11:GLN:HG2	1:B:12:THR:H	1.10	1.11
1:A:10:TRP:HA	1:A:14:ARG:HB2	1.33	1.10
1:C:221:GLY:HA3	1:D:441:ARG:CD	1.80	1.10
1:C:221:GLY:HA3	1:D:441:ARG:HD3	1.15	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLN:HG2	1:A:12:THR:H	1.06	1.07
1:D:338:ALA:HB3	1:D:500:PRO:HG2	1.12	1.07
1:C:10:TRP:HA	1:C:14:ARG:HB2	1.37	1.07
1:C:338:ALA:HB3	1:C:500:PRO:HG2	1.12	1.06
1:C:221:GLY:CA	1:D:441:ARG:HD3	1.85	1.06
1:A:441:ARG:CD	1:B:221:GLY:HA3	1.84	1.06
1:C:441:ARG:HD3	1:D:221:GLY:HA3	1.09	1.05
1:B:10:TRP:HA	1:B:14:ARG:HB2	1.37	1.05
1:D:10:TRP:HA	1:D:14:ARG:HB2	1.37	1.05
1:A:220:PHE:HA	1:B:497:ARG:HH21	1.22	1.04
1:A:338:ALA:HB3	1:A:500:PRO:HG2	1.08	1.03
1:D:351:TYR:HB3	1:D:352:PRO:HD3	1.41	1.02
1:A:351:TYR:HB3	1:A:352:PRO:HD3	1.42	1.01
1:B:338:ALA:O	1:B:339:THR:C	2.02	1.01
1:B:351:TYR:HB3	1:B:352:PRO:HD3	1.41	1.01
1:C:351:TYR:HB3	1:C:352:PRO:HD3	1.41	1.01
1:A:441:ARG:HD3	1:B:221:GLY:CA	1.91	1.00
1:C:497:ARG:HH21	1:D:220:PHE:HA	1.26	1.00
1:C:338:ALA:O	1:C:339:THR:C	2.02	0.99
1:B:80:ILE:O	1:B:84:ILE:HG12	1.63	0.99
1:B:11:GLN:N	1:B:14:ARG:HB3	1.78	0.98
1:D:11:GLN:N	1:D:14:ARG:HB3	1.78	0.98
1:D:80:ILE:O	1:D:84:ILE:HG12	1.63	0.98
1:C:512:ASP:OD1	1:D:377:ARG:HA	1.61	0.98
1:C:395:ILE:HG12	1:C:396:ASP:H	1.28	0.98
1:B:395:ILE:HG12	1:B:396:ASP:H	1.27	0.98
1:A:338:ALA:HB3	1:A:500:PRO:CG	1.93	0.97
1:A:80:ILE:O	1:A:84:ILE:HG12	1.63	0.97
1:A:91:TRP:HA	1:B:242:MET:HE1	1.46	0.97
1:C:80:ILE:O	1:C:84:ILE:HG12	1.63	0.97
1:D:338:ALA:O	1:D:339:THR:C	2.02	0.97
1:A:395:ILE:HG12	1:A:396:ASP:H	1.28	0.97
1:D:395:ILE:HG12	1:D:396:ASP:H	1.27	0.97
1:C:11:GLN:N	1:C:14:ARG:HB3	1.78	0.96
1:A:91:TRP:HA	1:B:242:MET:CE	1.95	0.96
1:B:347:VAL:HG13	1:B:395:ILE:HD11	1.47	0.96
1:D:347:VAL:HG13	1:D:395:ILE:HD11	1.47	0.96
1:C:347:VAL:HG13	1:C:395:ILE:HD11	1.47	0.95
1:A:539:LEU:HA	1:A:542:ILE:HD13	1.46	0.95
1:A:272:PHE:HB2	1:A:273:PRO:HD3	1.49	0.94
1:C:377:ARG:HA	1:D:512:ASP:OD1	1.65	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:VAL:HG13	1:A:395:ILE:HD11	1.44	0.94
1:B:338:ALA:HB3	1:B:500:PRO:CG	1.97	0.94
1:D:272:PHE:HB2	1:D:273:PRO:HD3	1.50	0.93
1:D:338:ALA:HB3	1:D:500:PRO:CG	1.97	0.93
1:C:338:ALA:HB3	1:C:500:PRO:CG	1.97	0.93
1:A:220:PHE:HA	1:B:497:ARG:NH2	1.83	0.93
1:C:497:ARG:NH2	1:D:220:PHE:HA	1.83	0.93
1:A:220:PHE:CZ	1:B:429:PHE:HE1	1.87	0.93
1:B:272:PHE:HB2	1:B:273:PRO:HD3	1.50	0.93
1:A:11:GLN:N	1:A:14:ARG:CB	2.32	0.92
1:A:74:LEU:HD22	1:A:75:MET:HE2	1.50	0.92
1:B:539:LEU:HA	1:B:542:ILE:HD13	1.51	0.92
1:A:98:MET:HB3	1:B:238:ARG:NH2	1.83	0.92
1:B:74:LEU:HD22	1:B:75:MET:HE2	1.52	0.91
1:C:74:LEU:HD22	1:C:75:MET:HE2	1.52	0.91
1:C:272:PHE:HB2	1:C:273:PRO:HD3	1.50	0.91
1:A:11:GLN:HG2	1:A:12:THR:N	1.85	0.91
1:D:74:LEU:HD22	1:D:75:MET:HE2	1.52	0.91
1:C:242:MET:HE1	1:D:91:TRP:HA	1.53	0.90
1:A:470:LEU:HD12	1:A:470:LEU:H	1.36	0.90
1:A:429:PHE:HE1	1:B:220:PHE:CZ	1.90	0.90
1:C:220:PHE:HA	1:D:497:ARG:HH21	1.36	0.89
1:A:116:PHE:HE1	1:B:211:LEU:HD12	1.37	0.89
1:C:116:PHE:HE1	1:D:211:LEU:HD12	1.38	0.89
1:C:539:LEU:HA	1:C:542:ILE:HD13	1.53	0.89
1:A:466:MET:HE2	1:A:472:THR:HG21	1.55	0.89
1:B:466:MET:HE2	1:B:472:THR:HG21	1.54	0.89
1:D:539:LEU:HA	1:D:542:ILE:HD13	1.53	0.89
1:A:98:MET:HB3	1:B:238:ARG:CZ	2.03	0.89
1:A:10:TRP:CA	1:A:14:ARG:HB2	2.03	0.88
1:D:466:MET:HE2	1:D:472:THR:HG21	1.54	0.88
1:A:21:ALA:HB3	1:A:22:PRO:HD3	1.56	0.87
1:A:20:ILE:HD13	1:A:96:VAL:HG21	1.56	0.87
1:C:466:MET:HE2	1:C:472:THR:HG21	1.54	0.87
1:A:221:GLY:HA3	1:B:441:ARG:NE	1.89	0.87
1:A:211:LEU:HD12	1:B:116:PHE:HE1	1.40	0.87
1:A:220:PHE:CZ	1:B:439:TYR:HB3	2.08	0.87
1:C:459:ALA:O	1:C:463:ILE:HG12	1.75	0.87
1:B:21:ALA:HB3	1:B:22:PRO:HD3	1.57	0.87
1:D:11:GLN:HG2	1:D:12:THR:N	1.90	0.87
1:B:459:ALA:O	1:B:463:ILE:HG12	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLY:HA3	1:B:441:ARG:HD3	0.90	0.86
1:D:459:ALA:O	1:D:463:ILE:HG12	1.75	0.86
1:C:439:TYR:HB3	1:D:220:PHE:CZ	2.10	0.86
1:A:497:ARG:HH21	1:B:220:PHE:HA	1.37	0.86
1:C:21:ALA:HB3	1:C:22:PRO:HD3	1.57	0.86
1:A:242:MET:HE1	1:B:91:TRP:HA	1.57	0.86
1:C:505:ASP:HA	1:C:535:ILE:HG23	1.57	0.86
1:A:238:ARG:NH2	1:B:98:MET:HB3	1.90	0.86
1:C:11:GLN:HG2	1:C:12:THR:N	1.90	0.85
1:D:505:ASP:HA	1:D:535:ILE:HG23	1.57	0.85
1:A:459:ALA:O	1:A:463:ILE:HG12	1.74	0.85
1:B:426:VAL:HG11	1:B:490:ALA:HB2	1.59	0.85
1:A:433:VAL:HG11	1:A:463:ILE:HD12	1.59	0.85
1:D:433:VAL:HG11	1:D:463:ILE:HD12	1.58	0.85
1:A:470:LEU:HD12	1:A:470:LEU:N	1.91	0.85
1:C:433:VAL:HG11	1:C:463:ILE:HD12	1.59	0.85
1:C:292:ILE:HD12	1:D:48:LEU:HD12	1.59	0.85
1:B:433:VAL:HG11	1:B:463:ILE:HD12	1.57	0.85
1:C:292:ILE:HD12	1:D:48:LEU:CD1	2.07	0.84
1:D:436:ASN:ND2	1:D:474:ILE:HG21	1.91	0.84
1:A:436:ASN:ND2	1:A:474:ILE:HG21	1.92	0.84
1:B:505:ASP:HA	1:B:535:ILE:HG23	1.57	0.84
1:D:113:VAL:HG22	1:D:114:ALA:H	1.42	0.84
1:D:174:LEU:HD22	1:D:262:ALA:HB2	1.59	0.84
1:A:505:ASP:HA	1:A:535:ILE:HG23	1.59	0.84
1:D:21:ALA:HB3	1:D:22:PRO:HD3	1.57	0.84
1:B:67:MET:O	1:B:70:VAL:HG12	1.78	0.84
1:C:436:ASN:ND2	1:C:474:ILE:HG21	1.91	0.84
1:B:436:ASN:ND2	1:B:474:ILE:HG21	1.91	0.84
1:A:67:MET:O	1:A:70:VAL:HG12	1.78	0.84
1:B:113:VAL:HG22	1:B:114:ALA:H	1.42	0.84
1:C:113:VAL:HG22	1:C:114:ALA:H	1.42	0.84
1:C:119:GLN:HE21	1:C:119:GLN:H	1.26	0.84
1:A:316:GLN:OE1	1:A:319:PHE:HD1	1.61	0.83
1:D:470:LEU:HD12	1:D:470:LEU:H	1.42	0.83
1:C:426:VAL:HG11	1:C:490:ALA:HB2	1.59	0.83
1:C:470:LEU:H	1:C:470:LEU:HD12	1.42	0.83
1:C:211:LEU:HD12	1:D:116:PHE:HE1	1.42	0.83
1:D:67:MET:O	1:D:70:VAL:HG12	1.78	0.83
1:B:174:LEU:HD22	1:B:262:ALA:HB2	1.60	0.83
1:C:67:MET:O	1:C:70:VAL:HG12	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ILE:HG12	1:A:396:ASP:N	1.94	0.83
1:A:238:ARG:CZ	1:B:98:MET:HB3	2.08	0.83
1:B:11:GLN:HG2	1:B:12:THR:N	1.90	0.83
1:B:470:LEU:H	1:B:470:LEU:HD12	1.42	0.83
1:D:119:GLN:HE21	1:D:119:GLN:H	1.26	0.83
1:A:113:VAL:HG22	1:A:114:ALA:H	1.44	0.83
1:D:426:VAL:HG11	1:D:490:ALA:HB2	1.59	0.83
1:A:470:LEU:H	1:A:470:LEU:CD1	1.92	0.83
1:C:512:ASP:HB2	1:D:378:SER:H	1.43	0.83
1:B:20:ILE:HD13	1:B:96:VAL:HG21	1.61	0.83
1:D:284:ILE:O	1:D:284:ILE:HD13	1.79	0.82
1:A:242:MET:CE	1:B:91:TRP:HA	2.09	0.82
1:A:426:VAL:HG11	1:A:490:ALA:HB2	1.62	0.82
1:A:174:LEU:HD22	1:A:262:ALA:HB2	1.60	0.82
1:A:284:ILE:O	1:A:284:ILE:HD13	1.80	0.82
1:C:284:ILE:O	1:C:284:ILE:HD13	1.80	0.82
1:B:284:ILE:O	1:B:284:ILE:HD13	1.79	0.82
1:C:174:LEU:HD22	1:C:262:ALA:HB2	1.59	0.82
1:A:56:PHE:HA	1:A:59:THR:HG23	1.62	0.81
1:C:220:PHE:HA	1:D:497:ARG:NH2	1.93	0.81
1:A:438:ALA:C	1:A:440:ALA:H	1.87	0.81
1:A:512:ASP:OD1	1:B:377:ARG:HA	1.81	0.81
1:B:438:ALA:C	1:B:440:ALA:H	1.88	0.81
1:D:151:ALA:HA	1:D:154:ILE:HD12	1.62	0.81
1:B:345:ARG:HD2	1:B:345:ARG:N	1.96	0.81
1:C:220:PHE:CZ	1:D:429:PHE:HE1	1.99	0.81
1:C:378:SER:H	1:D:512:ASP:HB2	1.45	0.81
1:A:151:ALA:HA	1:A:154:ILE:HD12	1.61	0.81
1:A:221:GLY:CA	1:B:441:ARG:CD	2.42	0.81
1:B:119:GLN:HE21	1:B:119:GLN:H	1.26	0.81
1:D:20:ILE:HD13	1:D:96:VAL:HG21	1.61	0.81
1:D:345:ARG:N	1:D:345:ARG:HD2	1.96	0.81
1:D:412:LEU:HD21	1:D:416:ARG:NH1	1.96	0.81
1:C:20:ILE:HD13	1:C:96:VAL:HG21	1.61	0.81
1:C:441:ARG:NE	1:D:221:GLY:HA3	1.96	0.81
1:D:10:TRP:CA	1:D:14:ARG:HB2	2.11	0.81
1:A:344:PHE:HD1	1:A:400:ILE:HG12	1.44	0.80
1:C:220:PHE:CZ	1:D:439:TYR:HB3	2.15	0.80
1:D:344:PHE:HD1	1:D:400:ILE:HG12	1.47	0.80
1:B:412:LEU:HD21	1:B:416:ARG:NH1	1.97	0.80
1:C:221:GLY:HA3	1:D:441:ARG:NE	1.97	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:LYS:HZ3	1:D:58:LYS:HA	1.47	0.80
1:A:441:ARG:HD3	1:B:220:PHE:O	1.81	0.80
1:B:395:ILE:HG12	1:B:396:ASP:N	1.96	0.80
1:A:119:GLN:HE21	1:A:119:GLN:H	1.27	0.80
1:A:412:LEU:HD21	1:A:416:ARG:NH1	1.97	0.80
1:A:497:ARG:NH2	1:B:220:PHE:HA	1.96	0.80
1:C:426:VAL:HG11	1:C:490:ALA:CB	2.12	0.80
1:A:156:LEU:HB2	1:A:294:LEU:HD13	1.64	0.80
1:B:151:ALA:HA	1:B:154:ILE:HD12	1.62	0.80
1:C:220:PHE:O	1:D:441:ARG:HD3	1.81	0.80
1:C:349:PHE:HA	1:C:396:ASP:HB2	1.63	0.80
1:A:210:MET:HG3	1:A:211:LEU:HD13	1.62	0.80
1:A:345:ARG:N	1:A:345:ARG:HD2	1.97	0.80
1:B:382:LYS:HB2	2:B:5002:ANP:O1B	1.82	0.80
1:D:210:MET:HG3	1:D:211:LEU:HD13	1.64	0.80
1:D:351:TYR:CB	1:D:352:PRO:HD3	2.12	0.80
1:B:460:MET:HE2	1:B:460:MET:HA	1.63	0.79
1:C:10:TRP:CA	1:C:14:ARG:HB2	2.11	0.79
1:B:344:PHE:HD1	1:B:400:ILE:HG12	1.46	0.79
1:C:412:LEU:HD21	1:C:416:ARG:NH1	1.96	0.79
1:D:395:ILE:HG12	1:D:396:ASP:N	1.96	0.79
1:D:470:LEU:HD12	1:D:470:LEU:N	1.97	0.79
1:A:112:PRO:O	1:A:113:VAL:HG12	1.82	0.79
1:C:344:PHE:HD1	1:C:400:ILE:HG12	1.47	0.79
1:C:438:ALA:C	1:C:440:ALA:H	1.88	0.79
1:B:351:TYR:CB	1:B:352:PRO:HD3	2.12	0.79
1:C:345:ARG:N	1:C:345:ARG:HD2	1.96	0.79
1:B:349:PHE:HA	1:B:396:ASP:HB2	1.63	0.79
1:A:350:THR:HG22	1:A:396:ASP:OD2	1.83	0.79
1:A:460:MET:HE2	1:A:460:MET:HA	1.63	0.79
1:D:56:PHE:HA	1:D:59:THR:HG23	1.63	0.79
1:D:349:PHE:HA	1:D:396:ASP:HB2	1.63	0.79
1:D:438:ALA:C	1:D:440:ALA:H	1.88	0.79
1:B:16:LEU:HD12	1:B:315:CYS:SG	2.23	0.79
1:B:426:VAL:HG11	1:B:490:ALA:CB	2.12	0.79
1:C:151:ALA:HA	1:C:154:ILE:HD12	1.62	0.79
1:C:349:PHE:HA	1:C:396:ASP:CB	2.13	0.79
1:C:429:PHE:HE1	1:D:220:PHE:CZ	2.01	0.79
1:C:210:MET:HG3	1:C:211:LEU:HD13	1.64	0.79
1:D:349:PHE:HA	1:D:396:ASP:CB	2.13	0.79
1:D:426:VAL:HG11	1:D:490:ALA:CB	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LEU:HB2	1:B:294:LEU:HD13	1.65	0.79
1:C:351:TYR:CB	1:C:352:PRO:HD3	2.12	0.79
1:D:460:MET:HE2	1:D:460:MET:HA	1.63	0.79
1:C:460:MET:HA	1:C:460:MET:HE2	1.63	0.79
1:B:10:TRP:CA	1:B:14:ARG:HB2	2.11	0.78
1:B:478:GLY:O	1:B:486:ARG:HD2	1.83	0.78
1:C:91:TRP:HA	1:D:242:MET:HE1	1.64	0.78
1:D:348:THR:O	1:D:396:ASP:HB3	1.84	0.78
1:A:349:PHE:HA	1:A:396:ASP:CB	2.13	0.78
1:C:16:LEU:HD12	1:C:315:CYS:SG	2.23	0.78
1:D:16:LEU:HD12	1:D:315:CYS:SG	2.23	0.78
1:D:93:SER:HB3	1:D:140:SER:HB3	1.65	0.78
1:B:56:PHE:HA	1:B:59:THR:HG23	1.63	0.78
1:B:348:THR:O	1:B:396:ASP:HB3	1.83	0.78
1:C:56:PHE:HA	1:C:59:THR:HG23	1.63	0.78
1:C:93:SER:HB3	1:C:140:SER:HB3	1.65	0.78
1:C:395:ILE:HG12	1:C:396:ASP:N	1.96	0.78
1:A:154:ILE:HA	1:A:157:PHE:CE2	2.18	0.78
1:A:377:ARG:HA	1:B:512:ASP:OD1	1.83	0.78
1:C:48:LEU:CD1	1:D:292:ILE:HD12	2.14	0.78
1:C:470:LEU:HD12	1:C:470:LEU:N	1.97	0.78
1:C:478:GLY:O	1:C:486:ARG:HD2	1.84	0.78
1:A:349:PHE:HA	1:A:396:ASP:HB2	1.63	0.78
1:D:154:ILE:HA	1:D:157:PHE:CE2	2.19	0.78
1:A:426:VAL:HG11	1:A:490:ALA:CB	2.14	0.78
1:B:349:PHE:HA	1:B:396:ASP:CB	2.13	0.78
1:C:242:MET:CE	1:D:91:TRP:HA	2.13	0.78
1:C:350:THR:HG22	1:C:396:ASP:OD2	1.84	0.78
1:B:112:PRO:O	1:B:113:VAL:HG12	1.84	0.77
1:C:100:MET:HA	1:C:100:MET:HE3	1.66	0.77
1:D:156:LEU:HB2	1:D:294:LEU:HD13	1.65	0.77
1:B:470:LEU:HD12	1:B:470:LEU:N	1.97	0.77
1:D:112:PRO:O	1:D:113:VAL:HG12	1.84	0.77
1:D:478:GLY:O	1:D:486:ARG:HD2	1.84	0.77
1:C:112:PRO:O	1:C:113:VAL:HG12	1.84	0.77
1:A:93:SER:HB3	1:A:140:SER:HB3	1.65	0.77
1:B:100:MET:HA	1:B:100:MET:HE3	1.66	0.77
1:A:439:TYR:HB3	1:B:220:PHE:CZ	2.20	0.77
1:C:156:LEU:HB2	1:C:294:LEU:HD13	1.65	0.77
1:D:100:MET:HA	1:D:100:MET:HE3	1.66	0.77
1:A:220:PHE:CE1	1:B:439:TYR:HB3	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:CYS:SG	1:A:316:GLN:NE2	2.57	0.77
1:C:154:ILE:HA	1:C:157:PHE:CE2	2.19	0.77
1:C:348:THR:O	1:C:396:ASP:HB3	1.83	0.77
1:A:316:GLN:OE1	1:A:319:PHE:CD1	2.37	0.77
1:B:93:SER:HB3	1:B:140:SER:HB3	1.65	0.77
1:B:210:MET:HG3	1:B:211:LEU:HD13	1.64	0.77
1:A:348:THR:O	1:A:396:ASP:HB3	1.84	0.77
1:B:350:THR:HG22	1:B:396:ASP:OD2	1.84	0.77
1:A:476:GLU:O	1:A:479:VAL:HG23	1.85	0.77
1:A:20:ILE:CD1	1:A:96:VAL:HG21	2.15	0.76
1:A:100:MET:HA	1:A:100:MET:HE3	1.66	0.76
1:A:478:GLY:O	1:A:486:ARG:HD2	1.84	0.76
1:C:441:ARG:CZ	1:D:221:GLY:O	2.33	0.76
1:D:26:GLY:HA2	1:D:88:CYS:SG	2.25	0.76
1:A:401:LEU:HD23	1:A:401:LEU:N	2.00	0.76
1:B:26:GLY:HA2	1:B:88:CYS:SG	2.25	0.76
1:C:68:PRO:O	1:C:72:ILE:HD13	1.86	0.76
1:D:350:THR:HG22	1:D:396:ASP:OD2	1.84	0.76
1:D:119:GLN:H	1:D:119:GLN:NE2	1.84	0.76
1:B:119:GLN:H	1:B:119:GLN:NE2	1.84	0.76
1:B:535:ILE:O	1:B:535:ILE:HD13	1.86	0.76
1:D:476:GLU:O	1:D:479:VAL:HG23	1.86	0.76
1:A:256:GLN:HA	1:A:299:LYS:HD3	1.68	0.76
1:A:351:TYR:CB	1:A:352:PRO:HD3	2.14	0.76
1:B:58:LYS:HB3	1:B:62:SER:HB3	1.68	0.76
1:C:535:ILE:O	1:C:535:ILE:HD13	1.86	0.76
1:C:316:GLN:OE1	1:C:319:PHE:HD1	1.69	0.76
1:B:68:PRO:O	1:B:72:ILE:HD13	1.86	0.75
1:C:470:LEU:H	1:C:470:LEU:CD1	1.98	0.75
1:C:58:LYS:HB3	1:C:62:SER:HB3	1.68	0.75
1:D:68:PRO:O	1:D:72:ILE:HD13	1.86	0.75
1:B:154:ILE:HA	1:B:157:PHE:CE2	2.19	0.75
1:C:26:GLY:HA2	1:C:88:CYS:SG	2.25	0.75
1:C:218:LEU:HD23	1:D:416:ARG:NH1	2.02	0.75
1:C:238:ARG:NH2	1:D:98:MET:HB3	2.01	0.75
1:A:58:LYS:HB3	1:A:62:SER:HB3	1.68	0.75
1:A:63:VAL:HG12	1:B:271:SER:HB2	1.66	0.75
1:C:48:LEU:HD12	1:D:292:ILE:HD12	1.67	0.75
1:C:281:ALA:CB	1:D:56:PHE:HB3	2.13	0.75
1:B:252:ASP:HB2	1:B:253:PRO:HD3	1.69	0.75
1:A:83:TYR:O	1:A:87:TYR:HB3	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:PHE:O	1:B:441:ARG:HD3	1.87	0.75
1:C:476:GLU:O	1:C:479:VAL:HG23	1.86	0.75
1:B:58:LYS:HZ3	1:B:58:LYS:HA	1.50	0.75
1:B:470:LEU:H	1:B:470:LEU:CD1	1.98	0.75
1:C:67:MET:HB3	1:C:68:PRO:HD3	1.69	0.75
1:D:58:LYS:HB3	1:D:62:SER:HB3	1.68	0.75
1:D:470:LEU:H	1:D:470:LEU:CD1	1.98	0.75
1:B:476:GLU:O	1:B:479:VAL:HG23	1.86	0.75
1:C:119:GLN:H	1:C:119:GLN:NE2	1.84	0.75
1:D:252:ASP:HB2	1:D:253:PRO:HD3	1.69	0.75
1:C:441:ARG:HH11	1:C:441:ARG:HA	1.52	0.74
1:D:316:GLN:OE1	1:D:319:PHE:HD1	1.69	0.74
1:B:134:GLN:HE22	1:B:310:ARG:HE	1.35	0.74
1:D:535:ILE:HD13	1:D:535:ILE:O	1.86	0.74
1:A:119:GLN:H	1:A:119:GLN:NE2	1.83	0.74
1:A:26:GLY:HA2	1:A:88:CYS:SG	2.27	0.74
1:B:114:ALA:HA	1:B:117:ASP:OD1	1.88	0.74
1:B:174:LEU:HD21	1:B:261:LEU:HD22	1.70	0.74
1:B:256:GLN:HA	1:B:299:LYS:HD3	1.70	0.74
1:A:16:LEU:HD12	1:A:315:CYS:SG	2.26	0.74
1:A:114:ALA:HA	1:A:117:ASP:OD1	1.87	0.74
1:A:213:GLY:O	1:A:217:VAL:HG23	1.88	0.74
1:B:67:MET:HB3	1:B:68:PRO:HD3	1.69	0.74
1:C:83:TYR:O	1:C:87:TYR:HB3	1.88	0.74
1:C:114:ALA:HA	1:C:117:ASP:OD1	1.88	0.74
1:B:20:ILE:CD1	1:B:96:VAL:HG21	2.17	0.74
1:B:316:GLN:OE1	1:B:319:PHE:HD1	1.69	0.74
1:B:390:THR:HG22	1:B:419:VAL:HG11	1.70	0.74
1:C:20:ILE:CD1	1:C:96:VAL:HG21	2.17	0.74
1:C:252:ASP:HB2	1:C:253:PRO:HD3	1.69	0.74
1:D:114:ALA:HA	1:D:117:ASP:OD1	1.88	0.74
1:D:134:GLN:HE22	1:D:310:ARG:HE	1.35	0.74
1:A:390:THR:HG22	1:A:419:VAL:HG11	1.70	0.73
1:A:441:ARG:NE	1:B:221:GLY:HA3	2.03	0.73
1:C:97:VAL:HB	1:C:136:ALA:HB2	1.69	0.73
1:C:221:GLY:O	1:D:441:ARG:CZ	2.37	0.73
1:D:20:ILE:CD1	1:D:96:VAL:HG21	2.17	0.73
1:B:83:TYR:O	1:B:87:TYR:HB3	1.88	0.73
1:C:441:ARG:HD3	1:D:220:PHE:O	1.87	0.73
1:B:97:VAL:HB	1:B:136:ALA:HB2	1.69	0.73
1:B:380:SER:OG	1:B:551:VAL:HG22	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:VAL:HB	1:D:136:ALA:HB2	1.69	0.73
1:D:83:TYR:O	1:D:87:TYR:HB3	1.88	0.73
1:D:401:LEU:HD23	1:D:401:LEU:N	2.04	0.73
1:A:271:SER:HB2	1:B:63:VAL:HG12	1.70	0.73
1:A:344:PHE:CD1	1:A:400:ILE:HG12	2.22	0.73
1:C:11:GLN:N	1:C:14:ARG:CB	2.52	0.73
1:C:134:GLN:HE22	1:C:310:ARG:HE	1.35	0.73
1:D:256:GLN:HA	1:D:299:LYS:HD3	1.70	0.73
1:D:390:THR:HG22	1:D:419:VAL:HG11	1.70	0.73
1:B:441:ARG:HH11	1:B:441:ARG:HA	1.52	0.73
1:A:134:GLN:HE22	1:A:310:ARG:HE	1.34	0.73
1:B:401:LEU:N	1:B:401:LEU:HD23	2.04	0.73
1:A:380:SER:OG	1:A:551:VAL:HG22	1.89	0.72
1:A:447:ARG:HD2	1:A:450:ILE:HD11	1.71	0.72
1:C:401:LEU:N	1:C:401:LEU:HD23	2.04	0.72
1:D:67:MET:HB3	1:D:68:PRO:HD3	1.69	0.72
1:A:401:LEU:HD23	1:A:401:LEU:H	1.55	0.72
1:B:213:GLY:O	1:B:217:VAL:HG23	1.89	0.72
1:C:447:ARG:HD2	1:C:450:ILE:HD11	1.71	0.72
1:D:174:LEU:HD21	1:D:261:LEU:HD22	1.70	0.72
1:B:113:VAL:HG13	1:B:114:ALA:N	2.04	0.72
1:C:213:GLY:O	1:C:217:VAL:HG23	1.89	0.72
1:C:380:SER:OG	1:C:551:VAL:HG22	1.89	0.72
1:C:416:ARG:CZ	1:D:218:LEU:HD23	2.20	0.72
1:B:11:GLN:CG	1:B:12:THR:H	1.96	0.72
1:C:390:THR:HG22	1:C:419:VAL:HG11	1.70	0.72
1:D:213:GLY:O	1:D:217:VAL:HG23	1.89	0.72
1:A:97:VAL:HB	1:A:136:ALA:HB2	1.70	0.72
1:A:174:LEU:HD21	1:A:261:LEU:HD22	1.71	0.72
1:A:441:ARG:HA	1:A:441:ARG:HH11	1.54	0.72
1:A:535:ILE:O	1:A:535:ILE:HD13	1.89	0.72
1:C:416:ARG:NH1	1:D:218:LEU:HD23	2.04	0.72
1:B:447:ARG:HD2	1:B:450:ILE:HD11	1.71	0.72
1:D:11:GLN:N	1:D:14:ARG:CB	2.52	0.72
1:D:113:VAL:HG13	1:D:114:ALA:N	2.04	0.72
1:D:566:LEU:HD21	1:D:576:HIS:CD2	2.25	0.72
1:C:256:GLN:HA	1:C:299:LYS:HD3	1.70	0.71
1:D:380:SER:OG	1:D:551:VAL:HG22	1.89	0.71
1:D:441:ARG:HA	1:D:441:ARG:HH11	1.53	0.71
1:C:174:LEU:HD21	1:C:261:LEU:HD22	1.70	0.71
1:A:113:VAL:HG13	1:A:114:ALA:N	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:PHE:CD1	1:C:400:ILE:HG12	2.25	0.71
1:A:98:MET:SD	1:A:101:ARG:HD3	2.30	0.71
1:C:116:PHE:CE1	1:D:211:LEU:HD12	2.25	0.71
1:A:178:VAL:HA	1:A:258:ILE:HD13	1.71	0.71
1:A:566:LEU:HD21	1:A:576:HIS:CD2	2.26	0.71
1:B:103:ARG:HG2	1:B:322:LEU:HD11	1.73	0.71
1:B:344:PHE:CD1	1:B:400:ILE:HG12	2.25	0.71
1:C:103:ARG:HG2	1:C:322:LEU:HD11	1.73	0.71
1:D:447:ARG:HD2	1:D:450:ILE:HD11	1.71	0.71
1:A:103:ARG:HG2	1:A:322:LEU:HD11	1.73	0.71
1:A:221:GLY:O	1:B:441:ARG:NH1	2.24	0.71
1:B:11:GLN:N	1:B:14:ARG:CB	2.52	0.71
1:B:566:LEU:HD21	1:B:576:HIS:CD2	2.25	0.71
1:A:10:TRP:C	1:A:14:ARG:CB	2.63	0.70
1:A:68:PRO:O	1:A:72:ILE:HD13	1.90	0.70
1:A:74:LEU:HD13	1:B:260:SER:OG	1.90	0.70
1:A:252:ASP:HB2	1:A:253:PRO:HD3	1.71	0.70
1:A:382:LYS:HB2	2:A:5001:ANP:O1B	1.91	0.70
1:C:44:MET:O	1:C:48:LEU:HD23	1.91	0.70
1:C:354:ARG:O	1:C:355:GLU:HG3	1.91	0.70
1:A:212:LYS:HE3	1:B:212:LYS:HE3	1.74	0.70
1:B:354:ARG:O	1:B:355:GLU:HG3	1.91	0.70
1:D:44:MET:O	1:D:48:LEU:HD23	1.91	0.70
1:D:103:ARG:HG2	1:D:322:LEU:HD11	1.73	0.70
1:D:344:PHE:CD1	1:D:400:ILE:HG12	2.25	0.70
1:D:354:ARG:O	1:D:355:GLU:HG3	1.91	0.70
1:A:67:MET:HB3	1:A:68:PRO:HD3	1.73	0.70
1:A:381:GLY:O	1:A:385:ILE:HG22	1.91	0.70
1:A:385:ILE:O	1:A:389:ILE:HD12	1.91	0.70
1:B:351:TYR:HB3	1:B:352:PRO:CD	2.20	0.70
1:D:343:GLU:HG2	1:D:365:LYS:HG3	1.72	0.70
1:A:337:ARG:HD2	1:A:338:ALA:H	1.56	0.70
1:D:455:ARG:HD2	1:D:456:MET:HE2	1.74	0.70
1:A:89:ILE:HD12	1:A:144:ILE:HG21	1.73	0.70
1:C:113:VAL:HG13	1:C:114:ALA:N	2.04	0.70
1:C:343:GLU:HG2	1:C:365:LYS:HG3	1.72	0.70
1:A:391:ARG:O	1:A:393:TYR:N	2.24	0.70
1:A:446:SER:HB2	1:A:449:GLN:OE1	1.91	0.70
1:C:455:ARG:HD2	1:C:456:MET:HE2	1.74	0.70
1:C:566:LEU:HD21	1:C:576:HIS:CD2	2.25	0.70
1:A:455:ARG:HD2	1:A:456:MET:HE2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:MET:SD	1:B:101:ARG:HD3	2.32	0.70
1:B:343:GLU:HG2	1:B:365:LYS:HG3	1.72	0.70
1:C:446:SER:HB2	1:C:449:GLN:OE1	1.92	0.70
1:A:108:MET:HE1	1:A:124:LEU:HB3	1.73	0.70
1:A:445:TYR:CD2	1:A:496:LEU:HD11	2.26	0.70
1:D:446:SER:HB2	1:D:449:GLN:OE1	1.92	0.70
1:A:221:GLY:O	1:B:441:ARG:CZ	2.40	0.70
1:A:223:GLN:OE1	1:A:223:GLN:N	2.21	0.70
1:A:440:ALA:HB1	1:A:497:ARG:HG3	1.72	0.70
1:B:455:ARG:HD2	1:B:456:MET:HE2	1.74	0.70
1:C:58:LYS:HA	1:C:58:LYS:HZ3	1.57	0.70
1:D:98:MET:SD	1:D:101:ARG:HD3	2.32	0.70
1:B:446:SER:HB2	1:B:449:GLN:OE1	1.92	0.69
1:C:14:ARG:O	1:C:18:PRO:HD3	1.93	0.69
1:D:455:ARG:C	1:D:457:ALA:H	2.00	0.69
1:A:343:GLU:HG2	1:A:365:LYS:HG3	1.73	0.69
1:B:44:MET:O	1:B:48:LEU:HD23	1.91	0.69
1:C:188:ARG:O	1:C:192:ILE:HG12	1.93	0.69
1:C:337:ARG:HD2	1:C:338:ALA:H	1.57	0.69
1:D:316:GLN:OE1	1:D:319:PHE:CD1	2.46	0.69
1:B:188:ARG:O	1:B:192:ILE:HG12	1.93	0.69
1:C:91:TRP:HA	1:D:242:MET:CE	2.22	0.69
1:C:98:MET:SD	1:C:101:ARG:HD3	2.32	0.69
1:D:440:ALA:HB1	1:D:497:ARG:HG3	1.74	0.69
1:B:14:ARG:O	1:B:18:PRO:HD3	1.93	0.69
1:C:391:ARG:O	1:C:393:TYR:N	2.26	0.69
1:D:178:VAL:HA	1:D:258:ILE:HD13	1.75	0.69
1:A:89:ILE:O	1:A:92:VAL:HG12	1.93	0.69
1:C:108:MET:HE1	1:C:124:LEU:HB3	1.73	0.69
1:C:178:VAL:HA	1:C:258:ILE:HD13	1.75	0.69
1:C:210:MET:SD	1:D:109:MET:HB3	2.32	0.69
1:B:97:VAL:HG13	1:B:98:MET:H	1.58	0.69
1:B:337:ARG:HD2	1:B:338:ALA:H	1.57	0.69
1:C:98:MET:HB3	1:D:238:ARG:NH2	2.08	0.69
1:C:455:ARG:C	1:C:457:ALA:H	2.00	0.69
1:D:97:VAL:HG13	1:D:98:MET:H	1.58	0.69
1:D:188:ARG:O	1:D:192:ILE:HG12	1.93	0.69
1:D:401:LEU:HD23	1:D:401:LEU:H	1.58	0.69
1:B:108:MET:HE1	1:B:124:LEU:HB3	1.73	0.69
1:B:391:ARG:O	1:B:393:TYR:N	2.26	0.69
1:A:218:LEU:HD23	1:B:416:ARG:NH1	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:TYR:HB3	1:A:352:PRO:CD	2.21	0.69
1:A:48:LEU:HD12	1:B:292:ILE:HD12	1.76	0.68
1:A:110:GLY:C	1:A:112:PRO:HD3	2.18	0.68
1:A:354:ARG:O	1:A:355:GLU:HG3	1.92	0.68
1:B:315:CYS:SG	1:B:316:GLN:NE2	2.66	0.68
1:B:316:GLN:OE1	1:B:319:PHE:CD1	2.46	0.68
1:B:401:LEU:HD23	1:B:401:LEU:H	1.58	0.68
1:B:505:ASP:HA	1:B:535:ILE:CG2	2.23	0.68
1:D:108:MET:HE1	1:D:124:LEU:HB3	1.73	0.68
1:D:315:CYS:SG	1:D:316:GLN:NE2	2.66	0.68
1:A:256:GLN:HG2	1:A:299:LYS:CE	2.23	0.68
1:C:385:ILE:O	1:C:389:ILE:HD12	1.94	0.68
1:D:385:ILE:O	1:D:389:ILE:HD12	1.93	0.68
1:A:10:TRP:C	1:A:14:ARG:HB3	2.18	0.68
1:A:188:ARG:O	1:A:192:ILE:HG12	1.93	0.68
1:B:385:ILE:O	1:B:389:ILE:HD12	1.94	0.68
1:B:455:ARG:C	1:B:457:ALA:H	2.00	0.68
1:C:316:GLN:OE1	1:C:319:PHE:CD1	2.46	0.68
1:D:351:TYR:HB3	1:D:352:PRO:CD	2.20	0.68
1:A:366:ILE:HG12	1:A:372:VAL:HG21	1.75	0.68
1:B:110:GLY:C	1:B:112:PRO:HD3	2.19	0.68
1:B:433:VAL:HB	1:B:470:LEU:HA	1.76	0.68
1:B:467:ASP:O	1:B:468:ASN:HB2	1.94	0.68
1:C:218:LEU:HD23	1:D:416:ARG:CZ	2.23	0.68
1:C:433:VAL:HB	1:C:470:LEU:HA	1.76	0.68
1:D:391:ARG:O	1:D:393:TYR:N	2.26	0.68
1:D:433:VAL:HB	1:D:470:LEU:HA	1.76	0.68
1:A:119:GLN:HE21	1:A:119:GLN:N	1.90	0.68
1:A:316:GLN:HA	1:A:319:PHE:HB2	1.76	0.68
1:B:366:ILE:HG12	1:B:372:VAL:HG21	1.75	0.68
1:C:441:ARG:NH1	1:D:221:GLY:O	2.26	0.68
1:D:381:GLY:O	1:D:385:ILE:HG22	1.94	0.68
1:A:44:MET:O	1:A:48:LEU:HD23	1.93	0.68
1:C:467:ASP:O	1:C:468:ASN:HB2	1.93	0.68
1:D:14:ARG:O	1:D:18:PRO:HD3	1.93	0.68
1:A:220:PHE:CZ	1:B:429:PHE:CE1	2.76	0.68
1:C:110:GLY:C	1:C:112:PRO:HD3	2.19	0.68
1:C:315:CYS:SG	1:C:316:GLN:NE2	2.66	0.68
1:B:381:GLY:O	1:B:385:ILE:HG22	1.94	0.68
1:D:11:GLN:O	1:D:14:ARG:HB3	1.94	0.68
1:D:119:GLN:HE21	1:D:119:GLN:N	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:SER:HB2	2:D:5004:ANP:O1A	1.94	0.68
1:A:435:ASN:HA	1:A:438:ALA:HB3	1.76	0.68
1:B:89:ILE:O	1:B:92:VAL:HG12	1.94	0.68
1:B:316:GLN:HA	1:B:319:PHE:HB2	1.75	0.68
1:B:440:ALA:HB1	1:B:497:ARG:HG3	1.74	0.68
1:C:344:PHE:CB	1:C:400:ILE:HA	2.24	0.68
1:A:433:VAL:HB	1:A:470:LEU:HA	1.76	0.68
1:C:440:ALA:HB1	1:C:497:ARG:HG3	1.74	0.68
1:D:344:PHE:CB	1:D:400:ILE:HA	2.24	0.68
1:A:11:GLN:CG	1:A:12:THR:H	1.92	0.67
1:A:505:ASP:HA	1:A:535:ILE:CG2	2.24	0.67
1:C:67:MET:HA	1:D:267:LEU:HD22	1.76	0.67
1:C:89:ILE:HD12	1:C:144:ILE:HG21	1.77	0.67
1:C:159:MET:O	1:C:163:TYR:HB3	1.94	0.67
1:C:366:ILE:HG12	1:C:372:VAL:HG21	1.75	0.67
1:A:83:TYR:HA	1:B:249:SER:OG	1.94	0.67
1:A:159:MET:O	1:A:163:TYR:HB3	1.94	0.67
1:B:178:VAL:HA	1:B:258:ILE:HD13	1.75	0.67
1:D:159:MET:O	1:D:163:TYR:HB3	1.94	0.67
1:D:316:GLN:HA	1:D:319:PHE:HB2	1.75	0.67
1:B:119:GLN:HE21	1:B:119:GLN:N	1.92	0.67
1:B:344:PHE:CB	1:B:400:ILE:HA	2.24	0.67
1:C:11:GLN:O	1:C:14:ARG:HB3	1.94	0.67
1:C:449:GLN:HB3	1:C:496:LEU:HD13	1.76	0.67
1:D:110:GLY:C	1:D:112:PRO:HD3	2.19	0.67
1:D:337:ARG:HD2	1:D:338:ALA:H	1.57	0.67
1:A:11:GLN:O	1:A:14:ARG:HB3	1.93	0.67
1:B:326:GLN:C	1:B:328:LYS:H	2.03	0.67
1:D:89:ILE:O	1:D:92:VAL:HG12	1.94	0.67
1:D:89:ILE:HD12	1:D:144:ILE:HG21	1.77	0.67
1:B:89:ILE:HD12	1:B:144:ILE:HG21	1.77	0.67
1:C:441:ARG:CD	1:D:221:GLY:CA	2.53	0.67
1:A:256:GLN:HG2	1:A:299:LYS:HE2	1.74	0.67
1:C:89:ILE:O	1:C:92:VAL:HG12	1.94	0.67
1:C:97:VAL:HG13	1:C:98:MET:H	1.58	0.67
1:C:401:LEU:HD23	1:C:401:LEU:H	1.58	0.67
1:D:505:ASP:HA	1:D:535:ILE:CG2	2.23	0.67
1:B:159:MET:O	1:B:163:TYR:HB3	1.94	0.67
1:B:165:TRP:O	1:B:169:ILE:HG13	1.95	0.67
1:C:165:TRP:O	1:C:169:ILE:HG13	1.95	0.67
1:C:221:GLY:CA	1:D:441:ARG:CD	2.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:505:ASP:HA	1:C:535:ILE:CG2	2.23	0.67
1:D:445:TYR:CD2	1:D:496:LEU:HD11	2.30	0.67
1:C:256:GLN:HG2	1:C:299:LYS:CE	2.25	0.67
1:D:366:ILE:HG12	1:D:372:VAL:HG21	1.75	0.67
1:A:326:GLN:C	1:A:328:LYS:H	2.02	0.67
1:B:11:GLN:O	1:B:14:ARG:HB3	1.94	0.67
1:C:267:LEU:HD22	1:D:67:MET:HA	1.77	0.67
1:C:382:LYS:HB2	2:C:5003:ANP:O1B	1.95	0.67
1:A:344:PHE:CB	1:A:400:ILE:HA	2.25	0.66
1:B:445:TYR:CD2	1:B:496:LEU:HD11	2.30	0.66
1:D:467:ASP:O	1:D:468:ASN:HB2	1.94	0.66
1:A:63:VAL:CG1	1:B:271:SER:HB2	2.24	0.66
1:A:455:ARG:C	1:A:457:ALA:H	1.99	0.66
1:C:109:MET:HB3	1:D:210:MET:SD	2.35	0.66
1:C:119:GLN:HE21	1:C:119:GLN:N	1.92	0.66
1:C:381:GLY:O	1:C:385:ILE:HG22	1.94	0.66
1:A:271:SER:HB2	1:B:63:VAL:CG1	2.25	0.66
1:C:238:ARG:CZ	1:D:98:MET:HB3	2.25	0.66
1:D:216:GLU:C	1:D:220:PHE:HB2	2.20	0.66
1:D:256:GLN:HG2	1:D:299:LYS:CE	2.25	0.66
1:D:435:ASN:HA	1:D:438:ALA:HB3	1.77	0.66
1:A:74:LEU:HD22	1:A:75:MET:CE	2.25	0.66
1:B:216:GLU:C	1:B:220:PHE:HB2	2.20	0.66
1:B:256:GLN:HG2	1:B:299:LYS:CE	2.25	0.66
1:A:14:ARG:O	1:A:18:PRO:HD3	1.96	0.66
1:A:97:VAL:HG13	1:A:98:MET:H	1.59	0.66
1:A:269:ALA:O	1:A:273:PRO:HB2	1.96	0.66
1:C:56:PHE:HA	1:C:59:THR:CG2	2.26	0.66
1:C:216:GLU:C	1:C:220:PHE:HB2	2.20	0.66
1:C:316:GLN:HA	1:C:319:PHE:HB2	1.75	0.66
1:A:439:TYR:HB3	1:B:220:PHE:CE1	2.30	0.66
1:C:223:GLN:OE1	1:C:223:GLN:N	2.25	0.66
1:C:326:GLN:C	1:C:328:LYS:H	2.03	0.66
1:C:445:TYR:CD2	1:C:496:LEU:HD11	2.29	0.66
1:D:449:GLN:HB3	1:D:496:LEU:HD13	1.76	0.66
1:A:440:ALA:HB1	1:A:497:ARG:CG	2.26	0.66
1:C:56:PHE:CB	1:D:281:ALA:HB2	2.16	0.66
1:C:344:PHE:HB3	1:C:400:ILE:HA	1.78	0.66
1:D:223:GLN:OE1	1:D:223:GLN:N	2.25	0.66
1:A:109:MET:HB3	1:B:210:MET:SD	2.36	0.66
1:A:467:ASP:O	1:A:468:ASN:HB2	1.92	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:ASN:HA	1:B:438:ALA:HB3	1.77	0.66
1:D:165:TRP:O	1:D:169:ILE:HG13	1.95	0.66
1:C:207:ALA:O	1:C:211:LEU:HD22	1.95	0.66
1:D:256:GLN:HG2	1:D:299:LYS:HE2	1.78	0.66
1:A:85:SER:O	1:A:89:ILE:HG22	1.95	0.65
1:A:165:TRP:O	1:A:169:ILE:HG13	1.97	0.65
1:B:449:GLN:HB3	1:B:496:LEU:HD13	1.76	0.65
1:C:115:PHE:HB2	1:C:327:GLU:OE1	1.97	0.65
1:C:435:ASN:HA	1:C:438:ALA:HB3	1.77	0.65
1:A:322:LEU:HD23	1:A:322:LEU:O	1.96	0.65
1:B:141:GLY:O	1:B:144:ILE:HG12	1.97	0.65
1:D:56:PHE:HA	1:D:59:THR:CG2	2.26	0.65
1:A:216:GLU:C	1:A:220:PHE:HB2	2.21	0.65
1:A:416:ARG:NH1	1:B:218:LEU:HD23	2.11	0.65
1:C:256:GLN:HG2	1:C:299:LYS:HE2	1.78	0.65
1:D:207:ALA:O	1:D:211:LEU:HD22	1.95	0.65
1:B:85:SER:O	1:B:89:ILE:HG22	1.96	0.65
1:B:570:GLY:O	1:B:572:TYR:N	2.28	0.65
1:C:237:MET:HE3	1:C:237:MET:HA	1.78	0.65
1:D:141:GLY:O	1:D:144:ILE:HG12	1.97	0.65
1:D:216:GLU:O	1:D:220:PHE:HB2	1.97	0.65
1:A:449:GLN:HB3	1:A:496:LEU:HD13	1.78	0.65
1:A:512:ASP:HB2	1:B:378:SER:H	1.62	0.65
1:A:115:PHE:HB2	1:A:327:GLU:OE1	1.96	0.65
1:B:56:PHE:HA	1:B:59:THR:CG2	2.26	0.65
1:B:115:PHE:HB2	1:B:327:GLU:OE1	1.97	0.65
1:B:216:GLU:O	1:B:220:PHE:HB2	1.97	0.65
1:D:224:GLU:OE2	1:D:225:VAL:HG23	1.97	0.65
1:A:141:GLY:O	1:A:144:ILE:HG12	1.96	0.65
1:A:207:ALA:O	1:A:211:LEU:HD22	1.96	0.65
1:C:269:ALA:O	1:C:273:PRO:HB2	1.96	0.65
1:C:351:TYR:HB3	1:C:352:PRO:CD	2.20	0.65
1:D:322:LEU:HD23	1:D:322:LEU:O	1.97	0.65
1:A:29:VAL:HG11	1:A:87:TYR:HE2	1.62	0.65
1:B:207:ALA:O	1:B:211:LEU:HD22	1.95	0.65
1:B:256:GLN:HG2	1:B:299:LYS:HE2	1.78	0.65
1:C:64:LEU:HB2	1:D:271:SER:OG	1.97	0.65
1:C:216:GLU:O	1:C:220:PHE:HB2	1.97	0.65
1:B:368:ALA:HA	1:B:531:THR:OG1	1.97	0.65
1:C:141:GLY:O	1:C:144:ILE:HG12	1.97	0.65
1:D:326:GLN:C	1:D:328:LYS:H	2.03	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ALA:O	1:A:340:GLY:N	2.28	0.65
1:A:570:GLY:O	1:A:572:TYR:N	2.28	0.65
1:C:322:LEU:O	1:C:322:LEU:HD23	1.97	0.64
1:A:362:ILE:CD1	1:A:556:ILE:H	2.09	0.64
1:B:29:VAL:HG11	1:B:87:TYR:HE2	1.62	0.64
1:C:29:VAL:HG11	1:C:87:TYR:HE2	1.62	0.64
1:C:211:LEU:HD12	1:D:116:PHE:CE1	2.30	0.64
1:D:85:SER:O	1:D:89:ILE:HG22	1.96	0.64
1:D:115:PHE:HB2	1:D:327:GLU:OE1	1.97	0.64
1:A:56:PHE:HA	1:A:59:THR:CG2	2.26	0.64
1:B:269:ALA:O	1:B:273:PRO:HB2	1.96	0.64
1:C:85:SER:O	1:C:89:ILE:HG22	1.96	0.64
1:C:74:LEU:HD22	1:C:75:MET:CE	2.27	0.64
1:C:97:VAL:HG13	1:C:98:MET:N	2.12	0.64
1:C:224:GLU:OE2	1:C:225:VAL:HG23	1.97	0.64
1:D:74:LEU:HD22	1:D:75:MET:CE	2.27	0.64
1:D:368:ALA:HA	1:D:531:THR:OG1	1.97	0.64
1:A:58:LYS:HZ1	1:A:61:ARG:HD3	1.62	0.64
1:A:156:LEU:CB	1:A:294:LEU:HD13	2.27	0.64
1:A:475:GLY:N	1:A:480:LEU:CD1	2.61	0.64
1:C:138:SER:O	1:C:142:ALA:HB3	1.98	0.64
1:B:351:TYR:CB	1:B:352:PRO:CD	2.75	0.64
1:C:56:PHE:HB3	1:D:281:ALA:CB	2.17	0.64
1:C:351:TYR:CB	1:C:352:PRO:CD	2.75	0.64
1:C:570:GLY:O	1:C:572:TYR:N	2.28	0.64
1:A:185:VAL:HG11	1:A:251:SER:OG	1.97	0.64
1:B:237:MET:HA	1:B:237:MET:HE3	1.78	0.64
1:C:98:MET:HB3	1:D:238:ARG:CZ	2.28	0.64
1:C:220:PHE:CE1	1:D:439:TYR:HB3	2.32	0.64
1:D:29:VAL:HG11	1:D:87:TYR:HE2	1.62	0.64
1:D:237:MET:HA	1:D:237:MET:HE3	1.78	0.64
1:A:15:ARG:O	1:A:18:PRO:HD2	1.97	0.64
1:A:116:PHE:CE1	1:B:211:LEU:HD12	2.27	0.64
1:A:378:SER:H	1:B:512:ASP:HB2	1.63	0.64
1:B:74:LEU:HD22	1:B:75:MET:CE	2.27	0.64
1:C:221:GLY:O	1:D:441:ARG:NH1	2.30	0.64
1:D:344:PHE:HB3	1:D:400:ILE:HA	1.78	0.64
1:A:218:LEU:HD23	1:B:416:ARG:CZ	2.28	0.64
1:A:429:PHE:CE1	1:B:220:PHE:CZ	2.81	0.64
1:B:58:LYS:HZ1	1:B:61:ARG:HD3	1.62	0.64
1:B:97:VAL:HG13	1:B:98:MET:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:SER:O	1:B:142:ALA:HB3	1.98	0.64
1:B:224:GLU:OE2	1:B:225:VAL:HG23	1.97	0.64
1:B:438:ALA:O	1:B:443:GLU:HA	1.98	0.64
1:C:368:ALA:HA	1:C:531:THR:OG1	1.97	0.64
1:D:97:VAL:HG13	1:D:98:MET:N	2.12	0.64
1:D:438:ALA:C	1:D:440:ALA:N	2.56	0.64
1:A:234:SER:O	1:A:237:MET:HB3	1.98	0.63
1:C:58:LYS:HZ1	1:C:61:ARG:HD3	1.62	0.63
1:D:269:ALA:O	1:D:273:PRO:HB2	1.96	0.63
1:A:441:ARG:CZ	1:B:221:GLY:O	2.46	0.63
1:D:351:TYR:CB	1:D:352:PRO:CD	2.75	0.63
1:D:440:ALA:HB1	1:D:497:ARG:CG	2.28	0.63
1:A:505:ASP:OD2	1:A:535:ILE:HD12	1.99	0.63
1:B:322:LEU:O	1:B:322:LEU:HD23	1.97	0.63
1:C:10:TRP:C	1:C:14:ARG:HB3	2.23	0.63
1:C:439:TYR:HB3	1:D:220:PHE:CE1	2.33	0.63
1:A:236:LYS:O	1:A:240:GLN:HB2	1.99	0.63
1:A:374:LEU:HD23	1:A:533:LEU:HD21	1.80	0.63
1:B:111:MET:HA	1:B:111:MET:HE2	1.80	0.63
1:B:344:PHE:HB3	1:B:400:ILE:HA	1.78	0.63
1:D:269:ALA:C	1:D:273:PRO:HD2	2.24	0.63
1:A:380:SER:O	2:A:5001:ANP:O2A	2.17	0.63
1:B:438:ALA:C	1:B:440:ALA:N	2.56	0.63
1:C:156:LEU:CB	1:C:294:LEU:HD13	2.29	0.63
1:D:138:SER:O	1:D:142:ALA:HB3	1.98	0.63
1:A:224:GLU:OE2	1:A:225:VAL:HG23	1.98	0.63
1:B:10:TRP:C	1:B:14:ARG:HB3	2.24	0.63
1:D:111:MET:HE2	1:D:111:MET:HA	1.80	0.63
1:C:383:SER:HB2	2:C:5003:ANP:O1A	1.98	0.63
1:D:10:TRP:C	1:D:14:ARG:HB3	2.24	0.63
1:A:342:LEU:HD23	1:A:342:LEU:C	2.24	0.63
1:A:566:LEU:HD21	1:A:576:HIS:HD2	1.64	0.63
1:A:20:ILE:HD13	1:A:96:VAL:CG2	2.29	0.63
1:A:351:TYR:CB	1:A:352:PRO:CD	2.77	0.63
1:A:383:SER:OG	2:A:5001:ANP:O2B	2.10	0.63
1:A:97:VAL:HG13	1:A:98:MET:N	2.13	0.62
1:A:111:MET:HE2	1:A:111:MET:HA	1.80	0.62
1:A:344:PHE:HB3	1:A:400:ILE:HA	1.80	0.62
1:C:10:TRP:C	1:C:14:ARG:CB	2.72	0.62
1:C:67:MET:HB2	1:D:267:LEU:HB3	1.81	0.62
1:D:192:ILE:CG2	1:D:244:MET:HB2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:LYS:O	1:D:240:GLN:HB2	1.99	0.62
1:D:438:ALA:O	1:D:443:GLU:HA	1.98	0.62
1:A:10:TRP:C	1:A:14:ARG:HB2	2.22	0.62
1:A:150:GLY:O	1:A:154:ILE:HG13	1.99	0.62
1:A:211:LEU:HD12	1:B:116:PHE:CE1	2.28	0.62
1:B:338:ALA:O	1:B:340:GLY:N	2.32	0.62
1:C:269:ALA:C	1:C:273:PRO:HD2	2.24	0.62
1:B:156:LEU:CB	1:B:294:LEU:HD13	2.29	0.62
1:B:269:ALA:C	1:B:273:PRO:HD2	2.24	0.62
1:C:236:LYS:O	1:C:240:GLN:HB2	1.99	0.62
1:D:10:TRP:C	1:D:14:ARG:CB	2.72	0.62
1:A:438:ALA:C	1:A:440:ALA:N	2.55	0.62
1:D:58:LYS:HZ1	1:D:61:ARG:HD3	1.63	0.62
1:B:192:ILE:CG2	1:B:244:MET:HB2	2.29	0.62
1:C:438:ALA:O	1:C:443:GLU:HA	1.99	0.62
1:C:440:ALA:HB1	1:C:497:ARG:CG	2.28	0.62
1:D:541:THR:C	1:D:542:ILE:HD12	2.25	0.62
1:D:342:LEU:HD23	1:D:342:LEU:C	2.25	0.62
1:A:368:ALA:HA	1:A:531:THR:OG1	1.98	0.62
1:B:374:LEU:HD23	1:B:533:LEU:HD21	1.80	0.62
1:C:512:ASP:HB2	1:D:378:SER:CB	2.30	0.62
1:D:156:LEU:CB	1:D:294:LEU:HD13	2.28	0.62
1:D:338:ALA:O	1:D:340:GLY:N	2.32	0.62
1:D:570:GLY:O	1:D:572:TYR:N	2.28	0.62
1:A:63:VAL:HG11	1:B:271:SER:N	2.13	0.62
1:A:83:TYR:O	1:A:87:TYR:CB	2.48	0.62
1:A:216:GLU:O	1:A:220:PHE:HB2	2.00	0.62
1:A:237:MET:HA	1:A:237:MET:HE3	1.80	0.62
1:B:10:TRP:C	1:B:14:ARG:CB	2.72	0.62
1:B:185:VAL:HG11	1:B:251:SER:OG	2.00	0.62
1:C:271:SER:OG	1:D:64:LEU:HB2	1.99	0.62
1:A:192:ILE:CG2	1:A:244:MET:HB2	2.30	0.62
1:A:438:ALA:O	1:A:443:GLU:HA	1.99	0.62
1:C:374:LEU:HD23	1:C:533:LEU:HD21	1.80	0.62
1:D:333:ARG:NH1	1:D:333:ARG:HB3	2.15	0.62
1:B:236:LYS:O	1:B:240:GLN:HB2	1.99	0.61
1:C:249:SER:OG	1:D:83:TYR:HA	2.00	0.61
1:C:338:ALA:O	1:C:340:GLY:N	2.31	0.61
1:C:342:LEU:HD23	1:C:342:LEU:C	2.25	0.61
1:D:566:LEU:HD21	1:D:576:HIS:HD2	1.64	0.61
1:B:15:ARG:O	1:B:18:PRO:HD2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:ALA:HB1	1:B:497:ARG:CG	2.29	0.61
1:C:438:ALA:C	1:C:440:ALA:N	2.56	0.61
1:C:541:THR:C	1:C:542:ILE:HD12	2.25	0.61
1:C:566:LEU:HD21	1:C:576:HIS:HD2	1.64	0.61
1:D:374:LEU:HD23	1:D:533:LEU:HD21	1.80	0.61
1:A:383:SER:HB2	2:A:5001:ANP:O1A	2.00	0.61
1:C:111:MET:HE2	1:C:111:MET:HA	1.80	0.61
1:C:192:ILE:CG2	1:C:244:MET:HB2	2.29	0.61
1:C:267:LEU:HB3	1:D:67:MET:HB2	1.82	0.61
1:B:59:THR:HA	1:B:63:VAL:HG21	1.82	0.61
1:B:333:ARG:HB3	1:B:333:ARG:NH1	2.15	0.61
1:C:164:SER:OG	1:C:167:LEU:HD23	2.00	0.61
1:D:144:ILE:HG13	1:D:145:THR:N	2.15	0.61
1:A:213:GLY:HA2	1:B:427:HIS:HD2	1.66	0.61
1:C:185:VAL:HG11	1:C:251:SER:OG	1.99	0.61
1:A:144:ILE:HG13	1:A:145:THR:N	2.15	0.61
1:A:508:THR:HA	1:A:511:LEU:HD12	1.83	0.61
1:B:196:MET:HA	1:B:240:GLN:HG2	1.83	0.61
1:B:342:LEU:C	1:B:342:LEU:HD23	2.25	0.61
1:B:548:ILE:HB	1:B:565:LEU:HD11	1.82	0.61
1:C:150:GLY:O	1:C:154:ILE:HG13	2.01	0.61
1:A:138:SER:O	1:A:142:ALA:HB3	2.00	0.61
1:A:164:SER:OG	1:A:167:LEU:HD23	2.00	0.61
1:C:15:ARG:O	1:C:18:PRO:HD2	2.00	0.61
1:D:164:SER:OG	1:D:167:LEU:HD23	2.00	0.61
1:D:185:VAL:HG11	1:D:251:SER:OG	2.00	0.61
1:B:164:SER:OG	1:B:167:LEU:HD23	2.00	0.61
1:B:223:GLN:OE1	1:B:223:GLN:N	2.25	0.61
1:A:131:ASP:HB3	1:A:318:LEU:HD23	1.83	0.61
1:A:269:ALA:C	1:A:273:PRO:HD2	2.25	0.61
1:A:341:ASP:HB3	1:A:403:ASP:OD1	2.01	0.61
1:C:333:ARG:NH1	1:C:333:ARG:HB3	2.15	0.61
1:A:223:GLN:H	1:A:223:GLN:CD	2.08	0.60
1:A:557:VAL:O	1:A:557:VAL:HG12	2.00	0.60
1:C:212:LYS:HE3	1:D:212:LYS:HE3	1.83	0.60
1:D:15:ARG:O	1:D:18:PRO:HD2	2.00	0.60
1:D:150:GLY:O	1:D:154:ILE:HG13	2.00	0.60
1:A:333:ARG:NH1	1:A:333:ARG:HB3	2.16	0.60
1:A:416:ARG:CZ	1:B:218:LEU:HD23	2.30	0.60
1:C:508:THR:HA	1:C:511:LEU:HD12	1.83	0.60
1:B:150:GLY:O	1:B:154:ILE:HG13	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:SER:O	1:B:237:MET:HB3	2.01	0.60
1:C:196:MET:HA	1:C:240:GLN:HG2	1.83	0.60
1:D:59:THR:HA	1:D:63:VAL:HG21	1.83	0.60
1:A:114:ALA:HA	1:A:117:ASP:CG	2.25	0.60
1:A:548:ILE:HB	1:A:565:LEU:HD11	1.83	0.60
1:B:482:SER:HB3	1:B:485:GLN:HG3	1.84	0.60
1:B:505:ASP:OD2	1:B:535:ILE:HD12	2.02	0.60
1:A:196:MET:HA	1:A:240:GLN:HG2	1.84	0.60
1:B:566:LEU:HD21	1:B:576:HIS:HD2	1.64	0.60
1:D:114:ALA:HA	1:D:117:ASP:CG	2.26	0.60
1:C:144:ILE:HG13	1:C:145:THR:N	2.15	0.60
1:A:284:ILE:O	1:A:284:ILE:CD1	2.49	0.60
1:B:114:ALA:HA	1:B:117:ASP:CG	2.26	0.60
1:B:333:ARG:HB3	1:B:333:ARG:HH11	1.67	0.60
1:C:114:ALA:HA	1:C:117:ASP:CG	2.26	0.60
1:C:172:VAL:O	1:C:172:VAL:HG12	2.02	0.60
1:C:548:ILE:HB	1:C:565:LEU:HD11	1.83	0.60
1:D:196:MET:HA	1:D:240:GLN:HG2	1.83	0.60
1:D:234:SER:O	1:D:237:MET:HB3	2.01	0.60
1:B:172:VAL:O	1:B:172:VAL:HG12	2.02	0.60
1:B:475:GLY:N	1:B:480:LEU:CD1	2.65	0.60
1:B:508:THR:HA	1:B:511:LEU:HD12	1.83	0.60
1:C:61:ARG:HG3	1:C:62:SER:H	1.67	0.60
1:D:172:VAL:HG12	1:D:172:VAL:O	2.02	0.60
1:A:172:VAL:O	1:A:172:VAL:HG12	2.01	0.60
1:A:558:GLU:HG3	1:A:565:LEU:HD23	1.84	0.60
1:C:475:GLY:N	1:C:480:LEU:CD1	2.65	0.60
1:D:362:ILE:HD11	1:D:555:ILE:HA	1.84	0.60
1:A:58:LYS:HZ1	1:A:61:ARG:CD	2.15	0.59
1:A:220:PHE:HZ	1:B:439:TYR:HD2	1.47	0.59
1:A:383:SER:O	1:A:386:ALA:HB3	2.02	0.59
1:B:362:ILE:HD11	1:B:555:ILE:HA	1.84	0.59
1:C:59:THR:HA	1:C:63:VAL:HG21	1.83	0.59
1:C:436:ASN:HD21	1:C:474:ILE:HG21	1.65	0.59
1:D:475:GLY:N	1:D:480:LEU:CD1	2.65	0.59
1:D:508:THR:HA	1:D:511:LEU:HD12	1.83	0.59
1:D:548:ILE:HB	1:D:565:LEU:HD11	1.83	0.59
1:D:557:VAL:O	1:D:557:VAL:HG12	2.02	0.59
1:D:382:LYS:HB2	2:D:5004:ANP:O1B	2.02	0.59
1:A:105:PHE:CZ	1:B:210:MET:HE3	2.37	0.59
1:A:393:TYR:O	1:A:395:ILE:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ALA:N	1:B:176:PRO:HD2	2.18	0.59
1:D:333:ARG:HB3	1:D:333:ARG:HH11	1.67	0.59
1:A:475:GLY:HA3	1:A:480:LEU:H	1.67	0.59
1:C:20:ILE:HD13	1:C:96:VAL:CG2	2.33	0.59
1:A:58:LYS:HZ3	1:A:58:LYS:HA	1.68	0.59
1:B:380:SER:O	2:B:5002:ANP:O2A	2.21	0.59
1:C:234:SER:O	1:C:237:MET:HB3	2.01	0.59
1:C:557:VAL:O	1:C:557:VAL:HG12	2.02	0.59
1:C:558:GLU:HG3	1:C:565:LEU:HD23	1.84	0.59
1:A:105:PHE:O	1:A:108:MET:HB2	2.02	0.59
1:A:374:LEU:HB2	1:A:535:ILE:HB	1.84	0.59
1:B:83:TYR:O	1:B:87:TYR:CB	2.50	0.59
1:C:440:ALA:HB2	1:C:493:ARG:HG3	1.84	0.59
1:A:59:THR:HA	1:A:63:VAL:HG21	1.83	0.59
1:A:421:LEU:HD12	1:A:503:ILE:O	2.03	0.59
1:B:440:ALA:HB2	1:B:493:ARG:HG3	1.84	0.59
1:C:333:ARG:HB3	1:C:333:ARG:HH11	1.67	0.59
1:D:61:ARG:HG3	1:D:62:SER:H	1.67	0.59
1:D:505:ASP:OD2	1:D:535:ILE:HD12	2.02	0.59
1:D:558:GLU:HG3	1:D:565:LEU:HD23	1.84	0.59
1:B:144:ILE:HG13	1:B:145:THR:N	2.15	0.59
1:C:175:ALA:N	1:C:176:PRO:HD2	2.18	0.59
1:C:505:ASP:OD2	1:C:535:ILE:HD12	2.02	0.59
1:D:482:SER:HB3	1:D:485:GLN:HG3	1.83	0.59
1:A:210:MET:SD	1:B:109:MET:HB3	2.42	0.59
1:C:131:ASP:HB3	1:C:318:LEU:HD23	1.85	0.59
1:D:167:LEU:HG	1:D:287:VAL:HG11	1.85	0.59
1:A:482:SER:HB3	1:A:485:GLN:HG3	1.85	0.58
1:B:374:LEU:HB2	1:B:535:ILE:HB	1.85	0.58
1:B:558:GLU:HG3	1:B:565:LEU:HD23	1.84	0.58
1:D:342:LEU:HD13	1:D:366:ILE:HD12	1.85	0.58
1:A:440:ALA:HB1	1:A:497:ARG:CD	2.33	0.58
1:C:83:TYR:O	1:C:87:TYR:CB	2.50	0.58
1:C:482:SER:HB3	1:C:485:GLN:HG3	1.84	0.58
1:D:436:ASN:HD21	1:D:474:ILE:HG21	1.65	0.58
1:A:98:MET:HB3	1:B:238:ARG:NE	2.17	0.58
1:B:58:LYS:HB3	1:B:62:SER:CB	2.34	0.58
1:B:61:ARG:HG3	1:B:62:SER:H	1.67	0.58
1:B:342:LEU:HD13	1:B:366:ILE:HD12	1.85	0.58
1:B:475:GLY:HA3	1:B:480:LEU:H	1.68	0.58
1:C:105:PHE:O	1:C:108:MET:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:LEU:HB2	1:C:535:ILE:HB	1.85	0.58
1:D:341:ASP:HB3	1:D:403:ASP:OD1	2.03	0.58
1:A:362:ILE:HD11	1:A:555:ILE:HA	1.84	0.58
1:B:167:LEU:HG	1:B:287:VAL:HG11	1.85	0.58
1:C:341:ASP:HB3	1:C:403:ASP:OD1	2.03	0.58
1:D:58:LYS:HB3	1:D:62:SER:CB	2.34	0.58
1:D:83:TYR:O	1:D:87:TYR:CB	2.50	0.58
1:D:475:GLY:HA3	1:D:480:LEU:H	1.68	0.58
1:B:249:SER:O	1:B:253:PRO:HD2	2.04	0.58
1:B:382:LYS:NZ	2:B:5002:ANP:O1B	2.35	0.58
1:C:362:ILE:HD11	1:C:555:ILE:HA	1.84	0.58
1:D:175:ALA:N	1:D:176:PRO:HD2	2.18	0.58
1:A:11:GLN:H	1:A:14:ARG:CB	2.14	0.58
1:A:56:PHE:HB3	1:B:281:ALA:HB2	1.85	0.58
1:A:260:SER:OG	1:B:74:LEU:HD13	2.03	0.58
1:A:503:ILE:HG23	1:A:533:LEU:HD12	1.86	0.58
1:C:249:SER:O	1:C:253:PRO:HD2	2.04	0.58
1:D:421:LEU:HD12	1:D:503:ILE:O	2.04	0.58
1:A:31:GLY:O	1:A:35:ILE:HD13	2.03	0.58
1:A:221:GLY:CA	1:B:441:ARG:NE	2.61	0.58
1:C:167:LEU:HG	1:C:287:VAL:HG11	1.85	0.58
1:C:249:SER:HG	1:D:83:TYR:HD1	1.51	0.58
1:C:475:GLY:HA3	1:C:480:LEU:H	1.68	0.58
1:D:105:PHE:O	1:D:108:MET:HB2	2.03	0.58
1:A:84:ILE:O	1:A:87:TYR:HD2	1.87	0.58
1:A:394:ASP:O	1:A:395:ILE:HG22	2.04	0.58
1:B:421:LEU:HD12	1:B:503:ILE:O	2.04	0.58
1:B:557:VAL:O	1:B:557:VAL:HG12	2.02	0.58
1:D:374:LEU:HB2	1:D:535:ILE:HB	1.85	0.58
1:A:169:ILE:O	1:A:169:ILE:HG22	2.04	0.58
1:A:263:LEU:HD13	1:A:263:LEU:C	2.29	0.58
1:A:440:ALA:HB2	1:A:493:ARG:HG3	1.85	0.58
1:A:442:THR:O	1:A:443:GLU:HB2	2.02	0.58
1:C:11:GLN:CG	1:C:12:THR:H	1.95	0.58
1:D:249:SER:O	1:D:253:PRO:HD2	2.04	0.58
1:D:440:ALA:HB2	1:D:493:ARG:HG3	1.84	0.58
1:A:98:MET:SD	1:A:101:ARG:NH1	2.73	0.58
1:C:429:PHE:CE1	1:D:220:PHE:CZ	2.89	0.58
1:D:223:GLN:H	1:D:223:GLN:CD	2.12	0.58
1:D:394:ASP:O	1:D:395:ILE:HG22	2.04	0.58
1:A:296:ARG:C	1:A:296:ARG:HD3	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:GLY:HA3	1:A:408:ARG:O	2.04	0.57
1:A:401:LEU:HD12	1:A:404:GLY:HA2	1.86	0.57
1:B:131:ASP:HB3	1:B:318:LEU:HD23	1.85	0.57
1:B:503:ILE:HG23	1:B:533:LEU:HD12	1.86	0.57
1:D:393:TYR:O	1:D:395:ILE:N	2.37	0.57
1:D:503:ILE:HG23	1:D:533:LEU:HD12	1.86	0.57
1:A:210:MET:HE2	1:A:210:MET:HA	1.86	0.57
1:A:333:ARG:HB3	1:A:333:ARG:HH11	1.68	0.57
1:A:576:HIS:O	1:A:579:GLN:HB2	2.04	0.57
1:B:508:THR:HG21	1:B:516:GLU:OE2	2.04	0.57
1:C:393:TYR:O	1:C:395:ILE:N	2.37	0.57
1:D:131:ASP:HB3	1:D:318:LEU:HD23	1.85	0.57
1:A:167:LEU:HG	1:A:287:VAL:HG11	1.85	0.57
1:B:105:PHE:O	1:B:108:MET:HB2	2.03	0.57
1:B:238:ARG:O	1:B:242:MET:HB2	2.04	0.57
1:B:436:ASN:HD21	1:B:474:ILE:HG21	1.65	0.57
1:C:210:MET:HE3	1:D:105:PHE:CZ	2.39	0.57
1:C:503:ILE:HG23	1:C:533:LEU:HD12	1.86	0.57
1:D:373:ALA:HA	1:D:534:VAL:O	2.04	0.57
1:B:20:ILE:HD13	1:B:96:VAL:CG2	2.33	0.57
1:B:341:ASP:HB3	1:B:403:ASP:OD1	2.03	0.57
1:B:487:GLN:HE22	1:B:510:ALA:H	1.53	0.57
1:C:15:ARG:C	1:C:18:PRO:HD2	2.29	0.57
1:C:342:LEU:HD13	1:C:366:ILE:HD12	1.85	0.57
1:B:98:MET:SD	1:B:101:ARG:NH1	2.77	0.57
1:D:424:GLN:H	1:D:424:GLN:CD	2.12	0.57
1:B:176:PRO:O	1:B:180:ILE:HG12	2.05	0.57
1:B:393:TYR:O	1:B:395:ILE:N	2.37	0.57
1:B:424:GLN:H	1:B:424:GLN:CD	2.12	0.57
1:C:238:ARG:O	1:C:242:MET:HB2	2.04	0.57
1:C:455:ARG:HB2	1:C:460:MET:HG3	1.87	0.57
1:D:49:LYS:HD2	1:D:49:LYS:O	2.05	0.57
1:A:15:ARG:C	1:A:18:PRO:HD2	2.30	0.57
1:A:58:LYS:HB3	1:A:62:SER:CB	2.33	0.57
1:A:175:ALA:N	1:A:176:PRO:HD2	2.19	0.57
1:A:541:THR:O	1:A:542:ILE:HG13	2.03	0.57
1:B:15:ARG:C	1:B:18:PRO:HD2	2.29	0.57
1:B:394:ASP:O	1:B:395:ILE:HG22	2.04	0.57
1:C:383:SER:O	1:C:386:ALA:HB3	2.05	0.57
1:C:49:LYS:HD2	1:C:49:LYS:O	2.05	0.57
1:C:134:GLN:HE22	1:C:310:ARG:NE	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:ARG:HB2	1:B:460:MET:HG3	1.87	0.57
1:B:576:HIS:O	1:B:579:GLN:HB2	2.05	0.57
1:C:576:HIS:O	1:C:579:GLN:HB2	2.05	0.57
1:D:176:PRO:O	1:D:180:ILE:HG12	2.04	0.57
1:D:238:ARG:O	1:D:242:MET:HB2	2.04	0.57
1:A:49:LYS:HD2	1:A:49:LYS:O	2.05	0.57
1:A:58:LYS:HA	1:A:58:LYS:NZ	2.20	0.57
1:A:112:PRO:HG2	1:A:328:LYS:HB3	1.87	0.57
1:A:249:SER:O	1:A:253:PRO:HD2	2.05	0.57
1:B:331:GLY:HA3	1:B:408:ARG:O	2.05	0.57
1:B:383:SER:HB2	2:B:5002:ANP:O1A	2.04	0.57
1:B:541:THR:C	1:B:542:ILE:HD12	2.30	0.57
1:C:169:ILE:O	1:C:169:ILE:HG22	2.05	0.57
1:C:269:ALA:HA	1:C:273:PRO:HD2	1.87	0.57
1:C:373:ALA:HA	1:C:534:VAL:O	2.04	0.57
1:C:394:ASP:O	1:C:395:ILE:HG22	2.04	0.57
1:A:176:PRO:O	1:A:180:ILE:HG12	2.05	0.56
1:A:373:ALA:HA	1:A:534:VAL:O	2.04	0.56
1:A:439:TYR:HD2	1:B:220:PHE:HZ	1.51	0.56
1:B:344:PHE:HE2	1:B:364:LEU:HB3	1.70	0.56
1:B:373:ALA:HA	1:B:534:VAL:O	2.04	0.56
1:C:58:LYS:HB3	1:C:62:SER:CB	2.33	0.56
1:C:220:PHE:CZ	1:D:429:PHE:CE1	2.88	0.56
1:D:269:ALA:HA	1:D:273:PRO:HD2	1.87	0.56
1:D:383:SER:O	1:D:386:ALA:HB3	2.05	0.56
1:D:455:ARG:HB2	1:D:460:MET:HG3	1.87	0.56
1:D:508:THR:HG21	1:D:516:GLU:OE2	2.04	0.56
1:A:11:GLN:O	1:A:12:THR:C	2.46	0.56
1:A:57:GLY:O	1:A:58:LYS:HD2	2.06	0.56
1:B:16:LEU:HA	1:B:319:PHE:HZ	1.70	0.56
1:B:49:LYS:O	1:B:49:LYS:HD2	2.05	0.56
1:B:374:LEU:O	1:B:535:ILE:HG12	2.05	0.56
1:C:478:GLY:HA3	1:C:486:ARG:HD2	1.88	0.56
1:D:15:ARG:C	1:D:18:PRO:HD2	2.29	0.56
1:D:216:GLU:O	1:D:218:LEU:N	2.38	0.56
1:D:374:LEU:CD2	1:D:533:LEU:HD21	2.35	0.56
1:A:29:VAL:HB	1:A:88:CYS:SG	2.45	0.56
1:A:216:GLU:O	1:A:218:LEU:N	2.39	0.56
1:A:238:ARG:O	1:A:242:MET:HB2	2.05	0.56
1:A:424:GLN:H	1:A:424:GLN:CD	2.11	0.56
1:A:455:ARG:HB2	1:A:460:MET:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:THR:O	1:B:443:GLU:HB2	2.04	0.56
1:C:45:LEU:HD23	1:C:45:LEU:O	2.05	0.56
1:C:508:THR:HG21	1:C:516:GLU:OE2	2.04	0.56
1:D:20:ILE:HD13	1:D:96:VAL:CG2	2.33	0.56
1:D:45:LEU:O	1:D:45:LEU:HD23	2.06	0.56
1:D:284:ILE:O	1:D:284:ILE:CD1	2.52	0.56
1:A:214:HIS:O	1:A:218:LEU:HD13	2.06	0.56
1:A:292:ILE:HD12	1:B:48:LEU:HD12	1.88	0.56
1:B:296:ARG:C	1:B:296:ARG:HD3	2.30	0.56
1:B:374:LEU:CD2	1:B:533:LEU:HD21	2.35	0.56
1:C:220:PHE:O	1:D:441:ARG:CD	2.52	0.56
1:C:362:ILE:CD1	1:C:556:ILE:H	2.19	0.56
1:D:362:ILE:CD1	1:D:556:ILE:H	2.19	0.56
1:A:61:ARG:HG3	1:A:62:SER:H	1.69	0.56
1:A:547:GLU:OE2	1:A:559:ARG:HB3	2.06	0.56
1:B:134:GLN:HE22	1:B:310:ARG:NE	2.03	0.56
1:C:176:PRO:O	1:C:180:ILE:HG12	2.05	0.56
1:C:296:ARG:HD3	1:C:296:ARG:C	2.30	0.56
1:C:442:THR:O	1:C:443:GLU:HB2	2.04	0.56
1:D:98:MET:SD	1:D:101:ARG:NH1	2.77	0.56
1:D:576:HIS:O	1:D:579:GLN:HB2	2.05	0.56
1:A:11:GLN:O	1:A:15:ARG:N	2.35	0.56
1:A:45:LEU:O	1:A:45:LEU:HD23	2.06	0.56
1:A:269:ALA:HA	1:A:273:PRO:HD2	1.86	0.56
1:A:432:THR:HA	1:A:472:THR:O	2.06	0.56
1:C:210:MET:HE2	1:C:210:MET:HA	1.87	0.56
1:C:214:HIS:O	1:C:218:LEU:HD13	2.06	0.56
1:C:235:ASN:O	1:C:238:ARG:HG2	2.05	0.56
1:C:401:LEU:HD12	1:C:404:GLY:HA2	1.88	0.56
1:C:421:LEU:HD12	1:C:503:ILE:O	2.04	0.56
1:A:16:LEU:HA	1:A:319:PHE:HZ	1.71	0.56
1:A:134:GLN:HE22	1:A:310:ARG:NE	2.03	0.56
1:A:441:ARG:NH1	1:B:221:GLY:O	2.39	0.56
1:A:508:THR:HG21	1:A:516:GLU:OE2	2.05	0.56
1:B:58:LYS:HA	1:B:58:LYS:NZ	2.21	0.56
1:B:214:HIS:O	1:B:218:LEU:HD13	2.06	0.56
1:B:235:ASN:O	1:B:238:ARG:HG2	2.05	0.56
1:B:326:GLN:C	1:B:328:LYS:N	2.64	0.56
1:C:216:GLU:O	1:C:218:LEU:N	2.38	0.56
1:D:235:ASN:O	1:D:238:ARG:HG2	2.05	0.56
1:A:291:MET:HE2	1:A:291:MET:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:MET:HA	1:B:210:MET:HE2	1.88	0.56
1:B:423:SER:O	1:B:424:GLN:C	2.49	0.56
1:C:29:VAL:HB	1:C:88:CYS:SG	2.46	0.56
1:C:374:LEU:CD2	1:C:533:LEU:HD21	2.35	0.56
1:C:454:ALA:CB	1:C:460:MET:HE3	2.36	0.56
1:C:487:GLN:HE22	1:C:510:ALA:H	1.53	0.56
1:D:442:THR:O	1:D:443:GLU:HB2	2.04	0.56
1:A:478:GLY:HA3	1:A:486:ARG:HD2	1.87	0.56
1:B:454:ALA:CB	1:B:460:MET:HE3	2.36	0.56
1:C:58:LYS:HA	1:C:58:LYS:NZ	2.21	0.56
1:C:97:VAL:HB	1:C:136:ALA:CB	2.36	0.56
1:C:108:MET:CE	1:C:124:LEU:HB3	2.36	0.56
1:C:331:GLY:HA3	1:C:408:ARG:O	2.05	0.56
1:C:344:PHE:HE2	1:C:364:LEU:HB3	1.70	0.56
1:C:374:LEU:O	1:C:535:ILE:HG12	2.06	0.56
1:C:424:GLN:CD	1:C:424:GLN:H	2.12	0.56
1:D:374:LEU:O	1:D:535:ILE:HG12	2.06	0.56
1:D:382:LYS:NZ	2:D:5004:ANP:O1B	2.39	0.56
1:D:423:SER:O	1:D:424:GLN:C	2.49	0.56
1:D:454:ALA:CB	1:D:460:MET:HE3	2.36	0.56
1:A:11:GLN:CA	1:A:14:ARG:HB3	2.36	0.56
1:A:438:ALA:O	1:A:440:ALA:N	2.39	0.56
1:B:169:ILE:HG22	1:B:169:ILE:O	2.05	0.56
1:B:216:GLU:O	1:B:218:LEU:N	2.38	0.56
1:D:487:GLN:HE22	1:D:510:ALA:H	1.53	0.56
1:A:389:ILE:O	1:A:407:LEU:HD21	2.06	0.55
1:B:269:ALA:HA	1:B:273:PRO:HD2	1.87	0.55
1:C:57:GLY:O	1:C:58:LYS:HD2	2.06	0.55
1:C:102:ARG:NH2	1:D:238:ARG:NH2	2.54	0.55
1:D:16:LEU:HA	1:D:319:PHE:HZ	1.70	0.55
1:D:57:GLY:O	1:D:58:LYS:HD2	2.06	0.55
1:D:58:LYS:HA	1:D:58:LYS:NZ	2.21	0.55
1:D:214:HIS:O	1:D:218:LEU:HD13	2.06	0.55
1:D:296:ARG:C	1:D:296:ARG:HD3	2.30	0.55
1:D:432:THR:HA	1:D:472:THR:O	2.06	0.55
1:A:235:ASN:O	1:A:238:ARG:HG2	2.06	0.55
1:B:362:ILE:CD1	1:B:556:ILE:H	2.19	0.55
1:D:344:PHE:HE2	1:D:364:LEU:HB3	1.70	0.55
1:A:220:PHE:O	1:B:441:ARG:CD	2.54	0.55
1:A:391:ARG:C	1:A:393:TYR:H	2.13	0.55
1:A:436:ASN:HD21	1:A:474:ILE:HG21	1.67	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:GLN:HE22	1:A:510:ALA:H	1.52	0.55
1:B:45:LEU:O	1:B:45:LEU:HD23	2.06	0.55
1:C:440:ALA:HB1	1:C:497:ARG:CD	2.36	0.55
1:A:342:LEU:HD13	1:A:366:ILE:HD12	1.87	0.55
1:A:400:ILE:O	1:A:407:LEU:HD13	2.06	0.55
1:A:454:ALA:CB	1:A:460:MET:HE3	2.36	0.55
1:B:97:VAL:HB	1:B:136:ALA:CB	2.36	0.55
1:C:441:ARG:CD	1:D:221:GLY:O	2.54	0.55
1:D:29:VAL:HB	1:D:88:CYS:SG	2.46	0.55
1:D:376:GLY:HA3	1:D:551:VAL:O	2.07	0.55
1:A:263:LEU:HD13	1:A:263:LEU:O	2.06	0.55
1:B:440:ALA:HB1	1:B:497:ARG:CD	2.36	0.55
1:C:432:THR:HA	1:C:472:THR:O	2.07	0.55
1:D:76:ILE:O	1:D:80:ILE:HB	2.06	0.55
1:D:331:GLY:HA3	1:D:408:ARG:O	2.05	0.55
1:A:11:GLN:H	1:A:14:ARG:HB3	1.65	0.55
1:A:108:MET:CE	1:A:124:LEU:HB3	2.36	0.55
1:A:291:MET:HA	1:A:291:MET:CE	2.36	0.55
1:B:31:GLY:O	1:B:35:ILE:HD13	2.06	0.55
1:B:76:ILE:O	1:B:80:ILE:HB	2.06	0.55
1:B:203:VAL:HG22	1:B:233:VAL:HG12	1.89	0.55
1:B:383:SER:O	1:B:386:ALA:HB3	2.05	0.55
1:B:432:THR:HA	1:B:472:THR:O	2.06	0.55
1:C:31:GLY:O	1:C:35:ILE:HD13	2.07	0.55
1:C:196:MET:HA	1:C:240:GLN:CG	2.37	0.55
1:C:284:ILE:O	1:C:284:ILE:CD1	2.52	0.55
1:C:416:ARG:HD3	1:D:218:LEU:HB3	1.88	0.55
1:C:423:SER:O	1:C:424:GLN:C	2.49	0.55
1:D:11:GLN:O	1:D:15:ARG:N	2.36	0.55
1:D:108:MET:CE	1:D:124:LEU:HB3	2.36	0.55
1:D:152:SER:O	1:D:156:LEU:HD23	2.07	0.55
1:D:169:ILE:O	1:D:169:ILE:HG22	2.05	0.55
1:A:210:MET:HE3	1:B:105:PHE:CZ	2.41	0.55
1:A:374:LEU:CD2	1:A:533:LEU:HD21	2.36	0.55
1:A:423:SER:O	1:A:424:GLN:C	2.50	0.55
1:B:101:ARG:HH21	1:B:129:THR:HA	1.72	0.55
1:B:284:ILE:O	1:B:284:ILE:CD1	2.52	0.55
1:B:376:GLY:HA3	1:B:551:VAL:O	2.07	0.55
1:B:401:LEU:HD12	1:B:404:GLY:HA2	1.88	0.55
1:C:83:TYR:HD1	1:D:249:SER:HG	1.53	0.55
1:D:31:GLY:O	1:D:35:ILE:HD13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:VAL:HB	1:D:136:ALA:CB	2.36	0.55
1:D:326:GLN:C	1:D:328:LYS:N	2.64	0.55
1:D:439:TYR:HA	1:D:443:GLU:HG3	1.89	0.55
1:D:440:ALA:HB1	1:D:497:ARG:CD	2.36	0.55
1:D:446:SER:HB2	1:D:449:GLN:CD	2.32	0.55
1:A:201:GLY:O	1:A:204:THR:HB	2.07	0.55
1:A:315:CYS:SG	1:A:319:PHE:CD1	3.00	0.55
1:C:16:LEU:HA	1:C:319:PHE:HZ	1.70	0.55
1:A:474:ILE:C	1:A:480:LEU:HD11	2.32	0.55
1:B:344:PHE:HZ	1:B:385:ILE:HD12	1.72	0.55
1:C:427:HIS:HD2	1:D:213:GLY:HA2	1.71	0.55
1:C:446:SER:HB2	1:C:449:GLN:CD	2.32	0.55
1:D:210:MET:HE2	1:D:210:MET:HA	1.88	0.55
1:D:434:ALA:HB2	1:D:470:LEU:HB3	1.89	0.55
1:D:547:GLU:OE2	1:D:559:ARG:HB3	2.07	0.55
1:A:441:ARG:CD	1:B:221:GLY:CA	2.66	0.55
1:A:446:SER:HB2	1:A:449:GLN:CD	2.31	0.55
1:B:439:TYR:HA	1:B:443:GLU:HG3	1.89	0.55
1:B:446:SER:HB2	1:B:449:GLN:CD	2.32	0.55
1:C:291:MET:CE	1:C:291:MET:HA	2.37	0.55
1:C:326:GLN:C	1:C:328:LYS:N	2.64	0.55
1:D:133:GLU:O	1:D:136:ALA:HB3	2.07	0.55
1:D:478:GLY:HA3	1:D:486:ARG:HD2	1.87	0.55
1:A:97:VAL:HB	1:A:136:ALA:CB	2.37	0.54
1:A:152:SER:O	1:A:156:LEU:HD23	2.06	0.54
1:A:315:CYS:SG	1:A:319:PHE:CE1	3.00	0.54
1:A:362:ILE:HD11	1:A:556:ILE:H	1.72	0.54
1:A:455:ARG:HH11	1:A:456:MET:CE	2.20	0.54
1:B:108:MET:CE	1:B:124:LEU:HB3	2.36	0.54
1:C:166:GLN:OE1	1:C:166:GLN:HA	2.07	0.54
1:C:441:ARG:HG2	1:D:220:PHE:O	2.07	0.54
1:D:401:LEU:HD12	1:D:404:GLY:HA2	1.88	0.54
1:A:76:ILE:O	1:A:80:ILE:HB	2.07	0.54
1:B:344:PHE:CE2	1:B:364:LEU:HB3	2.43	0.54
1:B:547:GLU:OE2	1:B:559:ARG:HB3	2.07	0.54
1:C:58:LYS:HZ1	1:C:61:ARG:CD	2.20	0.54
1:D:196:MET:HA	1:D:240:GLN:CG	2.37	0.54
1:D:201:GLY:O	1:D:204:THR:HB	2.07	0.54
1:D:344:PHE:HZ	1:D:385:ILE:HD12	1.72	0.54
1:A:63:VAL:CG1	1:B:267:LEU:O	2.55	0.54
1:A:167:LEU:HD12	1:A:266:VAL:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:HD21	1:A:261:LEU:HB3	1.89	0.54
1:A:402:MET:O	1:A:403:ASP:HB2	2.06	0.54
1:C:112:PRO:HG2	1:C:328:LYS:HB3	1.89	0.54
1:C:438:ALA:O	1:C:440:ALA:N	2.41	0.54
1:D:59:THR:HA	1:D:63:VAL:CG2	2.38	0.54
1:D:111:MET:CE	1:D:326:GLN:HA	2.38	0.54
1:D:344:PHE:CE2	1:D:364:LEU:HB3	2.43	0.54
1:B:57:GLY:O	1:B:58:LYS:HD2	2.06	0.54
1:B:111:MET:CE	1:B:326:GLN:HA	2.38	0.54
1:C:344:PHE:HZ	1:C:385:ILE:HD12	1.72	0.54
1:D:101:ARG:HH21	1:D:129:THR:HA	1.72	0.54
1:B:152:SER:O	1:B:156:LEU:HD23	2.07	0.54
1:B:166:GLN:HA	1:B:166:GLN:OE1	2.07	0.54
1:B:174:LEU:HD21	1:B:261:LEU:HB3	1.88	0.54
1:B:291:MET:HA	1:B:291:MET:CE	2.37	0.54
1:C:76:ILE:O	1:C:80:ILE:HB	2.06	0.54
1:C:376:GLY:HA3	1:C:551:VAL:O	2.07	0.54
1:C:441:ARG:CD	1:D:220:PHE:O	2.55	0.54
1:D:174:LEU:HD21	1:D:261:LEU:HB3	1.89	0.54
1:A:48:LEU:CD1	1:B:292:ILE:HD12	2.37	0.54
1:A:86:SER:CB	1:B:249:SER:HB2	2.38	0.54
1:A:213:GLY:HA2	1:B:427:HIS:CD2	2.42	0.54
1:B:173:VAL:HG12	1:B:174:LEU:HD12	1.90	0.54
1:B:196:MET:HA	1:B:240:GLN:CG	2.37	0.54
1:C:101:ARG:HH21	1:C:129:THR:HA	1.72	0.54
1:C:111:MET:CE	1:C:326:GLN:HA	2.38	0.54
1:C:174:LEU:HD21	1:C:261:LEU:HB3	1.89	0.54
1:C:203:VAL:HG22	1:C:233:VAL:HG12	1.89	0.54
1:C:434:ALA:HB2	1:C:470:LEU:HB3	1.89	0.54
1:D:87:TYR:CG	1:D:88:CYS:N	2.76	0.54
1:D:134:GLN:HE22	1:D:310:ARG:NE	2.03	0.54
1:D:400:ILE:O	1:D:407:LEU:HD13	2.07	0.54
1:A:196:MET:HA	1:A:240:GLN:CG	2.37	0.54
1:B:29:VAL:HB	1:B:88:CYS:SG	2.46	0.54
1:B:59:THR:HA	1:B:63:VAL:CG2	2.37	0.54
1:C:59:THR:HA	1:C:63:VAL:CG2	2.38	0.54
1:C:344:PHE:CE2	1:C:364:LEU:HB3	2.43	0.54
1:C:550:VAL:HG21	1:C:572:TYR:HB2	1.90	0.54
1:D:291:MET:HA	1:D:291:MET:CE	2.37	0.54
1:D:402:MET:O	1:D:403:ASP:HB2	2.07	0.54
1:B:168:SER:O	1:B:172:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ASN:HA	1:B:238:ARG:NE	2.23	0.54
1:B:478:GLY:HA3	1:B:486:ARG:HD2	1.88	0.54
1:C:98:MET:SD	1:C:101:ARG:NH1	2.77	0.54
1:C:441:ARG:NE	1:D:221:GLY:CA	2.68	0.54
1:C:547:GLU:OE2	1:C:559:ARG:HB3	2.07	0.54
1:D:84:ILE:O	1:D:87:TYR:HD2	1.91	0.54
1:A:10:TRP:O	1:A:11:GLN:HB3	2.08	0.54
1:A:133:GLU:O	1:A:136:ALA:HB3	2.07	0.54
1:A:302:THR:HG23	1:A:303:ASN:N	2.23	0.54
1:A:376:GLY:HA3	1:A:551:VAL:O	2.08	0.54
1:A:493:ARG:HD3	1:A:497:ARG:NH1	2.23	0.54
1:A:541:THR:C	1:A:542:ILE:HD12	2.32	0.54
1:A:542:ILE:O	1:A:544:GLN:N	2.40	0.54
1:B:112:PRO:HG2	1:B:328:LYS:HB3	1.89	0.54
1:B:434:ALA:HB2	1:B:470:LEU:HB3	1.89	0.54
1:C:89:ILE:HG23	1:C:90:SER:N	2.23	0.54
1:C:389:ILE:O	1:C:407:LEU:HD21	2.08	0.54
1:D:112:PRO:HG2	1:D:328:LYS:HB3	1.89	0.54
1:A:101:ARG:HH21	1:A:129:THR:HA	1.73	0.54
1:A:344:PHE:HE2	1:A:364:LEU:HB3	1.72	0.54
1:B:87:TYR:CG	1:B:88:CYS:N	2.76	0.54
1:B:154:ILE:HA	1:B:157:PHE:CD2	2.43	0.54
1:B:295:MET:O	1:B:299:LYS:HG3	2.08	0.54
1:C:133:GLU:O	1:C:136:ALA:HB3	2.07	0.54
1:C:152:SER:O	1:C:156:LEU:HD23	2.07	0.54
1:C:201:GLY:O	1:C:204:THR:HB	2.07	0.54
1:D:168:SER:O	1:D:172:VAL:HG23	2.08	0.54
1:A:168:SER:O	1:A:172:VAL:HG23	2.07	0.53
1:A:439:TYR:HA	1:A:443:GLU:HG3	1.90	0.53
1:C:214:HIS:CE1	1:C:218:LEU:HD11	2.43	0.53
1:C:235:ASN:HA	1:C:238:ARG:NE	2.23	0.53
1:C:263:LEU:HD13	1:C:263:LEU:C	2.33	0.53
1:C:400:ILE:O	1:C:407:LEU:HD13	2.07	0.53
1:C:402:MET:O	1:C:403:ASP:HB2	2.07	0.53
1:A:111:MET:CE	1:A:326:GLN:HA	2.38	0.53
1:A:368:ALA:HA	1:A:531:THR:HG1	1.73	0.53
1:B:11:GLN:O	1:B:15:ARG:N	2.36	0.53
1:B:133:GLU:O	1:B:136:ALA:HB3	2.07	0.53
1:C:11:GLN:O	1:C:15:ARG:N	2.36	0.53
1:C:220:PHE:C	1:D:441:ARG:HD3	2.33	0.53
1:C:302:THR:HG23	1:C:303:ASN:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:HIS:CE1	1:D:218:LEU:HD11	2.43	0.53
1:A:154:ILE:HA	1:A:157:PHE:CD2	2.42	0.53
1:A:561:THR:HG22	1:A:562:HIS:N	2.24	0.53
1:B:84:ILE:O	1:B:87:TYR:HD2	1.91	0.53
1:B:214:HIS:CE1	1:B:218:LEU:HD11	2.44	0.53
1:B:263:LEU:C	1:B:263:LEU:HD13	2.33	0.53
1:C:173:VAL:HG12	1:C:174:LEU:HD12	1.90	0.53
1:C:291:MET:HA	1:C:291:MET:HE2	1.90	0.53
1:D:203:VAL:HG22	1:D:233:VAL:HG12	1.89	0.53
1:D:550:VAL:HG21	1:D:572:TYR:HB2	1.90	0.53
1:A:173:VAL:HG12	1:A:174:LEU:HD12	1.90	0.53
1:A:347:VAL:HG13	1:A:395:ILE:CD1	2.29	0.53
1:B:346:ASN:N	1:B:363:ASN:OD1	2.38	0.53
1:B:438:ALA:O	1:B:440:ALA:N	2.41	0.53
1:C:11:GLN:O	1:C:12:THR:C	2.52	0.53
1:C:439:TYR:HA	1:C:443:GLU:HG3	1.89	0.53
1:D:302:THR:HG23	1:D:303:ASN:H	1.74	0.53
1:A:98:MET:HB3	1:B:238:ARG:HH21	1.68	0.53
1:A:203:VAL:HG22	1:A:233:VAL:HG12	1.90	0.53
1:A:281:ALA:HA	1:A:284:ILE:HG22	1.91	0.53
1:A:338:ALA:CB	1:A:500:PRO:HG2	2.04	0.53
1:A:434:ALA:HB2	1:A:470:LEU:HB3	1.91	0.53
1:A:441:ARG:CD	1:B:220:PHE:O	2.54	0.53
1:B:302:THR:HG23	1:B:303:ASN:N	2.23	0.53
1:B:542:ILE:O	1:B:544:GLN:N	2.42	0.53
1:C:223:GLN:H	1:C:223:GLN:CD	2.12	0.53
1:C:295:MET:O	1:C:299:LYS:HG3	2.09	0.53
1:C:428:LEU:HD23	1:C:493:ARG:NH2	2.24	0.53
1:C:441:ARG:HD3	1:D:220:PHE:C	2.34	0.53
1:C:548:ILE:HD12	1:C:548:ILE:N	2.22	0.53
1:D:16:LEU:HD23	1:D:16:LEU:O	2.08	0.53
1:D:89:ILE:HG23	1:D:90:SER:N	2.23	0.53
1:D:438:ALA:O	1:D:440:ALA:N	2.41	0.53
1:D:513:THR:HG23	1:D:514:GLU:N	2.24	0.53
1:A:428:LEU:HD23	1:A:493:ARG:NH2	2.24	0.53
1:A:492:ALA:O	1:A:493:ARG:C	2.51	0.53
1:A:561:THR:HG22	1:A:563:SER:H	1.73	0.53
1:B:89:ILE:HG23	1:B:90:SER:N	2.23	0.53
1:B:201:GLY:O	1:B:204:THR:HB	2.07	0.53
1:B:400:ILE:O	1:B:407:LEU:HD13	2.07	0.53
1:B:402:MET:O	1:B:403:ASP:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:TYR:CG	1:C:88:CYS:N	2.76	0.53
1:D:412:LEU:HD21	1:D:416:ARG:HH11	1.73	0.53
1:D:542:ILE:O	1:D:544:GLN:N	2.42	0.53
1:A:219:ILE:HG13	1:A:220:PHE:N	2.22	0.53
1:A:220:PHE:O	1:B:441:ARG:HG2	2.07	0.53
1:A:235:ASN:HA	1:A:238:ARG:NE	2.24	0.53
1:A:455:ARG:HH11	1:A:456:MET:HE2	1.74	0.53
1:B:389:ILE:O	1:B:407:LEU:HD21	2.08	0.53
1:D:166:GLN:OE1	1:D:166:GLN:HA	2.07	0.53
1:D:263:LEU:HD13	1:D:263:LEU:C	2.33	0.53
1:D:291:MET:HA	1:D:291:MET:HE2	1.90	0.53
1:B:252:ASP:HB2	1:B:253:PRO:CD	2.38	0.53
1:B:441:ARG:HA	1:B:441:ARG:NH1	2.23	0.53
1:B:561:THR:HG22	1:B:563:SER:H	1.74	0.53
1:C:221:GLY:CA	1:D:441:ARG:NE	2.71	0.53
1:C:575:LEU:HD22	1:D:513:THR:HG22	1.91	0.53
1:A:214:HIS:CE1	1:A:218:LEU:HD11	2.43	0.53
1:A:424:GLN:CD	1:A:424:GLN:N	2.67	0.53
1:C:512:ASP:HB2	1:D:378:SER:N	2.20	0.53
1:D:154:ILE:HA	1:D:157:PHE:CD2	2.43	0.53
1:D:235:ASN:HA	1:D:238:ARG:NE	2.23	0.53
1:D:389:ILE:O	1:D:407:LEU:HD21	2.08	0.53
1:A:220:PHE:C	1:B:441:ARG:HD3	2.33	0.53
1:A:382:LYS:NZ	2:A:5001:ANP:O1B	2.42	0.53
1:C:383:SER:OG	2:C:5003:ANP:O2B	2.15	0.53
1:C:512:ASP:CB	1:D:378:SER:H	2.19	0.53
1:A:166:GLN:OE1	1:A:166:GLN:HA	2.07	0.52
1:A:326:GLN:C	1:A:328:LYS:N	2.64	0.52
1:A:550:VAL:HG21	1:A:572:TYR:HB2	1.91	0.52
1:B:16:LEU:O	1:B:16:LEU:HD23	2.08	0.52
1:B:428:LEU:HD23	1:B:493:ARG:NH2	2.24	0.52
1:B:455:ARG:HH11	1:B:456:MET:CE	2.22	0.52
1:B:550:VAL:HG21	1:B:572:TYR:HB2	1.90	0.52
1:C:134:GLN:NE2	1:C:310:ARG:HE	2.06	0.52
1:C:217:VAL:HA	1:C:220:PHE:CB	2.39	0.52
1:C:298:LEU:HD23	1:C:298:LEU:C	2.34	0.52
1:C:513:THR:HG23	1:C:514:GLU:N	2.24	0.52
1:D:47:LEU:HD13	1:D:47:LEU:O	2.10	0.52
1:D:173:VAL:HG12	1:D:174:LEU:HD12	1.90	0.52
1:A:40:SER:O	1:A:44:MET:HG2	2.09	0.52
1:A:59:THR:HA	1:A:63:VAL:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:THR:HG23	1:A:303:ASN:H	1.73	0.52
1:B:513:THR:HG23	1:B:514:GLU:N	2.24	0.52
1:C:67:MET:HA	1:D:267:LEU:CD2	2.39	0.52
1:C:83:TYR:HA	1:D:249:SER:OG	2.09	0.52
1:C:154:ILE:HA	1:C:157:PHE:CD2	2.43	0.52
1:C:168:SER:O	1:C:172:VAL:HG23	2.08	0.52
1:C:302:THR:HG23	1:C:303:ASN:H	1.74	0.52
1:C:346:ASN:N	1:C:363:ASN:OD1	2.38	0.52
1:C:455:ARG:HH11	1:C:456:MET:CE	2.22	0.52
1:D:298:LEU:HD23	1:D:298:LEU:C	2.34	0.52
1:D:474:ILE:HA	1:D:480:LEU:HD11	1.91	0.52
1:A:59:THR:O	1:A:60:ASP:HB2	2.10	0.52
1:A:346:ASN:N	1:A:363:ASN:OD1	2.38	0.52
1:A:378:SER:CB	1:B:512:ASP:HB2	2.39	0.52
1:A:388:LEU:HD23	1:A:388:LEU:O	2.08	0.52
1:B:548:ILE:HD12	1:B:548:ILE:N	2.24	0.52
1:C:156:LEU:HB3	1:C:294:LEU:HD22	1.92	0.52
1:C:475:GLY:O	1:C:476:GLU:C	2.52	0.52
1:C:542:ILE:O	1:C:544:GLN:N	2.42	0.52
1:D:217:VAL:HA	1:D:220:PHE:CB	2.39	0.52
1:D:441:ARG:HA	1:D:441:ARG:NH1	2.24	0.52
1:A:47:LEU:HD13	1:A:47:LEU:O	2.10	0.52
1:A:144:ILE:HG13	1:A:145:THR:HG23	1.91	0.52
1:A:149:GLU:O	1:A:153:ILE:HD13	2.10	0.52
1:A:441:ARG:HA	1:A:441:ARG:NH1	2.23	0.52
1:A:513:THR:HG23	1:A:514:GLU:N	2.24	0.52
1:B:169:ILE:C	1:B:170:ILE:HD13	2.34	0.52
1:B:217:VAL:HA	1:B:220:PHE:CB	2.39	0.52
1:C:84:ILE:O	1:C:87:TYR:HD2	1.91	0.52
1:D:252:ASP:HB2	1:D:253:PRO:CD	2.38	0.52
1:D:428:LEU:HD23	1:D:493:ARG:NH2	2.24	0.52
1:A:67:MET:HE2	1:A:68:PRO:HG3	1.91	0.52
1:A:127:ARG:O	1:A:131:ASP:HB2	2.10	0.52
1:A:298:LEU:HD23	1:A:298:LEU:C	2.34	0.52
1:A:342:LEU:C	1:A:343:GLU:HG3	2.34	0.52
1:B:98:MET:HA	1:B:101:ARG:CD	2.40	0.52
1:B:368:ALA:HA	1:B:531:THR:HG1	1.73	0.52
1:C:167:LEU:HD12	1:C:266:VAL:HG22	1.91	0.52
1:C:342:LEU:C	1:C:343:GLU:HG3	2.34	0.52
1:C:512:ASP:HB2	1:D:378:SER:HB3	1.90	0.52
1:D:59:THR:O	1:D:60:ASP:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:LEU:HD12	1:D:266:VAL:HG22	1.91	0.52
1:D:219:ILE:HG13	1:D:220:PHE:N	2.25	0.52
1:A:20:ILE:HD12	1:A:139:SER:OG	2.10	0.52
1:A:87:TYR:CG	1:A:88:CYS:N	2.77	0.52
1:A:219:ILE:HD13	1:B:421:LEU:HB3	1.92	0.52
1:A:427:HIS:HD2	1:B:213:GLY:HA2	1.75	0.52
1:B:291:MET:HA	1:B:291:MET:HE2	1.90	0.52
1:B:347:VAL:HG13	1:B:395:ILE:CD1	2.31	0.52
1:C:242:MET:O	1:C:245:VAL:HG22	2.10	0.52
1:D:10:TRP:C	1:D:14:ARG:HB2	2.35	0.52
1:D:40:SER:O	1:D:44:MET:HG2	2.10	0.52
1:D:242:MET:O	1:D:245:VAL:HG22	2.10	0.52
1:D:426:VAL:HG11	1:D:490:ALA:HB1	1.92	0.52
1:D:475:GLY:O	1:D:476:GLU:C	2.52	0.52
1:A:242:MET:O	1:A:245:VAL:HG22	2.09	0.52
1:A:562:HIS:O	1:A:566:LEU:HB2	2.10	0.52
1:B:383:SER:OG	2:B:5002:ANP:O2B	2.16	0.52
1:B:460:MET:HA	1:B:460:MET:CE	2.38	0.52
1:C:16:LEU:O	1:C:16:LEU:HD23	2.08	0.52
1:C:279:LEU:O	1:C:283:THR:HB	2.10	0.52
1:C:388:LEU:HD23	1:C:388:LEU:O	2.10	0.52
1:C:441:ARG:NE	1:D:221:GLY:O	2.42	0.52
1:D:347:VAL:HG13	1:D:395:ILE:CD1	2.31	0.52
1:A:79:GLY:HA2	1:B:253:PRO:HB3	1.91	0.52
1:A:87:TYR:CE2	1:A:88:CYS:SG	3.03	0.52
1:A:130:TYR:CD2	1:A:200:MET:HG2	2.45	0.52
1:A:238:ARG:NE	1:B:98:MET:HB3	2.25	0.52
1:A:401:LEU:N	1:A:401:LEU:CD2	2.72	0.52
1:B:134:GLN:NE2	1:B:310:ARG:HE	2.06	0.52
1:B:388:LEU:O	1:B:388:LEU:HD23	2.10	0.52
1:C:474:ILE:HA	1:C:480:LEU:HD11	1.92	0.52
1:D:98:MET:HA	1:D:101:ARG:CD	2.40	0.52
1:D:127:ARG:O	1:D:131:ASP:HB2	2.10	0.52
1:D:144:ILE:HG13	1:D:145:THR:HG23	1.92	0.52
1:D:279:LEU:O	1:D:283:THR:HB	2.10	0.52
1:D:295:MET:O	1:D:299:LYS:HG3	2.08	0.52
1:D:368:ALA:HA	1:D:531:THR:HG1	1.73	0.52
1:D:380:SER:O	2:D:5004:ANP:O2A	2.27	0.52
1:A:62:SER:HA	1:A:66:TRP:CD1	2.44	0.52
1:A:475:GLY:N	1:A:480:LEU:HD11	2.25	0.52
1:A:548:ILE:N	1:A:548:ILE:HD12	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ILE:HG13	1:B:145:THR:HG23	1.92	0.52
1:B:298:LEU:C	1:B:298:LEU:HD23	2.34	0.52
1:B:391:ARG:C	1:B:393:TYR:H	2.18	0.52
1:C:62:SER:HA	1:C:66:TRP:CD1	2.45	0.52
1:C:226:GLU:HA	1:C:226:GLU:OE2	2.10	0.52
1:C:264:ALA:O	1:D:67:MET:SD	2.68	0.52
1:D:169:ILE:C	1:D:170:ILE:HD13	2.35	0.52
1:D:342:LEU:C	1:D:343:GLU:HG3	2.34	0.52
1:A:196:MET:O	1:A:237:MET:HE1	2.10	0.52
1:A:337:ARG:HD2	1:A:338:ALA:N	2.24	0.52
1:A:344:PHE:CE2	1:A:364:LEU:HB3	2.45	0.52
1:B:62:SER:HA	1:B:66:TRP:CD1	2.45	0.52
1:B:256:GLN:HG2	1:B:299:LYS:CD	2.40	0.52
1:B:492:ALA:O	1:B:493:ARG:C	2.53	0.52
1:D:49:LYS:O	1:D:52:LEU:HB3	2.10	0.52
1:D:67:MET:HE2	1:D:68:PRO:HG3	1.92	0.52
1:D:388:LEU:O	1:D:388:LEU:HD23	2.10	0.52
1:D:391:ARG:C	1:D:393:TYR:H	2.18	0.52
1:D:424:GLN:CD	1:D:424:GLN:N	2.68	0.52
1:A:167:LEU:HD22	1:A:167:LEU:N	2.25	0.51
1:A:217:VAL:HA	1:A:220:PHE:CB	2.40	0.51
1:A:284:ILE:O	1:A:284:ILE:HG23	2.10	0.51
1:A:342:LEU:HD22	1:A:366:ILE:HD12	1.91	0.51
1:B:58:LYS:HZ1	1:B:61:ARG:CD	2.23	0.51
1:B:104:LEU:HD11	1:B:318:LEU:HD22	1.93	0.51
1:B:127:ARG:O	1:B:131:ASP:HB2	2.10	0.51
1:B:475:GLY:O	1:B:476:GLU:C	2.52	0.51
1:C:40:SER:O	1:C:44:MET:HG2	2.10	0.51
1:D:156:LEU:HB3	1:D:294:LEU:HD22	1.92	0.51
1:D:226:GLU:HA	1:D:226:GLU:OE2	2.10	0.51
1:D:274:SER:C	1:D:276:MET:H	2.18	0.51
1:D:561:THR:HG22	1:D:563:SER:H	1.74	0.51
1:A:49:LYS:O	1:A:52:LEU:HB3	2.11	0.51
1:A:455:ARG:C	1:A:457:ALA:N	2.69	0.51
1:B:40:SER:O	1:B:44:MET:HG2	2.10	0.51
1:B:315:CYS:O	1:B:319:PHE:N	2.42	0.51
1:C:47:LEU:O	1:C:47:LEU:HD13	2.09	0.51
1:C:49:LYS:O	1:C:52:LEU:HB3	2.10	0.51
1:C:98:MET:HA	1:C:101:ARG:CD	2.40	0.51
1:D:11:GLN:O	1:D:12:THR:C	2.52	0.51
1:D:104:LEU:HD11	1:D:318:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:GLN:HG2	1:D:299:LYS:CD	2.41	0.51
1:D:302:THR:HG23	1:D:303:ASN:N	2.23	0.51
1:D:455:ARG:HH11	1:D:456:MET:CE	2.22	0.51
1:D:489:ILE:O	1:D:492:ALA:HB3	2.10	0.51
1:A:79:GLY:CA	1:B:253:PRO:HB3	2.40	0.51
1:A:198:ASN:HD22	1:A:198:ASN:N	2.08	0.51
1:A:364:LEU:HD12	1:A:365:LYS:H	1.76	0.51
1:B:149:GLU:O	1:B:153:ILE:HD13	2.11	0.51
1:B:279:LEU:O	1:B:283:THR:HB	2.10	0.51
1:B:342:LEU:C	1:B:343:GLU:HG3	2.34	0.51
1:B:424:GLN:CD	1:B:424:GLN:N	2.68	0.51
1:C:167:LEU:N	1:C:167:LEU:HD22	2.26	0.51
1:C:274:SER:C	1:C:276:MET:H	2.18	0.51
1:C:391:ARG:C	1:C:393:TYR:H	2.18	0.51
1:C:513:THR:HG22	1:D:575:LEU:HD22	1.93	0.51
1:D:62:SER:HA	1:D:66:TRP:CD1	2.45	0.51
1:D:130:TYR:CD2	1:D:200:MET:HG2	2.45	0.51
1:A:424:GLN:H	1:A:424:GLN:NE2	2.08	0.51
1:A:475:GLY:O	1:A:476:GLU:C	2.52	0.51
1:C:127:ARG:O	1:C:131:ASP:HB2	2.10	0.51
1:C:144:ILE:HG13	1:C:145:THR:HG23	1.92	0.51
1:C:169:ILE:C	1:C:170:ILE:HD13	2.35	0.51
1:C:256:GLN:HG2	1:C:299:LYS:CD	2.40	0.51
1:C:441:ARG:HA	1:C:441:ARG:NH1	2.23	0.51
1:A:89:ILE:HG23	1:A:90:SER:N	2.24	0.51
1:B:59:THR:O	1:B:60:ASP:HB2	2.09	0.51
1:B:167:LEU:HD22	1:B:167:LEU:N	2.26	0.51
1:B:274:SER:C	1:B:276:MET:H	2.18	0.51
1:C:67:MET:HE2	1:C:68:PRO:HG3	1.92	0.51
1:C:220:PHE:HZ	1:D:439:TYR:HD2	1.57	0.51
1:C:338:ALA:HB2	1:C:418:GLN:HG3	1.93	0.51
1:C:424:GLN:CD	1:C:424:GLN:N	2.68	0.51
1:C:562:HIS:O	1:C:566:LEU:HB2	2.11	0.51
1:D:198:ASN:N	1:D:198:ASN:HD22	2.09	0.51
1:A:98:MET:HA	1:A:101:ARG:CD	2.40	0.51
1:A:226:GLU:HA	1:A:226:GLU:OE2	2.09	0.51
1:A:489:ILE:O	1:A:492:ALA:HB3	2.11	0.51
1:C:59:THR:O	1:C:60:ASP:HB2	2.09	0.51
1:C:281:ALA:HA	1:C:284:ILE:HG22	1.92	0.51
1:D:346:ASN:N	1:D:363:ASN:OD1	2.38	0.51
1:D:424:GLN:H	1:D:424:GLN:NE2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:ARG:C	1:D:457:ALA:N	2.69	0.51
1:A:309:GLN:O	1:A:310:ARG:C	2.53	0.51
1:B:156:LEU:HB3	1:B:294:LEU:HD22	1.92	0.51
1:B:242:MET:O	1:B:245:VAL:HG22	2.10	0.51
1:B:263:LEU:HD13	1:B:263:LEU:O	2.11	0.51
1:B:489:ILE:O	1:B:492:ALA:HB3	2.10	0.51
1:C:475:GLY:CA	1:C:480:LEU:HG	2.41	0.51
1:D:475:GLY:CA	1:D:480:LEU:HG	2.41	0.51
1:A:63:VAL:HG13	1:B:267:LEU:O	2.10	0.51
1:A:295:MET:O	1:A:299:LYS:HG3	2.10	0.51
1:A:315:CYS:O	1:A:319:PHE:N	2.43	0.51
1:A:374:LEU:O	1:A:535:ILE:HG12	2.11	0.51
1:B:47:LEU:O	1:B:47:LEU:HD13	2.10	0.51
1:B:219:ILE:HG13	1:B:220:PHE:N	2.25	0.51
1:D:283:THR:C	1:D:285:THR:H	2.18	0.51
1:D:338:ALA:HB2	1:D:418:GLN:HG3	1.93	0.51
1:A:16:LEU:HD23	1:A:16:LEU:O	2.10	0.51
1:A:252:ASP:HB2	1:A:253:PRO:CD	2.38	0.51
1:A:362:ILE:HD13	1:A:556:ILE:HG22	1.93	0.51
1:B:10:TRP:C	1:B:14:ARG:HB2	2.35	0.51
1:B:49:LYS:O	1:B:52:LEU:HB3	2.10	0.51
1:B:167:LEU:HD12	1:B:266:VAL:HG22	1.91	0.51
1:C:378:SER:CB	1:D:512:ASP:HB2	2.40	0.51
1:C:441:ARG:CD	1:D:221:GLY:C	2.83	0.51
1:C:455:ARG:HH11	1:C:456:MET:HE2	1.76	0.51
1:C:561:THR:HG22	1:C:563:SER:H	1.74	0.51
1:A:274:SER:C	1:A:276:MET:H	2.18	0.51
1:A:339:THR:HG23	1:A:403:ASP:OD2	2.11	0.51
1:B:226:GLU:OE2	1:B:226:GLU:HA	2.10	0.51
1:B:275:VAL:O	1:B:275:VAL:HG12	2.11	0.51
1:B:302:THR:HG23	1:B:303:ASN:H	1.74	0.51
1:B:337:ARG:HD2	1:B:338:ALA:N	2.26	0.51
1:B:342:LEU:HD22	1:B:366:ILE:HD12	1.93	0.51
1:B:561:THR:HG22	1:B:562:HIS:N	2.26	0.51
1:C:198:ASN:HD22	1:C:198:ASN:N	2.09	0.51
1:C:421:LEU:HB3	1:D:219:ILE:HD13	1.92	0.51
1:C:489:ILE:O	1:C:492:ALA:HB3	2.10	0.51
1:D:167:LEU:HD22	1:D:167:LEU:N	2.26	0.51
1:A:16:LEU:HD12	1:A:315:CYS:CB	2.41	0.50
1:A:343:GLU:HB3	1:A:345:ARG:NH2	2.26	0.50
1:B:276:MET:SD	1:B:276:MET:O	2.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:LEU:N	1:B:401:LEU:CD2	2.74	0.50
1:B:562:HIS:O	1:B:566:LEU:HB2	2.11	0.50
1:C:219:ILE:HG13	1:C:220:PHE:N	2.25	0.50
1:C:492:ALA:O	1:C:493:ARG:C	2.53	0.50
1:C:493:ARG:HD3	1:C:497:ARG:NH1	2.26	0.50
1:D:149:GLU:O	1:D:153:ILE:HD13	2.11	0.50
1:D:275:VAL:O	1:D:275:VAL:HG12	2.11	0.50
1:A:156:LEU:HB3	1:A:294:LEU:HD22	1.94	0.50
1:A:193:SER:O	1:A:196:MET:HB3	2.11	0.50
1:A:279:LEU:O	1:A:283:THR:HB	2.11	0.50
1:A:558:GLU:OE1	1:A:559:ARG:N	2.44	0.50
1:B:130:TYR:CD2	1:B:200:MET:HG2	2.45	0.50
1:C:149:GLU:O	1:C:153:ILE:HD13	2.11	0.50
1:C:174:LEU:HD23	1:C:258:ILE:O	2.11	0.50
1:D:468:ASN:O	1:D:471:ASP:HB2	2.11	0.50
1:A:35:ILE:O	1:A:38:ALA:HB3	2.11	0.50
1:A:249:SER:OG	1:B:83:TYR:HA	2.10	0.50
1:B:67:MET:HE2	1:B:68:PRO:HG3	1.93	0.50
1:B:242:MET:HA	1:B:245:VAL:HG22	1.93	0.50
1:B:474:ILE:HA	1:B:480:LEU:HD11	1.91	0.50
1:C:10:TRP:C	1:C:14:ARG:HB2	2.35	0.50
1:C:276:MET:O	1:C:276:MET:SD	2.70	0.50
1:C:561:THR:HG22	1:C:562:HIS:N	2.26	0.50
1:D:342:LEU:HD22	1:D:366:ILE:HD12	1.93	0.50
1:D:492:ALA:O	1:D:493:ARG:C	2.53	0.50
1:D:493:ARG:HD3	1:D:497:ARG:NH1	2.26	0.50
1:A:120:SER:OG	1:A:205:THR:HG23	2.11	0.50
1:A:174:LEU:HD23	1:A:258:ILE:O	2.11	0.50
1:A:256:GLN:HA	1:A:299:LYS:CD	2.39	0.50
1:A:256:GLN:HG2	1:A:299:LYS:CD	2.41	0.50
1:A:283:THR:C	1:A:285:THR:H	2.19	0.50
1:A:315:CYS:SG	1:A:319:PHE:CZ	3.05	0.50
1:A:382:LYS:HB2	1:A:382:LYS:NZ	2.26	0.50
1:B:11:GLN:O	1:B:12:THR:C	2.52	0.50
1:B:343:GLU:HB3	1:B:345:ARG:NH2	2.27	0.50
1:C:283:THR:C	1:C:285:THR:H	2.18	0.50
1:D:93:SER:O	1:D:96:VAL:HG12	2.12	0.50
1:D:242:MET:HA	1:D:245:VAL:HG22	1.93	0.50
1:A:281:ALA:HB2	1:B:56:PHE:HB3	1.92	0.50
1:A:362:ILE:CD1	1:A:556:ILE:HG22	2.41	0.50
1:B:424:GLN:H	1:B:424:GLN:NE2	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:VAL:O	1:C:275:VAL:HG12	2.11	0.50
1:D:281:ALA:HA	1:D:284:ILE:HG22	1.92	0.50
1:D:337:ARG:HD2	1:D:338:ALA:N	2.26	0.50
1:D:562:HIS:O	1:D:566:LEU:HB2	2.11	0.50
1:A:194:LYS:O	1:A:197:GLN:HB2	2.12	0.50
1:A:474:ILE:HA	1:A:480:LEU:HD11	1.93	0.50
1:A:475:GLY:CA	1:A:480:LEU:HG	2.42	0.50
1:B:70:VAL:CG1	1:B:71:VAL:N	2.75	0.50
1:C:70:VAL:CG1	1:C:71:VAL:N	2.75	0.50
1:C:93:SER:O	1:C:96:VAL:HG12	2.12	0.50
1:C:130:TYR:CD2	1:C:200:MET:HG2	2.45	0.50
1:C:157:PHE:CD1	1:C:157:PHE:C	2.89	0.50
1:C:326:GLN:HB3	1:C:328:LYS:HG2	1.94	0.50
1:C:412:LEU:HD21	1:C:416:ARG:HH11	1.74	0.50
1:C:449:GLN:HB3	1:C:496:LEU:CD1	2.41	0.50
1:D:326:GLN:HB3	1:D:328:LYS:HG2	1.94	0.50
1:A:33:ALA:HB2	1:A:84:ILE:CG2	2.41	0.50
1:A:90:SER:HB3	1:B:245:VAL:HG21	1.93	0.50
1:A:169:ILE:C	1:A:170:ILE:HD13	2.37	0.50
1:A:192:ILE:HG21	1:A:244:MET:HB2	1.94	0.50
1:B:326:GLN:HB3	1:B:328:LYS:HG2	1.94	0.50
1:B:426:VAL:HG11	1:B:490:ALA:HB1	1.92	0.50
1:C:242:MET:HA	1:C:245:VAL:HG22	1.93	0.50
1:C:315:CYS:O	1:C:319:PHE:N	2.42	0.50
1:C:401:LEU:N	1:C:401:LEU:CD2	2.74	0.50
1:C:424:GLN:H	1:C:424:GLN:NE2	2.09	0.50
1:C:484:GLY:O	1:C:488:ARG:HG3	2.12	0.50
1:D:33:ALA:HB2	1:D:84:ILE:CG2	2.42	0.50
1:D:157:PHE:C	1:D:157:PHE:CD1	2.90	0.50
1:D:174:LEU:HD23	1:D:258:ILE:O	2.11	0.50
1:D:450:ILE:HG13	1:D:451:GLU:H	1.77	0.50
1:D:548:ILE:N	1:D:548:ILE:HD12	2.26	0.50
1:A:271:SER:N	1:B:63:VAL:HG11	2.27	0.50
1:A:315:CYS:SG	1:A:319:PHE:CG	3.05	0.50
1:B:174:LEU:CD2	1:B:261:LEU:HB3	2.42	0.50
1:B:281:ALA:HA	1:B:284:ILE:HG22	1.92	0.50
1:B:475:GLY:CA	1:B:480:LEU:HG	2.41	0.50
1:C:174:LEU:CD2	1:C:261:LEU:HB3	2.42	0.50
1:C:342:LEU:HD22	1:C:366:ILE:HD12	1.93	0.50
1:C:369:GLY:HA2	1:C:529:ASN:O	2.12	0.50
1:D:276:MET:SD	1:D:276:MET:O	2.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:CYS:O	1:D:319:PHE:N	2.42	0.50
1:D:455:ARG:HH11	1:D:456:MET:HE2	1.76	0.50
1:A:93:SER:O	1:A:96:VAL:HG12	2.12	0.50
1:A:280:THR:O	1:A:284:ILE:HG22	2.12	0.50
1:A:468:ASN:O	1:A:471:ASP:HB2	2.11	0.50
1:C:20:ILE:HD12	1:C:139:SER:OG	2.12	0.50
1:C:252:ASP:HB2	1:C:253:PRO:CD	2.38	0.50
1:A:460:MET:HA	1:A:460:MET:CE	2.38	0.49
1:B:104:LEU:O	1:B:105:PHE:C	2.55	0.49
1:B:157:PHE:CD1	1:B:157:PHE:C	2.89	0.49
1:B:344:PHE:HZ	1:B:385:ILE:CD1	2.25	0.49
1:B:468:ASN:O	1:B:471:ASP:HB2	2.11	0.49
1:C:281:ALA:HB2	1:D:56:PHE:CB	2.16	0.49
1:C:450:ILE:HG13	1:C:451:GLU:H	1.77	0.49
1:D:58:LYS:HZ1	1:D:61:ARG:CD	2.25	0.49
1:D:120:SER:OG	1:D:205:THR:HG23	2.12	0.49
1:D:343:GLU:HB3	1:D:345:ARG:NH2	2.27	0.49
1:D:460:MET:HA	1:D:460:MET:CE	2.38	0.49
1:A:11:GLN:O	1:A:14:ARG:N	2.45	0.49
1:A:220:PHE:HZ	1:B:439:TYR:CD2	2.27	0.49
1:B:174:LEU:HD23	1:B:258:ILE:O	2.12	0.49
1:B:192:ILE:HG21	1:B:244:MET:HB2	1.94	0.49
1:B:223:GLN:H	1:B:223:GLN:CD	2.12	0.49
1:B:369:GLY:HA2	1:B:529:ASN:O	2.12	0.49
1:B:450:ILE:HG13	1:B:451:GLU:H	1.77	0.49
1:B:455:ARG:HH11	1:B:456:MET:HE2	1.76	0.49
1:C:104:LEU:HD11	1:C:318:LEU:HD22	1.93	0.49
1:C:218:LEU:HB3	1:D:416:ARG:HD3	1.93	0.49
1:C:450:ILE:HG13	1:C:451:GLU:N	2.27	0.49
1:D:474:ILE:C	1:D:480:LEU:HD11	2.37	0.49
1:B:20:ILE:HD12	1:B:139:SER:OG	2.12	0.49
1:B:28:ILE:HG23	1:B:29:VAL:N	2.27	0.49
1:B:93:SER:O	1:B:96:VAL:HG12	2.12	0.49
1:B:198:ASN:HD22	1:B:198:ASN:N	2.09	0.49
1:B:280:THR:O	1:B:284:ILE:HG22	2.13	0.49
1:B:493:ARG:HD3	1:B:497:ARG:NH1	2.27	0.49
1:C:104:LEU:O	1:C:105:PHE:C	2.55	0.49
1:C:238:ARG:NH2	1:D:102:ARG:NH2	2.60	0.49
1:D:561:THR:HG22	1:D:562:HIS:N	2.26	0.49
1:A:220:PHE:CZ	1:B:439:TYR:HD2	2.29	0.49
1:B:338:ALA:HB2	1:B:418:GLN:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:LEU:HD21	1:B:416:ARG:HH11	1.74	0.49
1:B:450:ILE:HG13	1:B:451:GLU:N	2.27	0.49
1:B:474:ILE:C	1:B:480:LEU:HD11	2.37	0.49
1:C:263:LEU:HD13	1:C:263:LEU:O	2.11	0.49
1:C:460:MET:HA	1:C:460:MET:CE	2.38	0.49
1:C:468:ASN:O	1:C:471:ASP:HB2	2.11	0.49
1:C:558:GLU:OE1	1:C:559:ARG:N	2.46	0.49
1:D:70:VAL:CG1	1:D:71:VAL:N	2.75	0.49
1:D:263:LEU:HD13	1:D:263:LEU:O	2.11	0.49
1:D:364:LEU:HD12	1:D:365:LYS:H	1.77	0.49
1:A:104:LEU:HD11	1:A:318:LEU:HD22	1.94	0.49
1:A:326:GLN:HB3	1:A:328:LYS:CG	2.43	0.49
1:C:33:ALA:HB2	1:C:84:ILE:CG2	2.42	0.49
1:D:192:ILE:HG21	1:D:244:MET:HB2	1.93	0.49
1:A:16:LEU:CA	1:A:319:PHE:HZ	2.26	0.49
1:A:450:ILE:HG13	1:A:451:GLU:H	1.78	0.49
1:B:283:THR:C	1:B:285:THR:H	2.18	0.49
1:B:461:ASP:O	1:B:465:LYS:HG3	2.13	0.49
1:B:484:GLY:O	1:B:488:ARG:HG3	2.12	0.49
1:B:558:GLU:OE1	1:B:559:ARG:N	2.46	0.49
1:C:196:MET:O	1:C:237:MET:HE1	2.13	0.49
1:D:344:PHE:HZ	1:D:385:ILE:CD1	2.25	0.49
1:A:484:GLY:O	1:A:488:ARG:HG3	2.13	0.49
1:B:33:ALA:HB2	1:B:84:ILE:CG2	2.42	0.49
1:C:193:SER:O	1:C:196:MET:HB3	2.13	0.49
1:C:280:THR:O	1:C:284:ILE:HG22	2.13	0.49
1:D:450:ILE:HG13	1:D:451:GLU:N	2.27	0.49
1:A:242:MET:HA	1:A:245:VAL:HG22	1.94	0.49
1:A:338:ALA:HB2	1:A:418:GLN:HG3	1.94	0.49
1:A:369:GLY:HA2	1:A:529:ASN:O	2.12	0.49
1:A:377:ARG:O	1:A:379:GLY:N	2.46	0.49
1:A:548:ILE:HB	1:A:565:LEU:CD1	2.43	0.49
1:B:309:GLN:O	1:B:310:ARG:C	2.56	0.49
1:C:256:GLN:HE22	1:D:78:ARG:CG	2.25	0.49
1:C:360:ARG:O	1:C:362:ILE:HG12	2.13	0.49
1:D:28:ILE:HG23	1:D:29:VAL:N	2.27	0.49
1:D:178:VAL:HA	1:D:258:ILE:CD1	2.43	0.49
1:D:326:GLN:HB3	1:D:328:LYS:CG	2.43	0.49
1:D:484:GLY:O	1:D:488:ARG:HG3	2.12	0.49
1:A:74:LEU:O	1:A:75:MET:C	2.55	0.49
1:A:75:MET:SD	1:B:257:LEU:HD13	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLY:O	1:A:144:ILE:CG1	2.61	0.49
1:A:454:ALA:HB1	1:A:460:MET:HE3	1.95	0.49
1:B:179:SER:O	1:B:182:ILE:HG22	2.13	0.49
1:B:193:SER:O	1:B:196:MET:HB3	2.13	0.49
1:C:35:ILE:O	1:C:38:ALA:HB3	2.13	0.49
1:C:194:LYS:O	1:C:197:GLN:HB2	2.13	0.49
1:C:343:GLU:HB3	1:C:345:ARG:NH2	2.26	0.49
1:C:364:LEU:HD12	1:C:365:LYS:H	1.78	0.49
1:C:366:ILE:HG12	1:C:372:VAL:CG2	2.43	0.49
1:D:20:ILE:HD12	1:D:139:SER:OG	2.12	0.49
1:D:71:VAL:O	1:D:75:MET:HG2	2.13	0.49
1:D:548:ILE:HB	1:D:565:LEU:CD1	2.43	0.49
1:A:104:LEU:O	1:A:105:PHE:C	2.54	0.49
1:B:194:LYS:O	1:B:197:GLN:HB2	2.13	0.49
1:B:377:ARG:O	1:B:379:GLY:N	2.46	0.49
1:C:28:ILE:HG23	1:C:29:VAL:N	2.27	0.49
1:C:192:ILE:HG21	1:C:244:MET:HB2	1.94	0.49
1:C:474:ILE:C	1:C:480:LEU:HD11	2.37	0.49
1:D:194:LYS:O	1:D:197:GLN:HB2	2.13	0.49
1:A:157:PHE:CD1	1:A:157:PHE:C	2.90	0.48
1:A:450:ILE:O	1:A:451:GLU:C	2.56	0.48
1:B:360:ARG:O	1:B:362:ILE:HG12	2.13	0.48
1:C:120:SER:OG	1:C:205:THR:HG23	2.12	0.48
1:C:179:SER:O	1:C:182:ILE:HG22	2.13	0.48
1:C:326:GLN:HB3	1:C:328:LYS:CG	2.42	0.48
1:C:426:VAL:HG11	1:C:490:ALA:HB1	1.92	0.48
1:D:11:GLN:O	1:D:14:ARG:N	2.46	0.48
1:D:366:ILE:HG12	1:D:372:VAL:CG2	2.43	0.48
1:D:369:GLY:HA2	1:D:529:ASN:O	2.12	0.48
1:A:62:SER:HA	1:A:66:TRP:HD1	1.78	0.48
1:A:174:LEU:CD2	1:A:261:LEU:HB3	2.43	0.48
1:A:275:VAL:O	1:A:275:VAL:HG12	2.12	0.48
1:A:334:VAL:HG13	1:A:334:VAL:O	2.13	0.48
1:B:120:SER:OG	1:B:205:THR:HG23	2.12	0.48
1:C:87:TYR:CE2	1:C:88:CYS:SG	3.07	0.48
1:C:335:ILE:HB	1:C:410:TYR:HE1	1.79	0.48
1:D:174:LEU:CD2	1:D:261:LEU:HB3	2.42	0.48
1:D:196:MET:O	1:D:237:MET:HE1	2.13	0.48
1:D:335:ILE:HB	1:D:410:TYR:HE1	1.78	0.48
1:D:449:GLN:HB3	1:D:496:LEU:CD1	2.41	0.48
1:D:460:MET:HE2	1:D:463:ILE:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:VAL:O	1:A:75:MET:HG2	2.12	0.48
1:A:335:ILE:HB	1:A:410:TYR:HE1	1.78	0.48
1:A:441:ARG:HD3	1:B:220:PHE:C	2.38	0.48
1:B:160:MET:HE2	1:B:160:MET:HA	1.95	0.48
1:B:326:GLN:HB3	1:B:328:LYS:CG	2.43	0.48
1:B:449:GLN:HB3	1:B:496:LEU:CD1	2.41	0.48
1:B:548:ILE:HB	1:B:565:LEU:CD1	2.42	0.48
1:C:256:GLN:HA	1:C:299:LYS:CD	2.41	0.48
1:C:344:PHE:HZ	1:C:385:ILE:CD1	2.25	0.48
1:C:377:ARG:O	1:C:379:GLY:N	2.46	0.48
1:C:390:THR:CG2	1:C:419:VAL:HG11	2.42	0.48
1:A:28:ILE:HG23	1:A:29:VAL:N	2.28	0.48
1:A:326:GLN:HB3	1:A:328:LYS:HG2	1.94	0.48
1:A:450:ILE:HG13	1:A:451:GLU:N	2.28	0.48
1:B:35:ILE:O	1:B:38:ALA:HB3	2.13	0.48
1:B:460:MET:HE2	1:B:463:ILE:HB	1.95	0.48
1:C:421:LEU:HB3	1:D:219:ILE:CD1	2.44	0.48
1:C:461:ASP:O	1:C:465:LYS:HG3	2.13	0.48
1:D:377:ARG:O	1:D:379:GLY:N	2.46	0.48
1:D:390:THR:CG2	1:D:419:VAL:HG11	2.42	0.48
1:A:113:VAL:HG12	1:A:327:GLU:CD	2.38	0.48
1:A:134:GLN:NE2	1:A:310:ARG:HE	2.06	0.48
1:A:401:LEU:HD12	1:A:404:GLY:CA	2.44	0.48
1:A:419:VAL:HG23	1:A:501:ILE:O	2.13	0.48
1:A:492:ALA:O	1:A:495:LEU:N	2.45	0.48
1:B:143:LEU:HA	1:B:146:VAL:HG12	1.96	0.48
1:C:105:PHE:CZ	1:D:210:MET:HE3	2.48	0.48
1:C:213:GLY:HA2	1:D:427:HIS:HD2	1.79	0.48
1:C:292:ILE:HD12	1:D:48:LEU:CG	2.42	0.48
1:D:74:LEU:HD23	1:D:78:ARG:HB3	1.96	0.48
1:D:104:LEU:O	1:D:105:PHE:C	2.56	0.48
1:A:460:MET:HE2	1:A:463:ILE:HB	1.95	0.48
1:B:74:LEU:HD23	1:B:78:ARG:HB3	1.96	0.48
1:C:71:VAL:O	1:C:75:MET:HG2	2.13	0.48
1:C:74:LEU:HD23	1:C:78:ARG:HB3	1.96	0.48
1:C:368:ALA:HA	1:C:531:THR:HG1	1.78	0.48
1:C:382:LYS:HB2	1:C:382:LYS:NZ	2.29	0.48
1:C:475:GLY:N	1:C:480:LEU:HD11	2.29	0.48
1:C:548:ILE:HB	1:C:565:LEU:CD1	2.42	0.48
1:D:35:ILE:O	1:D:38:ALA:HB3	2.13	0.48
1:D:179:SER:O	1:D:182:ILE:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ALA:CA	1:A:273:PRO:HD2	2.44	0.48
1:A:342:LEU:CD1	1:A:366:ILE:HD12	2.43	0.48
1:A:412:LEU:HD21	1:A:416:ARG:CZ	2.44	0.48
1:C:178:VAL:HA	1:C:258:ILE:CD1	2.43	0.48
1:C:284:ILE:O	1:C:284:ILE:HG23	2.14	0.48
1:C:309:GLN:O	1:C:310:ARG:C	2.56	0.48
1:C:419:VAL:HG23	1:C:501:ILE:O	2.14	0.48
1:C:455:ARG:C	1:C:457:ALA:N	2.69	0.48
1:D:87:TYR:CE2	1:D:88:CYS:SG	3.07	0.48
1:D:143:LEU:HA	1:D:146:VAL:HG12	1.96	0.48
1:D:256:GLN:HA	1:D:299:LYS:CD	2.41	0.48
1:D:309:GLN:O	1:D:310:ARG:C	2.56	0.48
1:D:558:GLU:OE1	1:D:559:ARG:N	2.46	0.48
1:A:21:ALA:HB3	1:A:22:PRO:CD	2.35	0.48
1:A:110:GLY:O	1:A:112:PRO:HD3	2.14	0.48
1:A:344:PHE:HZ	1:A:385:ILE:HD12	1.79	0.48
1:A:412:LEU:HD21	1:A:416:ARG:HH11	1.75	0.48
1:A:421:LEU:HD13	1:A:503:ILE:HB	1.96	0.48
1:B:11:GLN:O	1:B:14:ARG:N	2.46	0.48
1:B:76:ILE:HG22	1:B:77:LEU:N	2.28	0.48
1:B:196:MET:O	1:B:237:MET:HE1	2.13	0.48
1:B:364:LEU:HD12	1:B:365:LYS:H	1.77	0.48
1:B:454:ALA:HB1	1:B:460:MET:HE3	1.96	0.48
1:D:110:GLY:O	1:D:112:PRO:HD3	2.14	0.48
1:D:269:ALA:CA	1:D:273:PRO:HD2	2.44	0.48
1:D:360:ARG:O	1:D:362:ILE:HG12	2.13	0.48
1:D:461:ASP:O	1:D:465:LYS:HG3	2.13	0.48
1:A:70:VAL:CG1	1:A:71:VAL:N	2.76	0.48
1:A:160:MET:HE2	1:A:160:MET:HA	1.94	0.48
1:A:475:GLY:H	1:A:480:LEU:HD12	1.78	0.48
1:B:269:ALA:CA	1:B:273:PRO:HD2	2.44	0.48
1:C:11:GLN:O	1:C:14:ARG:N	2.46	0.48
1:C:74:LEU:O	1:C:75:MET:C	2.57	0.48
1:C:165:TRP:CH2	1:C:166:GLN:HG2	2.49	0.48
1:C:214:HIS:O	1:C:215:LYS:C	2.57	0.48
1:C:220:PHE:O	1:D:441:ARG:HG2	2.13	0.48
1:D:74:LEU:O	1:D:75:MET:C	2.57	0.48
1:D:134:GLN:NE2	1:D:310:ARG:HE	2.06	0.48
1:D:280:THR:O	1:D:284:ILE:HG22	2.13	0.48
1:D:523:LEU:O	1:D:527:GLN:HG2	2.14	0.48
1:A:74:LEU:HD23	1:A:78:ARG:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:PRO:O	1:A:277:ASP:O	2.32	0.48
1:A:437:ILE:HG23	1:A:493:ARG:HA	1.96	0.48
1:A:475:GLY:O	1:A:478:GLY:N	2.47	0.48
1:B:71:VAL:O	1:B:75:MET:HG2	2.13	0.48
1:B:366:ILE:HG12	1:B:372:VAL:CG2	2.43	0.48
1:B:561:THR:O	1:B:562:HIS:C	2.57	0.48
1:C:76:ILE:HG22	1:C:77:LEU:N	2.28	0.48
1:D:193:SER:O	1:D:196:MET:HB3	2.13	0.48
1:D:454:ALA:HB1	1:D:460:MET:HE3	1.96	0.48
1:A:561:THR:O	1:A:562:HIS:C	2.57	0.47
1:B:87:TYR:CE2	1:B:88:CYS:SG	3.07	0.47
1:B:254:ILE:O	1:B:257:LEU:HB3	2.14	0.47
1:B:577:LYS:C	1:B:579:GLN:N	2.72	0.47
1:C:110:GLY:O	1:C:112:PRO:HD3	2.14	0.47
1:C:160:MET:HA	1:C:160:MET:HE2	1.95	0.47
1:D:160:MET:HE2	1:D:160:MET:HA	1.95	0.47
1:A:165:TRP:CH2	1:A:166:GLN:HG2	2.49	0.47
1:A:411:THR:O	1:A:412:LEU:C	2.57	0.47
1:B:113:VAL:HG12	1:B:327:GLU:CD	2.39	0.47
1:B:335:ILE:HB	1:B:410:TYR:HE1	1.78	0.47
1:C:432:THR:HB	1:C:470:LEU:O	2.15	0.47
1:C:467:ASP:O	1:C:468:ASN:CB	2.62	0.47
1:D:113:VAL:HG12	1:D:327:GLU:CD	2.39	0.47
1:D:467:ASP:O	1:D:468:ASN:CB	2.62	0.47
1:A:235:ASN:C	1:A:237:MET:N	2.73	0.47
1:A:276:MET:O	1:A:276:MET:SD	2.72	0.47
1:A:348:THR:HG23	1:A:360:ARG:HA	1.96	0.47
1:B:21:ALA:HB3	1:B:22:PRO:CD	2.36	0.47
1:B:70:VAL:HG13	1:B:71:VAL:N	2.29	0.47
1:C:254:ILE:O	1:C:257:LEU:HB3	2.14	0.47
1:D:165:TRP:CH2	1:D:166:GLN:HG2	2.49	0.47
1:D:334:VAL:O	1:D:334:VAL:HG13	2.14	0.47
1:D:466:MET:HE2	1:D:472:THR:CG2	2.37	0.47
1:A:52:LEU:HD11	1:B:289:SER:HB2	1.96	0.47
1:A:197:GLN:O	1:A:198:ASN:C	2.57	0.47
1:A:461:ASP:O	1:A:465:LYS:HG3	2.14	0.47
1:B:541:THR:O	1:B:542:ILE:HG13	2.13	0.47
1:C:252:ASP:CB	1:C:253:PRO:HD3	2.42	0.47
1:C:412:LEU:HD21	1:C:416:ARG:CZ	2.44	0.47
1:D:76:ILE:HG22	1:D:77:LEU:N	2.28	0.47
1:A:179:SER:O	1:A:182:ILE:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLY:C	1:B:441:ARG:CD	2.87	0.47
1:B:110:GLY:O	1:B:112:PRO:HD3	2.14	0.47
1:B:178:VAL:HA	1:B:258:ILE:CD1	2.43	0.47
1:B:334:VAL:O	1:B:334:VAL:HG13	2.15	0.47
1:C:62:SER:HA	1:C:66:TRP:HD1	1.80	0.47
1:C:185:VAL:HG12	1:C:189:PHE:CE2	2.50	0.47
1:C:475:GLY:O	1:C:478:GLY:N	2.47	0.47
1:C:482:SER:HB2	2:D:5004:ANP:H5'1	1.96	0.47
1:D:284:ILE:O	1:D:284:ILE:HG23	2.14	0.47
1:D:372:VAL:O	1:D:533:LEU:HD22	2.15	0.47
1:D:382:LYS:HB2	1:D:382:LYS:NZ	2.29	0.47
1:A:143:LEU:HA	1:A:146:VAL:HG12	1.96	0.47
1:A:475:GLY:N	1:A:480:LEU:HD12	2.30	0.47
1:B:74:LEU:O	1:B:75:MET:C	2.57	0.47
1:B:192:ILE:HG22	1:B:244:MET:HB2	1.97	0.47
1:B:273:PRO:O	1:B:276:MET:HB3	2.15	0.47
1:B:466:MET:HE2	1:B:472:THR:CG2	2.37	0.47
1:C:339:THR:HG23	1:C:403:ASP:OD2	2.15	0.47
1:C:342:LEU:CD1	1:C:366:ILE:HD12	2.44	0.47
1:C:523:LEU:O	1:C:527:GLN:HG2	2.14	0.47
1:D:21:ALA:HB3	1:D:22:PRO:CD	2.36	0.47
1:D:339:THR:HG23	1:D:403:ASP:OD2	2.15	0.47
1:D:342:LEU:CD1	1:D:366:ILE:HD12	2.44	0.47
1:D:419:VAL:HG23	1:D:501:ILE:O	2.14	0.47
1:A:221:GLY:O	1:B:441:ARG:CD	2.63	0.47
1:A:441:ARG:HA	1:A:441:ARG:HD2	1.69	0.47
1:A:577:LYS:C	1:A:579:GLN:N	2.72	0.47
1:B:89:ILE:CD1	1:B:144:ILE:HD13	2.45	0.47
1:B:141:GLY:O	1:B:144:ILE:CG1	2.63	0.47
1:B:185:VAL:HG12	1:B:189:PHE:CE2	2.50	0.47
1:B:256:GLN:HA	1:B:299:LYS:CD	2.41	0.47
1:B:506:GLU:N	1:B:535:ILE:O	2.48	0.47
1:C:98:MET:HA	1:C:101:ARG:HD3	1.97	0.47
1:C:235:ASN:C	1:C:237:MET:N	2.73	0.47
1:C:269:ALA:CA	1:C:273:PRO:HD2	2.44	0.47
1:C:308:PHE:C	1:C:308:PHE:CD1	2.93	0.47
1:C:348:THR:HG23	1:C:360:ARG:HA	1.97	0.47
1:C:372:VAL:O	1:C:533:LEU:HD22	2.15	0.47
1:C:427:HIS:CD2	1:D:213:GLY:HA2	2.49	0.47
1:C:460:MET:HE2	1:C:463:ILE:HB	1.95	0.47
1:D:185:VAL:HG12	1:D:189:PHE:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:PRO:O	1:D:276:MET:HB3	2.15	0.47
1:D:308:PHE:CD1	1:D:308:PHE:C	2.93	0.47
1:D:348:THR:HG23	1:D:360:ARG:HA	1.97	0.47
1:D:475:GLY:N	1:D:480:LEU:HD11	2.29	0.47
1:D:492:ALA:O	1:D:495:LEU:N	2.47	0.47
1:A:512:ASP:HB3	1:A:515:SER:OG	2.15	0.47
1:B:16:LEU:CA	1:B:319:PHE:HZ	2.27	0.47
1:B:98:MET:HA	1:B:101:ARG:HD3	1.96	0.47
1:B:284:ILE:O	1:B:284:ILE:HG23	2.14	0.47
1:B:308:PHE:CD1	1:B:308:PHE:C	2.93	0.47
1:B:354:ARG:C	1:B:355:GLU:HG3	2.39	0.47
1:B:475:GLY:N	1:B:480:LEU:HD11	2.29	0.47
1:C:113:VAL:HG12	1:C:327:GLU:CD	2.39	0.47
1:C:421:LEU:HD13	1:C:503:ILE:HB	1.97	0.47
1:D:98:MET:HA	1:D:101:ARG:HD3	1.97	0.47
1:D:254:ILE:O	1:D:257:LEU:HB3	2.14	0.47
1:A:449:GLN:HB3	1:A:496:LEU:CD1	2.44	0.47
1:A:542:ILE:C	1:A:544:GLN:N	2.73	0.47
1:B:214:HIS:O	1:B:215:LYS:C	2.57	0.47
1:B:475:GLY:O	1:B:478:GLY:N	2.47	0.47
1:C:21:ALA:HB3	1:C:22:PRO:CD	2.36	0.47
1:C:89:ILE:CD1	1:C:144:ILE:HD13	2.45	0.47
1:C:273:PRO:O	1:C:276:MET:HB3	2.15	0.47
1:C:512:ASP:HB3	1:C:515:SER:OG	2.14	0.47
1:C:543:GLU:HG2	1:C:562:HIS:CE1	2.50	0.47
1:D:354:ARG:C	1:D:355:GLU:HG3	2.39	0.47
1:D:512:ASP:HB3	1:D:515:SER:OG	2.14	0.47
1:A:11:GLN:CG	1:A:12:THR:N	2.59	0.47
1:A:433:VAL:O	1:A:434:ALA:C	2.58	0.47
1:B:165:TRP:CH2	1:B:166:GLN:HG2	2.49	0.47
1:B:372:VAL:O	1:B:533:LEU:HD22	2.15	0.47
1:C:132:SER:O	1:C:135:VAL:HG12	2.15	0.47
1:C:221:GLY:O	1:D:441:ARG:NE	2.48	0.47
1:C:334:VAL:HG13	1:C:334:VAL:O	2.15	0.47
1:D:192:ILE:HG22	1:D:244:MET:HB2	1.97	0.47
1:A:96:VAL:O	1:A:99:THR:HG22	2.15	0.46
1:A:219:ILE:O	1:A:220:PHE:C	2.58	0.46
1:B:17:TRP:N	1:B:18:PRO:CD	2.79	0.46
1:B:342:LEU:CD1	1:B:366:ILE:HD12	2.44	0.46
1:B:348:THR:HG23	1:B:360:ARG:HA	1.97	0.46
1:B:419:VAL:HG23	1:B:501:ILE:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:ASP:O	1:B:468:ASN:CB	2.63	0.46
1:B:523:LEU:O	1:B:527:GLN:HG2	2.14	0.46
1:C:354:ARG:C	1:C:355:GLU:HG3	2.39	0.46
1:D:70:VAL:HG13	1:D:71:VAL:N	2.29	0.46
1:D:89:ILE:CD1	1:D:144:ILE:HD13	2.45	0.46
1:D:401:LEU:HD12	1:D:404:GLY:CA	2.45	0.46
1:D:475:GLY:O	1:D:478:GLY:N	2.47	0.46
1:D:565:LEU:HD13	1:D:572:TYR:CD2	2.50	0.46
1:A:390:THR:CG2	1:A:419:VAL:HG11	2.43	0.46
1:A:496:LEU:HD12	1:A:496:LEU:O	2.15	0.46
1:A:523:LEU:O	1:A:527:GLN:HG2	2.16	0.46
1:A:557:VAL:O	1:A:557:VAL:CG1	2.64	0.46
1:B:450:ILE:O	1:B:451:GLU:C	2.58	0.46
1:B:565:LEU:HD13	1:B:572:TYR:CD2	2.50	0.46
1:C:70:VAL:HG13	1:C:71:VAL:N	2.29	0.46
1:C:221:GLY:O	1:D:441:ARG:CD	2.63	0.46
1:C:401:LEU:HD12	1:C:404:GLY:CA	2.45	0.46
1:C:454:ALA:HB1	1:C:460:MET:HE3	1.96	0.46
1:C:520:GLN:HA	1:C:520:GLN:NE2	2.30	0.46
1:D:17:TRP:N	1:D:18:PRO:CD	2.79	0.46
1:D:214:HIS:O	1:D:215:LYS:C	2.57	0.46
1:A:214:HIS:O	1:A:215:LYS:C	2.58	0.46
1:A:296:ARG:HD3	1:A:297:PRO:N	2.31	0.46
1:A:316:GLN:NE2	1:A:319:PHE:CD1	2.83	0.46
1:A:316:GLN:CD	1:A:319:PHE:CD1	2.93	0.46
1:A:372:VAL:O	1:A:533:LEU:HD22	2.15	0.46
1:B:132:SER:O	1:B:135:VAL:HG12	2.15	0.46
1:B:256:GLN:HG2	1:B:299:LYS:HD2	1.98	0.46
1:B:339:THR:HG23	1:B:403:ASP:OD2	2.15	0.46
1:B:344:PHE:HB2	1:B:400:ILE:HA	1.97	0.46
1:B:520:GLN:NE2	1:B:520:GLN:HA	2.30	0.46
1:B:561:THR:C	1:B:563:SER:N	2.73	0.46
1:C:267:LEU:CD2	1:D:67:MET:HA	2.44	0.46
1:D:421:LEU:HD13	1:D:503:ILE:HB	1.97	0.46
1:D:543:GLU:HG2	1:D:562:HIS:CE1	2.50	0.46
1:A:64:LEU:HB2	1:B:271:SER:OG	2.15	0.46
1:A:76:ILE:HG22	1:A:77:LEU:N	2.29	0.46
1:A:89:ILE:CD1	1:A:144:ILE:HD13	2.46	0.46
1:A:344:PHE:HB2	1:A:400:ILE:HA	1.96	0.46
1:A:426:VAL:HG11	1:A:490:ALA:HB1	1.94	0.46
1:B:252:ASP:CB	1:B:253:PRO:HD3	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:LEU:HD13	1:B:503:ILE:HB	1.97	0.46
1:B:512:ASP:HB3	1:B:515:SER:OG	2.14	0.46
1:C:17:TRP:N	1:C:18:PRO:CD	2.79	0.46
1:D:16:LEU:CA	1:D:319:PHE:HZ	2.28	0.46
1:D:132:SER:O	1:D:135:VAL:HG12	2.15	0.46
1:D:197:GLN:O	1:D:198:ASN:C	2.59	0.46
1:D:432:THR:HB	1:D:470:LEU:O	2.15	0.46
1:A:308:PHE:CD1	1:A:308:PHE:C	2.93	0.46
1:C:192:ILE:HG22	1:C:244:MET:HB2	1.97	0.46
1:C:344:PHE:HB2	1:C:400:ILE:HA	1.97	0.46
1:C:535:ILE:O	1:C:535:ILE:CD1	2.62	0.46
1:C:542:ILE:C	1:C:544:GLN:N	2.74	0.46
1:D:541:THR:O	1:D:542:ILE:HG13	2.15	0.46
1:A:164:SER:HG	1:A:167:LEU:HD23	1.81	0.46
1:A:185:VAL:HG12	1:A:189:PHE:CE2	2.50	0.46
1:A:506:GLU:N	1:A:535:ILE:O	2.48	0.46
1:A:543:GLU:HG2	1:A:562:HIS:CE1	2.51	0.46
1:B:543:GLU:HG2	1:B:562:HIS:CE1	2.50	0.46
1:C:143:LEU:HA	1:C:146:VAL:HG12	1.96	0.46
1:C:535:ILE:HD13	1:C:535:ILE:C	2.41	0.46
1:C:577:LYS:C	1:C:579:GLN:N	2.72	0.46
1:D:412:LEU:HD21	1:D:416:ARG:CZ	2.44	0.46
1:A:217:VAL:O	1:A:217:VAL:HG12	2.16	0.46
1:A:331:GLY:C	1:A:332:LYS:HG3	2.41	0.46
1:A:535:ILE:O	1:A:535:ILE:CD1	2.61	0.46
1:B:432:THR:HB	1:B:470:LEU:O	2.15	0.46
1:B:542:ILE:C	1:B:544:GLN:N	2.74	0.46
1:C:16:LEU:CA	1:C:319:PHE:HZ	2.27	0.46
1:C:492:ALA:O	1:C:495:LEU:N	2.47	0.46
1:C:541:THR:O	1:C:542:ILE:HG13	2.15	0.46
1:D:256:GLN:HG2	1:D:299:LYS:HD2	1.98	0.46
1:D:326:GLN:O	1:D:328:LYS:N	2.49	0.46
1:D:437:ILE:HG23	1:D:493:ARG:HA	1.98	0.46
1:D:520:GLN:HA	1:D:520:GLN:NE2	2.30	0.46
1:A:63:VAL:HG11	1:B:271:SER:CA	2.46	0.46
1:A:98:MET:HA	1:A:101:ARG:HD3	1.97	0.46
1:A:112:PRO:O	1:A:113:VAL:CG1	2.60	0.46
1:A:131:ASP:CB	1:A:318:LEU:HD23	2.46	0.46
1:A:132:SER:O	1:A:135:VAL:HG12	2.16	0.46
1:A:366:ILE:HG12	1:A:372:VAL:CG2	2.42	0.46
1:A:427:HIS:CD2	1:B:213:GLY:HA2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:GLN:HA	1:A:520:GLN:NE2	2.29	0.46
1:B:16:LEU:HD12	1:B:315:CYS:CB	2.46	0.46
1:B:235:ASN:C	1:B:237:MET:N	2.73	0.46
1:C:141:GLY:O	1:C:144:ILE:CG1	2.63	0.46
1:D:112:PRO:O	1:D:113:VAL:CG1	2.62	0.46
1:A:326:GLN:O	1:A:328:LYS:N	2.49	0.46
1:B:382:LYS:HB2	1:B:382:LYS:NZ	2.30	0.46
1:B:437:ILE:HG23	1:B:493:ARG:HA	1.98	0.46
1:C:67:MET:SD	1:D:264:ALA:O	2.73	0.46
1:C:256:GLN:HE22	1:D:78:ARG:HG2	1.80	0.46
1:C:437:ILE:HG23	1:C:493:ARG:HA	1.98	0.46
1:C:450:ILE:O	1:C:451:GLU:C	2.58	0.46
1:D:62:SER:HA	1:D:66:TRP:HD1	1.80	0.46
1:D:344:PHE:HB2	1:D:400:ILE:HA	1.97	0.46
1:A:108:MET:O	1:A:111:MET:HB2	2.16	0.46
1:A:218:LEU:N	1:A:218:LEU:HD12	2.31	0.46
1:A:223:GLN:O	1:A:226:GLU:HB2	2.16	0.46
1:A:354:ARG:C	1:A:355:GLU:HG3	2.41	0.46
1:A:432:THR:HB	1:A:470:LEU:O	2.16	0.46
1:A:459:ALA:HB1	1:A:462:PHE:CE1	2.51	0.46
1:C:96:VAL:O	1:C:99:THR:HG22	2.16	0.46
1:C:561:THR:O	1:C:562:HIS:C	2.57	0.46
1:D:506:GLU:N	1:D:535:ILE:O	2.48	0.46
1:A:70:VAL:HG13	1:A:71:VAL:N	2.30	0.45
1:A:344:PHE:HZ	1:A:385:ILE:CD1	2.29	0.45
1:B:62:SER:HA	1:B:66:TRP:HD1	1.79	0.45
1:B:401:LEU:HD12	1:B:404:GLY:CA	2.45	0.45
1:C:10:TRP:O	1:C:11:GLN:HB3	2.16	0.45
1:C:145:THR:HA	1:C:148:ARG:HB3	1.98	0.45
1:C:565:LEU:HD13	1:C:572:TYR:CD2	2.50	0.45
1:D:219:ILE:O	1:D:220:PHE:C	2.59	0.45
1:D:401:LEU:N	1:D:401:LEU:CD2	2.74	0.45
1:D:450:ILE:O	1:D:451:GLU:C	2.58	0.45
1:A:63:VAL:HG12	1:A:64:LEU:N	2.30	0.45
1:A:96:VAL:C	1:A:99:THR:HG22	2.41	0.45
1:A:108:MET:HE1	1:A:124:LEU:CB	2.45	0.45
1:A:254:ILE:O	1:A:257:LEU:HB3	2.16	0.45
1:A:273:PRO:O	1:A:276:MET:HB3	2.17	0.45
1:A:474:ILE:CG1	1:A:475:GLY:N	2.80	0.45
1:B:11:GLN:CA	1:B:14:ARG:HB3	2.46	0.45
1:B:296:ARG:HD3	1:B:297:PRO:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:ILE:HD13	1:B:535:ILE:C	2.41	0.45
1:C:326:GLN:O	1:C:328:LYS:N	2.49	0.45
1:C:349:PHE:HA	1:C:396:ASP:HB3	1.97	0.45
1:C:572:TYR:C	1:C:572:TYR:CD1	2.94	0.45
1:A:343:GLU:HB3	1:A:345:ARG:HH21	1.81	0.45
1:A:437:ILE:O	1:A:440:ALA:HB3	2.16	0.45
1:B:10:TRP:O	1:B:11:GLN:HB3	2.16	0.45
1:B:326:GLN:O	1:B:328:LYS:N	2.49	0.45
1:B:412:LEU:HD21	1:B:416:ARG:CZ	2.44	0.45
1:B:441:ARG:HA	1:B:441:ARG:HD2	1.60	0.45
1:C:463:ILE:O	1:C:466:MET:HG2	2.17	0.45
1:A:118:LYS:NZ	1:A:352:PRO:HG3	2.32	0.45
1:A:174:LEU:HD22	1:A:262:ALA:CB	2.40	0.45
1:A:192:ILE:HG22	1:A:244:MET:HB2	1.98	0.45
1:A:558:GLU:CD	1:A:559:ARG:N	2.74	0.45
1:B:190:ARG:HA	1:B:313:ALA:HB2	1.98	0.45
1:B:508:THR:O	1:B:510:ALA:N	2.50	0.45
1:C:197:GLN:O	1:C:198:ASN:C	2.59	0.45
1:C:296:ARG:HD3	1:C:297:PRO:N	2.31	0.45
1:C:439:TYR:HD2	1:D:220:PHE:HZ	1.63	0.45
1:C:441:ARG:HD3	1:D:221:GLY:C	2.37	0.45
1:D:207:ALA:O	1:D:210:MET:HB3	2.17	0.45
1:D:366:ILE:HG23	1:D:372:VAL:HG23	1.99	0.45
1:A:112:PRO:O	1:A:327:GLU:OE1	2.34	0.45
1:A:277:ASP:C	1:A:279:LEU:H	2.25	0.45
1:A:467:ASP:O	1:A:468:ASN:CB	2.61	0.45
1:A:565:LEU:HD13	1:A:572:TYR:CD2	2.51	0.45
1:A:572:TYR:CD1	1:A:572:TYR:C	2.94	0.45
1:B:277:ASP:C	1:B:279:LEU:H	2.24	0.45
1:C:219:ILE:O	1:C:220:PHE:C	2.59	0.45
1:C:343:GLU:HB3	1:C:345:ARG:HH21	1.81	0.45
1:D:96:VAL:O	1:D:99:THR:HG22	2.16	0.45
1:D:441:ARG:HA	1:D:441:ARG:HD2	1.62	0.45
1:D:561:THR:O	1:D:562:HIS:C	2.57	0.45
1:A:190:ARG:HA	1:A:313:ALA:HB2	1.97	0.45
1:A:315:CYS:SG	1:A:319:PHE:CE2	3.10	0.45
1:A:401:LEU:HD12	1:A:404:GLY:C	2.42	0.45
1:B:207:ALA:O	1:B:210:MET:HB3	2.17	0.45
1:B:219:ILE:O	1:B:220:PHE:C	2.59	0.45
1:B:558:GLU:CD	1:B:559:ARG:N	2.75	0.45
1:C:74:LEU:HD23	1:C:74:LEU:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:LEU:HD23	1:C:171:LEU:C	2.41	0.45
1:C:175:ALA:N	1:C:176:PRO:CD	2.80	0.45
1:C:253:PRO:HG3	1:D:79:GLY:HA2	1.99	0.45
1:A:75:MET:CE	1:B:257:LEU:HA	2.46	0.45
1:A:252:ASP:CB	1:A:253:PRO:HD3	2.44	0.45
1:B:74:LEU:HD23	1:B:74:LEU:C	2.42	0.45
1:B:431:ASP:HB3	1:B:435:ASN:HB2	1.99	0.45
1:B:463:ILE:O	1:B:466:MET:HG2	2.17	0.45
1:B:492:ALA:O	1:B:495:LEU:N	2.47	0.45
1:B:535:ILE:O	1:B:535:ILE:CD1	2.62	0.45
1:C:16:LEU:HD12	1:C:315:CYS:CB	2.46	0.45
1:C:164:SER:HG	1:C:167:LEU:HD23	1.82	0.45
1:C:273:PRO:O	1:C:277:ASP:O	2.35	0.45
1:C:347:VAL:HG13	1:C:395:ILE:CD1	2.31	0.45
1:C:439:TYR:O	1:D:220:PHE:CE1	2.69	0.45
1:D:74:LEU:HD23	1:D:74:LEU:C	2.42	0.45
1:D:164:SER:HG	1:D:167:LEU:HD23	1.80	0.45
1:D:171:LEU:HD23	1:D:171:LEU:C	2.41	0.45
1:D:235:ASN:C	1:D:237:MET:N	2.73	0.45
1:D:277:ASP:C	1:D:279:LEU:H	2.24	0.45
1:D:299:LYS:CB	1:D:299:LYS:HZ2	2.29	0.45
1:D:339:THR:HG23	1:D:339:THR:O	2.17	0.45
1:D:431:ASP:HB3	1:D:435:ASN:HB2	1.99	0.45
1:D:459:ALA:HB1	1:D:462:PHE:CE1	2.52	0.45
1:A:141:GLY:C	1:A:144:ILE:HG12	2.42	0.45
1:A:178:VAL:CA	1:A:258:ILE:HD13	2.45	0.45
1:B:273:PRO:O	1:B:277:ASP:O	2.35	0.45
1:B:343:GLU:HB3	1:B:345:ARG:HH21	1.81	0.45
1:B:572:TYR:CD1	1:B:572:TYR:C	2.94	0.45
1:D:10:TRP:O	1:D:11:GLN:HB3	2.16	0.45
1:D:11:GLN:CA	1:D:14:ARG:HB3	2.46	0.45
1:D:74:LEU:O	1:D:78:ARG:HB3	2.17	0.45
1:D:190:ARG:HA	1:D:313:ALA:HB2	1.98	0.45
1:D:273:PRO:O	1:D:277:ASP:O	2.35	0.45
1:D:296:ARG:HD3	1:D:297:PRO:N	2.31	0.45
1:D:572:TYR:CD1	1:D:572:TYR:C	2.94	0.45
1:A:11:GLN:C	1:A:14:ARG:HB3	2.42	0.45
1:A:74:LEU:HD23	1:A:74:LEU:C	2.42	0.45
1:A:437:ILE:HA	1:A:493:ARG:HB2	1.99	0.45
1:A:466:MET:HE2	1:A:472:THR:CG2	2.39	0.45
1:A:508:THR:O	1:A:510:ALA:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:ILE:HG23	1:A:535:ILE:O	2.16	0.45
1:B:96:VAL:O	1:B:99:THR:HG22	2.16	0.45
1:B:108:MET:HE1	1:B:124:LEU:CB	2.45	0.45
1:B:197:GLN:O	1:B:198:ASN:C	2.59	0.45
1:C:337:ARG:HD2	1:C:338:ALA:N	2.26	0.45
1:C:508:THR:O	1:C:510:ALA:N	2.50	0.45
1:C:512:ASP:HB3	1:C:515:SER:CB	2.47	0.45
1:C:558:GLU:CD	1:C:559:ARG:N	2.75	0.45
1:D:331:GLY:C	1:D:332:LYS:HG3	2.41	0.45
1:A:145:THR:HA	1:A:148:ARG:HB3	1.99	0.45
1:A:197:GLN:O	1:A:200:MET:N	2.50	0.45
1:B:111:MET:HE1	1:B:325:GLU:O	2.16	0.45
1:B:217:VAL:O	1:B:217:VAL:HG12	2.17	0.45
1:B:223:GLN:O	1:B:226:GLU:HB2	2.17	0.45
1:B:382:LYS:HB2	1:B:382:LYS:HZ2	1.81	0.45
1:C:207:ALA:O	1:C:210:MET:HB3	2.17	0.45
1:C:439:TYR:HB3	1:D:220:PHE:HZ	1.75	0.45
1:D:16:LEU:HD12	1:D:315:CYS:CB	2.46	0.45
1:D:175:ALA:N	1:D:176:PRO:CD	2.80	0.45
1:D:468:ASN:HB2	1:D:472:THR:OG1	2.17	0.45
1:D:535:ILE:HD13	1:D:535:ILE:C	2.41	0.45
1:A:93:SER:OG	1:A:94:GLY:N	2.50	0.44
1:A:249:SER:HB2	1:B:86:SER:CB	2.47	0.44
1:A:316:GLN:OE1	1:A:316:GLN:HA	2.17	0.44
1:A:445:TYR:HD2	1:A:496:LEU:HD21	1.83	0.44
1:A:468:ASN:HB2	1:A:472:THR:OG1	2.17	0.44
1:B:96:VAL:C	1:B:99:THR:HG22	2.42	0.44
1:B:339:THR:HG23	1:B:339:THR:O	2.17	0.44
1:B:431:ASP:HB3	1:B:432:THR:H	1.46	0.44
1:B:459:ALA:HB1	1:B:462:PHE:CE1	2.52	0.44
1:B:468:ASN:HB2	1:B:472:THR:OG1	2.17	0.44
1:C:256:GLN:HG2	1:C:299:LYS:HD2	1.98	0.44
1:C:260:SER:OG	1:D:74:LEU:HD13	2.17	0.44
1:C:331:GLY:C	1:C:332:LYS:HG3	2.41	0.44
1:C:395:ILE:CG1	1:C:396:ASP:H	2.14	0.44
1:D:316:GLN:OE1	1:D:316:GLN:HA	2.17	0.44
1:D:391:ARG:C	1:D:393:TYR:N	2.75	0.44
1:A:56:PHE:HD2	1:B:274:SER:HG	1.65	0.44
1:B:390:THR:CG2	1:B:419:VAL:HG11	2.42	0.44
1:C:561:THR:C	1:C:563:SER:N	2.73	0.44
1:D:108:MET:O	1:D:111:MET:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:GLU:HB3	1:D:345:ARG:HH21	1.81	0.44
1:D:455:ARG:HD2	1:D:456:MET:CE	2.46	0.44
1:D:558:GLU:CD	1:D:559:ARG:N	2.75	0.44
1:A:37:ASN:HD22	1:A:37:ASN:HA	1.53	0.44
1:A:178:VAL:HA	1:A:258:ILE:CD1	2.42	0.44
1:A:209:GLN:O	1:A:210:MET:C	2.60	0.44
1:A:322:LEU:HD23	1:A:322:LEU:C	2.42	0.44
1:B:109:MET:C	1:B:111:MET:H	2.26	0.44
1:B:171:LEU:HD23	1:B:171:LEU:C	2.41	0.44
1:B:331:GLY:C	1:B:332:LYS:HG3	2.41	0.44
1:C:10:TRP:CG	1:C:11:GLN:N	2.85	0.44
1:C:108:MET:O	1:C:111:MET:HB2	2.17	0.44
1:C:111:MET:HE1	1:C:325:GLU:O	2.16	0.44
1:C:277:ASP:C	1:C:279:LEU:H	2.24	0.44
1:C:437:ILE:O	1:C:440:ALA:HB3	2.18	0.44
1:C:506:GLU:N	1:C:535:ILE:O	2.48	0.44
1:D:111:MET:HE1	1:D:325:GLU:O	2.16	0.44
1:D:463:ILE:O	1:D:466:MET:HG2	2.17	0.44
1:A:520:GLN:HA	1:A:520:GLN:HE21	1.82	0.44
1:A:539:LEU:HA	1:A:542:ILE:CD1	2.31	0.44
1:B:10:TRP:CG	1:B:11:GLN:N	2.85	0.44
1:C:96:VAL:C	1:C:99:THR:HG22	2.42	0.44
1:C:223:GLN:O	1:C:226:GLU:HB2	2.18	0.44
1:C:468:ASN:HB2	1:C:472:THR:OG1	2.17	0.44
1:D:10:TRP:CG	1:D:11:GLN:N	2.85	0.44
1:D:96:VAL:C	1:D:99:THR:HG22	2.42	0.44
1:A:512:ASP:HB2	1:B:378:SER:CB	2.48	0.44
1:A:512:ASP:HB3	1:A:515:SER:CB	2.47	0.44
1:B:74:LEU:O	1:B:78:ARG:HB3	2.17	0.44
1:B:142:ALA:HB1	1:B:308:PHE:HD2	1.83	0.44
1:B:145:THR:HA	1:B:148:ARG:HB3	1.98	0.44
1:B:411:THR:O	1:B:412:LEU:C	2.60	0.44
1:C:11:GLN:CA	1:C:14:ARG:HB3	2.46	0.44
1:C:74:LEU:O	1:C:78:ARG:HB3	2.17	0.44
1:C:97:VAL:CG1	1:C:98:MET:N	2.81	0.44
1:D:141:GLY:O	1:D:144:ILE:CG1	2.63	0.44
1:D:145:THR:HA	1:D:148:ARG:HB3	1.98	0.44
1:D:218:LEU:N	1:D:218:LEU:HD12	2.32	0.44
1:D:380:SER:O	1:D:382:LYS:N	2.49	0.44
1:A:111:MET:HE1	1:A:325:GLU:O	2.17	0.44
1:A:256:GLN:HG2	1:A:299:LYS:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ILE:HG23	1:A:372:VAL:HG23	2.00	0.44
1:A:558:GLU:CD	1:A:558:GLU:C	2.86	0.44
1:B:437:ILE:O	1:B:440:ALA:HB3	2.17	0.44
1:B:512:ASP:HB3	1:B:515:SER:CB	2.47	0.44
1:B:557:VAL:O	1:B:557:VAL:CG1	2.66	0.44
1:C:238:ARG:HG3	1:D:95:LYS:NZ	2.33	0.44
1:C:339:THR:HG23	1:C:339:THR:O	2.17	0.44
1:D:508:THR:HG22	1:D:538:ARG:NH2	2.33	0.44
1:A:315:CYS:SG	1:A:319:PHE:CD2	3.10	0.44
1:A:431:ASP:HB3	1:A:435:ASN:HB2	1.98	0.44
1:A:455:ARG:HD2	1:A:456:MET:CE	2.45	0.44
1:A:512:ASP:HB3	1:A:515:SER:HB2	2.00	0.44
1:B:108:MET:O	1:B:111:MET:HB2	2.17	0.44
1:B:111:MET:HE1	1:B:326:GLN:HA	1.99	0.44
1:B:508:THR:HG22	1:B:538:ARG:NH2	2.33	0.44
1:B:520:GLN:HA	1:B:520:GLN:HE21	1.82	0.44
1:C:21:ALA:CB	1:C:22:PRO:HD3	2.40	0.44
1:D:142:ALA:HB1	1:D:308:PHE:HD2	1.83	0.44
1:D:520:GLN:HA	1:D:520:GLN:HE21	1.82	0.44
1:A:29:VAL:CG1	1:A:87:TYR:HE2	2.28	0.44
1:A:171:LEU:C	1:A:171:LEU:HD23	2.43	0.44
1:B:170:ILE:HD13	1:B:170:ILE:N	2.33	0.44
1:B:218:LEU:N	1:B:218:LEU:HD12	2.32	0.44
1:C:190:ARG:HA	1:C:313:ALA:HB2	1.98	0.44
1:C:435:ASN:C	1:C:437:ILE:N	2.75	0.44
1:C:459:ALA:HB1	1:C:462:PHE:CE1	2.52	0.44
1:D:252:ASP:CB	1:D:253:PRO:HD3	2.43	0.44
1:D:445:TYR:HD2	1:D:496:LEU:HD21	1.83	0.44
1:A:97:VAL:CG1	1:A:98:MET:H	2.30	0.44
1:A:342:LEU:CD2	1:A:366:ILE:HD12	2.48	0.44
1:B:49:LYS:HB3	1:B:50:PRO:HD3	2.00	0.44
1:B:67:MET:CB	1:B:68:PRO:HD3	2.45	0.44
1:B:435:ASN:C	1:B:437:ILE:N	2.75	0.44
1:C:102:ARG:NH2	1:D:238:ARG:CZ	2.81	0.44
1:C:170:ILE:HD13	1:C:170:ILE:N	2.33	0.44
1:C:378:SER:N	1:D:512:ASP:HB2	2.23	0.44
1:C:475:GLY:O	1:C:477:ASN:N	2.51	0.44
1:C:508:THR:HG22	1:C:538:ARG:NH2	2.33	0.44
1:C:551:VAL:HG23	1:C:555:ILE:C	2.43	0.44
1:D:37:ASN:HD22	1:D:37:ASN:HA	1.54	0.44
1:D:435:ASN:C	1:D:437:ILE:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:475:GLY:O	1:D:477:ASN:N	2.51	0.44
1:D:542:ILE:C	1:D:544:GLN:N	2.74	0.44
1:A:95:LYS:NZ	1:B:239:LEU:HD21	2.33	0.43
1:B:294:LEU:C	1:B:297:PRO:HD2	2.43	0.43
1:B:316:GLN:OE1	1:B:316:GLN:HA	2.17	0.43
1:B:475:GLY:O	1:B:477:ASN:N	2.51	0.43
1:B:496:LEU:HD12	1:B:496:LEU:O	2.18	0.43
1:B:580:PHE:HB2	1:B:581:GLY:H	1.68	0.43
1:C:111:MET:HE1	1:C:326:GLN:HA	1.99	0.43
1:C:218:LEU:N	1:C:218:LEU:HD12	2.32	0.43
1:C:380:SER:O	1:C:382:LYS:N	2.50	0.43
1:C:401:LEU:HD12	1:C:404:GLY:C	2.43	0.43
1:C:520:GLN:HA	1:C:520:GLN:HE21	1.82	0.43
1:C:557:VAL:O	1:C:557:VAL:CG1	2.66	0.43
1:D:203:VAL:HA	1:D:233:VAL:HG11	2.00	0.43
1:D:551:VAL:HG23	1:D:555:ILE:C	2.43	0.43
1:A:218:LEU:HB3	1:B:416:ARG:HD3	2.00	0.43
1:A:463:ILE:O	1:A:466:MET:HG2	2.17	0.43
1:B:445:TYR:HD2	1:B:496:LEU:HD21	1.83	0.43
1:B:551:VAL:HG23	1:B:555:ILE:C	2.43	0.43
1:C:112:PRO:O	1:C:113:VAL:CG1	2.62	0.43
1:D:111:MET:HE1	1:D:326:GLN:HA	1.99	0.43
1:D:474:ILE:CG1	1:D:475:GLY:N	2.81	0.43
1:A:10:TRP:CG	1:A:11:GLN:N	2.86	0.43
1:A:384:THR:O	1:A:388:LEU:HB2	2.18	0.43
1:A:408:ARG:O	1:A:409:GLU:C	2.61	0.43
1:A:416:ARG:HD3	1:B:218:LEU:HB3	2.00	0.43
1:A:439:TYR:CD2	1:B:220:PHE:HZ	2.33	0.43
1:A:488:ARG:O	1:A:491:ILE:HB	2.18	0.43
1:B:72:ILE:N	1:B:72:ILE:CD1	2.81	0.43
1:B:333:ARG:HH11	1:B:333:ARG:CB	2.30	0.43
1:C:10:TRP:CG	1:C:11:GLN:H	2.37	0.43
1:C:63:VAL:HG12	1:C:64:LEU:N	2.32	0.43
1:C:72:ILE:N	1:C:72:ILE:CD1	2.81	0.43
1:C:408:ARG:O	1:C:409:GLU:C	2.61	0.43
1:C:416:ARG:NH1	1:D:218:LEU:CD2	2.78	0.43
1:C:455:ARG:HD2	1:C:456:MET:CE	2.46	0.43
1:D:178:VAL:CA	1:D:258:ILE:HD13	2.47	0.43
1:D:183:ARG:HD2	1:D:183:ARG:HA	1.84	0.43
1:D:508:THR:O	1:D:510:ALA:N	2.50	0.43
1:D:512:ASP:HB3	1:D:515:SER:CB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:HIS:CE1	1:A:111:MET:HE3	2.53	0.43
1:B:401:LEU:HD12	1:B:404:GLY:C	2.43	0.43
1:C:96:VAL:HA	1:C:99:THR:HG22	2.01	0.43
1:C:131:ASP:CB	1:C:318:LEU:HD23	2.48	0.43
1:C:365:LYS:HE2	1:C:367:PRO:HG3	2.01	0.43
1:C:513:THR:CG2	1:D:575:LEU:HD22	2.49	0.43
1:D:437:ILE:O	1:D:440:ALA:HB3	2.18	0.43
1:D:475:GLY:H	1:D:480:LEU:HD12	1.83	0.43
1:A:17:TRP:N	1:A:18:PRO:CD	2.81	0.43
1:A:84:ILE:O	1:A:87:TYR:CD2	2.69	0.43
1:A:109:MET:C	1:A:111:MET:H	2.25	0.43
1:A:235:ASN:C	1:A:237:MET:H	2.26	0.43
1:A:480:LEU:O	1:A:481:LEU:HB3	2.17	0.43
1:B:10:TRP:CG	1:B:11:GLN:H	2.37	0.43
1:B:96:VAL:HA	1:B:99:THR:HG22	2.01	0.43
1:B:131:ASP:CB	1:B:318:LEU:HD23	2.48	0.43
1:B:175:ALA:N	1:B:176:PRO:CD	2.80	0.43
1:B:322:LEU:HD23	1:B:322:LEU:C	2.43	0.43
1:B:366:ILE:HG23	1:B:372:VAL:HG23	1.99	0.43
1:B:474:ILE:CG1	1:B:475:GLY:N	2.81	0.43
1:C:174:LEU:HD22	1:C:262:ALA:CB	2.39	0.43
1:C:474:ILE:CG1	1:C:475:GLY:N	2.81	0.43
1:C:512:ASP:HB3	1:C:515:SER:HB2	2.01	0.43
1:D:63:VAL:HG12	1:D:64:LEU:N	2.32	0.43
1:D:294:LEU:C	1:D:297:PRO:HD2	2.43	0.43
1:D:496:LEU:HD12	1:D:496:LEU:O	2.18	0.43
1:D:577:LYS:C	1:D:579:GLN:N	2.72	0.43
1:A:49:LYS:HB3	1:A:50:PRO:HD3	2.01	0.43
1:A:175:ALA:N	1:A:176:PRO:CD	2.82	0.43
1:A:473:ILE:HG23	1:A:473:ILE:O	2.19	0.43
1:B:512:ASP:O	1:B:513:THR:C	2.62	0.43
1:C:49:LYS:HB3	1:C:50:PRO:HD3	2.00	0.43
1:C:366:ILE:HG23	1:C:372:VAL:HG23	1.99	0.43
1:C:378:SER:HB3	1:D:512:ASP:HB2	2.01	0.43
1:C:441:ARG:CG	1:D:220:PHE:O	2.66	0.43
1:D:217:VAL:HG12	1:D:217:VAL:O	2.17	0.43
1:D:223:GLN:O	1:D:226:GLU:HB2	2.18	0.43
1:D:401:LEU:HD12	1:D:404:GLY:C	2.43	0.43
1:A:97:VAL:CG1	1:A:98:MET:N	2.81	0.43
1:A:333:ARG:HH11	1:A:333:ARG:CB	2.32	0.43
1:A:475:GLY:O	1:A:477:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ARG:CG	1:D:256:GLN:HE22	2.31	0.43
1:C:87:TYR:CZ	1:C:88:CYS:SG	3.09	0.43
1:C:437:ILE:HA	1:C:493:ARG:HB2	2.01	0.43
1:D:72:ILE:N	1:D:72:ILE:CD1	2.81	0.43
1:D:411:THR:O	1:D:412:LEU:C	2.60	0.43
1:D:412:LEU:HD21	1:D:416:ARG:HD2	2.01	0.43
1:A:203:VAL:HA	1:A:233:VAL:HG11	2.00	0.43
1:A:445:TYR:HB3	1:A:446:SER:H	1.73	0.43
1:B:63:VAL:HG12	1:B:64:LEU:N	2.32	0.43
1:B:512:ASP:HB3	1:B:515:SER:HB2	2.01	0.43
1:C:218:LEU:CD2	1:D:416:ARG:NH1	2.79	0.43
1:C:316:GLN:OE1	1:C:316:GLN:HA	2.17	0.43
1:C:475:GLY:H	1:C:480:LEU:HD12	1.83	0.43
1:C:558:GLU:CD	1:C:558:GLU:C	2.87	0.43
1:D:97:VAL:CG1	1:D:98:MET:H	2.30	0.43
1:D:380:SER:HG	1:D:551:VAL:HG22	1.80	0.43
1:A:74:LEU:O	1:A:78:ARG:HB3	2.18	0.43
1:A:339:THR:HG23	1:A:339:THR:O	2.18	0.43
1:B:113:VAL:CG2	1:B:114:ALA:H	2.15	0.43
1:B:437:ILE:HA	1:B:493:ARG:HB2	2.01	0.43
1:B:558:GLU:CD	1:B:558:GLU:C	2.87	0.43
1:C:112:PRO:O	1:C:327:GLU:OE1	2.37	0.43
1:C:322:LEU:HD23	1:C:322:LEU:C	2.43	0.43
1:C:333:ARG:HH11	1:C:333:ARG:CB	2.30	0.43
1:C:411:THR:O	1:C:412:LEU:C	2.60	0.43
1:C:431:ASP:HB3	1:C:435:ASN:HB2	1.99	0.43
1:C:513:THR:O	1:C:516:GLU:HB3	2.19	0.43
1:D:112:PRO:O	1:D:327:GLU:OE1	2.37	0.43
1:D:131:ASP:CB	1:D:318:LEU:HD23	2.48	0.43
1:D:235:ASN:C	1:D:237:MET:H	2.27	0.43
1:D:557:VAL:O	1:D:557:VAL:CG1	2.66	0.43
1:D:558:GLU:CD	1:D:558:GLU:C	2.87	0.43
1:A:16:LEU:HD11	1:A:135:VAL:CG2	2.48	0.43
1:A:33:ALA:O	1:A:81:THR:CG2	2.66	0.43
1:A:412:LEU:HD21	1:A:416:ARG:HD2	2.01	0.43
1:B:178:VAL:HB	1:B:258:ILE:HG21	2.01	0.43
1:B:315:CYS:SG	1:B:319:PHE:CD1	3.12	0.43
1:B:408:ARG:O	1:B:409:GLU:C	2.62	0.43
1:B:513:THR:O	1:B:516:GLU:HB3	2.19	0.43
1:C:107:HIS:CE1	1:C:111:MET:HE3	2.54	0.43
1:C:294:LEU:C	1:C:297:PRO:HD2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:LEU:HD12	1:C:496:LEU:O	2.18	0.43
1:D:29:VAL:CG1	1:D:87:TYR:HE2	2.30	0.43
1:D:49:LYS:HB3	1:D:50:PRO:HD3	2.00	0.43
1:D:93:SER:OG	1:D:94:GLY:N	2.52	0.43
1:D:109:MET:C	1:D:111:MET:H	2.26	0.43
1:D:512:ASP:O	1:D:513:THR:C	2.62	0.43
1:A:142:ALA:HB1	1:A:308:PHE:HD2	1.84	0.42
1:A:371:THR:HA	1:A:532:SER:O	2.19	0.42
1:B:93:SER:OG	1:B:94:GLY:N	2.52	0.42
1:B:475:GLY:H	1:B:480:LEU:HD12	1.83	0.42
1:C:217:VAL:O	1:C:217:VAL:HG12	2.17	0.42
1:C:315:CYS:SG	1:C:319:PHE:CD1	3.12	0.42
1:C:441:ARG:HA	1:C:441:ARG:HD2	1.61	0.42
1:C:445:TYR:HD2	1:C:496:LEU:HD21	1.83	0.42
1:D:209:GLN:O	1:D:210:MET:C	2.62	0.42
1:D:433:VAL:O	1:D:434:ALA:C	2.61	0.42
1:A:220:PHE:O	1:B:441:ARG:CG	2.67	0.42
1:A:280:THR:O	1:A:284:ILE:CG2	2.67	0.42
1:B:112:PRO:O	1:B:327:GLU:OE1	2.37	0.42
1:C:29:VAL:CG1	1:C:87:TYR:HE2	2.30	0.42
1:C:109:MET:C	1:C:111:MET:H	2.26	0.42
1:C:125:LEU:HD21	1:D:125:LEU:HD23	2.01	0.42
1:C:299:LYS:HZ2	1:C:299:LYS:CB	2.32	0.42
1:C:391:ARG:C	1:C:393:TYR:N	2.75	0.42
1:C:580:PHE:HB2	1:C:581:GLY:H	1.68	0.42
1:D:107:HIS:CE1	1:D:111:MET:HE3	2.55	0.42
1:D:178:VAL:HB	1:D:258:ILE:HG21	2.01	0.42
1:D:315:CYS:SG	1:D:319:PHE:CD1	3.12	0.42
1:A:95:LYS:NZ	1:B:238:ARG:HG3	2.34	0.42
1:A:111:MET:HE3	1:A:326:GLN:OE1	2.20	0.42
1:B:209:GLN:O	1:B:210:MET:C	2.62	0.42
1:B:235:ASN:C	1:B:237:MET:H	2.27	0.42
1:B:389:ILE:C	1:B:391:ARG:H	2.28	0.42
1:C:93:SER:HA	1:C:96:VAL:HG12	2.01	0.42
1:C:102:ARG:HH21	1:D:238:ARG:NH2	2.17	0.42
1:C:203:VAL:HA	1:C:233:VAL:HG11	2.00	0.42
1:C:220:PHE:CE1	1:D:439:TYR:O	2.71	0.42
1:C:221:GLY:C	1:D:441:ARG:CD	2.93	0.42
1:C:412:LEU:HD21	1:C:416:ARG:HD2	2.01	0.42
1:D:170:ILE:HD13	1:D:170:ILE:N	2.33	0.42
1:D:197:GLN:O	1:D:200:MET:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:CYS:SG	1:D:319:PHE:CE1	3.13	0.42
1:D:322:LEU:HD23	1:D:322:LEU:C	2.43	0.42
1:D:488:ARG:O	1:D:491:ILE:HB	2.20	0.42
1:D:513:THR:O	1:D:516:GLU:HB3	2.19	0.42
1:A:93:SER:HA	1:A:96:VAL:HG12	2.01	0.42
1:A:508:THR:HG22	1:A:538:ARG:NH2	2.34	0.42
1:B:97:VAL:CG1	1:B:98:MET:H	2.30	0.42
1:B:197:GLN:O	1:B:200:MET:N	2.52	0.42
1:B:203:VAL:HA	1:B:233:VAL:HG11	2.00	0.42
1:B:315:CYS:SG	1:B:319:PHE:CE1	3.13	0.42
1:C:389:ILE:C	1:C:391:ARG:H	2.28	0.42
1:C:570:GLY:C	1:C:572:TYR:H	2.24	0.42
1:D:349:PHE:CD2	1:D:388:LEU:HD11	2.55	0.42
1:D:389:ILE:C	1:D:391:ARG:H	2.27	0.42
1:D:515:SER:O	1:D:518:ALA:HB3	2.20	0.42
1:A:96:VAL:HA	1:A:99:THR:HG22	2.01	0.42
1:A:183:ARG:HD2	1:A:183:ARG:HA	1.85	0.42
1:A:360:ARG:O	1:A:362:ILE:HG12	2.20	0.42
1:A:378:SER:HB3	1:B:512:ASP:HB2	2.02	0.42
1:A:551:VAL:HG23	1:A:555:ILE:C	2.44	0.42
1:B:93:SER:HA	1:B:96:VAL:HG12	2.01	0.42
1:B:349:PHE:CD2	1:B:388:LEU:HD11	2.55	0.42
1:B:365:LYS:HE2	1:B:367:PRO:HG3	2.01	0.42
1:B:412:LEU:HD21	1:B:416:ARG:HD2	2.01	0.42
1:B:433:VAL:O	1:B:434:ALA:C	2.61	0.42
1:C:48:LEU:CG	1:D:292:ILE:HD12	2.48	0.42
1:C:482:SER:HB3	1:C:485:GLN:CG	2.50	0.42
1:C:488:ARG:O	1:C:491:ILE:HB	2.20	0.42
1:D:107:HIS:CD2	1:D:322:LEU:HA	2.54	0.42
1:D:535:ILE:HG23	1:D:535:ILE:O	2.20	0.42
1:A:271:SER:CA	1:B:63:VAL:HG11	2.49	0.42
1:B:167:LEU:O	1:B:170:ILE:HB	2.20	0.42
1:A:111:MET:HE1	1:A:326:GLN:HA	2.00	0.42
1:A:389:ILE:C	1:A:391:ARG:H	2.28	0.42
1:A:441:ARG:NE	1:B:221:GLY:CA	2.79	0.42
1:B:15:ARG:HH21	1:B:319:PHE:HD1	1.68	0.42
1:B:107:HIS:CE1	1:B:111:MET:HE3	2.54	0.42
1:B:384:THR:N	2:B:5002:ANP:O1A	2.53	0.42
1:C:209:GLN:O	1:C:210:MET:C	2.62	0.42
1:C:476:GLU:O	1:C:477:ASN:HB3	2.20	0.42
1:D:10:TRP:CG	1:D:11:GLN:H	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:MET:HE1	1:D:124:LEU:CB	2.45	0.42
1:D:141:GLY:C	1:D:144:ILE:HG12	2.44	0.42
1:A:140:SER:OG	1:A:141:GLY:N	2.53	0.42
1:A:163:TYR:OH	1:A:286:VAL:HB	2.20	0.42
1:A:349:PHE:CD2	1:A:388:LEU:HD11	2.55	0.42
1:A:561:THR:C	1:A:563:SER:N	2.72	0.42
1:B:29:VAL:CG1	1:B:87:TYR:HE2	2.30	0.42
1:B:141:GLY:C	1:B:144:ILE:HG12	2.44	0.42
1:B:535:ILE:HG23	1:B:535:ILE:O	2.20	0.42
1:C:20:ILE:HD11	1:C:96:VAL:HG21	1.99	0.42
1:C:433:VAL:O	1:C:434:ALA:C	2.61	0.42
1:D:93:SER:HA	1:D:96:VAL:HG12	2.01	0.42
1:D:421:LEU:HD12	1:D:422:VAL:H	1.85	0.42
1:A:97:VAL:O	1:A:100:MET:HB3	2.20	0.42
1:A:391:ARG:O	1:A:394:ASP:OD1	2.38	0.42
1:B:107:HIS:CD2	1:B:322:LEU:HA	2.54	0.42
1:B:349:PHE:HA	1:B:396:ASP:HB3	1.97	0.42
1:C:15:ARG:HH21	1:C:319:PHE:HD1	1.68	0.42
1:C:93:SER:OG	1:C:94:GLY:N	2.52	0.42
1:C:197:GLN:O	1:C:200:MET:N	2.52	0.42
1:D:478:GLY:HA3	1:D:486:ARG:CD	2.50	0.42
1:A:107:HIS:CD2	1:A:322:LEU:HA	2.55	0.42
1:A:421:LEU:HD12	1:A:422:VAL:H	1.85	0.42
1:A:435:ASN:C	1:A:437:ILE:N	2.75	0.42
1:A:512:ASP:O	1:A:513:THR:C	2.63	0.42
1:B:16:LEU:HD11	1:B:135:VAL:CG2	2.50	0.42
1:B:163:TYR:OH	1:B:286:VAL:HB	2.20	0.42
1:B:421:LEU:HD12	1:B:422:VAL:H	1.85	0.42
1:B:488:ARG:O	1:B:491:ILE:HB	2.20	0.42
1:C:142:ALA:HB1	1:C:308:PHE:HD2	1.83	0.42
1:C:167:LEU:O	1:C:170:ILE:HB	2.20	0.42
1:C:269:ALA:HA	1:C:273:PRO:CD	2.50	0.42
1:C:391:ARG:O	1:C:394:ASP:OD1	2.38	0.42
1:C:511:LEU:H	1:C:538:ARG:HH22	1.68	0.42
1:D:33:ALA:HB2	1:D:84:ILE:HG22	2.02	0.42
1:D:113:VAL:CG2	1:D:114:ALA:H	2.15	0.42
1:D:365:LYS:HE2	1:D:367:PRO:HG3	2.01	0.42
1:A:446:SER:HB2	1:A:449:GLN:NE2	2.35	0.41
1:A:491:ILE:O	1:A:492:ALA:C	2.63	0.41
1:A:535:ILE:HD13	1:A:535:ILE:C	2.44	0.41
1:C:338:ALA:HB3	1:C:500:PRO:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:LEU:HD11	1:D:135:VAL:CG2	2.50	0.41
1:D:445:TYR:HB3	1:D:446:SER:H	1.76	0.41
1:D:512:ASP:HB3	1:D:515:SER:HB2	2.01	0.41
1:A:338:ALA:O	1:A:339:THR:O	2.32	0.41
1:A:426:VAL:O	1:A:486:ARG:NH2	2.53	0.41
1:A:542:ILE:C	1:A:544:GLN:H	2.28	0.41
1:B:371:THR:HA	1:B:532:SER:O	2.21	0.41
1:C:16:LEU:HD11	1:C:135:VAL:CG2	2.50	0.41
1:C:101:ARG:HB2	1:C:128:ILE:HG23	2.03	0.41
1:C:219:ILE:HD13	1:D:421:LEU:HB3	2.02	0.41
1:C:280:THR:O	1:C:284:ILE:CG2	2.68	0.41
1:C:315:CYS:SG	1:C:319:PHE:CE1	3.13	0.41
1:C:349:PHE:CD2	1:C:388:LEU:HD11	2.55	0.41
1:C:480:LEU:O	1:C:481:LEU:HB3	2.20	0.41
1:D:28:ILE:O	1:D:32:ILE:HG12	2.21	0.41
1:D:97:VAL:O	1:D:100:MET:HB3	2.20	0.41
1:D:167:LEU:O	1:D:170:ILE:HB	2.20	0.41
1:D:408:ARG:O	1:D:409:GLU:C	2.61	0.41
1:A:15:ARG:HH21	1:A:319:PHE:HD1	1.68	0.41
1:A:226:GLU:O	1:A:227:THR:C	2.62	0.41
1:C:28:ILE:O	1:C:32:ILE:HG12	2.20	0.41
1:C:33:ALA:HB2	1:C:84:ILE:HG22	2.02	0.41
1:C:107:HIS:CD2	1:C:322:LEU:HA	2.54	0.41
1:C:235:ASN:C	1:C:237:MET:H	2.27	0.41
1:C:421:LEU:HD12	1:C:422:VAL:H	1.85	0.41
1:D:96:VAL:HA	1:D:99:THR:HG22	2.00	0.41
1:D:101:ARG:HB2	1:D:128:ILE:HG23	2.03	0.41
1:D:437:ILE:HA	1:D:493:ARG:HB2	2.01	0.41
1:D:476:GLU:O	1:D:477:ASN:HB3	2.20	0.41
1:D:511:LEU:H	1:D:538:ARG:HH22	1.68	0.41
1:A:33:ALA:HB2	1:A:84:ILE:HG22	2.03	0.41
1:A:225:VAL:HG21	1:B:443:GLU:HG2	2.02	0.41
1:A:365:LYS:HE2	1:A:367:PRO:HG3	2.01	0.41
1:B:294:LEU:O	1:B:297:PRO:HD2	2.20	0.41
1:B:380:SER:O	1:B:382:LYS:N	2.49	0.41
1:C:163:TYR:OH	1:C:286:VAL:HB	2.20	0.41
1:C:535:ILE:HG23	1:C:535:ILE:O	2.20	0.41
1:D:391:ARG:O	1:D:394:ASP:OD1	2.38	0.41
1:D:460:MET:HE1	1:D:470:LEU:HD11	2.02	0.41
1:A:157:PHE:HB2	1:A:171:LEU:HD11	2.02	0.41
1:A:267:LEU:O	1:B:63:VAL:CG1	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:ARG:O	1:A:492:ALA:N	2.51	0.41
1:B:455:ARG:HD2	1:B:456:MET:CE	2.46	0.41
1:B:455:ARG:C	1:B:457:ALA:N	2.69	0.41
1:C:178:VAL:HB	1:C:258:ILE:HG21	2.01	0.41
1:C:460:MET:HE1	1:C:470:LEU:HD11	2.02	0.41
1:D:13:PHE:CE1	1:D:312:MET:HE2	2.55	0.41
1:D:20:ILE:HD11	1:D:96:VAL:HG21	1.99	0.41
1:D:28:ILE:CG2	1:D:29:VAL:N	2.83	0.41
1:D:33:ALA:O	1:D:81:THR:CG2	2.69	0.41
1:D:111:MET:HE3	1:D:326:GLN:OE1	2.20	0.41
1:D:280:THR:O	1:D:284:ILE:CG2	2.69	0.41
1:D:333:ARG:HH11	1:D:333:ARG:CB	2.30	0.41
1:A:415:LEU:O	1:A:418:GLN:HB2	2.20	0.41
1:A:513:THR:O	1:A:516:GLU:HB3	2.21	0.41
1:B:192:ILE:O	1:B:196:MET:HB2	2.21	0.41
1:C:33:ALA:O	1:C:81:THR:CG2	2.69	0.41
1:C:296:ARG:N	1:C:297:PRO:HD2	2.36	0.41
1:C:371:THR:HA	1:C:532:SER:O	2.21	0.41
1:C:478:GLY:HA3	1:C:486:ARG:CD	2.50	0.41
1:A:23:PHE:CZ	1:A:95:LYS:HB3	2.55	0.41
1:A:28:ILE:CG2	1:A:29:VAL:N	2.83	0.41
1:A:549:VAL:HG13	1:A:556:ILE:CD1	2.50	0.41
1:B:13:PHE:CE1	1:B:312:MET:HE2	2.55	0.41
1:B:33:ALA:O	1:B:81:THR:CG2	2.69	0.41
1:B:111:MET:HE3	1:B:326:GLN:OE1	2.20	0.41
1:B:480:LEU:O	1:B:481:LEU:HB3	2.20	0.41
1:C:13:PHE:CE1	1:C:312:MET:HE2	2.55	0.41
1:C:141:GLY:C	1:C:144:ILE:HG12	2.44	0.41
1:C:512:ASP:H	1:D:378:SER:HB2	1.85	0.41
1:C:515:SER:O	1:C:518:ALA:HB3	2.20	0.41
1:C:575:LEU:HD22	1:D:513:THR:CG2	2.50	0.41
1:D:84:ILE:O	1:D:87:TYR:CD2	2.72	0.41
1:D:118:LYS:NZ	1:D:352:PRO:HG3	2.36	0.41
1:D:343:GLU:OE2	1:D:365:LYS:HE3	2.21	0.41
1:A:47:LEU:CD1	1:A:51:LEU:HD12	2.50	0.41
1:A:192:ILE:O	1:A:196:MET:HB2	2.20	0.41
1:A:292:ILE:HD12	1:B:48:LEU:CD1	2.49	0.41
1:B:280:THR:O	1:B:284:ILE:CG2	2.68	0.41
1:B:411:THR:O	1:B:411:THR:HG23	2.21	0.41
1:C:28:ILE:CG2	1:C:29:VAL:N	2.83	0.41
1:C:97:VAL:O	1:C:100:MET:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:ILE:O	1:C:196:MET:HB2	2.21	0.41
1:C:220:PHE:HZ	1:D:439:TYR:CD2	2.38	0.41
1:C:347:VAL:HA	1:C:398:GLY:HA3	2.03	0.41
1:C:512:ASP:O	1:C:513:THR:C	2.62	0.41
1:D:15:ARG:HH21	1:D:319:PHE:HD1	1.68	0.41
1:D:269:ALA:HA	1:D:273:PRO:CD	2.50	0.41
1:A:13:PHE:CE1	1:A:312:MET:HE2	2.55	0.41
1:A:20:ILE:HD11	1:A:96:VAL:HG21	2.00	0.41
1:A:87:TYR:CD2	1:A:88:CYS:N	2.89	0.41
1:A:167:LEU:O	1:A:170:ILE:HB	2.20	0.41
1:A:391:ARG:NH2	1:A:408:ARG:HA	2.36	0.41
1:A:411:THR:O	1:A:411:THR:HG23	2.21	0.41
1:A:445:TYR:CE2	1:A:496:LEU:HD11	2.55	0.41
1:A:511:LEU:H	1:A:538:ARG:HH22	1.69	0.41
1:A:515:SER:O	1:A:518:ALA:HB3	2.21	0.41
1:A:550:VAL:HB	1:A:558:GLU:HB3	2.03	0.41
1:B:28:ILE:CG2	1:B:29:VAL:N	2.83	0.41
1:B:33:ALA:HB2	1:B:84:ILE:HG22	2.02	0.41
1:B:87:TYR:CD2	1:B:88:CYS:N	2.89	0.41
1:B:97:VAL:CG1	1:B:98:MET:N	2.81	0.41
1:B:457:ALA:O	1:B:458:TYR:C	2.64	0.41
1:B:478:GLY:HA3	1:B:486:ARG:CD	2.50	0.41
1:B:515:SER:O	1:B:518:ALA:HB3	2.20	0.41
1:B:570:GLY:C	1:B:572:TYR:H	2.24	0.41
1:C:213:GLY:HA2	1:D:427:HIS:CD2	2.55	0.41
1:C:220:PHE:O	1:D:441:ARG:CG	2.69	0.41
1:C:226:GLU:O	1:C:227:THR:C	2.64	0.41
1:C:343:GLU:OE2	1:C:365:LYS:HE3	2.21	0.41
1:C:344:PHE:C	1:C:345:ARG:HD2	2.46	0.41
1:C:362:ILE:HD11	1:C:556:ILE:H	1.86	0.41
1:D:87:TYR:CD2	1:D:88:CYS:N	2.89	0.41
1:D:93:SER:HB3	1:D:140:SER:CB	2.44	0.41
1:D:248:SER:O	1:D:251:SER:HB3	2.21	0.41
1:D:360:ARG:HB3	1:D:361:ASN:H	1.73	0.41
1:D:480:LEU:O	1:D:481:LEU:HB3	2.20	0.41
1:D:535:ILE:O	1:D:535:ILE:CD1	2.62	0.41
1:A:98:MET:CB	1:B:238:ARG:NE	2.82	0.41
1:A:198:ASN:N	1:A:198:ASN:ND2	2.69	0.41
1:A:269:ALA:HA	1:A:273:PRO:CD	2.49	0.41
1:A:347:VAL:HA	1:A:398:GLY:HA3	2.03	0.41
1:B:342:LEU:CD2	1:B:366:ILE:HD12	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:GLU:OE2	1:B:365:LYS:HE3	2.21	0.41
1:B:542:ILE:C	1:B:544:GLN:H	2.29	0.41
1:C:140:SER:OG	1:C:141:GLY:N	2.53	0.41
1:C:384:THR:O	1:C:388:LEU:HB2	2.21	0.41
1:C:496:LEU:O	1:C:497:ARG:C	2.64	0.41
1:D:294:LEU:O	1:D:297:PRO:HD2	2.20	0.41
1:A:111:MET:O	1:A:112:PRO:C	2.64	0.40
1:A:146:VAL:O	1:A:150:GLY:HA3	2.21	0.40
1:A:235:ASN:OD1	1:A:238:ARG:HD2	2.21	0.40
1:A:294:LEU:C	1:A:297:PRO:HD2	2.45	0.40
1:A:439:TYR:O	1:A:443:GLU:OE2	2.39	0.40
1:A:474:ILE:CA	1:A:480:LEU:HD11	2.51	0.40
1:B:101:ARG:HB2	1:B:128:ILE:HG23	2.03	0.40
1:B:174:LEU:HD22	1:B:262:ALA:CB	2.40	0.40
1:B:296:ARG:N	1:B:297:PRO:HD2	2.36	0.40
1:B:344:PHE:C	1:B:345:ARG:HD2	2.46	0.40
1:B:391:ARG:O	1:B:394:ASP:OD1	2.38	0.40
1:B:473:ILE:HG23	1:B:473:ILE:O	2.22	0.40
1:C:67:MET:CB	1:C:68:PRO:HD3	2.45	0.40
1:C:87:TYR:CD2	1:C:88:CYS:N	2.89	0.40
1:C:342:LEU:CD2	1:C:366:ILE:HD12	2.51	0.40
1:C:491:ILE:O	1:C:495:LEU:HB2	2.21	0.40
1:D:97:VAL:CG1	1:D:98:MET:N	2.81	0.40
1:D:163:TYR:OH	1:D:286:VAL:HB	2.20	0.40
1:D:495:LEU:HD12	1:D:495:LEU:HA	1.95	0.40
1:D:542:ILE:C	1:D:544:GLN:H	2.29	0.40
1:A:98:MET:HE3	1:B:237:MET:HG3	2.02	0.40
1:A:317:THR:O	1:A:320:ALA:HB3	2.22	0.40
1:A:486:ARG:O	1:A:487:GLN:C	2.63	0.40
1:A:558:GLU:OE2	1:A:565:LEU:CD2	2.69	0.40
1:B:84:ILE:O	1:B:87:TYR:CD2	2.73	0.40
1:B:118:LYS:NZ	1:B:352:PRO:HG3	2.36	0.40
1:B:193:SER:O	1:B:197:GLN:HG3	2.21	0.40
1:B:476:GLU:O	1:B:477:ASN:HB3	2.20	0.40
1:C:445:TYR:HB3	1:C:446:SER:H	1.76	0.40
1:C:446:SER:HB2	1:C:449:GLN:NE2	2.36	0.40
1:D:296:ARG:N	1:D:297:PRO:HD2	2.36	0.40
1:D:371:THR:HA	1:D:532:SER:O	2.21	0.40
1:D:384:THR:O	1:D:388:LEU:HB2	2.21	0.40
1:A:93:SER:HB3	1:A:140:SER:CB	2.44	0.40
1:A:236:LYS:O	1:A:236:LYS:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:VAL:O	1:B:150:GLY:HA3	2.22	0.40
1:B:384:THR:O	1:B:388:LEU:HB2	2.21	0.40
1:C:84:ILE:O	1:C:87:TYR:CD2	2.73	0.40
1:C:111:MET:HE3	1:C:326:GLN:OE1	2.21	0.40
1:C:118:LYS:NZ	1:C:352:PRO:HG3	2.36	0.40
1:C:126:SER:O	1:C:127:ARG:C	2.64	0.40
1:C:272:PHE:HB2	1:C:273:PRO:CD	2.37	0.40
1:C:378:SER:H	1:D:512:ASP:CB	2.24	0.40
1:C:473:ILE:O	1:C:473:ILE:HG23	2.21	0.40
1:C:550:VAL:HB	1:C:558:GLU:HB3	2.03	0.40
1:D:319:PHE:HD2	1:D:319:PHE:HA	1.82	0.40
1:D:491:ILE:O	1:D:495:LEU:HB2	2.21	0.40
1:A:101:ARG:HB2	1:A:128:ILE:HG23	2.03	0.40
1:B:28:ILE:O	1:B:32:ILE:HG12	2.20	0.40
1:B:97:VAL:O	1:B:100:MET:HB3	2.20	0.40
1:B:248:SER:O	1:B:251:SER:HB3	2.21	0.40
1:B:315:CYS:O	1:B:319:PHE:HB2	2.22	0.40
1:C:178:VAL:CA	1:C:258:ILE:HD13	2.48	0.40
1:C:391:ARG:NH2	1:C:408:ARG:HA	2.36	0.40
1:D:342:LEU:CD2	1:D:366:ILE:HD12	2.51	0.40
1:D:347:VAL:HA	1:D:398:GLY:HA3	2.03	0.40
1:D:440:ALA:HB1	1:D:497:ARG:NE	2.37	0.40
1:D:446:SER:HB2	1:D:449:GLN:NE2	2.36	0.40
1:A:100:MET:HE3	1:A:100:MET:CA	2.46	0.40
1:A:102:ARG:CD	1:B:231:ASP:OD1	2.69	0.40
1:A:248:SER:O	1:A:251:SER:HB3	2.22	0.40
1:A:338:ALA:HB3	1:A:500:PRO:CB	2.48	0.40
1:A:400:ILE:HG22	1:A:407:LEU:HD11	2.03	0.40
1:A:457:ALA:O	1:A:458:TYR:C	2.63	0.40
1:B:126:SER:O	1:B:127:ARG:C	2.64	0.40
1:B:338:ALA:HB3	1:B:500:PRO:CB	2.50	0.40
1:B:444:GLU:HA	1:B:444:GLU:OE1	2.21	0.40
1:B:460:MET:HE1	1:B:470:LEU:HD11	2.02	0.40
1:B:491:ILE:O	1:B:495:LEU:HB2	2.21	0.40
1:B:496:LEU:O	1:B:497:ARG:C	2.64	0.40
1:C:11:GLN:CG	1:C:12:THR:N	2.63	0.40
1:C:125:LEU:HD23	1:D:125:LEU:HD21	2.03	0.40
1:C:143:LEU:HA	1:C:143:LEU:HD23	1.96	0.40
1:C:248:SER:O	1:C:251:SER:HB3	2.21	0.40
1:C:411:THR:O	1:C:411:THR:HG23	2.21	0.40
1:C:542:ILE:C	1:C:544:GLN:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:GLN:CG	1:D:12:THR:N	2.63	0.40
1:D:192:ILE:O	1:D:196:MET:HB2	2.21	0.40
1:D:226:GLU:O	1:D:227:THR:C	2.64	0.40
1:D:411:THR:O	1:D:411:THR:HG23	2.21	0.40
1:D:415:LEU:O	1:D:418:GLN:HB2	2.22	0.40
1:D:561:THR:C	1:D:563:SER:N	2.73	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	570/582 (98%)	414 (73%)	102 (18%)	54 (10%)	0	7
1	B	570/582 (98%)	413 (72%)	107 (19%)	50 (9%)	0	8
1	C	570/582 (98%)	413 (72%)	107 (19%)	50 (9%)	0	8
1	D	570/582 (98%)	414 (73%)	106 (19%)	50 (9%)	0	8
All	All	2280/2328 (98%)	1654 (72%)	422 (18%)	204 (9%)	0	8

All (204) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASP
1	A	113	VAL
1	A	161	PHE
1	A	217	VAL
1	A	351	TYR
1	A	392	PHE
1	A	394	ASP
1	A	395	ILE
1	A	509	SER

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Mol	Chain	Res	Type
1	A	571	VAL
1	B	60	ASP
1	B	113	VAL
1	B	161	PHE
1	B	217	VAL
1	B	351	TYR
1	B	392	PHE
1	B	394	ASP
1	B	395	ILE
1	B	509	SER
1	B	571	VAL
1	C	60	ASP
1	C	113	VAL
1	C	161	PHE
1	C	217	VAL
1	C	351	TYR
1	C	392	PHE
1	C	394	ASP
1	C	395	ILE
1	C	509	SER
1	C	571	VAL
1	D	60	ASP
1	D	113	VAL
1	D	161	PHE
1	D	217	VAL
1	D	351	TYR
1	D	392	PHE
1	D	394	ASP
1	D	395	ILE
1	D	509	SER
1	D	571	VAL
1	A	63	VAL
1	A	76	ILE
1	A	114	ALA
1	A	140	SER
1	A	339	THR
1	A	353	GLY
1	A	361	ASN
1	A	378	SER
1	A	381	GLY
1	A	382	LYS
1	A	439	TYR

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Mol	Chain	Res	Type
1	A	539	LEU
1	A	543	GLU
1	B	63	VAL
1	B	76	ILE
1	B	114	ALA
1	B	140	SER
1	B	353	GLY
1	B	361	ASN
1	B	378	SER
1	B	381	GLY
1	B	382	LYS
1	B	439	TYR
1	B	442	THR
1	B	539	LEU
1	B	543	GLU
1	C	63	VAL
1	C	114	ALA
1	C	140	SER
1	C	353	GLY
1	C	361	ASN
1	C	378	SER
1	C	381	GLY
1	C	382	LYS
1	C	439	TYR
1	C	442	THR
1	C	539	LEU
1	C	543	GLU
1	D	63	VAL
1	D	76	ILE
1	D	114	ALA
1	D	140	SER
1	D	353	GLY
1	D	361	ASN
1	D	378	SER
1	D	381	GLY
1	D	382	LYS
1	D	439	TYR
1	D	442	THR
1	D	539	LEU
1	D	543	GLU
1	A	52	LEU
1	A	57	GLY

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Mol	Chain	Res	Type
1	A	59	THR
1	A	118	LYS
1	A	129	THR
1	A	276	MET
1	A	327	GLU
1	A	346	ASN
1	A	413	ALA
1	A	492	ALA
1	B	52	LEU
1	B	57	GLY
1	B	59	THR
1	B	118	LYS
1	B	129	THR
1	B	276	MET
1	B	280	THR
1	B	327	GLU
1	B	339	THR
1	B	346	ASN
1	B	413	ALA
1	B	476	GLU
1	B	492	ALA
1	C	52	LEU
1	C	57	GLY
1	C	59	THR
1	C	76	ILE
1	C	118	LYS
1	C	129	THR
1	C	276	MET
1	C	280	THR
1	C	327	GLU
1	C	339	THR
1	C	346	ASN
1	C	413	ALA
1	C	492	ALA
1	D	52	LEU
1	D	57	GLY
1	D	59	THR
1	D	118	LYS
1	D	129	THR
1	D	276	MET
1	D	280	THR
1	D	327	GLU

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Mol	Chain	Res	Type
1	D	339	THR
1	D	346	ASN
1	D	413	ALA
1	D	476	GLU
1	D	492	ALA
1	A	11	GLN
1	A	216	GLU
1	A	280	THR
1	A	324	SER
1	A	424	GLN
1	A	442	THR
1	A	456	MET
1	A	459	ALA
1	A	476	GLU
1	A	527	GLN
1	B	216	GLU
1	B	424	GLN
1	B	456	MET
1	B	459	ALA
1	C	216	GLU
1	C	424	GLN
1	C	456	MET
1	C	459	ALA
1	C	476	GLU
1	D	216	GLU
1	D	424	GLN
1	D	456	MET
1	D	459	ALA
1	A	47	LEU
1	A	272	PHE
1	A	391	ARG
1	A	441	ARG
1	A	458	TYR
1	B	47	LEU
1	B	272	PHE
1	B	324	SER
1	B	458	TYR
1	B	527	GLN
1	C	47	LEU
1	C	272	PHE
1	C	324	SER
1	C	458	TYR

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Mol	Chain	Res	Type
1	C	527	GLN
1	D	47	LEU
1	D	272	PHE
1	D	324	SER
1	D	458	TYR
1	D	527	GLN
1	A	87	TYR
1	B	391	ARG
1	C	391	ARG
1	D	391	ARG
1	A	111	MET
1	B	111	MET
1	C	111	MET
1	D	111	MET
1	A	112	PRO
1	A	542	ILE
1	B	542	ILE
1	C	542	ILE
1	D	542	ILE
1	A	275	VAL
1	B	128	ILE
1	B	275	VAL
1	C	128	ILE
1	C	275	VAL
1	D	128	ILE
1	D	275	VAL
1	A	128	ILE

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	483/493 (98%)	442 (92%)	41 (8%)	10	35
1	B	483/493 (98%)	446 (92%)	37 (8%)	12	38
1	C	483/493 (98%)	445 (92%)	38 (8%)	11	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	483/493 (98%)	445 (92%)	38 (8%)	11	37
All	All	1932/1972 (98%)	1778 (92%)	154 (8%)	11	37

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	37	ASN
1	A	58	LYS
1	A	72	ILE
1	A	80	ILE
1	A	87	TYR
1	A	88	CYS
1	A	98	MET
1	A	108	MET
1	A	113	VAL
1	A	119	GLN
1	A	165	TRP
1	A	170	ILE
1	A	187	LYS
1	A	211	LEU
1	A	224	GLU
1	A	237	MET
1	A	253	PRO
1	A	255	ILE
1	A	284	ILE
1	A	291	MET
1	A	292	ILE
1	A	299	LYS
1	A	315	CYS
1	A	319	PHE
1	A	342	LEU
1	A	344	PHE
1	A	345	ARG
1	A	385	ILE
1	A	389	ILE
1	A	401	LEU
1	A	424	GLN
1	A	431	ASP
1	A	460	MET
1	A	470	LEU
1	A	480	LEU

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Mol	Chain	Res	Type
1	A	496	LEU
1	A	535	ILE
1	A	537	HIS
1	A	558	GLU
1	A	566	LEU
1	B	34	LEU
1	B	37	ASN
1	B	58	LYS
1	B	72	ILE
1	B	87	TYR
1	B	88	CYS
1	B	98	MET
1	B	113	VAL
1	B	119	GLN
1	B	165	TRP
1	B	170	ILE
1	B	187	LYS
1	B	211	LEU
1	B	224	GLU
1	B	253	PRO
1	B	255	ILE
1	B	284	ILE
1	B	291	MET
1	B	292	ILE
1	B	299	LYS
1	B	319	PHE
1	B	339	THR
1	B	342	LEU
1	B	344	PHE
1	B	345	ARG
1	B	385	ILE
1	B	389	ILE
1	B	401	LEU
1	B	424	GLN
1	B	431	ASP
1	B	460	MET
1	B	470	LEU
1	B	480	LEU
1	B	535	ILE
1	B	537	HIS
1	B	558	GLU
1	B	566	LEU

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Mol	Chain	Res	Type
1	C	34	LEU
1	C	37	ASN
1	C	58	LYS
1	C	72	ILE
1	C	87	TYR
1	C	88	CYS
1	C	98	MET
1	C	108	MET
1	C	113	VAL
1	C	119	GLN
1	C	165	TRP
1	C	170	ILE
1	C	187	LYS
1	C	211	LEU
1	C	224	GLU
1	C	253	PRO
1	C	255	ILE
1	C	284	ILE
1	C	291	MET
1	C	292	ILE
1	C	299	LYS
1	C	319	PHE
1	C	339	THR
1	C	342	LEU
1	C	344	PHE
1	C	345	ARG
1	C	385	ILE
1	C	389	ILE
1	C	401	LEU
1	C	424	GLN
1	C	431	ASP
1	C	460	MET
1	C	470	LEU
1	C	480	LEU
1	C	535	ILE
1	C	537	HIS
1	C	558	GLU
1	C	566	LEU
1	D	34	LEU
1	D	37	ASN
1	D	58	LYS
1	D	72	ILE

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Mol	Chain	Res	Type
1	D	87	TYR
1	D	88	CYS
1	D	98	MET
1	D	108	MET
1	D	113	VAL
1	D	119	GLN
1	D	165	TRP
1	D	170	ILE
1	D	187	LYS
1	D	211	LEU
1	D	224	GLU
1	D	253	PRO
1	D	255	ILE
1	D	284	ILE
1	D	291	MET
1	D	292	ILE
1	D	299	LYS
1	D	319	PHE
1	D	339	THR
1	D	342	LEU
1	D	344	PHE
1	D	345	ARG
1	D	385	ILE
1	D	389	ILE
1	D	401	LEU
1	D	424	GLN
1	D	431	ASP
1	D	460	MET
1	D	470	LEU
1	D	480	LEU
1	D	535	ILE
1	D	537	HIS
1	D	558	GLU
1	D	566	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	107	HIS
1	A	119	GLN
1	A	134	GLN

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Mol	Chain	Res	Type
1	A	198	ASN
1	A	202	GLN
1	A	214	HIS
1	A	256	GLN
1	A	316	GLN
1	A	427	HIS
1	A	435	ASN
1	A	464	ASN
1	A	468	ASN
1	A	520	GLN
1	A	537	HIS
1	A	568	GLN
1	A	576	HIS
1	B	37	ASN
1	B	107	HIS
1	B	119	GLN
1	B	134	GLN
1	B	198	ASN
1	B	202	GLN
1	B	214	HIS
1	B	256	GLN
1	B	316	GLN
1	B	427	HIS
1	B	435	ASN
1	B	464	ASN
1	B	468	ASN
1	B	520	GLN
1	B	537	HIS
1	B	568	GLN
1	B	576	HIS
1	C	37	ASN
1	C	107	HIS
1	C	119	GLN
1	C	134	GLN
1	C	198	ASN
1	C	214	HIS
1	C	256	GLN
1	C	316	GLN
1	C	427	HIS
1	C	435	ASN
1	C	464	ASN
1	C	468	ASN

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Mol	Chain	Res	Type
1	C	520	GLN
1	C	568	GLN
1	C	576	HIS
1	D	37	ASN
1	D	107	HIS
1	D	119	GLN
1	D	134	GLN
1	D	198	ASN
1	D	256	GLN
1	D	316	GLN
1	D	427	HIS
1	D	435	ASN
1	D	464	ASN
1	D	468	ASN
1	D	520	GLN
1	D	537	HIS
1	D	568	GLN
1	D	576	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	ANP	C	5003	-	33,33,33	1.99	10 (30%)	45,52,52	1.72	6 (13%)
2	ANP	A	5001	-	33,33,33	2.15	10 (30%)	45,52,52	1.80	7 (15%)
2	ANP	B	5002	-	33,33,33	2.11	10 (30%)	45,52,52	1.68	8 (17%)
2	ANP	D	5004	-	33,33,33	1.84	8 (24%)	45,52,52	1.68	7 (15%)

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	ANP	C	5003	-	-	4/18/38/38	0/3/3/3
2	ANP	A	5001	-	-	4/18/38/38	0/3/3/3
2	ANP	B	5002	-	-	5/18/38/38	0/3/3/3
2	ANP	D	5004	-	-	5/18/38/38	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5002	ANP	PB-O3A	-6.74	1.50	1.59
2	A	5001	ANP	PB-O3A	-6.71	1.50	1.59
2	C	5003	ANP	PB-O3A	-5.72	1.52	1.59
2	D	5004	ANP	PB-O3A	-5.48	1.52	1.59
2	C	5003	ANP	PA-O3A	-4.79	1.54	1.59
2	B	5002	ANP	PA-O3A	-4.26	1.54	1.59
2	A	5001	ANP	PA-O3A	-4.21	1.54	1.59
2	B	5002	ANP	PB-O2B	-3.88	1.46	1.56
2	A	5001	ANP	PB-O2B	-3.84	1.46	1.56
2	D	5004	ANP	PG-O2G	-3.52	1.47	1.56
2	B	5002	ANP	PG-O2G	-3.43	1.47	1.56
2	A	5001	ANP	PG-O2G	-3.40	1.47	1.56
2	C	5003	ANP	PG-O2G	-3.14	1.48	1.56
2	A	5001	ANP	PG-N3B	-3.12	1.55	1.63
2	D	5004	ANP	PB-O2B	-3.08	1.48	1.56
2	C	5003	ANP	PB-O2B	-3.06	1.48	1.56
2	D	5004	ANP	PA-O3A	-2.95	1.56	1.59
2	A	5001	ANP	C4-N3	2.75	1.39	1.34
2	C	5003	ANP	PA-O5'	-2.58	1.49	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	5004	ANP	PG-O3G	-2.57	1.50	1.56
2	C	5003	ANP	PG-O3G	-2.51	1.50	1.56
2	A	5001	ANP	PB-N3B	-2.51	1.56	1.63
2	B	5002	ANP	PG-O3G	-2.50	1.50	1.56
2	A	5001	ANP	PG-O3G	-2.43	1.50	1.56
2	C	5003	ANP	C4-N3	2.43	1.39	1.34
2	B	5002	ANP	PG-O1G	2.42	1.49	1.46
2	D	5004	ANP	C4-N3	2.38	1.38	1.34
2	B	5002	ANP	C1'-N9	2.37	1.52	1.46
2	A	5001	ANP	C1'-N9	2.32	1.52	1.46
2	A	5001	ANP	PA-O5'	-2.31	1.50	1.59
2	D	5004	ANP	PG-N3B	-2.21	1.57	1.63
2	C	5003	ANP	PB-N3B	-2.17	1.57	1.63
2	D	5004	ANP	C1'-N9	2.16	1.52	1.46
2	C	5003	ANP	PA-O1A	-2.14	1.43	1.50
2	B	5002	ANP	PA-O5'	-2.14	1.51	1.59
2	C	5003	ANP	PG-N3B	-2.11	1.57	1.63
2	B	5002	ANP	C3'-C4'	-2.10	1.47	1.53
2	B	5002	ANP	PG-N3B	-2.00	1.58	1.63

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5001	ANP	O1G-PG-N3B	-6.08	102.82	111.77
2	B	5002	ANP	O1G-PG-N3B	-5.81	103.22	111.77
2	D	5004	ANP	O1G-PG-N3B	-5.58	103.56	111.77
2	C	5003	ANP	O1G-PG-N3B	-5.39	103.84	111.77
2	A	5001	ANP	O2B-PB-O1B	4.62	119.77	109.87
2	C	5003	ANP	O2B-PB-O1B	4.60	119.73	109.87
2	D	5004	ANP	O2B-PB-O1B	4.49	119.49	109.87
2	B	5002	ANP	O2B-PB-O1B	4.46	119.42	109.87
2	A	5001	ANP	O1B-PB-N3B	-4.30	105.44	111.77
2	C	5003	ANP	O1B-PB-N3B	-4.24	105.53	111.77
2	C	5003	ANP	O2G-PG-O3G	3.80	117.81	107.59
2	A	5001	ANP	O2G-PG-O3G	3.71	117.57	107.59
2	D	5004	ANP	O2G-PG-O3G	3.49	116.97	107.59
2	B	5002	ANP	O2G-PG-O3G	3.23	116.27	107.59
2	D	5004	ANP	O2B-PB-O3A	3.09	114.96	104.64
2	C	5003	ANP	O2B-PB-O3A	3.03	114.76	104.64
2	A	5001	ANP	O2B-PB-O3A	3.00	114.64	104.64
2	B	5002	ANP	O2B-PB-O3A	2.94	114.46	104.64
2	B	5002	ANP	O1B-PB-N3B	-2.94	107.44	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	5004	ANP	O1B-PB-N3B	-2.77	107.69	111.77
2	D	5004	ANP	O3A-PB-N3B	-2.42	99.87	106.59
2	B	5002	ANP	O2A-PA-O3A	2.26	113.38	107.27
2	A	5001	ANP	O2A-PA-O3A	2.22	113.27	107.27
2	B	5002	ANP	O3A-PB-N3B	-2.17	100.58	106.59
2	D	5004	ANP	O2A-PA-O3A	2.13	113.03	107.27
2	A	5001	ANP	O3A-PB-N3B	-2.09	100.78	106.59
2	C	5003	ANP	O2A-PA-O3A	2.09	112.92	107.27
2	B	5002	ANP	C4-N9-C8	-2.03	103.61	105.74

There are no chirality outliers.

All (18) torsion outliers are listed below:

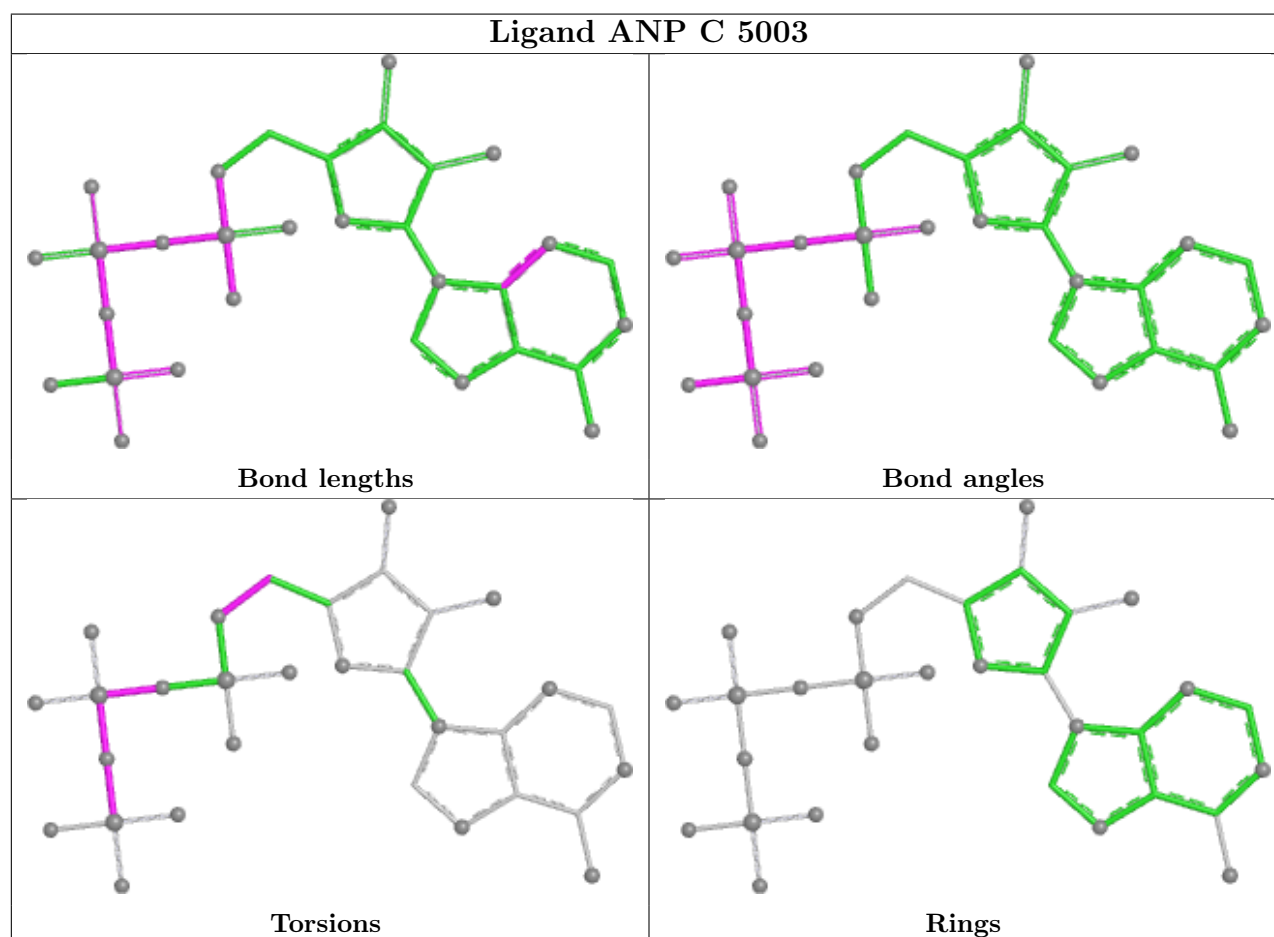
Mol	Chain	Res	Type	Atoms
2	A	5001	ANP	PB-N3B-PG-O1G
2	A	5001	ANP	PG-N3B-PB-O1B
2	B	5002	ANP	PB-N3B-PG-O1G
2	B	5002	ANP	PG-N3B-PB-O1B
2	C	5003	ANP	PB-N3B-PG-O1G
2	C	5003	ANP	PG-N3B-PB-O1B
2	D	5004	ANP	PB-N3B-PG-O1G
2	D	5004	ANP	PG-N3B-PB-O1B
2	B	5002	ANP	C4'-C5'-O5'-PA
2	A	5001	ANP	C4'-C5'-O5'-PA
2	C	5003	ANP	C4'-C5'-O5'-PA
2	D	5004	ANP	C4'-C5'-O5'-PA
2	A	5001	ANP	PA-O3A-PB-O2B
2	B	5002	ANP	PA-O3A-PB-O2B
2	C	5003	ANP	PA-O3A-PB-O2B
2	D	5004	ANP	PA-O3A-PB-O2B
2	B	5002	ANP	PA-O3A-PB-O1B
2	D	5004	ANP	PA-O3A-PB-O1B

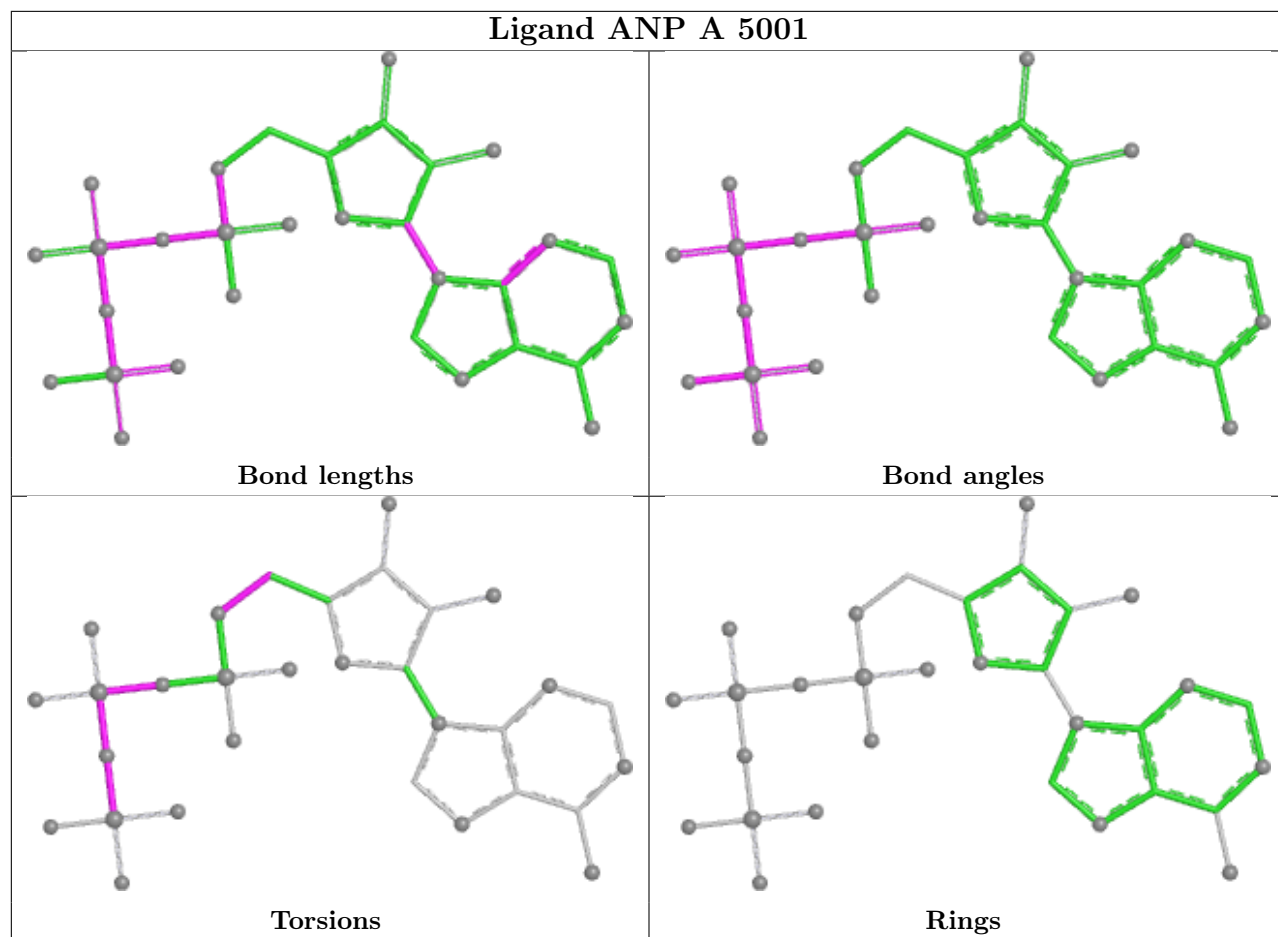
There are no ring outliers.

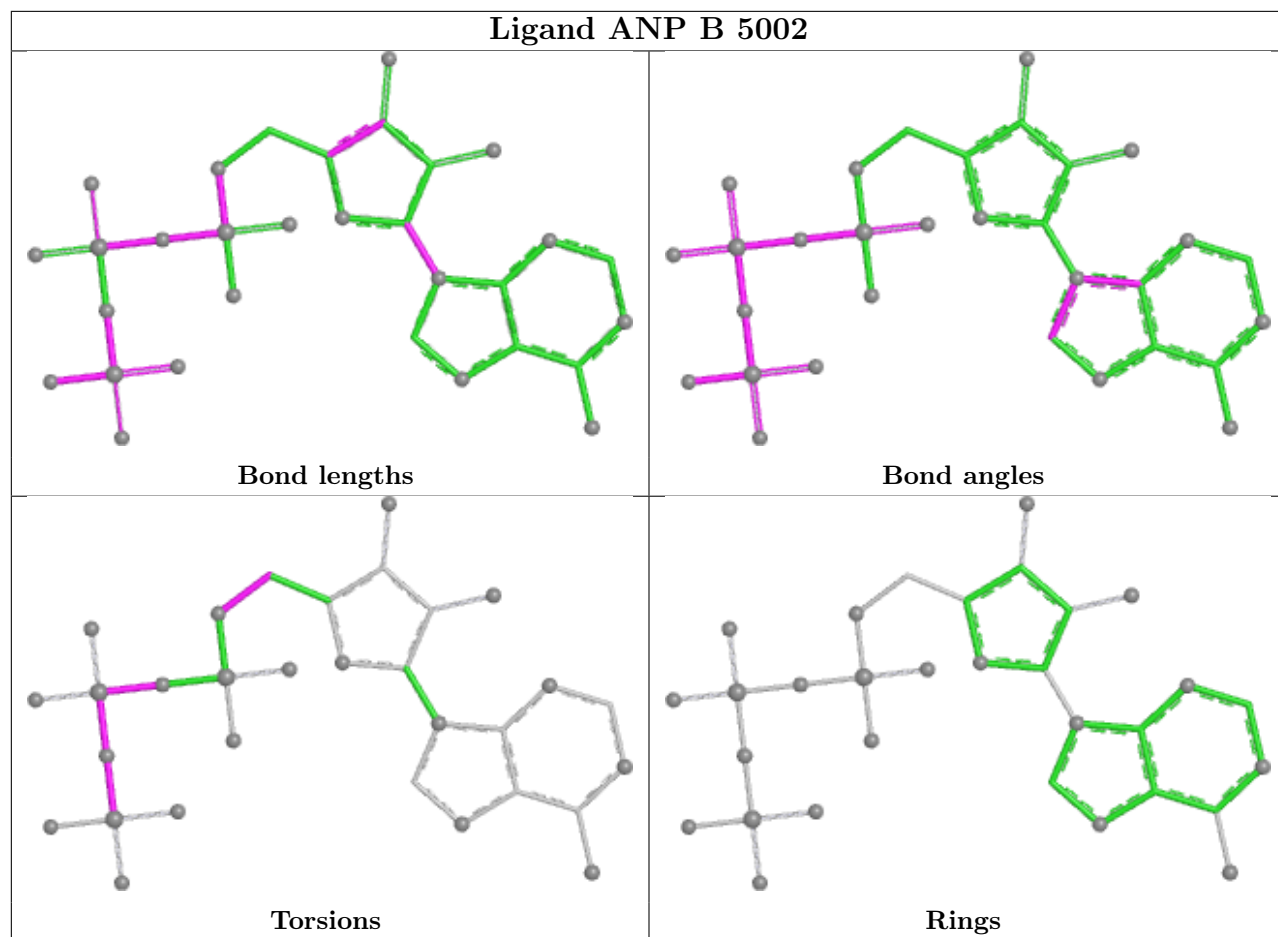
4 monomers are involved in 19 short contacts:

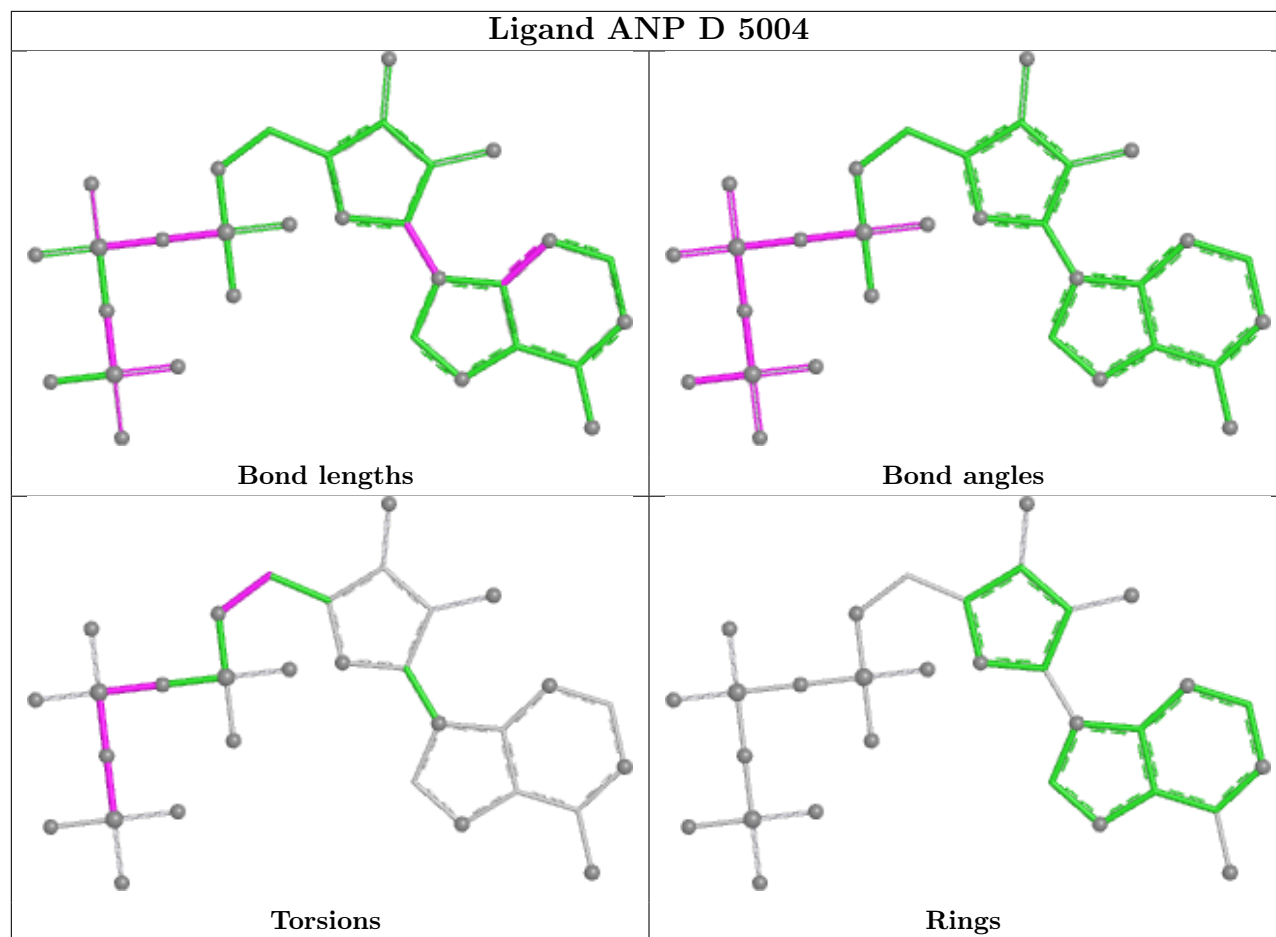
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	5003	ANP	3	0
2	A	5001	ANP	5	0
2	B	5002	ANP	6	0
2	D	5004	ANP	5	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	572/582 (98%)	0.36	33 (5%)	29	20	61, 154, 203, 205	0
1	B	572/582 (98%)	0.36	27 (4%)	36	23	55, 135, 200, 205	0
1	C	572/582 (98%)	0.28	27 (4%)	36	23	66, 137, 197, 205	0
1	D	572/582 (98%)	0.27	25 (4%)	39	25	59, 146, 201, 205	0
All	All	2288/2328 (98%)	0.32	112 (4%)	35	23	55, 143, 201, 205	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	51	LEU	8.2
1	A	279	LEU	5.3
1	A	295	MET	5.1
1	A	167	LEU	4.9
1	A	51	LEU	4.8
1	D	298	LEU	4.4
1	B	50	PRO	4.3
1	D	394	ASP	4.0
1	B	356	VAL	3.9
1	B	247	ALA	3.7
1	D	356	VAL	3.7
1	C	274	SER	3.7
1	D	163	TYR	3.6
1	C	298	LEU	3.6
1	B	266	VAL	3.4
1	C	441	ARG	3.4
1	B	570	GLY	3.4
1	A	448	GLU	3.4
1	C	379	GLY	3.3
1	C	270	ALA	3.2
1	A	60	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	60	ASP	3.0
1	B	181	ALA	3.0
1	D	266	VAL	2.9
1	D	284	ILE	2.9
1	D	279	LEU	2.9
1	C	394	ASP	2.8
1	C	442	THR	2.8
1	A	55	GLY	2.8
1	A	220	PHE	2.7
1	A	48	LEU	2.7
1	A	336	ASP	2.6
1	B	166	GLN	2.6
1	B	160	MET	2.6
1	B	267	LEU	2.6
1	B	255	ILE	2.6
1	A	70	VAL	2.6
1	D	440	ALA	2.6
1	D	245	VAL	2.5
1	C	526	LEU	2.5
1	C	70	VAL	2.5
1	A	288	PHE	2.5
1	A	204	THR	2.5
1	A	277	ASP	2.5
1	D	485	GLN	2.5
1	C	279	LEU	2.5
1	B	55	GLY	2.5
1	B	184	VAL	2.5
1	A	287	VAL	2.4
1	A	433	VAL	2.4
1	B	13	PHE	2.4
1	D	377	ARG	2.4
1	D	399	HIS	2.4
1	B	312	MET	2.4
1	B	442	THR	2.4
1	A	83	TYR	2.4
1	B	163	TYR	2.4
1	A	68	PRO	2.4
1	C	327	GLU	2.4
1	C	370	LYS	2.4
1	A	353	GLY	2.3
1	C	51	LEU	2.3
1	A	394	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	394	ASP	2.3
1	A	556	ILE	2.3
1	C	90	SER	2.3
1	D	287	VAL	2.3
1	A	351	TYR	2.3
1	C	338	ALA	2.3
1	D	338	ALA	2.3
1	C	60	ASP	2.3
1	D	357	PRO	2.3
1	B	56	PHE	2.3
1	C	22	PRO	2.3
1	D	94	GLY	2.3
1	C	220	PHE	2.3
1	C	62	SER	2.3
1	D	260	SER	2.3
1	D	184	VAL	2.3
1	C	440	ALA	2.2
1	A	276	MET	2.2
1	D	295	MET	2.2
1	A	270	ALA	2.2
1	B	295	MET	2.2
1	A	221	GLY	2.2
1	B	444	GLU	2.2
1	A	12	THR	2.2
1	D	512	ASP	2.2
1	D	159	MET	2.2
1	A	273	PRO	2.2
1	B	30	ALA	2.1
1	A	90	SER	2.1
1	B	333	ARG	2.1
1	B	192	ILE	2.1
1	B	286	VAL	2.1
1	C	59	THR	2.1
1	D	259	ALA	2.1
1	D	54	ASP	2.1
1	C	530	ARG	2.1
1	D	378	SER	2.1
1	A	445	TYR	2.1
1	D	376	GLY	2.1
1	B	291	MET	2.1
1	C	570	GLY	2.1
1	A	284	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	266	VAL	2.1
1	C	163	TYR	2.0
1	C	284	ILE	2.0
1	C	332	LYS	2.0
1	A	570	GLY	2.0
1	C	190	ARG	2.0
1	A	47	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

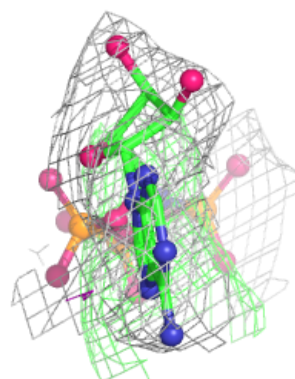
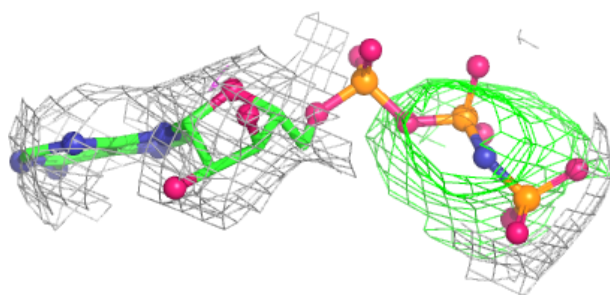
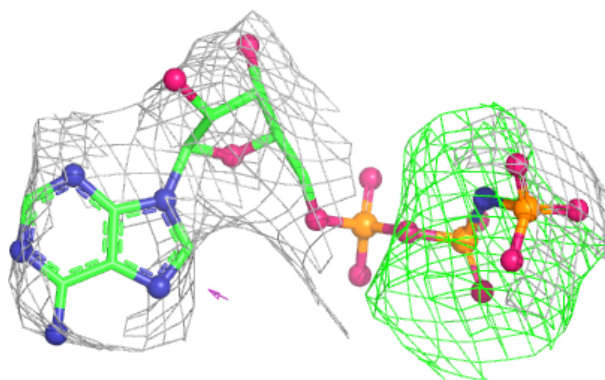
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ANP	A	5001	31/31	0.89	0.14	121,121,121,121	0
2	ANP	D	5004	31/31	0.92	0.13	139,139,139,139	0
2	ANP	C	5003	31/31	0.93	0.14	111,111,111,111	0
2	ANP	B	5002	31/31	0.93	0.14	124,124,124,124	0

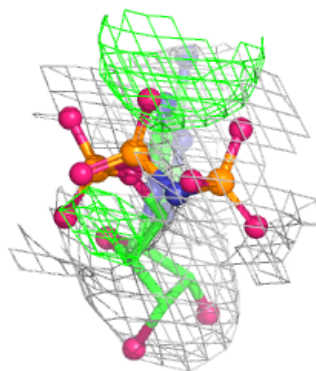
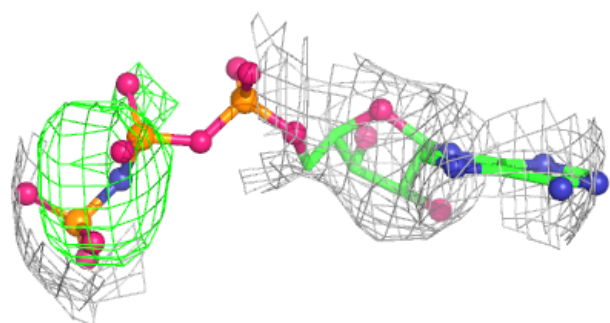
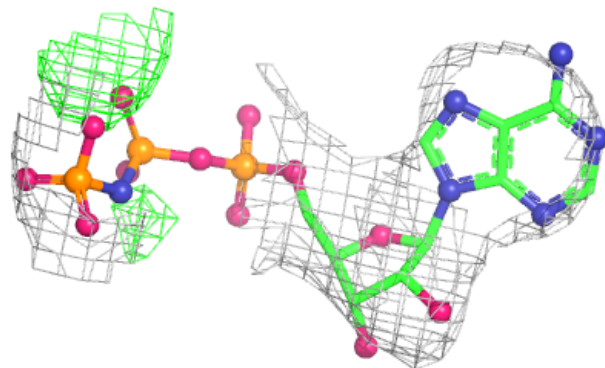
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP A 5001:

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

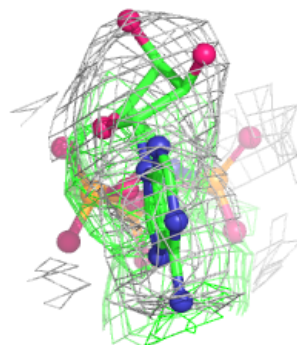
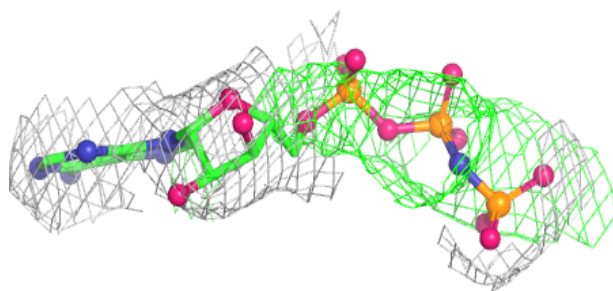
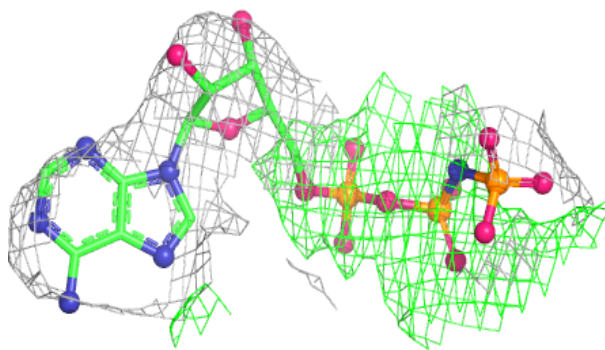
**Electron density around ANP D 5004:**

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

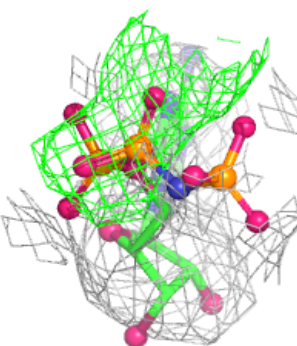
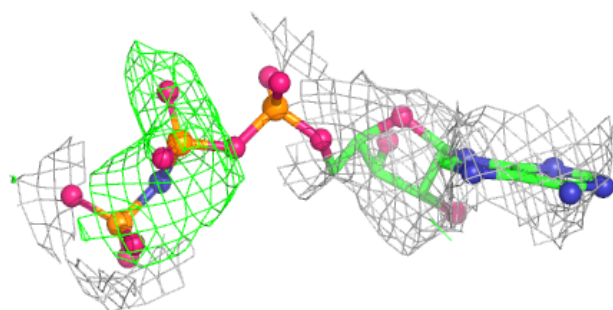
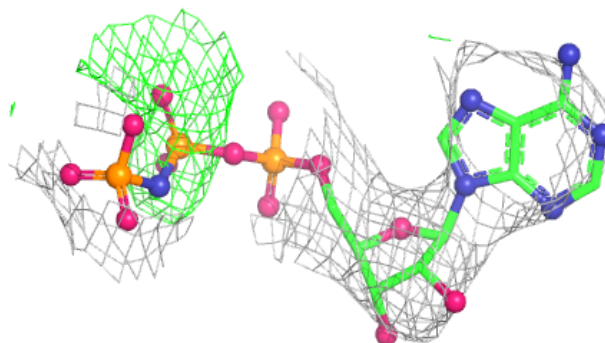


Electron density around ANP C 5003:

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

**Electron density around ANP B 5002:**

$2mF_o - DF_c$ (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.