



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:59 PM UTC

PDB ID : 1LKX / pdb_00001lkx
Title : MOTOR DOMAIN OF MYOE, A CLASS-I MYOSIN
Authors : Kollmar, M.; Durrwang, U.; Kliche, W.; Manstein, D.J.; Kull, F.J.
Deposited on : 2002-04-26
Resolution : 3.00 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

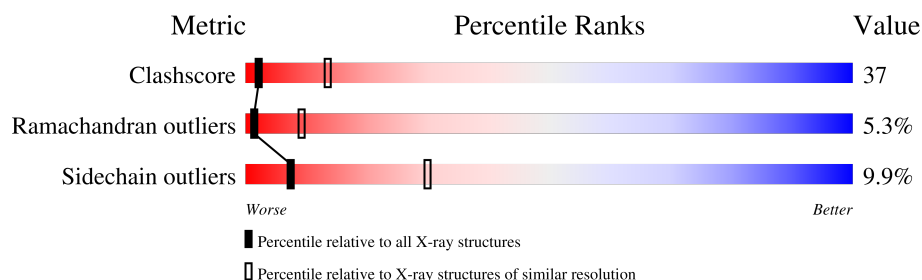
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	697	42% 41% 9% • 7%
1	B	697	43% 40% 9% • 7%
1	C	697	42% 43% 11% • •
1	D	697	42% 43% 7% • 5%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 21265 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MYOSIN IE HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	650	Total	C	N	O	S	0	0	0
			5192	3285	890	988	29			
1	B	650	Total	C	N	O	S	0	0	0
			5188	3282	889	988	29			
1	C	679	Total	C	N	O	S	0	0	0
			5422	3427	932	1033	30			
1	D	660	Total	C	N	O	S	0	0	0
			5267	3329	903	1005	30			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLU	ASP	SEE REMARK 999	UNP Q03479
A	48	THR	ARG	SEE REMARK 999	UNP Q03479
A	77	MET	ILE	SEE REMARK 999	UNP Q03479
A	?	-	ILE	SEE REMARK 999	UNP Q03479
A	?	-	ARG	SEE REMARK 999	UNP Q03479
A	137	LEU	PHE	SEE REMARK 999	UNP Q03479
A	138	ASP	GLN	SEE REMARK 999	UNP Q03479
A	215	ASP	ASN	SEE REMARK 999	UNP Q03479
A	371	ILE	LEU	SEE REMARK 999	UNP Q03479
A	372	ILE	SER	SEE REMARK 999	UNP Q03479
A	373	ASN	ILE	SEE REMARK 999	UNP Q03479
A	374	CYS	VAL	SEE REMARK 999	UNP Q03479
A	375	THR	HIS	SEE REMARK 999	UNP Q03479
A	376	THR	ARG	SEE REMARK 999	UNP Q03479
A	378	LYS	-	SEE REMARK 999	UNP Q03479
A	380	PRO	THR	SEE REMARK 999	UNP Q03479
A	427	VAL	-	SEE REMARK 999	UNP Q03479
A	428	ARG	-	SEE REMARK 999	UNP Q03479
A	429	GLU	LYS	SEE REMARK 999	UNP Q03479
A	440	ASN	-	SEE REMARK 999	UNP Q03479
A	498	ILE	ASN	SEE REMARK 999	UNP Q03479

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Chain	Residue	Modelled	Actual	Comment	Reference
A	604	VAL	ASP	SEE REMARK 999	UNP Q03479
A	681	ASN	ILE	SEE REMARK 999	UNP Q03479
A	683	THR	ARG	SEE REMARK 999	UNP Q03479
B	26	GLU	ASP	SEE REMARK 999	UNP Q03479
B	48	THR	ARG	SEE REMARK 999	UNP Q03479
B	77	MET	ILE	SEE REMARK 999	UNP Q03479
B	?	-	ILE	SEE REMARK 999	UNP Q03479
B	?	-	ARG	SEE REMARK 999	UNP Q03479
B	137	LEU	PHE	SEE REMARK 999	UNP Q03479
B	138	ASP	GLN	SEE REMARK 999	UNP Q03479
B	215	ASP	ASN	SEE REMARK 999	UNP Q03479
B	371	ILE	LEU	SEE REMARK 999	UNP Q03479
B	372	ILE	SER	SEE REMARK 999	UNP Q03479
B	373	ASN	ILE	SEE REMARK 999	UNP Q03479
B	374	CYS	VAL	SEE REMARK 999	UNP Q03479
B	375	THR	HIS	SEE REMARK 999	UNP Q03479
B	376	THR	ARG	SEE REMARK 999	UNP Q03479
B	378	LYS	-	SEE REMARK 999	UNP Q03479
B	380	PRO	THR	SEE REMARK 999	UNP Q03479
B	427	VAL	-	SEE REMARK 999	UNP Q03479
B	428	ARG	-	SEE REMARK 999	UNP Q03479
B	429	GLU	LYS	SEE REMARK 999	UNP Q03479
B	440	ASN	-	SEE REMARK 999	UNP Q03479
B	498	ILE	ASN	SEE REMARK 999	UNP Q03479
B	604	VAL	ASP	SEE REMARK 999	UNP Q03479
B	681	ASN	ILE	SEE REMARK 999	UNP Q03479
B	683	THR	ARG	SEE REMARK 999	UNP Q03479
C	26	GLU	ASP	SEE REMARK 999	UNP Q03479
C	48	THR	ARG	SEE REMARK 999	UNP Q03479
C	77	MET	ILE	SEE REMARK 999	UNP Q03479
C	?	-	ILE	SEE REMARK 999	UNP Q03479
C	?	-	ARG	SEE REMARK 999	UNP Q03479
C	137	LEU	PHE	SEE REMARK 999	UNP Q03479
C	138	ASP	GLN	SEE REMARK 999	UNP Q03479
C	215	ASP	ASN	SEE REMARK 999	UNP Q03479
C	371	ILE	LEU	SEE REMARK 999	UNP Q03479
C	372	ILE	SER	SEE REMARK 999	UNP Q03479
C	373	ASN	ILE	SEE REMARK 999	UNP Q03479
C	374	CYS	VAL	SEE REMARK 999	UNP Q03479
C	375	THR	HIS	SEE REMARK 999	UNP Q03479
C	376	THR	ARG	SEE REMARK 999	UNP Q03479
C	378	LYS	-	SEE REMARK 999	UNP Q03479

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Chain	Residue	Modelled	Actual	Comment	Reference
C	380	PRO	THR	SEE REMARK 999	UNP Q03479
C	427	VAL	-	SEE REMARK 999	UNP Q03479
C	428	ARG	-	SEE REMARK 999	UNP Q03479
C	429	GLU	LYS	SEE REMARK 999	UNP Q03479
C	440	ASN	-	SEE REMARK 999	UNP Q03479
C	498	ILE	ASN	SEE REMARK 999	UNP Q03479
C	604	VAL	ASP	SEE REMARK 999	UNP Q03479
C	681	ASN	ILE	SEE REMARK 999	UNP Q03479
C	683	THR	ARG	SEE REMARK 999	UNP Q03479
D	26	GLU	ASP	SEE REMARK 999	UNP Q03479
D	48	THR	ARG	SEE REMARK 999	UNP Q03479
D	77	MET	ILE	SEE REMARK 999	UNP Q03479
D	?	-	ILE	SEE REMARK 999	UNP Q03479
D	?	-	ARG	SEE REMARK 999	UNP Q03479
D	137	LEU	PHE	SEE REMARK 999	UNP Q03479
D	138	ASP	GLN	SEE REMARK 999	UNP Q03479
D	215	ASP	ASN	SEE REMARK 999	UNP Q03479
D	371	ILE	LEU	SEE REMARK 999	UNP Q03479
D	372	ILE	SER	SEE REMARK 999	UNP Q03479
D	373	ASN	ILE	SEE REMARK 999	UNP Q03479
D	374	CYS	VAL	SEE REMARK 999	UNP Q03479
D	375	THR	HIS	SEE REMARK 999	UNP Q03479
D	376	THR	ARG	SEE REMARK 999	UNP Q03479
D	378	LYS	-	SEE REMARK 999	UNP Q03479
D	380	PRO	THR	SEE REMARK 999	UNP Q03479
D	427	VAL	-	SEE REMARK 999	UNP Q03479
D	428	ARG	-	SEE REMARK 999	UNP Q03479
D	429	GLU	LYS	SEE REMARK 999	UNP Q03479
D	440	ASN	-	SEE REMARK 999	UNP Q03479
D	498	ILE	ASN	SEE REMARK 999	UNP Q03479
D	604	VAL	ASP	SEE REMARK 999	UNP Q03479
D	681	ASN	ILE	SEE REMARK 999	UNP Q03479
D	683	THR	ARG	SEE REMARK 999	UNP Q03479

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

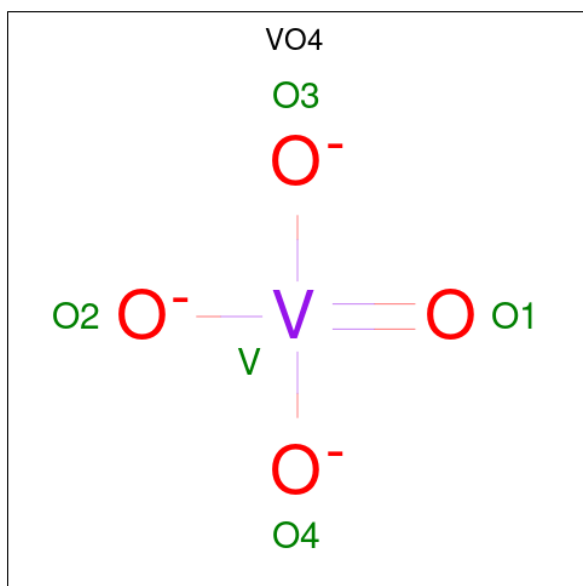
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

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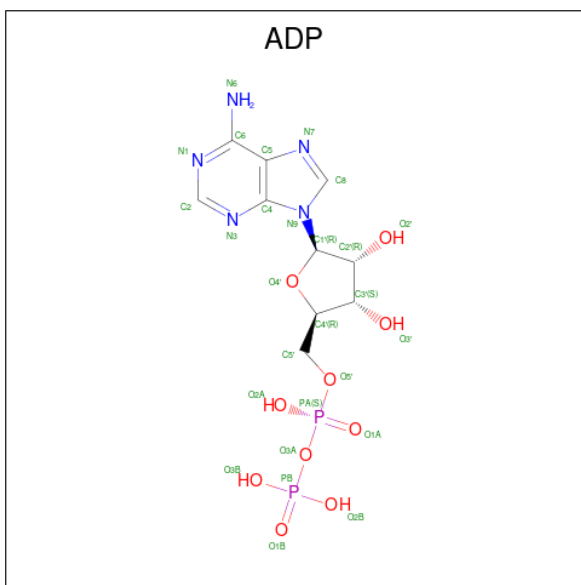
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is VANADATE ION (CCD ID: VO4) (formula: O_4V).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	V	0	0
			5	4	1		
3	B	1	Total	O	V	0	0
			5	4	1		
3	C	1	Total	O	V	0	0
			5	4	1		
3	D	1	Total	O	V	0	0
			5	4	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 5 is water.

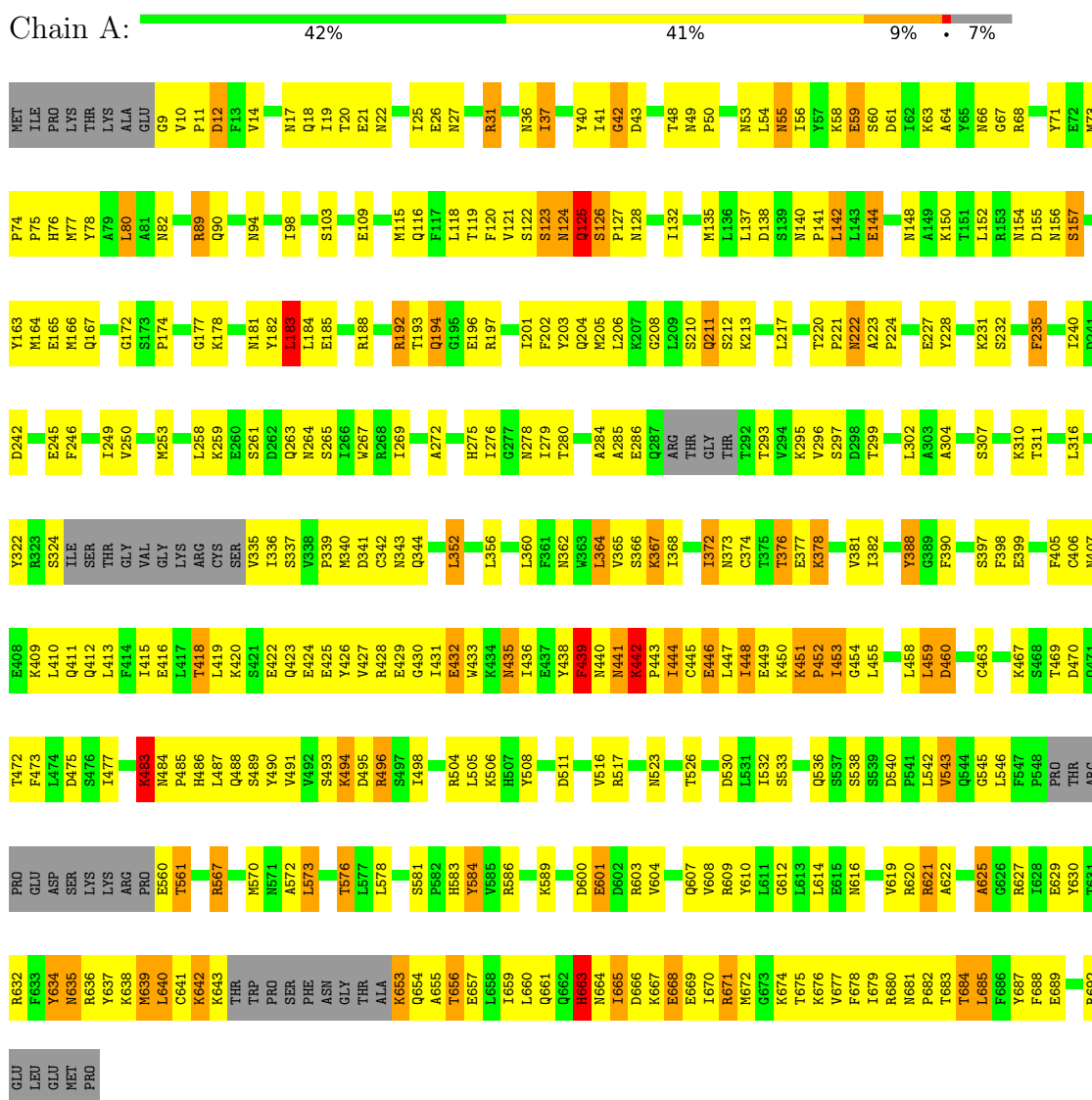
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	18	Total O 18 18	0	0
5	B	16	Total O 16 16	0	0
5	C	19	Total O 19 19	0	0
5	D	11	Total O 11 11	0	0

3 Residue-property plots

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

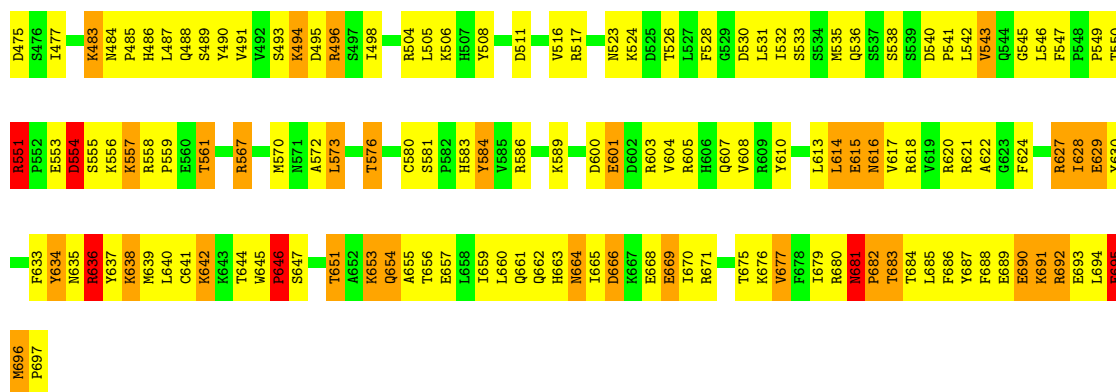
Note EDS was not executed.

• Molecule 1: MYOSIN IE HEAVY CHAIN



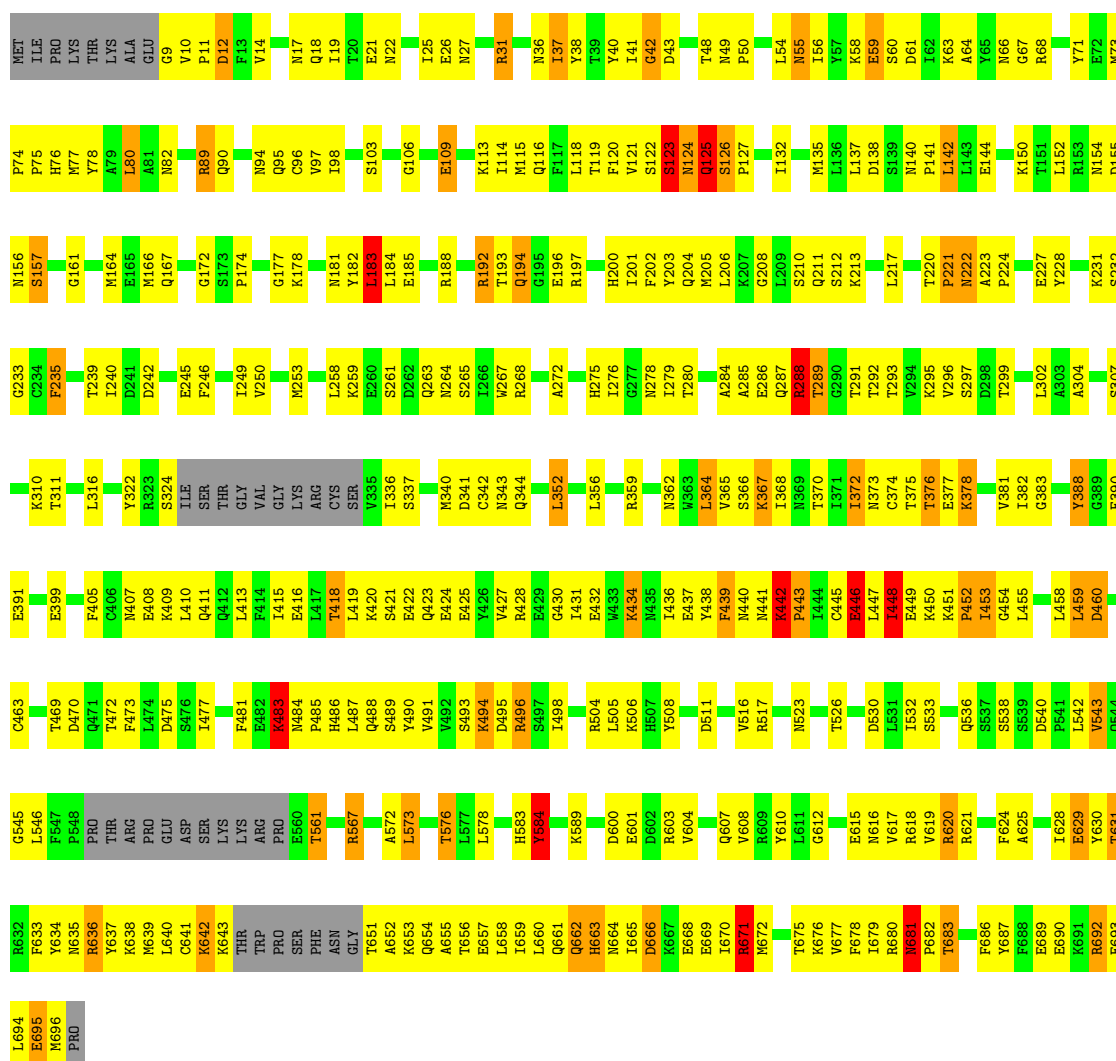
• Molecule 1: MYOSIN IE HEAVY CHAIN





Molecule 1: MYOSIN IE HEAVY CHAIN

Chain D: 42% 43% 7% 5%



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.82Å 143.67Å 236.05Å 90.00° 94.86° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	21265	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, VO4, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	0/5280	0.94	18/7108 (0.3%)
1	B	0.46	0/5276	0.91	13/7104 (0.2%)
1	C	0.53	0/5521	0.96	23/7442 (0.3%)
1	D	0.50	0/5356	0.94	18/7212 (0.2%)
All	All	0.50	0/21433	0.94	72/28866 (0.2%)

There are no bond length outliers.

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	441	ASN	N-CA-C	-10.71	100.26	113.97
1	A	125	GLN	N-CA-C	-10.57	100.93	114.04
1	B	125	GLN	N-CA-C	-9.98	101.67	114.04
1	D	125	GLN	N-CA-C	-9.84	101.04	113.43
1	C	125	GLN	N-CA-C	-9.77	101.92	114.04
1	D	289	THR	N-CA-C	-8.77	102.59	113.28
1	C	681	ASN	CA-C-N	8.47	130.43	119.84
1	C	681	ASN	C-N-CA	8.47	130.43	119.84
1	D	372	ILE	N-CA-C	8.28	118.93	111.81
1	A	483	LYS	N-CA-C	-8.22	93.30	110.80
1	D	483	LYS	N-CA-C	-8.13	93.49	110.80
1	B	483	LYS	N-CA-C	-8.02	93.72	110.80
1	C	483	LYS	N-CA-C	-7.99	93.77	110.80
1	A	372	ILE	N-CA-C	7.74	118.46	111.81
1	C	419	LEU	N-CA-C	7.71	123.44	113.18
1	B	372	ILE	N-CA-C	7.50	118.26	111.81
1	C	372	ILE	N-CA-C	7.22	118.02	111.81
1	D	443	PRO	N-CA-C	-7.15	105.23	114.03
1	A	685	LEU	N-CA-C	-7.04	106.59	114.62
1	D	442	LYS	N-CA-C	6.89	125.04	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	443	PRO	N-CA-C	-6.79	105.67	114.03
1	A	668	GLU	N-CA-C	-6.68	105.52	113.21
1	D	288	ARG	N-CA-C	-6.56	105.58	113.97
1	B	441	ASN	N-CA-C	-6.48	105.67	113.97
1	C	434	LYS	N-CA-C	-6.47	100.25	109.96
1	B	445	CYS	N-CA-C	-6.37	104.60	112.38
1	B	121	VAL	N-CA-C	-6.30	103.22	111.09
1	B	49	ASN	CA-C-N	6.18	125.75	119.19
1	B	49	ASN	C-N-CA	6.18	125.75	119.19
1	B	37	ILE	CB-CA-C	-6.13	104.03	111.88
1	C	547	PHE	CA-C-N	6.07	124.03	119.66
1	C	547	PHE	C-N-CA	6.07	124.03	119.66
1	C	37	ILE	CB-CA-C	-6.05	104.13	111.88
1	D	121	VAL	N-CA-C	-6.04	103.58	112.04
1	C	444	ILE	N-CA-C	-6.03	105.19	111.58
1	D	446	GLU	N-CA-C	-5.94	104.72	111.07
1	A	121	VAL	N-CA-C	-5.94	103.67	111.09
1	C	615	GLU	N-CA-C	-5.92	104.91	111.71
1	D	37	ILE	CB-CA-C	-5.90	104.33	111.88
1	C	121	VAL	N-CA-C	-5.89	103.73	111.09
1	A	441	ASN	N-CA-C	-5.85	105.98	113.23
1	A	442	LYS	CA-C-N	-5.83	113.64	120.12
1	A	442	LYS	C-N-CA	-5.83	113.64	120.12
1	D	681	ASN	CA-C-N	5.80	125.67	119.28
1	D	681	ASN	C-N-CA	5.80	125.67	119.28
1	C	581	SER	CA-C-N	5.73	125.64	119.85
1	C	581	SER	C-N-CA	5.73	125.64	119.85
1	A	446	GLU	N-CA-C	-5.70	103.89	111.24
1	D	442	LYS	CA-C-N	-5.69	113.96	119.87
1	D	442	LYS	C-N-CA	-5.69	113.96	119.87
1	B	636	ARG	N-CA-C	-5.58	105.58	112.38
1	C	628	ILE	N-CA-C	5.55	116.11	108.12
1	A	654	GLN	N-CA-C	-5.53	105.17	111.14
1	A	581	SER	CA-C-N	5.49	125.39	119.85
1	A	581	SER	C-N-CA	5.49	125.39	119.85
1	C	49	ASN	CA-C-N	5.48	124.83	118.85
1	C	49	ASN	C-N-CA	5.48	124.83	118.85
1	C	691	LYS	N-CA-C	-5.44	105.25	111.07
1	A	37	ILE	CB-CA-C	-5.41	104.96	111.88
1	C	251	LYS	N-CA-C	-5.41	105.28	111.07
1	B	451	LYS	N-CA-C	5.39	116.33	110.13
1	D	629	GLU	N-CA-C	-5.31	102.42	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	690	GLU	N-CA-C	-5.31	105.95	112.90
1	A	442	LYS	N-CA-C	5.21	121.31	109.81
1	B	584	TYR	N-CA-C	5.14	117.87	109.59
1	D	38	TYR	N-CA-C	5.13	118.58	109.96
1	A	451	LYS	CA-C-N	5.10	126.21	119.84
1	A	451	LYS	C-N-CA	5.10	126.21	119.84
1	A	240	ILE	N-CA-C	5.09	115.92	108.53
1	D	584	TYR	N-CA-C	5.05	117.73	109.59
1	D	671	ARG	N-CA-C	5.02	116.34	107.61
1	C	41	ILE	N-CA-C	-5.01	98.92	109.34

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	5192	0	5189	397	0
1	B	5188	0	5182	379	0
1	C	5422	0	5415	443	0
1	D	5267	0	5265	384	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
3	C	5	0	0	1	0
3	D	5	0	0	1	0
4	A	27	0	12	2	0
4	B	27	0	12	2	0
4	C	27	0	12	2	0
4	D	27	0	12	3	0
5	A	18	0	0	5	0
5	B	16	0	0	2	0
5	C	19	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	11	0	0	2	0
All	All	21265	0	21099	1570	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

All (1570) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ARG:HD3	1:D:259:LYS:HE2	1.24	1.17
1:C:635:ASN:HA	1:C:638:LYS:HD2	1.28	1.16
1:D:642:LYS:H	1:D:642:LYS:HD2	1.00	1.09
1:B:656:THR:HG21	1:B:677:VAL:HG21	1.37	1.06
1:C:288:ARG:HD3	1:C:288:ARG:H	1.22	1.03
1:C:629:GLU:CD	1:C:629:GLU:H	1.61	1.01
1:C:376:THR:HG23	1:D:373:ASN:O	1.60	1.01
1:B:76:HIS:HD2	1:B:78:TYR:H	1.00	1.00
1:B:635:ASN:HD22	1:B:636:ARG:H	1.09	0.99
1:A:125:GLN:NE2	1:C:68:ARG:HE	1.60	0.98
1:B:634:TYR:HB2	1:B:655:ALA:HB3	1.43	0.98
1:D:651:THR:HB	1:D:654:GLN:HG3	1.44	0.97
1:A:76:HIS:HD2	1:A:78:TYR:H	0.97	0.96
1:C:295:LYS:HD3	1:C:296:VAL:H	1.31	0.96
1:A:67:GLY:H	1:A:82:ASN:HD21	1.10	0.95
1:D:227:GLU:H	1:D:278:ASN:HD21	1.12	0.95
1:D:486:HIS:HA	1:D:506:LYS:HB2	1.49	0.95
1:A:37:ILE:HD11	1:A:54:LEU:HD22	1.49	0.95
1:C:67:GLY:H	1:C:82:ASN:HD21	1.12	0.94
1:A:125:GLN:HB3	1:C:68:ARG:NH2	1.81	0.94
1:C:76:HIS:HD2	1:C:78:TYR:H	1.00	0.94
1:A:295:LYS:HD3	1:A:296:VAL:H	1.30	0.94
1:B:295:LYS:HD3	1:B:296:VAL:H	1.31	0.93
1:B:67:GLY:H	1:B:82:ASN:HD21	1.11	0.93
1:B:627:ARG:HG2	1:B:676:LYS:HE2	1.48	0.93
1:D:295:LYS:HD3	1:D:296:VAL:H	1.32	0.92
1:B:37:ILE:HD11	1:B:54:LEU:HD22	1.52	0.92
1:D:76:HIS:HD2	1:D:78:TYR:H	0.96	0.92
1:D:642:LYS:HD2	1:D:642:LYS:N	1.84	0.92
1:B:132:ILE:HA	1:B:135:MET:HE3	1.51	0.92
1:B:227:GLU:H	1:B:278:ASN:HD21	1.17	0.91
1:C:227:GLU:H	1:C:278:ASN:HD21	1.15	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:ILE:HD11	1:D:54:LEU:HD22	1.52	0.91
1:D:67:GLY:H	1:D:82:ASN:HD21	1.10	0.91
1:D:448:ILE:HG12	1:D:448:ILE:O	1.71	0.91
1:D:291:THR:HG22	1:D:292:THR:HG22	1.52	0.91
1:B:620:ARG:HA	1:B:620:ARG:NE	1.84	0.91
1:D:76:HIS:CD2	1:D:78:TYR:H	1.88	0.90
1:C:181:ASN:HD21	1:C:362:ASN:ND2	1.70	0.90
1:A:589:LYS:H	1:A:607:GLN:HE22	1.19	0.89
1:A:486:HIS:HA	1:A:506:LYS:HB2	1.55	0.89
1:A:227:GLU:H	1:A:278:ASN:HD21	1.17	0.89
1:A:125:GLN:HB3	1:C:68:ARG:HH21	1.38	0.88
1:C:645:TRP:HB3	1:C:646:PRO:HD2	1.53	0.88
1:D:132:ILE:HA	1:D:135:MET:HE3	1.55	0.88
1:A:76:HIS:CD2	1:A:78:TYR:H	1.89	0.88
1:A:423:GLN:HE21	1:A:433:TRP:HE1	1.17	0.88
1:A:451:LYS:HB3	1:A:452:PRO:HD2	1.56	0.88
1:C:259:LYS:H	1:C:259:LYS:HD2	1.38	0.88
1:C:288:ARG:HD3	1:C:288:ARG:N	1.88	0.88
1:C:76:HIS:CD2	1:C:78:TYR:H	1.91	0.88
1:C:589:LYS:H	1:C:607:GLN:HE22	1.21	0.88
1:C:37:ILE:HD11	1:C:54:LEU:HD22	1.56	0.87
1:C:451:LYS:HB3	1:C:452:PRO:HD2	1.56	0.87
1:A:11:PRO:HA	1:A:31:ARG:HH21	1.40	0.87
1:D:451:LYS:HB3	1:D:452:PRO:HD2	1.56	0.86
1:A:132:ILE:HA	1:A:135:MET:HE3	1.58	0.86
1:B:76:HIS:CD2	1:B:78:TYR:H	1.92	0.86
1:B:486:HIS:HA	1:B:506:LYS:HB2	1.58	0.86
1:C:132:ILE:HA	1:C:135:MET:HE3	1.58	0.86
1:D:259:LYS:H	1:D:259:LYS:HD2	1.41	0.85
1:B:639:MET:O	1:B:640:LEU:HG	1.77	0.85
1:B:634:TYR:HB2	1:B:655:ALA:CB	2.06	0.85
1:C:486:HIS:HA	1:C:506:LYS:HB2	1.56	0.85
1:D:181:ASN:HD21	1:D:362:ASN:ND2	1.75	0.85
1:A:572:ALA:O	1:A:576:THR:HG22	1.76	0.85
1:B:377:GLU:HG2	1:D:681:ASN:OD1	1.77	0.84
1:B:451:LYS:HB3	1:B:452:PRO:HD2	1.57	0.84
1:D:418:THR:HG23	1:D:419:LEU:HG	1.58	0.84
1:A:259:LYS:H	1:A:259:LYS:HD2	1.43	0.84
1:D:11:PRO:HA	1:D:31:ARG:HH21	1.43	0.84
1:B:211:GLN:H	1:B:211:GLN:CD	1.83	0.84
1:C:572:ALA:O	1:C:576:THR:HG22	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:629:GLU:HA	1:D:675:THR:O	1.78	0.83
1:B:258:LEU:HD21	1:B:367:LYS:HD2	1.58	0.83
1:A:258:LEU:HD21	1:A:367:LYS:HD2	1.59	0.83
1:A:629:GLU:HA	1:A:676:LYS:HG2	1.58	0.83
1:D:211:GLN:CD	1:D:211:GLN:H	1.86	0.83
1:D:572:ALA:O	1:D:576:THR:HG22	1.78	0.83
1:C:696:MET:H	1:C:697:PRO:HA	1.44	0.82
1:C:408:GLU:HB3	1:C:446:GLU:OE1	1.79	0.82
1:B:11:PRO:HA	1:B:31:ARG:HH21	1.44	0.82
1:C:211:GLN:CD	1:C:211:GLN:H	1.87	0.82
1:D:258:LEU:HD21	1:D:367:LYS:HD2	1.62	0.82
1:B:589:LYS:H	1:B:607:GLN:HE22	1.24	0.82
1:C:635:ASN:HA	1:C:638:LYS:CD	2.08	0.81
1:B:572:ALA:O	1:B:576:THR:HG22	1.79	0.81
1:A:211:GLN:CD	1:A:211:GLN:H	1.87	0.81
1:C:660:LEU:HD13	1:C:670:ILE:HD13	1.62	0.81
1:B:12:ASP:HA	1:B:40:TYR:O	1.81	0.81
1:B:259:LYS:H	1:B:259:LYS:HD2	1.44	0.81
1:C:288:ARG:H	1:C:288:ARG:CD	1.89	0.81
1:D:288:ARG:HH11	1:D:288:ARG:HB2	1.46	0.81
1:D:12:ASP:HA	1:D:40:TYR:O	1.81	0.81
1:B:253:MET:HE3	1:B:263:GLN:HG2	1.61	0.80
1:D:642:LYS:NZ	1:D:662:GLN:HB3	1.96	0.80
1:C:80:LEU:HD11	1:C:583:HIS:HB3	1.64	0.80
1:A:156:ASN:ND2	4:A:791:ADP:O3'	2.13	0.80
1:A:439:PHE:HD1	1:A:440:ASN:N	1.79	0.80
1:A:10:VAL:HB	1:A:27:ASN:HD21	1.46	0.80
1:D:288:ARG:HB2	1:D:288:ARG:NH1	1.96	0.80
1:B:115:MET:O	1:B:119:THR:HG22	1.81	0.80
1:A:640:LEU:HD12	1:A:640:LEU:H	1.47	0.80
1:D:167:GLN:HE22	1:D:374:CYS:H	1.29	0.80
1:C:31:ARG:HH11	1:C:31:ARG:HB3	1.46	0.80
1:B:31:ARG:HH11	1:B:31:ARG:HB3	1.45	0.80
1:C:115:MET:O	1:C:119:THR:HG22	1.82	0.80
1:D:589:LYS:H	1:D:607:GLN:HE22	1.26	0.79
1:B:287:GLN:HB2	1:B:292:THR:HA	1.62	0.79
1:B:635:ASN:ND2	1:B:636:ARG:H	1.80	0.79
1:D:642:LYS:H	1:D:642:LYS:CD	1.84	0.79
1:C:10:VAL:HB	1:C:27:ASN:HD21	1.48	0.79
1:C:11:PRO:HA	1:C:31:ARG:HH21	1.48	0.79
1:D:288:ARG:CZ	1:D:288:ARG:H	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:LYS:HG2	1:B:511:ASP:OD1	1.84	0.78
1:B:635:ASN:HD22	1:B:636:ARG:N	1.80	0.78
1:C:258:LEU:HD21	1:C:367:LYS:HD2	1.65	0.78
1:B:181:ASN:HD21	1:B:362:ASN:ND2	1.82	0.78
1:A:441:ASN:C	1:A:443:PRO:HD3	2.09	0.77
1:D:506:LYS:HG2	1:D:511:ASP:OD1	1.83	0.77
1:C:131:ARG:HD3	1:D:259:LYS:CE	2.12	0.77
1:C:451:LYS:HB3	1:C:452:PRO:CD	2.15	0.77
1:A:67:GLY:H	1:A:82:ASN:ND2	1.83	0.77
1:A:119:THR:HG23	1:A:119:THR:O	1.84	0.77
1:A:442:LYS:HB2	1:A:442:LYS:NZ	2.00	0.77
1:A:115:MET:O	1:A:119:THR:HG22	1.85	0.77
1:A:669:GLU:C	1:A:670:ILE:HD12	2.08	0.77
1:B:418:THR:HG23	1:B:419:LEU:HG	1.68	0.76
1:B:10:VAL:HB	1:B:27:ASN:HD21	1.49	0.76
1:C:418:THR:CG2	1:C:616:ASN:HD21	1.97	0.76
1:D:431:ILE:HD12	1:D:671:ARG:HG2	1.65	0.76
1:C:441:ASN:O	1:C:442:LYS:HD3	1.85	0.76
1:D:642:LYS:HZ3	1:D:662:GLN:HB3	1.50	0.76
1:A:253:MET:HE3	1:A:263:GLN:HG2	1.67	0.76
1:D:67:GLY:H	1:D:82:ASN:ND2	1.83	0.76
1:A:12:ASP:HA	1:A:40:TYR:O	1.86	0.76
1:D:651:THR:HB	1:D:654:GLN:CG	2.14	0.76
1:D:10:VAL:HB	1:D:27:ASN:HD21	1.51	0.75
1:A:37:ILE:HG23	1:A:48:THR:O	1.85	0.75
1:A:436:ILE:HD12	1:A:619:VAL:HA	1.68	0.75
1:C:90:GLN:CD	1:C:636:ARG:HH21	1.95	0.75
1:D:115:MET:O	1:D:119:THR:HG22	1.87	0.75
1:D:434:LYS:O	1:D:434:LYS:HG2	1.86	0.75
1:D:451:LYS:HB3	1:D:452:PRO:CD	2.16	0.75
1:C:506:LYS:HG2	1:C:511:ASP:OD1	1.87	0.75
1:D:671:ARG:HB3	1:D:678:PHE:HB2	1.69	0.75
1:D:253:MET:HE3	1:D:263:GLN:HG2	1.69	0.74
1:C:287:GLN:HB3	1:C:291:THR:HG23	1.70	0.74
1:C:639:MET:HG2	1:C:640:LEU:HD12	1.68	0.74
1:A:10:VAL:HB	1:A:27:ASN:ND2	2.01	0.74
1:A:439:PHE:CD1	1:A:440:ASN:N	2.54	0.74
1:B:37:ILE:HG23	1:B:48:THR:O	1.87	0.74
1:B:451:LYS:HB3	1:B:452:PRO:CD	2.18	0.74
1:C:37:ILE:HG23	1:C:48:THR:O	1.88	0.74
1:C:636:ARG:HH11	1:C:636:ARG:HG2	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:660:LEU:HD13	1:D:670:ILE:CD1	2.17	0.74
1:B:67:GLY:H	1:B:82:ASN:ND2	1.85	0.74
1:D:119:THR:HG23	1:D:119:THR:O	1.87	0.74
1:D:641:CYS:HB2	1:D:659:ILE:HG12	1.69	0.74
1:C:119:THR:HG23	1:C:119:THR:O	1.86	0.73
1:A:177:GLY:O	1:A:372:ILE:HG22	1.88	0.73
1:C:418:THR:HG21	1:C:616:ASN:HD21	1.53	0.73
1:B:630:TYR:CE2	1:B:677:VAL:HG22	2.23	0.73
1:C:12:ASP:HA	1:C:40:TYR:O	1.89	0.73
1:C:167:GLN:HE22	1:C:374:CYS:H	1.34	0.73
1:A:636:ARG:HD2	1:A:636:ARG:O	1.89	0.73
1:B:423:GLN:HE22	1:B:436:ILE:H	1.37	0.73
1:C:177:GLY:O	1:C:372:ILE:HG22	1.89	0.73
1:A:181:ASN:HD21	1:A:362:ASN:ND2	1.86	0.73
1:A:451:LYS:HB3	1:A:452:PRO:CD	2.18	0.73
1:C:441:ASN:C	1:C:443:PRO:HD3	2.13	0.73
1:C:320:LEU:HD23	1:C:531:LEU:HD21	1.69	0.72
1:D:10:VAL:HB	1:D:27:ASN:ND2	2.04	0.72
1:D:31:ARG:HH11	1:D:31:ARG:HB3	1.52	0.72
1:A:80:LEU:HD11	1:A:583:HIS:HB3	1.69	0.72
1:A:125:GLN:HE21	1:C:68:ARG:HE	1.38	0.72
1:A:378:LYS:C	1:A:378:LYS:HD3	2.14	0.72
1:C:645:TRP:HB3	1:C:646:PRO:CD	2.18	0.72
1:C:634:TYR:O	1:C:638:LYS:HG3	1.88	0.72
1:D:27:ASN:O	1:D:31:ARG:HG2	1.89	0.72
1:C:636:ARG:O	1:C:636:ARG:HD3	1.89	0.72
1:C:443:PRO:O	1:C:447:LEU:HG	1.90	0.72
1:B:119:THR:HG23	1:B:119:THR:O	1.90	0.71
1:C:67:GLY:H	1:C:82:ASN:ND2	1.88	0.71
1:C:253:MET:HE3	1:C:263:GLN:HG2	1.72	0.71
1:D:620:ARG:CZ	1:D:620:ARG:HA	2.20	0.71
1:A:128:ASN:OD1	1:C:73:MET:HA	1.90	0.71
1:C:227:GLU:H	1:C:278:ASN:ND2	1.89	0.71
1:A:423:GLN:HE22	1:A:436:ILE:H	1.39	0.71
1:C:10:VAL:HB	1:C:27:ASN:ND2	2.05	0.71
1:B:448:ILE:HG12	1:B:448:ILE:O	1.89	0.71
1:B:684:THR:HG22	1:B:688:PHE:HE1	1.56	0.71
1:C:289:THR:O	1:C:291:THR:HG22	1.91	0.70
1:C:445:CYS:O	1:C:448:ILE:HG22	1.89	0.70
1:B:80:LEU:HD11	1:B:583:HIS:HB3	1.71	0.70
1:A:506:LYS:HG2	1:A:511:ASP:OD1	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:685:LEU:O	1:C:686:PHE:C	2.34	0.70
1:D:222:ASN:OD1	1:D:224:PRO:HD2	1.91	0.70
1:D:378:LYS:HD3	1:D:378:LYS:C	2.16	0.70
1:B:378:LYS:HG3	1:D:666:ASP:HB2	1.73	0.70
1:B:10:VAL:HB	1:B:27:ASN:ND2	2.05	0.70
1:B:227:GLU:H	1:B:278:ASN:ND2	1.90	0.70
1:C:222:ASN:OD1	1:C:224:PRO:HD2	1.92	0.70
1:A:227:GLU:H	1:A:278:ASN:ND2	1.90	0.70
1:A:637:TYR:O	1:A:659:ILE:HD13	1.92	0.70
1:C:444:ILE:HD12	1:C:444:ILE:H	1.57	0.70
1:C:637:TYR:CE2	1:C:688:PHE:HB3	2.27	0.70
1:A:31:ARG:HB3	1:A:31:ARG:HH11	1.56	0.69
1:D:37:ILE:HG23	1:D:48:THR:O	1.92	0.69
1:B:615:GLU:O	1:B:619:VAL:HG23	1.91	0.69
1:A:444:ILE:N	1:A:444:ILE:HD12	2.08	0.69
1:B:473:PHE:CZ	1:B:477:ILE:HD11	2.28	0.69
1:D:227:GLU:H	1:D:278:ASN:ND2	1.86	0.69
1:D:443:PRO:HA	1:D:446:GLU:HG2	1.75	0.69
1:C:473:PHE:CZ	1:C:477:ILE:HD11	2.27	0.69
1:D:181:ASN:HD21	1:D:362:ASN:HD21	1.40	0.69
1:D:142:LEU:HD11	1:D:364:LEU:HD21	1.75	0.69
1:A:671:ARG:HG2	1:A:671:ARG:HH11	1.58	0.69
1:C:416:GLU:OE2	1:C:420:LYS:HD3	1.93	0.69
1:A:477:ILE:HG22	1:A:487:LEU:HD21	1.75	0.68
1:B:177:GLY:O	1:B:372:ILE:HG22	1.93	0.68
1:A:144:GLU:HG3	5:A:798:HOH:O	1.94	0.68
1:B:692:ARG:HE	1:B:692:ARG:HA	1.58	0.68
1:A:431:ILE:O	1:A:432:GLU:C	2.35	0.68
1:B:642:LYS:HD2	1:B:642:LYS:N	2.08	0.68
1:C:311:THR:HG22	1:C:538:SER:HA	1.76	0.68
1:D:250:VAL:HA	1:D:253:MET:HG3	1.74	0.68
1:C:620:ARG:HA	1:C:620:ARG:CZ	2.24	0.68
1:D:493:SER:O	1:D:495:ASP:N	2.27	0.68
1:B:156:ASN:ND2	4:B:794:ADP:O3'	2.26	0.68
1:B:443:PRO:O	1:B:447:LEU:HG	1.94	0.68
1:C:493:SER:O	1:C:495:ASP:N	2.27	0.68
1:D:573:LEU:O	1:D:576:THR:HG23	1.94	0.68
1:B:27:ASN:O	1:B:31:ARG:HG2	1.94	0.68
1:B:504:ARG:HD2	1:B:511:ASP:HB3	1.75	0.68
1:A:641:CYS:HB2	1:A:659:ILE:HG12	1.76	0.67
1:B:477:ILE:HG22	1:B:487:LEU:HD21	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ASN:O	1:C:31:ARG:HG2	1.94	0.67
1:B:621:ARG:HH21	1:B:621:ARG:HG3	1.59	0.67
1:A:64:ALA:O	1:A:68:ARG:HD2	1.95	0.67
1:A:454:GLY:O	1:A:458:LEU:HD23	1.95	0.67
1:A:473:PHE:CZ	1:A:477:ILE:HD11	2.29	0.67
1:B:197:ARG:HG2	1:B:203:TYR:CZ	2.29	0.67
1:C:630:TYR:CE2	1:C:677:VAL:HG22	2.29	0.67
1:D:683:THR:HA	1:D:686:PHE:CD2	2.30	0.67
1:A:27:ASN:O	1:A:31:ARG:HG2	1.94	0.67
1:D:177:GLY:O	1:D:372:ILE:HG22	1.95	0.67
1:B:493:SER:O	1:B:495:ASP:N	2.28	0.67
1:A:666:ASP:HB3	1:A:668:GLU:HG2	1.77	0.66
1:A:669:GLU:O	1:A:670:ILE:HD12	1.95	0.66
1:C:436:ILE:HD12	1:C:436:ILE:H	1.61	0.66
1:B:378:LYS:HD3	1:B:378:LYS:C	2.20	0.66
1:C:311:THR:HG22	1:C:538:SER:CA	2.25	0.66
1:D:275:HIS:CE1	1:D:304:ALA:HB1	2.30	0.66
1:A:573:LEU:O	1:A:576:THR:HG23	1.95	0.66
1:C:122:SER:OG	1:C:174:PRO:HG3	1.94	0.66
1:C:181:ASN:HD21	1:C:362:ASN:HD21	1.40	0.66
1:C:573:LEU:O	1:C:576:THR:HG23	1.96	0.66
1:D:284:ALA:HB3	1:D:293:THR:C	2.21	0.66
1:D:630:TYR:HE2	1:D:672:MET:HE3	1.60	0.66
1:D:692:ARG:HG3	1:D:692:ARG:HH11	1.60	0.66
1:A:443:PRO:HD2	1:A:444:ILE:HD13	1.77	0.66
1:B:181:ASN:HD21	1:B:362:ASN:HD21	1.41	0.66
1:A:629:GLU:OE1	1:A:632:ARG:HD2	1.96	0.66
1:D:80:LEU:HD11	1:D:583:HIS:HB3	1.78	0.66
1:A:656:THR:CG2	1:A:672:MET:HE1	2.25	0.66
1:C:90:GLN:HE22	1:C:636:ARG:NH2	1.94	0.66
1:C:131:ARG:CD	1:D:259:LYS:HE2	2.15	0.66
1:A:493:SER:O	1:A:495:ASP:N	2.28	0.66
1:A:504:ARG:HD2	1:A:511:ASP:HB3	1.77	0.66
1:C:197:ARG:HG2	1:C:203:TYR:CZ	2.31	0.66
1:A:443:PRO:HG2	1:A:444:ILE:HD12	1.77	0.66
1:B:635:ASN:HA	1:B:638:LYS:HB2	1.78	0.66
1:D:504:ARG:HD2	1:D:511:ASP:HB3	1.78	0.66
1:A:197:ARG:HG2	1:A:203:TYR:CZ	2.30	0.65
1:B:573:LEU:O	1:B:576:THR:HG23	1.96	0.65
1:D:157:SER:N	5:D:905:HOH:O	2.29	0.65
1:A:423:GLN:HE22	1:A:436:ILE:N	1.93	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:LYS:HD3	1:C:378:LYS:C	2.20	0.65
1:D:454:GLY:O	1:D:458:LEU:HD23	1.96	0.65
1:C:644:THR:HG22	1:C:644:THR:O	1.95	0.65
1:C:443:PRO:HA	1:C:446:GLU:CG	2.26	0.65
1:D:324:SER:HA	1:D:336:ILE:O	1.96	0.65
1:A:665:ILE:HD11	1:A:688:PHE:HZ	1.62	0.65
1:B:662:GLN:C	1:B:664:ASN:H	2.04	0.65
1:C:194:GLN:CD	1:C:194:GLN:H	2.03	0.64
1:D:425:GLU:HA	1:D:428:ARG:NH2	2.12	0.64
1:A:670:ILE:HD11	1:A:679:ILE:HG23	1.78	0.64
1:D:119:THR:HG21	1:D:137:LEU:HD21	1.78	0.64
1:D:259:LYS:HD2	1:D:259:LYS:N	2.13	0.64
1:A:125:GLN:NE2	1:C:68:ARG:NE	2.39	0.64
1:C:259:LYS:HD2	1:C:259:LYS:N	2.11	0.64
1:C:423:GLN:HE21	1:C:433:TRP:HE1	1.44	0.64
1:D:89:ARG:HE	1:D:172:GLY:HA3	1.62	0.64
1:A:627:ARG:H	1:A:627:ARG:HD2	1.62	0.64
1:C:551:ARG:HD3	1:C:555:SER:OG	1.98	0.64
1:B:89:ARG:HE	1:B:172:GLY:HA3	1.63	0.64
1:A:295:LYS:HD3	1:A:296:VAL:N	2.09	0.64
1:A:423:GLN:NE2	1:A:436:ILE:H	1.95	0.64
1:C:679:ILE:HG21	1:C:684:THR:HB	1.80	0.64
1:B:17:ASN:CG	1:B:18:GLN:H	2.05	0.64
1:C:504:ARG:HD2	1:C:511:ASP:HB3	1.79	0.64
1:D:680:ARG:O	1:D:681:ASN:HB2	1.98	0.64
1:A:416:GLU:OE2	1:A:420:LYS:HD3	1.99	0.63
1:C:441:ASN:OD1	1:C:443:PRO:HD3	1.98	0.63
1:C:295:LYS:HD3	1:C:296:VAL:N	2.10	0.63
1:A:441:ASN:O	1:A:443:PRO:HD3	1.97	0.63
1:D:473:PHE:CZ	1:D:477:ILE:HD11	2.33	0.63
1:B:194:GLN:OE1	1:B:194:GLN:N	2.28	0.63
1:C:98:ILE:HD11	1:C:584:TYR:CD2	2.32	0.63
1:C:142:LEU:HD12	1:C:368:ILE:HD11	1.79	0.63
1:C:167:GLN:NE2	1:C:374:CYS:HB3	2.14	0.63
1:B:443:PRO:O	1:B:446:GLU:HB2	1.99	0.63
1:C:477:ILE:HG22	1:C:487:LEU:HD21	1.79	0.63
1:D:197:ARG:HG2	1:D:203:TYR:CZ	2.33	0.63
1:A:671:ARG:HG2	1:A:671:ARG:NH1	2.12	0.63
1:B:171:VAL:HG22	1:D:690:GLU:OE2	1.97	0.63
1:C:365:VAL:HG23	1:C:366:SER:N	2.14	0.63
1:C:412:GLN:HB2	1:C:442:LYS:HE2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:LYS:C	1:C:444:ILE:H	2.06	0.63
1:C:639:MET:HE2	1:C:696:MET:HE1	1.80	0.63
1:B:222:ASN:OD1	1:B:224:PRO:HD2	1.98	0.63
1:C:655:ALA:O	1:C:659:ILE:HG13	1.98	0.63
1:B:412:GLN:HB2	1:B:442:LYS:HE2	1.80	0.63
1:B:439:PHE:CG	1:B:440:ASN:N	2.67	0.63
1:A:103:SER:HA	3:A:792:VO4:O1	1.99	0.62
1:A:89:ARG:HE	1:A:172:GLY:HA3	1.64	0.62
1:C:613:LEU:O	1:C:617:VAL:HG23	1.98	0.62
1:C:694:LEU:O	1:C:695:GLU:HB3	1.98	0.62
1:A:22:ASN:O	1:A:26:GLU:HG3	1.98	0.62
1:B:454:GLY:O	1:B:458:LEU:HD23	1.99	0.62
1:A:683:THR:C	1:A:685:LEU:H	2.08	0.62
1:B:40:TYR:CZ	1:B:75:PRO:HA	2.33	0.62
1:C:259:LYS:H	1:C:259:LYS:CD	2.11	0.62
1:C:438:TYR:O	1:C:439:PHE:O	2.18	0.62
1:C:683:THR:HA	1:C:686:PHE:CD2	2.35	0.62
1:C:443:PRO:HA	1:C:446:GLU:HG2	1.81	0.62
1:A:259:LYS:HD2	1:A:259:LYS:N	2.13	0.62
1:A:444:ILE:N	1:A:444:ILE:CD1	2.61	0.62
1:C:17:ASN:CG	1:C:18:GLN:H	2.08	0.62
1:A:423:GLN:NE2	1:A:433:TRP:HE1	1.94	0.62
1:B:170:ALA:HB1	1:D:687:TYR:CD1	2.34	0.62
1:B:213:LYS:NZ	1:B:264:ASN:HD21	1.98	0.62
1:B:686:PHE:O	1:B:690:GLU:HG2	1.99	0.62
1:C:89:ARG:HE	1:C:172:GLY:HA3	1.65	0.62
1:A:127:PRO:HD2	1:C:73:MET:HG2	1.82	0.62
1:A:250:VAL:HA	1:A:253:MET:HG3	1.82	0.61
1:D:122:SER:OG	1:D:174:PRO:HG3	1.99	0.61
1:A:76:HIS:HD2	1:A:78:TYR:N	1.82	0.61
1:A:473:PHE:CE2	1:A:477:ILE:HD11	2.35	0.61
1:A:653:LYS:HZ2	1:A:653:LYS:HB2	1.65	0.61
1:B:451:LYS:HD2	1:B:451:LYS:N	2.16	0.61
1:C:40:TYR:CZ	1:C:75:PRO:HA	2.35	0.61
1:A:641:CYS:HB2	1:A:659:ILE:HG23	1.82	0.61
1:D:477:ILE:HG22	1:D:487:LEU:HD21	1.81	0.61
1:C:533:SER:HA	1:C:536:GLN:HE21	1.66	0.61
1:C:636:ARG:HG2	1:C:636:ARG:NH1	2.15	0.61
1:C:641:CYS:SG	1:C:662:GLN:NE2	2.74	0.61
1:B:64:ALA:O	1:B:68:ARG:HD2	2.00	0.61
1:B:211:GLN:CD	1:B:211:GLN:N	2.58	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:MET:HE3	1:C:77:MET:O	2.01	0.61
1:C:629:GLU:CD	1:C:629:GLU:N	2.44	0.61
1:D:17:ASN:CG	1:D:18:GLN:H	2.09	0.61
1:D:194:GLN:OE1	1:D:194:GLN:N	2.32	0.61
1:D:669:GLU:O	1:D:669:GLU:HG3	2.01	0.61
1:A:222:ASN:OD1	1:A:224:PRO:HD2	2.01	0.61
1:A:451:LYS:HD2	1:A:451:LYS:N	2.16	0.61
1:B:419:LEU:HD22	1:B:619:VAL:HG21	1.82	0.61
1:B:428:ARG:HG2	1:B:428:ARG:HH11	1.66	0.61
1:A:419:LEU:HD13	1:A:438:TYR:CB	2.30	0.61
1:A:448:ILE:HG12	1:A:448:ILE:O	2.00	0.61
1:A:667:LYS:C	1:A:669:GLU:H	2.09	0.61
1:D:439:PHE:CE2	1:D:612:GLY:HA3	2.35	0.61
1:D:680:ARG:O	1:D:681:ASN:CB	2.49	0.61
1:A:441:ASN:C	1:A:443:PRO:CD	2.74	0.61
1:B:142:LEU:HD11	1:B:364:LEU:HD21	1.81	0.61
1:D:64:ALA:O	1:D:68:ARG:HD2	2.01	0.61
1:B:409:LYS:HD2	1:B:446:GLU:OE1	2.01	0.60
1:B:22:ASN:O	1:B:26:GLU:HG3	2.00	0.60
1:B:667:LYS:O	1:B:669:GLU:N	2.34	0.60
1:C:473:PHE:CE2	1:C:477:ILE:HD11	2.36	0.60
1:D:40:TYR:CZ	1:D:75:PRO:HA	2.36	0.60
1:D:142:LEU:CD1	1:D:364:LEU:HD21	2.30	0.60
1:A:21:GLU:O	1:A:25:ILE:HD13	2.02	0.60
1:A:636:ARG:HG3	1:A:637:TYR:CD1	2.36	0.60
1:B:426:TYR:HE2	1:B:623:GLY:HA2	1.65	0.60
1:B:438:TYR:HA	1:B:615:GLU:HG2	1.82	0.60
1:C:443:PRO:HD2	1:C:444:ILE:CD1	2.31	0.60
1:D:55:ASN:HD21	1:D:58:LYS:HD3	1.65	0.60
1:D:473:PHE:CE2	1:D:477:ILE:HD11	2.36	0.60
1:A:40:TYR:CZ	1:A:75:PRO:HA	2.36	0.60
1:A:629:GLU:HG2	1:A:676:LYS:NZ	2.16	0.60
1:C:194:GLN:OE1	1:C:194:GLN:N	2.29	0.60
1:D:654:GLN:O	1:D:658:LEU:HG	2.02	0.60
1:A:280:THR:OG1	1:A:297:SER:HB2	2.02	0.60
1:A:148:ASN:ND2	5:A:798:HOH:O	2.34	0.60
1:B:250:VAL:HA	1:B:253:MET:HG3	1.84	0.60
1:D:55:ASN:ND2	1:D:58:LYS:HD3	2.16	0.60
1:B:122:SER:OG	1:B:174:PRO:HG3	2.02	0.60
1:B:621:ARG:HG3	1:B:621:ARG:NH2	2.17	0.60
1:A:17:ASN:CG	1:A:18:GLN:H	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:ASN:HD22	1:C:67:GLY:N	2.00	0.60
1:C:156:ASN:ND2	4:C:891:ADP:O3'	2.35	0.60
1:C:309:LEU:HD13	1:C:535:MET:HE1	1.84	0.60
1:D:451:LYS:N	1:D:451:LYS:HD2	2.17	0.60
1:B:442:LYS:HE3	1:B:442:LYS:O	2.02	0.60
1:B:473:PHE:CE2	1:B:477:ILE:HD11	2.37	0.60
1:B:504:ARG:HG2	1:B:504:ARG:HH11	1.67	0.60
1:A:670:ILE:HG13	1:A:679:ILE:HA	1.84	0.59
1:D:288:ARG:H	1:D:288:ARG:NE	1.99	0.59
1:D:416:GLU:OE2	1:D:420:LYS:HD3	2.01	0.59
1:B:295:LYS:HD3	1:B:296:VAL:N	2.11	0.59
1:C:64:ALA:O	1:C:68:ARG:HD2	2.02	0.59
1:C:376:THR:HG22	1:C:377:GLU:N	2.16	0.59
1:A:11:PRO:CA	1:A:31:ARG:HH21	2.13	0.59
1:A:409:LYS:HD2	1:A:446:GLU:OE1	2.02	0.59
1:A:412:GLN:HB2	1:A:442:LYS:HE3	1.83	0.59
1:A:533:SER:HA	1:A:536:GLN:HE21	1.67	0.59
1:A:653:LYS:HB2	1:A:653:LYS:NZ	2.17	0.59
1:A:678:PHE:C	1:A:679:ILE:HD12	2.27	0.59
1:B:125:GLN:O	1:B:126:SER:C	2.45	0.59
1:B:378:LYS:HG3	1:D:666:ASP:CB	2.32	0.59
1:C:41:ILE:HG22	1:C:41:ILE:O	2.03	0.59
1:C:90:GLN:NE2	1:C:636:ARG:HH21	2.00	0.59
1:C:98:ILE:HD11	1:C:584:TYR:HD2	1.66	0.59
1:D:441:ASN:O	1:D:442:LYS:HD3	2.02	0.59
1:A:620:ARG:HA	1:A:620:ARG:NE	2.17	0.59
1:B:77:MET:HE3	1:B:77:MET:HA	1.84	0.59
1:A:181:ASN:HD21	1:A:362:ASN:HD21	1.49	0.59
1:A:635:ASN:HB3	1:C:642:LYS:HG2	1.84	0.59
1:B:634:TYR:CB	1:B:655:ALA:HB3	2.28	0.59
1:C:142:LEU:HD11	1:C:364:LEU:HD21	1.84	0.59
1:C:158:SER:N	3:C:892:VO4:O2	2.33	0.59
1:D:295:LYS:HD3	1:D:296:VAL:N	2.11	0.59
1:A:411:GLN:HG2	1:A:508:TYR:CD2	2.37	0.59
1:A:440:ASN:ND2	1:A:442:LYS:HB3	2.18	0.59
1:A:679:ILE:HD12	1:A:679:ILE:N	2.18	0.59
1:B:390:PHE:N	1:B:407:ASN:OD1	2.36	0.59
1:A:55:ASN:HD21	1:A:58:LYS:HD3	1.68	0.59
1:B:73:MET:HE2	1:B:74:PRO:HD2	1.84	0.59
1:C:640:LEU:HD21	1:C:691:LYS:HB3	1.83	0.59
1:B:21:GLU:O	1:B:25:ILE:HD13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ASP:OD2	1:B:343:ASN:HB2	2.03	0.58
1:C:90:GLN:OE1	1:C:636:ARG:NH2	2.30	0.58
1:D:259:LYS:H	1:D:259:LYS:CD	2.13	0.58
1:A:140:ASN:HB2	1:A:141:PRO:HD3	1.84	0.58
1:B:119:THR:HG21	1:B:137:LEU:HD21	1.84	0.58
1:B:411:GLN:HG2	1:B:508:TYR:CD2	2.37	0.58
1:B:472:THR:HA	1:B:475:ASP:OD2	2.03	0.58
1:C:695:GLU:OE1	1:C:695:GLU:O	2.21	0.58
1:A:567:ARG:HG2	1:A:567:ARG:HH11	1.67	0.58
1:B:311:THR:HG22	1:B:538:SER:HA	1.86	0.58
1:C:309:LEU:HD13	1:C:535:MET:SD	2.43	0.58
1:C:472:THR:HA	1:C:475:ASP:OD2	2.03	0.58
1:A:341:ASP:OD2	1:A:343:ASN:HB2	2.03	0.58
1:B:140:ASN:HB2	1:B:141:PRO:HD3	1.85	0.58
1:B:486:HIS:O	1:B:505:LEU:HD12	2.03	0.58
1:C:341:ASP:OD2	1:C:343:ASN:HB2	2.04	0.58
1:C:438:TYR:HA	1:C:615:GLU:HG2	1.86	0.58
1:C:567:ARG:HG2	1:C:567:ARG:HH11	1.67	0.58
1:C:680:ARG:O	1:C:681:ASN:HB2	2.04	0.58
1:D:95:GLN:HB2	1:D:382:ILE:HG12	1.86	0.58
1:D:205:MET:HE3	1:D:267:TRP:CE3	2.39	0.58
1:D:634:TYR:C	1:D:634:TYR:CD2	2.81	0.58
1:A:55:ASN:ND2	1:A:58:LYS:HD3	2.19	0.58
1:B:259:LYS:HD2	1:B:259:LYS:N	2.14	0.58
1:C:213:LYS:NZ	1:C:264:ASN:HD21	2.00	0.58
1:D:192:ARG:HG3	1:D:232:SER:HB3	1.83	0.58
1:D:227:GLU:O	1:D:231:LYS:HG3	2.03	0.58
1:D:280:THR:OG1	1:D:297:SER:HB2	2.02	0.58
1:D:617:VAL:O	1:D:621:ARG:HB2	2.03	0.58
1:B:441:ASN:O	1:B:442:LYS:HD3	2.03	0.58
1:D:21:GLU:O	1:D:25:ILE:HD13	2.04	0.58
1:D:140:ASN:HB2	1:D:141:PRO:HD3	1.86	0.58
1:A:192:ARG:HG3	1:A:232:SER:HB3	1.86	0.58
1:D:284:ALA:HB3	1:D:293:THR:O	2.04	0.58
1:A:259:LYS:H	1:A:259:LYS:CD	2.14	0.58
1:B:378:LYS:HG3	1:D:666:ASP:CG	2.28	0.58
1:C:454:GLY:O	1:C:458:LEU:HD23	2.03	0.58
1:D:441:ASN:O	1:D:443:PRO:HD3	2.04	0.58
1:B:450:LYS:HB3	1:B:451:LYS:HD2	1.86	0.58
1:C:451:LYS:HD2	1:C:451:LYS:N	2.19	0.58
1:D:424:GLU:O	1:D:427:VAL:HG22	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:636:ARG:HG2	1:D:636:ARG:HH11	1.68	0.58
1:B:77:MET:HE3	1:B:77:MET:O	2.04	0.57
1:C:645:TRP:O	1:C:647:SER:N	2.37	0.57
1:A:418:THR:HG23	1:A:419:LEU:HG	1.85	0.57
1:D:533:SER:HA	1:D:536:GLN:HE21	1.68	0.57
1:B:670:ILE:HD12	1:B:670:ILE:N	2.20	0.57
1:D:295:LYS:CD	1:D:296:VAL:H	2.14	0.57
1:D:660:LEU:CD2	1:D:665:ILE:HD12	2.34	0.57
1:A:156:ASN:HD22	4:A:791:ADP:HO3'	1.52	0.57
1:A:442:LYS:HB2	1:A:442:LYS:HZ3	1.68	0.57
1:B:411:GLN:CG	1:B:442:LYS:HZ3	2.17	0.57
1:C:90:GLN:NE2	1:C:636:ARG:NH2	2.52	0.57
1:A:125:GLN:O	1:A:126:SER:C	2.47	0.57
1:A:423:GLN:HE21	1:A:433:TRP:NE1	1.97	0.57
1:B:259:LYS:H	1:B:259:LYS:CD	2.15	0.57
1:C:250:VAL:HA	1:C:253:MET:HG3	1.86	0.57
1:A:194:GLN:OE1	1:A:194:GLN:N	2.30	0.57
1:B:227:GLU:O	1:B:231:LYS:HG3	2.04	0.57
1:C:192:ARG:HG3	1:C:232:SER:HB3	1.86	0.57
1:C:696:MET:HB2	1:C:697:PRO:C	2.29	0.57
1:D:211:GLN:CD	1:D:211:GLN:N	2.61	0.57
1:D:504:ARG:HG2	1:D:504:ARG:HH11	1.70	0.57
1:C:324:SER:HA	1:C:336:ILE:O	2.04	0.57
1:D:249:ILE:O	1:D:253:MET:HG2	2.05	0.57
1:D:138:ASP:O	1:D:141:PRO:HD2	2.04	0.57
1:D:341:ASP:OD2	1:D:343:ASN:HB2	2.04	0.57
1:D:441:ASN:C	1:D:443:PRO:HD3	2.30	0.57
1:A:142:LEU:HD11	1:A:364:LEU:HD21	1.87	0.57
1:B:66:ASN:HD22	1:B:67:GLY:N	2.02	0.57
1:B:295:LYS:CD	1:B:296:VAL:H	2.13	0.57
1:B:452:PRO:O	1:B:453:ILE:HB	2.05	0.57
1:C:227:GLU:O	1:C:231:LYS:HG3	2.04	0.57
1:C:558:ARG:HB2	1:C:559:PRO:HD3	1.87	0.57
1:D:542:LEU:O	1:D:545:GLY:N	2.38	0.57
1:A:443:PRO:HG2	1:A:444:ILE:CD1	2.34	0.57
1:B:663:HIS:HB3	1:B:665:ILE:HG13	1.87	0.57
1:A:157:SER:N	5:A:808:HOH:O	2.37	0.56
1:B:633:PHE:O	1:B:637:TYR:HB2	2.04	0.56
1:C:434:LYS:H	1:C:434:LYS:CE	2.18	0.56
1:D:213:LYS:NZ	1:D:264:ASN:HD21	2.03	0.56
1:B:409:LYS:HZ2	1:B:450:LYS:HD3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:SER:HB3	1:C:531:LEU:HD11	1.86	0.56
1:C:629:GLU:HG3	1:C:676:LYS:HE3	1.87	0.56
1:D:94:ASN:ND2	1:D:381:VAL:H	2.03	0.56
1:D:365:VAL:HG23	1:D:366:SER:N	2.19	0.56
1:D:434:LYS:H	1:D:434:LYS:HD2	1.70	0.56
1:A:77:MET:HE3	1:A:77:MET:HA	1.88	0.56
1:A:122:SER:OG	1:A:174:PRO:HG3	2.05	0.56
1:A:125:GLN:HE22	1:C:68:ARG:HE	1.48	0.56
1:A:420:LYS:HE2	1:A:424:GLU:OE1	2.05	0.56
1:B:55:ASN:ND2	1:B:58:LYS:HD3	2.19	0.56
1:B:427:VAL:C	1:B:429:GLU:H	2.13	0.56
1:C:375:THR:O	1:D:376:THR:OG1	2.17	0.56
1:C:448:ILE:O	1:C:455:LEU:HG	2.04	0.56
1:C:485:PRO:O	1:C:486:HIS:HB2	2.05	0.56
1:C:557:LYS:N	1:C:557:LYS:HZ2	2.03	0.56
1:A:276:ILE:HD13	1:A:352:LEU:HD13	1.88	0.56
1:B:11:PRO:CA	1:B:31:ARG:HH21	2.18	0.56
1:C:197:ARG:NH1	1:C:242:ASP:OD1	2.39	0.56
1:C:504:ARG:HH11	1:C:504:ARG:HG2	1.70	0.56
1:A:211:GLN:CD	1:A:211:GLN:N	2.62	0.56
1:B:448:ILE:O	1:B:455:LEU:HG	2.05	0.56
1:D:660:LEU:HD23	1:D:665:ILE:HD12	1.87	0.56
1:D:695:GLU:O	1:D:696:MET:HB2	2.05	0.56
1:A:604:VAL:O	1:A:608:VAL:HG23	2.05	0.56
1:C:140:ASN:HB2	1:C:141:PRO:HD3	1.87	0.56
1:D:125:GLN:O	1:D:126:SER:C	2.49	0.56
1:D:438:TYR:O	1:D:440:ASN:N	2.39	0.56
1:D:642:LYS:HD3	1:D:662:GLN:HG2	1.86	0.56
1:B:167:GLN:HE22	1:B:374:CYS:H	1.53	0.56
1:C:22:ASN:O	1:C:26:GLU:HG3	2.06	0.56
1:C:486:HIS:O	1:C:505:LEU:HD12	2.06	0.56
1:D:54:LEU:O	1:D:56:ILE:N	2.39	0.56
1:A:227:GLU:O	1:A:231:LYS:HG3	2.05	0.56
1:B:653:LYS:H	1:B:653:LYS:CE	2.19	0.56
1:C:204:GLN:HE22	1:C:245:GLU:HG2	1.70	0.56
1:C:450:LYS:HB3	1:C:451:LYS:HD2	1.88	0.56
1:D:66:ASN:HD22	1:D:67:GLY:N	2.04	0.56
1:A:452:PRO:O	1:A:453:ILE:HB	2.06	0.56
1:C:488:GLN:HB2	1:C:504:ARG:HB3	1.87	0.56
1:C:656:THR:O	1:C:660:LEU:HG	2.05	0.56
1:C:690:GLU:O	1:C:694:LEU:HD23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:GLY:HA3	1:D:31:ARG:HD3	1.88	0.56
1:D:19:ILE:HD11	1:D:618:ARG:HG2	1.88	0.56
1:D:485:PRO:O	1:D:486:HIS:HB2	2.06	0.56
1:A:295:LYS:CD	1:A:296:VAL:H	2.12	0.55
1:B:194:GLN:CD	1:B:194:GLN:H	2.03	0.55
1:B:671:ARG:HG2	1:B:671:ARG:HH11	1.71	0.55
1:D:291:THR:HG22	1:D:292:THR:N	2.20	0.55
1:D:452:PRO:O	1:D:453:ILE:HB	2.06	0.55
1:D:484:ASN:OD1	1:D:485:PRO:O	2.24	0.55
1:B:118:LEU:O	1:B:122:SER:HB2	2.05	0.55
1:B:488:GLN:HB2	1:B:504:ARG:HB3	1.87	0.55
1:C:362:ASN:O	1:C:365:VAL:HG22	2.06	0.55
1:A:365:VAL:HG23	1:A:366:SER:N	2.21	0.55
1:B:55:ASN:HD21	1:B:58:LYS:HD3	1.71	0.55
1:B:567:ARG:HG2	1:B:567:ARG:HH11	1.71	0.55
1:C:624:PHE:CZ	1:C:680:ARG:NH2	2.73	0.55
1:C:634:TYR:CZ	1:C:638:LYS:HG2	2.41	0.55
1:D:422:GLU:HG2	1:D:619:VAL:HG11	1.87	0.55
1:D:472:THR:HA	1:D:475:ASP:OD2	2.06	0.55
1:B:211:GLN:H	1:B:211:GLN:NE2	2.04	0.55
1:C:31:ARG:NH1	1:C:36:ASN:HB3	2.21	0.55
1:A:194:GLN:CD	1:A:194:GLN:H	2.01	0.55
1:B:498:ILE:HD12	1:B:504:ARG:HB2	1.88	0.55
1:C:288:ARG:NH2	1:C:289:THR:OG1	2.39	0.55
1:C:670:ILE:HG22	1:C:671:ARG:H	1.71	0.55
1:D:567:ARG:HG2	1:D:567:ARG:HH11	1.70	0.55
1:A:419:LEU:HD13	1:A:438:TYR:HB2	1.88	0.55
1:B:533:SER:HA	1:B:536:GLN:HE21	1.72	0.55
1:B:675:THR:O	1:B:675:THR:HG22	2.05	0.55
1:C:679:ILE:HD12	1:C:685:LEU:HD21	1.88	0.55
1:A:150:LYS:HG3	1:A:155:ASP:HA	1.89	0.55
1:B:447:LEU:C	1:B:449:GLU:H	2.13	0.55
1:B:604:VAL:O	1:B:608:VAL:HG23	2.07	0.55
1:B:246:PHE:O	1:B:250:VAL:HG23	2.07	0.55
1:C:76:HIS:HD2	1:C:78:TYR:N	1.85	0.55
1:C:448:ILE:O	1:C:448:ILE:HG12	2.06	0.55
1:D:635:ASN:HA	1:D:638:LYS:HD3	1.89	0.55
1:A:213:LYS:NZ	1:A:264:ASN:HD21	2.04	0.55
1:B:523:ASN:OD1	1:B:561:THR:HB	2.07	0.55
1:B:652:ALA:O	1:B:654:GLN:N	2.40	0.55
1:C:125:GLN:O	1:C:126:SER:C	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:PRO:CA	1:D:31:ARG:HH21	2.14	0.55
1:D:150:LYS:HG3	1:D:155:ASP:HA	1.87	0.55
1:D:434:LYS:O	1:D:436:ILE:HD12	2.07	0.55
1:A:41:ILE:HG22	1:A:41:ILE:O	2.06	0.54
1:A:441:ASN:OD1	1:A:443:PRO:HD3	2.07	0.54
1:B:150:LYS:HG3	1:B:155:ASP:HA	1.88	0.54
1:B:637:TYR:HE2	1:B:688:PHE:HB3	1.72	0.54
1:B:680:ARG:HG2	1:B:681:ASN:OD1	2.07	0.54
1:C:211:GLN:H	1:C:211:GLN:NE2	2.05	0.54
1:D:661:GLN:C	1:D:663:HIS:H	2.15	0.54
1:A:442:LYS:HB2	1:A:442:LYS:HZ2	1.69	0.54
1:B:41:ILE:HG22	1:B:41:ILE:O	2.07	0.54
1:C:59:GLU:CD	1:C:60:SER:H	2.16	0.54
1:D:411:GLN:HG2	1:D:508:TYR:CD2	2.43	0.54
1:A:681:ASN:CG	1:A:682:PRO:HD2	2.32	0.54
1:C:484:ASN:OD1	1:C:485:PRO:O	2.25	0.54
1:D:376:THR:HG22	1:D:377:GLU:N	2.23	0.54
1:A:634:TYR:O	1:A:638:LYS:HG3	2.06	0.54
1:B:12:ASP:OD1	1:B:14:VAL:HG23	2.08	0.54
1:B:76:HIS:HD2	1:B:78:TYR:N	1.86	0.54
1:B:682:PRO:C	1:B:684:THR:H	2.15	0.54
1:D:436:ILE:HG12	1:D:618:ARG:HB3	1.89	0.54
1:D:447:LEU:C	1:D:449:GLU:H	2.16	0.54
1:A:58:LYS:HZ2	1:A:61:ASP:CG	2.16	0.54
1:A:211:GLN:H	1:A:211:GLN:NE2	2.06	0.54
1:A:459:LEU:HD13	1:A:523:ASN:ND2	2.23	0.54
1:A:655:ALA:O	1:A:656:THR:C	2.51	0.54
1:B:192:ARG:HG3	1:B:232:SER:HB3	1.90	0.54
1:B:272:ALA:O	1:B:276:ILE:HG13	2.07	0.54
1:B:276:ILE:HD13	1:B:352:LEU:HD13	1.90	0.54
1:C:434:LYS:H	1:C:434:LYS:HE3	1.71	0.54
1:D:489:SER:HA	1:D:498:ILE:HG21	1.89	0.54
1:A:485:PRO:O	1:A:486:HIS:HB2	2.08	0.54
1:B:59:GLU:OE1	1:B:60:SER:N	2.41	0.54
1:B:679:ILE:CG2	1:B:684:THR:HB	2.37	0.54
1:C:322:TYR:CE2	1:C:339:PRO:HG3	2.43	0.54
1:C:434:LYS:HD2	1:C:434:LYS:O	2.07	0.54
1:C:557:LYS:HZ2	1:C:557:LYS:H	1.55	0.54
1:C:376:THR:O	1:D:375:THR:HB	2.07	0.54
1:C:680:ARG:HG3	1:C:680:ARG:HH11	1.71	0.54
1:D:77:MET:HE3	1:D:77:MET:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:GLU:N	1:D:278:ASN:HD21	1.95	0.54
1:D:246:PHE:O	1:D:250:VAL:HG23	2.07	0.54
1:D:439:PHE:HD2	1:D:615:GLU:CD	2.16	0.54
1:A:31:ARG:NH1	1:A:36:ASN:HB3	2.23	0.54
1:A:472:THR:HA	1:A:475:ASP:OD2	2.08	0.54
1:C:21:GLU:O	1:C:25:ILE:HD13	2.08	0.54
1:C:418:THR:CG2	1:C:616:ASN:ND2	2.67	0.54
1:B:434:LYS:O	1:B:434:LYS:HG2	2.06	0.53
1:C:95:GLN:HB2	1:C:382:ILE:HG12	1.90	0.53
1:C:445:CYS:C	1:C:448:ILE:HG22	2.33	0.53
1:C:620:ARG:HA	1:C:620:ARG:NE	2.23	0.53
1:D:22:ASN:O	1:D:26:GLU:HG3	2.08	0.53
1:D:498:ILE:HD12	1:D:504:ARG:HB2	1.90	0.53
1:A:486:HIS:O	1:A:505:LEU:HD12	2.08	0.53
1:A:627:ARG:O	1:A:627:ARG:HG2	2.08	0.53
1:C:452:PRO:O	1:C:453:ILE:HB	2.08	0.53
1:D:14:VAL:HG13	1:D:621:ARG:HA	1.90	0.53
1:A:324:SER:HA	1:A:336:ILE:O	2.07	0.53
1:A:629:GLU:HG2	1:A:676:LYS:HZ1	1.72	0.53
1:C:636:ARG:HD2	1:C:637:TYR:CE1	2.43	0.53
1:D:388:TYR:CD1	1:D:388:TYR:N	2.77	0.53
1:B:59:GLU:CD	1:B:60:SER:H	2.16	0.53
1:C:272:ALA:O	1:C:276:ILE:HG13	2.09	0.53
1:C:295:LYS:CD	1:C:296:VAL:H	2.13	0.53
1:C:444:ILE:HD12	1:C:444:ILE:N	2.23	0.53
1:C:542:LEU:O	1:C:545:GLY:N	2.41	0.53
1:D:41:ILE:O	1:D:41:ILE:HG22	2.07	0.53
1:D:77:MET:HE3	1:D:77:MET:O	2.07	0.53
1:D:487:LEU:HD12	1:D:488:GLN:N	2.24	0.53
1:A:589:LYS:N	1:A:607:GLN:HE22	1.99	0.53
1:B:115:MET:HE1	1:B:140:ASN:HD21	1.74	0.53
1:C:498:ILE:HD12	1:C:504:ARG:HB2	1.89	0.53
1:C:182:TYR:OH	1:C:573:LEU:HD23	2.08	0.53
1:C:442:LYS:C	1:C:444:ILE:N	2.67	0.53
1:D:276:ILE:HD13	1:D:352:LEU:HD13	1.91	0.53
1:A:272:ALA:O	1:A:276:ILE:HG13	2.09	0.53
1:A:411:GLN:HG3	1:A:442:LYS:HE2	1.90	0.53
1:A:484:ASN:OD1	1:A:485:PRO:O	2.27	0.53
1:C:359:ARG:HB3	1:C:546:LEU:HD12	1.90	0.53
1:C:441:ASN:C	1:C:443:PRO:CD	2.80	0.53
1:C:629:GLU:HA	1:C:675:THR:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:THR:O	1:A:119:THR:CG2	2.56	0.53
1:C:88:MET:HG3	1:C:380:PRO:HB2	1.91	0.53
1:C:181:ASN:HD21	1:C:362:ASN:HD22	1.53	0.53
1:C:627:ARG:O	1:C:627:ARG:HG2	2.08	0.53
1:D:192:ARG:NH2	1:D:228:TYR:O	2.42	0.53
1:A:205:MET:HE3	1:A:267:TRP:CE3	2.44	0.53
1:B:204:GLN:HE22	1:B:245:GLU:HG2	1.73	0.53
1:B:205:MET:HE3	1:B:267:TRP:CE3	2.44	0.53
1:D:442:LYS:HE3	1:D:446:GLU:OE2	2.09	0.53
1:B:9:GLY:HA3	1:B:31:ARG:HD3	1.91	0.53
1:B:489:SER:HA	1:B:498:ILE:HG21	1.90	0.53
1:D:19:ILE:CD1	1:D:618:ARG:HG2	2.38	0.53
1:A:142:LEU:HD12	1:A:368:ILE:HD11	1.91	0.52
1:A:390:PHE:N	1:A:407:ASN:OD1	2.42	0.52
1:A:436:ILE:CD1	1:A:619:VAL:HA	2.37	0.52
1:A:681:ASN:ND2	1:A:682:PRO:HD2	2.24	0.52
1:B:416:GLU:OE2	1:B:420:LYS:HD3	2.09	0.52
1:C:11:PRO:CA	1:C:31:ARG:HH21	2.21	0.52
1:C:459:LEU:HD11	1:C:523:ASN:HB2	1.92	0.52
1:D:448:ILE:O	1:D:455:LEU:HG	2.08	0.52
1:D:572:ALA:O	1:D:576:THR:CG2	2.56	0.52
1:C:246:PHE:O	1:C:250:VAL:HG23	2.08	0.52
1:A:572:ALA:O	1:A:576:THR:CG2	2.53	0.52
1:B:17:ASN:CG	1:B:18:GLN:N	2.66	0.52
1:B:636:ARG:HD3	1:B:636:ARG:O	2.09	0.52
1:C:603:ARG:HG3	1:C:603:ARG:NH1	2.24	0.52
1:B:154:ASN:HB3	1:B:157:SER:HB2	1.91	0.52
1:B:459:LEU:HD13	1:B:523:ASN:ND2	2.24	0.52
1:C:142:LEU:CD1	1:C:364:LEU:HD21	2.40	0.52
1:C:589:LYS:N	1:C:607:GLN:HE22	2.00	0.52
1:A:9:GLY:HA3	1:A:31:ARG:HD3	1.91	0.52
1:A:59:GLU:O	1:A:63:LYS:HG3	2.10	0.52
1:A:118:LEU:O	1:A:122:SER:HB2	2.10	0.52
1:B:185:GLU:OE1	1:B:188:ARG:NE	2.34	0.52
1:B:484:ASN:OD1	1:B:485:PRO:O	2.28	0.52
1:A:448:ILE:O	1:A:455:LEU:HG	2.09	0.52
1:B:640:LEU:HD13	1:B:663:HIS:CD2	2.45	0.52
1:B:378:LYS:CG	1:D:666:ASP:HB2	2.39	0.52
1:B:408:GLU:HB3	1:B:446:GLU:OE2	2.09	0.52
1:D:204:GLN:HE22	1:D:245:GLU:HG2	1.75	0.52
1:D:603:ARG:NH1	1:D:603:ARG:HG3	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLN:HE21	1:C:68:ARG:NE	2.03	0.52
1:A:125:GLN:CB	1:C:68:ARG:HH21	2.17	0.52
1:A:422:GLU:OE1	1:A:620:ARG:NH2	2.43	0.52
1:A:429:GLU:O	1:A:674:LYS:HG3	2.10	0.52
1:B:125:GLN:O	1:B:127:PRO:N	2.43	0.52
1:B:653:LYS:H	1:B:653:LYS:HE2	1.74	0.52
1:C:204:GLN:NE2	1:C:245:GLU:HG2	2.24	0.52
1:C:320:LEU:CD2	1:C:531:LEU:HD21	2.39	0.52
1:B:197:ARG:NH1	1:B:242:ASP:OD1	2.43	0.52
1:C:138:ASP:O	1:C:141:PRO:HD2	2.09	0.52
1:C:669:GLU:HA	1:C:669:GLU:OE1	2.09	0.52
1:D:167:GLN:HE22	1:D:374:CYS:N	2.05	0.52
1:D:167:GLN:NE2	1:D:374:CYS:HB3	2.24	0.52
1:D:633:PHE:O	1:D:636:ARG:HB2	2.10	0.52
1:D:642:LYS:O	1:D:643:LYS:HB2	2.10	0.52
1:A:438:TYR:O	1:A:439:PHE:C	2.53	0.52
1:A:670:ILE:CG1	1:A:679:ILE:HG13	2.40	0.52
1:C:290:GLY:O	1:C:291:THR:HB	2.10	0.52
1:D:211:GLN:H	1:D:211:GLN:NE2	2.08	0.52
1:A:119:THR:HG21	1:A:137:LEU:HD21	1.91	0.51
1:A:204:GLN:HE22	1:A:245:GLU:HG2	1.75	0.51
1:B:31:ARG:NH1	1:B:36:ASN:HB3	2.23	0.51
1:B:376:THR:HG22	1:B:377:GLU:N	2.25	0.51
1:C:376:THR:HG21	1:D:370:THR:O	2.10	0.51
1:C:634:TYR:CE1	1:C:638:LYS:HG2	2.45	0.51
1:D:415:ILE:HD12	1:D:442:LYS:HD2	1.92	0.51
1:D:488:GLN:HB2	1:D:504:ARG:HB3	1.92	0.51
1:D:532:ILE:O	1:D:536:GLN:HG3	2.10	0.51
1:B:71:TYR:CD1	1:B:71:TYR:C	2.88	0.51
1:C:22:ASN:OD1	1:C:605:ARG:NH1	2.40	0.51
1:C:627:ARG:HA	1:C:677:VAL:O	2.11	0.51
1:D:73:MET:HE2	1:D:74:PRO:HD2	1.92	0.51
1:A:54:LEU:O	1:A:56:ILE:N	2.43	0.51
1:A:73:MET:HE2	1:A:74:PRO:HD2	1.92	0.51
1:B:490:TYR:O	1:B:494:LYS:HA	2.09	0.51
1:B:670:ILE:HG23	1:B:678:PHE:O	2.10	0.51
1:C:119:THR:HG21	1:C:137:LEU:HD21	1.93	0.51
1:C:572:ALA:O	1:C:576:THR:CG2	2.55	0.51
1:D:197:ARG:NH1	1:D:242:ASP:OD1	2.44	0.51
1:D:390:PHE:N	1:D:407:ASN:OD1	2.43	0.51
1:D:428:ARG:C	1:D:430:GLY:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:ILE:HD12	1:A:442:LYS:HD2	1.93	0.51
1:B:671:ARG:HG2	1:B:671:ARG:NH1	2.26	0.51
1:D:14:VAL:CG1	1:D:621:ARG:HA	2.40	0.51
1:D:405:PHE:CE1	1:D:409:LYS:HD3	2.46	0.51
1:D:604:VAL:O	1:D:608:VAL:HG23	2.10	0.51
1:B:459:LEU:HD11	1:B:523:ASN:HB2	1.93	0.51
1:C:77:MET:HE3	1:C:77:MET:HA	1.93	0.51
1:A:459:LEU:HD11	1:A:523:ASN:HB2	1.93	0.51
1:C:487:LEU:HD12	1:C:488:GLN:N	2.26	0.51
1:C:641:CYS:SG	1:C:644:THR:OG1	2.67	0.51
1:A:11:PRO:HA	1:A:31:ARG:NH2	2.19	0.51
1:A:17:ASN:CG	1:A:18:GLN:N	2.69	0.51
1:A:488:GLN:HB2	1:A:504:ARG:HB3	1.93	0.51
1:B:542:LEU:O	1:B:545:GLY:N	2.44	0.51
1:D:490:TYR:O	1:D:494:LYS:HA	2.10	0.51
1:D:517:ARG:HB2	1:D:517:ARG:CZ	2.41	0.51
1:A:267:TRP:HA	1:A:267:TRP:HE3	1.76	0.51
1:A:640:LEU:H	1:A:640:LEU:CD1	2.22	0.51
1:B:638:LYS:O	1:B:638:LYS:HD3	2.11	0.51
1:C:118:LEU:O	1:C:122:SER:HB2	2.10	0.51
1:C:436:ILE:HD12	1:C:436:ILE:N	2.25	0.51
1:C:600:ASP:HB3	1:C:603:ARG:HB3	1.93	0.51
1:D:450:LYS:HB3	1:D:451:LYS:HD2	1.92	0.51
1:D:523:ASN:OD1	1:D:561:THR:HB	2.11	0.51
1:A:641:CYS:CB	1:A:659:ILE:HG12	2.39	0.51
1:B:58:LYS:HZ2	1:B:58:LYS:HB2	1.75	0.51
1:C:71:TYR:CD1	1:C:71:TYR:C	2.89	0.51
1:C:418:THR:HG21	1:C:616:ASN:ND2	2.23	0.51
1:D:115:MET:HE1	1:D:140:ASN:HD21	1.76	0.51
1:D:123:SER:O	1:D:124:ASN:CG	2.53	0.51
1:D:636:ARG:NH2	1:D:689:GLU:OE2	2.44	0.51
1:B:59:GLU:O	1:B:63:LYS:HG3	2.12	0.51
1:B:426:TYR:HD2	1:B:433:TRP:CE3	2.29	0.51
1:A:490:TYR:O	1:A:494:LYS:HA	2.10	0.50
1:A:665:ILE:CD1	1:A:688:PHE:HZ	2.24	0.50
1:B:659:ILE:O	1:B:663:HIS:HB2	2.11	0.50
1:C:192:ARG:NH2	1:C:228:TYR:O	2.44	0.50
1:C:542:LEU:O	1:C:543:VAL:C	2.52	0.50
1:C:628:ILE:O	1:C:677:VAL:HG23	2.11	0.50
1:D:115:MET:CE	1:D:140:ASN:HD21	2.25	0.50
1:A:267:TRP:CE3	1:A:267:TRP:HA	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:LEU:HD12	1:B:368:ILE:HD11	1.93	0.50
1:B:572:ALA:O	1:B:576:THR:CG2	2.55	0.50
1:C:150:LYS:HG3	1:C:155:ASP:HA	1.92	0.50
1:C:434:LYS:O	1:C:436:ILE:HD12	2.11	0.50
1:D:284:ALA:O	1:D:286:GLU:N	2.45	0.50
1:A:427:VAL:HG23	1:A:428:ARG:N	2.26	0.50
1:A:450:LYS:HB3	1:A:451:LYS:HD2	1.93	0.50
1:B:409:LYS:NZ	1:B:450:LYS:HD3	2.27	0.50
1:C:445:CYS:O	1:C:448:ILE:CG2	2.58	0.50
1:D:17:ASN:CG	1:D:18:GLN:N	2.69	0.50
1:B:365:VAL:HG23	1:B:366:SER:N	2.26	0.50
1:D:192:ARG:CG	1:D:232:SER:HB3	2.42	0.50
1:A:310:LYS:HD2	1:A:540:ASP:HB2	1.93	0.50
1:A:446:GLU:O	1:A:449:GLU:N	2.45	0.50
1:D:636:ARG:O	1:D:692:ARG:NH1	2.44	0.50
1:A:197:ARG:NH1	1:A:242:ASP:OD1	2.44	0.50
1:A:438:TYR:O	1:A:439:PHE:O	2.30	0.50
1:B:115:MET:CE	1:B:140:ASN:HD21	2.25	0.50
1:B:438:TYR:O	1:B:439:PHE:C	2.54	0.50
1:B:452:PRO:O	1:B:453:ILE:CB	2.59	0.50
1:C:441:ASN:O	1:C:443:PRO:HD3	2.11	0.50
1:D:657:GLU:O	1:D:661:GLN:HG3	2.11	0.50
1:A:498:ILE:HD12	1:A:504:ARG:HB2	1.93	0.50
1:A:504:ARG:HG2	1:A:504:ARG:HH11	1.77	0.50
1:B:123:SER:O	1:B:124:ASN:CG	2.55	0.50
1:C:651:THR:HB	1:C:654:GLN:HB2	1.92	0.50
1:A:428:ARG:HH11	1:A:428:ARG:HG2	1.77	0.50
1:A:487:LEU:HD12	1:A:488:GLN:N	2.26	0.50
1:C:12:ASP:OD1	1:C:14:VAL:HG23	2.12	0.50
1:C:490:TYR:O	1:C:494:LYS:HA	2.11	0.50
1:C:532:ILE:O	1:C:536:GLN:HG3	2.12	0.50
1:D:154:ASN:HD21	4:D:894:ADP:H5'2	1.77	0.50
1:A:440:ASN:HD22	1:A:442:LYS:HB3	1.76	0.50
1:A:560:GLU:O	1:A:561:THR:O	2.30	0.50
1:C:203:TYR:HD2	5:C:907:HOH:O	1.94	0.50
1:C:433:TRP:HZ3	1:C:622:ALA:C	2.20	0.50
1:D:31:ARG:NH1	1:D:36:ASN:HB3	2.27	0.50
1:D:504:ARG:CD	1:D:511:ASP:HB3	2.42	0.50
1:A:19:ILE:HD12	1:A:621:ARG:HD2	1.92	0.49
1:A:376:THR:HG22	1:A:377:GLU:N	2.26	0.49
1:A:532:ILE:O	1:A:536:GLN:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:PRO:O	1:B:222:ASN:HB2	2.12	0.49
1:C:37:ILE:HG12	1:C:50:PRO:HG3	1.94	0.49
1:A:452:PRO:O	1:A:453:ILE:CB	2.60	0.49
1:B:42:GLY:O	1:B:43:ASP:HB2	2.12	0.49
1:C:55:ASN:ND2	1:C:58:LYS:HD3	2.28	0.49
1:C:284:ALA:O	1:C:286:GLU:N	2.45	0.49
1:C:459:LEU:HD13	1:C:523:ASN:ND2	2.26	0.49
1:C:670:ILE:HG22	1:C:671:ARG:N	2.27	0.49
1:D:154:ASN:HB3	1:D:157:SER:HB2	1.93	0.49
1:D:420:LYS:HE2	1:D:424:GLU:OE1	2.12	0.49
1:A:66:ASN:HD22	1:A:67:GLY:N	2.09	0.49
1:C:443:PRO:HD2	1:C:444:ILE:HD12	1.93	0.49
1:D:37:ILE:HG12	1:D:50:PRO:HG3	1.93	0.49
1:A:125:GLN:HE21	1:C:68:ARG:HH21	1.60	0.49
1:B:284:ALA:HB3	1:B:293:THR:O	2.13	0.49
1:B:436:ILE:O	1:B:436:ILE:HG22	2.13	0.49
1:C:388:TYR:CD1	1:C:388:TYR:N	2.79	0.49
1:D:452:PRO:O	1:D:453:ILE:CB	2.61	0.49
1:A:284:ALA:O	1:A:286:GLU:N	2.45	0.49
1:A:442:LYS:C	1:A:444:ILE:H	2.18	0.49
1:A:660:LEU:HD22	1:A:665:ILE:HD12	1.93	0.49
1:C:235:PHE:CD1	1:C:235:PHE:N	2.80	0.49
1:D:208:GLY:HA3	1:D:246:PHE:CD2	2.47	0.49
1:A:429:GLU:HA	1:A:429:GLU:OE2	2.13	0.49
1:A:439:PHE:CE2	1:A:612:GLY:HA2	2.47	0.49
1:A:630:TYR:HE2	1:A:677:VAL:HG22	1.76	0.49
1:C:211:GLN:CD	1:C:211:GLN:N	2.63	0.49
1:D:310:LYS:HD2	1:D:540:ASP:HB2	1.93	0.49
1:B:73:MET:HB3	1:B:74:PRO:CD	2.42	0.49
1:B:192:ARG:NH2	1:B:228:TYR:O	2.46	0.49
1:C:287:GLN:O	1:C:291:THR:O	2.30	0.49
1:C:441:ASN:CG	1:C:443:PRO:HD3	2.38	0.49
1:D:420:LYS:HG2	1:D:424:GLU:OE1	2.13	0.49
1:D:642:LYS:N	1:D:642:LYS:CD	2.58	0.49
1:A:246:PHE:O	1:A:250:VAL:HG23	2.12	0.49
1:C:489:SER:HA	1:C:498:ILE:HG21	1.94	0.49
1:D:288:ARG:NH2	1:D:289:THR:H	2.10	0.49
1:A:123:SER:O	1:A:124:ASN:CG	2.56	0.49
1:A:192:ARG:NH2	1:A:228:TYR:O	2.46	0.49
1:B:473:PHE:O	1:B:477:ILE:HG13	2.12	0.49
1:B:635:ASN:ND2	1:B:636:ARG:N	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:ASN:CG	1:C:18:GLN:N	2.69	0.49
1:C:125:GLN:O	1:C:127:PRO:N	2.45	0.49
1:D:603:ARG:HG3	1:D:603:ARG:HH11	1.77	0.49
1:D:630:TYR:CE2	1:D:653:LYS:HG3	2.48	0.49
1:A:71:TYR:CD1	1:A:71:TYR:C	2.91	0.49
1:A:441:ASN:C	1:A:442:LYS:HG3	2.38	0.49
1:A:453:ILE:HA	1:A:458:LEU:HD21	1.95	0.49
1:A:614:LEU:C	1:A:616:ASN:H	2.20	0.49
1:C:447:LEU:C	1:C:449:GLU:H	2.20	0.49
1:D:194:GLN:CD	1:D:194:GLN:H	2.07	0.49
1:D:311:THR:HG22	1:D:538:SER:HA	1.94	0.49
1:D:423:GLN:HE22	1:D:436:ILE:H	1.60	0.49
1:A:504:ARG:CD	1:A:511:ASP:HB3	2.42	0.48
1:A:637:TYR:CE2	1:A:688:PHE:HB3	2.48	0.48
1:B:340:MET:HB2	1:B:344:GLN:HB2	1.95	0.48
1:B:627:ARG:HG2	1:B:676:LYS:CE	2.32	0.48
1:C:55:ASN:HD21	1:C:58:LYS:HD3	1.77	0.48
1:C:59:GLU:OE1	1:C:60:SER:N	2.46	0.48
1:C:309:LEU:HD13	1:C:535:MET:CE	2.43	0.48
1:D:267:TRP:HE3	1:D:267:TRP:HA	1.78	0.48
1:A:367:LYS:O	1:A:367:LYS:HD3	2.13	0.48
1:A:636:ARG:NH2	1:A:689:GLU:OE1	2.46	0.48
1:B:485:PRO:O	1:B:486:HIS:HB2	2.13	0.48
1:C:59:GLU:CD	1:C:60:SER:N	2.71	0.48
1:C:447:LEU:C	1:C:449:GLU:N	2.70	0.48
1:D:71:TYR:CD1	1:D:71:TYR:C	2.92	0.48
1:A:188:ARG:O	1:A:192:ARG:NH1	2.47	0.48
1:A:523:ASN:OD1	1:A:561:THR:HB	2.13	0.48
1:B:54:LEU:O	1:B:56:ILE:N	2.46	0.48
1:B:235:PHE:CD1	1:B:235:PHE:N	2.80	0.48
1:B:282:ALA:HB2	1:B:297:SER:OG	2.13	0.48
1:B:310:LYS:HD2	1:B:540:ASP:HB2	1.95	0.48
1:B:362:ASN:O	1:B:365:VAL:HG22	2.13	0.48
1:B:409:LYS:HA	1:B:446:GLU:OE1	2.13	0.48
1:C:659:ILE:O	1:C:663:HIS:HD2	1.96	0.48
1:D:118:LEU:O	1:D:122:SER:HB2	2.12	0.48
1:B:311:THR:HG22	1:B:538:SER:CA	2.43	0.48
1:B:431:ILE:O	1:B:433:TRP:N	2.46	0.48
1:C:267:TRP:CE3	1:C:267:TRP:HA	2.48	0.48
1:C:633:PHE:C	1:C:633:PHE:CD2	2.90	0.48
1:C:665:ILE:O	1:C:666:ASP:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:ASP:O	1:B:463:CYS:HB2	2.13	0.48
1:B:663:HIS:C	1:B:665:ILE:H	2.21	0.48
1:B:687:TYR:CE1	1:B:691:LYS:HD3	2.48	0.48
1:C:417:LEU:HD12	1:C:584:TYR:HE2	1.78	0.48
1:C:614:LEU:HD12	1:C:614:LEU:O	2.13	0.48
1:D:473:PHE:O	1:D:477:ILE:HG13	2.14	0.48
1:A:489:SER:HA	1:A:498:ILE:HG21	1.95	0.48
1:A:542:LEU:O	1:A:546:LEU:HD22	2.14	0.48
1:B:37:ILE:HG12	1:B:50:PRO:HG3	1.94	0.48
1:B:267:TRP:CE3	1:B:267:TRP:HA	2.48	0.48
1:B:504:ARG:CD	1:B:511:ASP:HB3	2.42	0.48
1:C:323:ARG:NH2	1:C:528:PHE:CE1	2.81	0.48
1:D:267:TRP:CE3	1:D:267:TRP:HA	2.48	0.48
1:D:459:LEU:HD13	1:D:523:ASN:ND2	2.28	0.48
1:A:59:GLU:CD	1:A:60:SER:H	2.22	0.48
1:A:442:LYS:C	1:A:444:ILE:N	2.71	0.48
1:A:642:LYS:HE3	1:A:642:LYS:HA	1.96	0.48
1:A:669:GLU:HG2	1:A:684:THR:HG21	1.96	0.48
1:B:684:THR:HG22	1:B:688:PHE:CE1	2.44	0.48
1:C:267:TRP:HA	1:C:267:TRP:HE3	1.78	0.48
1:C:414:PHE:CD2	1:C:586:ARG:CZ	2.97	0.48
1:C:683:THR:HA	1:C:686:PHE:HD2	1.77	0.48
1:D:188:ARG:O	1:D:192:ARG:NH1	2.46	0.48
1:D:217:LEU:O	1:D:275:HIS:HE1	1.97	0.48
1:D:459:LEU:HD11	1:D:523:ASN:HB2	1.94	0.48
1:A:154:ASN:HB3	1:A:157:SER:HB2	1.95	0.48
1:B:267:TRP:HA	1:B:267:TRP:HE3	1.78	0.48
1:C:9:GLY:HA3	1:C:31:ARG:HD3	1.96	0.48
1:C:118:LEU:O	1:C:122:SER:CB	2.62	0.48
1:C:205:MET:HE3	1:C:267:TRP:CE3	2.48	0.48
1:D:279:ILE:HG23	1:D:296:VAL:HG13	1.96	0.48
1:D:446:GLU:HB2	1:D:450:LYS:HE2	1.96	0.48
1:A:688:PHE:HD1	1:A:688:PHE:H	1.61	0.48
1:B:532:ILE:O	1:B:536:GLN:HG3	2.14	0.48
1:C:504:ARG:CD	1:C:511:ASP:HB3	2.43	0.48
1:D:340:MET:HB2	1:D:344:GLN:HB2	1.96	0.48
1:D:486:HIS:O	1:D:505:LEU:HD12	2.13	0.48
1:D:542:LEU:O	1:D:543:VAL:C	2.57	0.48
1:A:542:LEU:O	1:A:545:GLY:N	2.47	0.48
1:B:208:GLY:HA3	1:B:246:PHE:CD2	2.49	0.48
1:B:284:ALA:O	1:B:286:GLU:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:ARG:NH1	1:B:603:ARG:HG3	2.28	0.48
1:C:167:GLN:HE22	1:C:374:CYS:N	2.09	0.48
1:C:442:LYS:O	1:C:446:GLU:HG2	2.13	0.48
1:A:37:ILE:HD11	1:A:54:LEU:CD2	2.34	0.47
1:A:59:GLU:OE1	1:A:60:SER:N	2.47	0.47
1:B:453:ILE:HA	1:B:458:LEU:HD21	1.96	0.47
1:C:192:ARG:CG	1:C:232:SER:HB3	2.43	0.47
1:D:421:SER:HA	1:D:424:GLU:OE2	2.14	0.47
1:A:600:ASP:HB3	1:A:603:ARG:HB3	1.97	0.47
1:B:653:LYS:O	1:B:655:ALA:N	2.47	0.47
1:C:276:ILE:HD13	1:C:352:LEU:HD13	1.95	0.47
1:B:119:THR:O	1:B:119:THR:CG2	2.61	0.47
1:B:487:LEU:HD12	1:B:488:GLN:N	2.28	0.47
1:C:436:ILE:H	1:C:436:ILE:CD1	2.27	0.47
1:C:694:LEU:O	1:C:695:GLU:CB	2.63	0.47
1:D:453:ILE:HA	1:D:458:LEU:HD21	1.95	0.47
1:C:181:ASN:ND2	1:C:362:ASN:ND2	2.52	0.47
1:C:411:GLN:HG2	1:C:508:TYR:CD2	2.49	0.47
1:C:460:ASP:O	1:C:463:CYS:HB2	2.14	0.47
1:C:633:PHE:O	1:C:634:TYR:C	2.57	0.47
1:D:625:ALA:HB1	1:D:682:PRO:HG3	1.96	0.47
1:D:692:ARG:HG3	1:D:692:ARG:NH1	2.26	0.47
1:A:208:GLY:HA3	1:A:246:PHE:CD2	2.49	0.47
1:B:59:GLU:CD	1:B:60:SER:N	2.72	0.47
1:B:441:ASN:C	1:B:443:PRO:HD3	2.40	0.47
1:C:123:SER:O	1:C:124:ASN:CG	2.57	0.47
1:A:603:ARG:NH1	1:A:603:ARG:HG3	2.30	0.47
1:B:204:GLN:NE2	1:B:245:GLU:HG2	2.29	0.47
1:B:600:ASP:HB3	1:B:603:ARG:HB3	1.97	0.47
1:C:58:LYS:HB2	1:C:58:LYS:HZ2	1.79	0.47
1:C:517:ARG:HB2	1:C:517:ARG:CZ	2.44	0.47
1:C:603:ARG:HG3	1:C:603:ARG:HH11	1.78	0.47
1:D:235:PHE:CD1	1:D:235:PHE:N	2.83	0.47
1:A:322:TYR:C	1:A:340:MET:HE2	2.40	0.47
1:A:420:LYS:O	1:A:424:GLU:HG3	2.15	0.47
1:A:446:GLU:HB3	1:A:450:LYS:HE2	1.96	0.47
1:A:460:ASP:O	1:A:463:CYS:HB2	2.15	0.47
1:B:142:LEU:CD1	1:B:364:LEU:HD21	2.44	0.47
1:B:506:LYS:HD3	5:B:804:HOH:O	2.15	0.47
1:B:542:LEU:O	1:B:543:VAL:C	2.58	0.47
1:C:54:LEU:O	1:C:56:ILE:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:MET:HE2	1:C:74:PRO:HD2	1.96	0.47
1:C:288:ARG:N	1:C:288:ARG:CD	2.58	0.47
1:C:310:LYS:HD2	1:C:540:ASP:HB2	1.97	0.47
1:D:59:GLU:CD	1:D:60:SER:H	2.22	0.47
1:D:96:CYS:HA	1:D:383:GLY:O	2.14	0.47
1:D:109:GLU:O	1:D:113:LYS:HG2	2.14	0.47
1:D:428:ARG:C	1:D:430:GLY:N	2.73	0.47
1:A:235:PHE:CD1	1:A:235:PHE:N	2.82	0.47
1:D:59:GLU:OE1	1:D:60:SER:N	2.48	0.47
1:A:185:GLU:OE1	1:A:188:ARG:NE	2.41	0.47
1:C:132:ILE:HD11	1:C:174:PRO:HB2	1.97	0.47
1:C:443:PRO:HD2	1:C:444:ILE:HD11	1.97	0.47
1:C:221:PRO:O	1:C:222:ASN:HB2	2.15	0.47
1:A:217:LEU:O	1:A:275:HIS:HE1	1.98	0.46
1:B:217:LEU:O	1:B:275:HIS:HE1	1.98	0.46
1:B:470:ASP:HB3	1:B:516:VAL:HG12	1.96	0.46
1:D:11:PRO:HA	1:D:31:ARG:NH2	2.22	0.46
1:A:37:ILE:HG12	1:A:50:PRO:HG3	1.97	0.46
1:A:443:PRO:O	1:A:447:LEU:HG	2.15	0.46
1:A:517:ARG:HB2	1:A:517:ARG:CZ	2.46	0.46
1:A:636:ARG:HD2	1:A:636:ARG:C	2.39	0.46
1:C:154:ASN:HB3	1:C:157:SER:HB2	1.96	0.46
1:C:322:TYR:N	1:C:340:MET:HE2	2.29	0.46
1:C:430:GLY:O	1:C:431:ILE:HD13	2.14	0.46
1:A:25:ILE:HD12	1:A:25:ILE:N	2.30	0.46
1:A:142:LEU:CD1	1:A:364:LEU:HD21	2.45	0.46
1:A:167:GLN:HE22	1:A:374:CYS:H	1.63	0.46
1:B:12:ASP:HA	1:B:40:TYR:C	2.39	0.46
1:C:144:GLU:O	1:C:148:ASN:HB2	2.15	0.46
1:C:689:GLU:O	1:C:693:GLU:HG3	2.14	0.46
1:D:118:LEU:O	1:D:122:SER:CB	2.63	0.46
1:A:77:MET:HE3	1:A:77:MET:O	2.16	0.46
1:B:405:PHE:CE1	1:B:409:LYS:HD3	2.51	0.46
1:B:660:LEU:C	1:B:660:LEU:HD23	2.40	0.46
1:B:684:THR:C	1:B:686:PHE:H	2.24	0.46
1:C:448:ILE:HD13	1:C:505:LEU:HD11	1.97	0.46
1:D:106:GLY:HA2	4:D:894:ADP:O1A	2.16	0.46
1:D:221:PRO:O	1:D:222:ASN:HB2	2.14	0.46
1:D:413:LEU:HD11	1:D:578:LEU:HD21	1.96	0.46
1:A:483:LYS:HD2	1:A:483:LYS:HA	1.76	0.46
1:B:154:ASN:CG	1:B:157:SER:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:MET:HB2	1:C:344:GLN:HB2	1.97	0.46
1:C:365:VAL:CG2	1:C:366:SER:N	2.78	0.46
1:D:142:LEU:HD12	1:D:368:ILE:HD11	1.96	0.46
1:D:442:LYS:HB2	1:D:442:LYS:NZ	2.29	0.46
1:D:600:ASP:HB3	1:D:603:ARG:HB3	1.98	0.46
1:D:634:TYR:O	1:D:638:LYS:HB3	2.15	0.46
1:A:639:MET:HG2	1:A:640:LEU:HD12	1.97	0.46
1:B:49:ASN:O	1:B:590:SER:OG	2.30	0.46
1:B:427:VAL:C	1:B:429:GLU:N	2.73	0.46
1:C:406:CYS:HA	1:C:570:MET:HE2	1.97	0.46
1:D:40:TYR:CE2	1:D:75:PRO:HA	2.50	0.46
1:D:201:ILE:HG23	1:D:202:PHE:N	2.30	0.46
1:D:425:GLU:HA	1:D:428:ARG:CZ	2.45	0.46
1:D:666:ASP:O	1:D:669:GLU:HB3	2.15	0.46
1:A:630:TYR:CD1	1:A:675:THR:HA	2.50	0.46
1:B:40:TYR:CE2	1:B:75:PRO:HA	2.50	0.46
1:B:92:GLN:NE2	1:D:687:TYR:CE1	2.83	0.46
1:B:388:TYR:CD1	1:B:388:TYR:N	2.77	0.46
1:C:473:PHE:O	1:C:477:ILE:HG13	2.16	0.46
1:C:604:VAL:O	1:C:608:VAL:HG23	2.16	0.46
1:D:125:GLN:O	1:D:127:PRO:N	2.49	0.46
1:D:442:LYS:HB2	1:D:442:LYS:HZ2	1.80	0.46
1:A:249:ILE:O	1:A:253:MET:HG2	2.15	0.46
1:A:362:ASN:O	1:A:365:VAL:HG22	2.16	0.46
1:A:667:LYS:C	1:A:669:GLU:N	2.74	0.46
1:B:37:ILE:HG22	1:B:48:THR:H	1.80	0.46
1:B:128:ASN:OD1	1:D:73:MET:HA	2.15	0.46
1:B:603:ARG:HG3	1:B:603:ARG:HH11	1.81	0.46
1:B:655:ALA:O	1:B:659:ILE:HG13	2.16	0.46
1:C:367:LYS:O	1:C:367:LYS:HD3	2.16	0.46
1:D:185:GLU:O	1:D:185:GLU:HG2	2.14	0.46
1:D:213:LYS:HZ2	1:D:264:ASN:HD21	1.63	0.46
1:A:204:GLN:NE2	1:A:245:GLU:HG2	2.31	0.46
1:A:340:MET:HB2	1:A:344:GLN:HB2	1.97	0.46
1:C:653:LYS:NZ	1:C:653:LYS:HB2	2.31	0.46
1:D:12:ASP:OD1	1:D:14:VAL:HG23	2.15	0.46
1:D:73:MET:HB3	1:D:74:PRO:CD	2.45	0.46
1:D:486:HIS:O	1:D:505:LEU:HA	2.16	0.46
1:D:681:ASN:HD22	1:D:681:ASN:HA	1.62	0.46
1:A:132:ILE:HD11	1:A:174:PRO:HB2	1.98	0.46
1:A:473:PHE:O	1:A:477:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:LYS:HB3	1:B:59:GLU:OE2	2.16	0.46
1:B:423:GLN:NE2	1:B:436:ILE:H	2.10	0.46
1:B:660:LEU:HD23	1:B:665:ILE:HB	1.97	0.46
1:C:453:ILE:HA	1:C:458:LEU:HD21	1.96	0.46
1:C:615:GLU:OE2	1:C:615:GLU:N	2.36	0.46
1:D:427:VAL:HG23	1:D:428:ARG:N	2.30	0.46
1:A:642:LYS:O	1:A:643:LYS:HB2	2.16	0.45
1:B:653:LYS:HG2	1:B:654:GLN:NE2	2.31	0.45
1:C:19:ILE:HD11	1:C:618:ARG:HG2	1.99	0.45
1:C:376:THR:HA	1:D:374:CYS:HA	1.98	0.45
1:D:287:GLN:HB2	1:D:292:THR:HA	1.97	0.45
1:A:12:ASP:OD1	1:A:14:VAL:HG23	2.16	0.45
1:A:132:ILE:HD11	1:A:174:PRO:C	2.41	0.45
1:A:197:ARG:HG2	1:A:203:TYR:CE1	2.51	0.45
1:A:625:ALA:HB3	1:A:679:ILE:O	2.16	0.45
1:C:556:LYS:C	1:C:557:LYS:HD3	2.41	0.45
1:A:118:LEU:O	1:A:122:SER:CB	2.65	0.45
1:A:304:ALA:O	1:A:307:SER:HB3	2.16	0.45
1:A:681:ASN:CG	1:A:682:PRO:CD	2.89	0.45
1:A:685:LEU:HD23	1:A:685:LEU:O	2.16	0.45
1:B:18:GLN:HG2	1:B:20:THR:HG23	1.97	0.45
1:D:59:GLU:O	1:D:63:LYS:HG3	2.17	0.45
1:A:221:PRO:O	1:A:222:ASN:HB2	2.15	0.45
1:A:322:TYR:CE2	1:A:339:PRO:HG3	2.51	0.45
1:A:427:VAL:CG2	1:A:428:ARG:N	2.80	0.45
1:A:542:LEU:O	1:A:543:VAL:C	2.58	0.45
1:A:656:THR:HG21	1:A:672:MET:HE1	1.97	0.45
1:A:670:ILE:HG13	1:A:679:ILE:HG13	1.99	0.45
1:B:481:PHE:CB	1:B:487:LEU:HD23	2.47	0.45
1:B:659:ILE:O	1:B:659:ILE:HG22	2.17	0.45
1:C:132:ILE:HD11	1:C:174:PRO:C	2.42	0.45
1:C:452:PRO:O	1:C:453:ILE:CB	2.64	0.45
1:C:524:LYS:NZ	5:C:911:HOH:O	2.48	0.45
1:D:193:THR:O	1:D:196:GLU:HB2	2.16	0.45
1:D:431:ILE:O	1:D:432:GLU:C	2.56	0.45
1:A:94:ASN:ND2	1:A:381:VAL:H	2.14	0.45
1:C:58:LYS:HB3	1:C:59:GLU:OE2	2.15	0.45
1:C:309:LEU:O	1:C:538:SER:OG	2.23	0.45
1:D:210:SER:C	1:D:212:SER:N	2.73	0.45
1:D:441:ASN:C	1:D:443:PRO:CD	2.90	0.45
1:A:125:GLN:O	1:A:127:PRO:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:PHE:CE1	1:A:409:LYS:HD3	2.52	0.45
1:B:154:ASN:HD21	4:B:794:ADP:H5'2	1.81	0.45
1:B:367:LYS:O	1:B:367:LYS:HD3	2.16	0.45
1:B:624:PHE:O	1:B:626:GLY:N	2.48	0.45
1:B:662:GLN:C	1:B:664:ASN:N	2.69	0.45
1:B:680:ARG:HG3	1:B:680:ARG:HH11	1.81	0.45
1:B:690:GLU:O	1:B:691:LYS:HD2	2.17	0.45
1:C:115:MET:HE1	1:C:140:ASN:HD21	1.81	0.45
1:C:201:ILE:HG23	1:C:202:PHE:N	2.30	0.45
1:C:217:LEU:O	1:C:275:HIS:HE1	1.98	0.45
1:C:635:ASN:CA	1:C:638:LYS:HD2	2.21	0.45
1:D:115:MET:O	1:D:116:GLN:C	2.60	0.45
1:D:359:ARG:HB3	1:D:546:LEU:HD12	1.99	0.45
1:A:18:GLN:HG2	1:A:20:THR:HG23	1.99	0.45
1:A:670:ILE:HG13	1:A:678:PHE:O	2.17	0.45
1:B:138:ASP:O	1:B:141:PRO:HD2	2.17	0.45
1:B:297:SER:O	1:B:299:THR:HG23	2.16	0.45
1:C:408:GLU:OE2	1:C:442:LYS:NZ	2.49	0.45
1:D:367:LYS:O	1:D:367:LYS:HD3	2.16	0.45
1:D:391:GLU:HA	5:D:897:HOH:O	2.17	0.45
1:D:483:LYS:HD2	1:D:483:LYS:HA	1.72	0.45
1:A:12:ASP:HA	1:A:40:TYR:C	2.42	0.45
1:A:98:ILE:HD11	1:A:584:TYR:HD2	1.82	0.45
1:B:73:MET:HB3	1:B:74:PRO:HD2	1.99	0.45
1:B:200:HIS:O	1:B:201:ILE:C	2.60	0.45
1:B:239:THR:C	1:B:240:ILE:HD13	2.42	0.45
1:B:517:ARG:HB2	1:B:517:ARG:CZ	2.46	0.45
1:B:607:GLN:HA	1:B:610:TYR:CE2	2.52	0.45
1:C:409:LYS:HD2	1:C:446:GLU:OE2	2.17	0.45
1:D:25:ILE:N	1:D:25:ILE:HD12	2.31	0.45
1:D:119:THR:O	1:D:119:THR:CG2	2.60	0.45
1:D:132:ILE:HD11	1:D:174:PRO:HB2	1.98	0.45
1:A:42:GLY:O	1:A:43:ASP:HB2	2.15	0.45
1:A:192:ARG:CG	1:A:232:SER:HB3	2.47	0.45
1:B:589:LYS:N	1:B:607:GLN:HE22	2.03	0.45
1:B:653:LYS:C	1:B:655:ALA:N	2.75	0.45
1:C:42:GLY:O	1:C:43:ASP:HB2	2.15	0.45
1:C:96:CYS:SG	1:C:580:CYS:HB2	2.57	0.45
1:C:551:ARG:HD2	1:C:551:ARG:O	2.17	0.45
1:D:272:ALA:O	1:D:276:ILE:HG13	2.17	0.45
1:D:439:PHE:CD1	1:D:440:ASN:N	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:SER:O	1:A:299:THR:N	2.46	0.45
1:A:367:LYS:HD3	1:A:367:LYS:C	2.42	0.45
1:B:157:SER:N	5:B:796:HOH:O	2.49	0.45
1:B:367:LYS:HD3	1:B:367:LYS:C	2.42	0.45
1:B:444:ILE:C	1:B:446:GLU:N	2.72	0.45
1:C:40:TYR:CE2	1:C:75:PRO:HA	2.51	0.45
1:C:73:MET:HB3	1:C:74:PRO:CD	2.47	0.45
1:C:210:SER:C	1:C:212:SER:N	2.73	0.45
1:C:488:GLN:OE1	1:C:504:ARG:NH1	2.50	0.45
1:C:657:GLU:O	1:C:661:GLN:HG2	2.17	0.45
1:D:449:GLU:HB3	1:D:455:LEU:HB2	1.99	0.45
1:A:419:LEU:HD13	1:A:438:TYR:HB3	1.99	0.44
1:B:426:TYR:O	1:B:431:ILE:HB	2.17	0.44
1:B:635:ASN:HD22	1:B:635:ASN:H	1.64	0.44
1:C:188:ARG:O	1:C:192:ARG:NH1	2.50	0.44
1:C:624:PHE:CE2	1:C:680:ARG:NH2	2.85	0.44
1:D:58:LYS:HZ2	1:D:61:ASP:CG	2.24	0.44
1:D:200:HIS:O	1:D:201:ILE:C	2.60	0.44
1:D:439:PHE:HE2	1:D:612:GLY:HA3	1.81	0.44
1:A:542:LEU:HG	1:A:546:LEU:HD21	1.98	0.44
1:A:600:ASP:O	1:A:601:GLU:C	2.60	0.44
1:C:322:TYR:HE2	1:C:339:PRO:HG3	1.82	0.44
1:C:335:VAL:HG22	1:C:335:VAL:O	2.17	0.44
1:C:441:ASN:C	1:C:442:LYS:HG3	2.41	0.44
1:D:447:LEU:C	1:D:449:GLU:N	2.75	0.44
1:D:488:GLN:OE1	1:D:504:ARG:NH1	2.51	0.44
1:A:152:LEU:HG	1:A:196:GLU:HG3	1.99	0.44
1:A:680:ARG:HB2	1:A:680:ARG:NH1	2.33	0.44
1:C:167:GLN:HE22	1:C:374:CYS:HB3	1.79	0.44
1:C:607:GLN:HA	1:C:610:TYR:CE2	2.52	0.44
1:D:460:ASP:O	1:D:463:CYS:HB2	2.17	0.44
1:A:40:TYR:CE2	1:A:75:PRO:HA	2.52	0.44
1:A:279:ILE:HD13	1:A:302:LEU:HD23	1.99	0.44
1:A:388:TYR:CD1	1:A:388:TYR:N	2.77	0.44
1:A:413:LEU:HD11	1:A:578:LEU:HD21	1.98	0.44
1:A:439:PHE:CE2	1:A:609:ARG:O	2.70	0.44
1:B:182:TYR:O	1:B:183:LEU:C	2.60	0.44
1:C:523:ASN:OD1	1:C:561:THR:HB	2.16	0.44
1:D:37:ILE:HG22	1:D:48:THR:H	1.83	0.44
1:D:364:LEU:O	1:D:368:ILE:HG13	2.17	0.44
1:D:367:LYS:HD3	1:D:367:LYS:C	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381:VAL:HG12	1:D:382:ILE:N	2.32	0.44
1:D:451:LYS:CB	1:D:452:PRO:CD	2.90	0.44
1:B:49:ASN:HA	1:B:50:PRO:HD3	1.83	0.44
1:B:118:LEU:O	1:B:122:SER:CB	2.66	0.44
1:D:185:GLU:HG3	1:D:399:GLU:HG2	2.00	0.44
1:A:37:ILE:HG22	1:A:48:THR:H	1.82	0.44
1:B:25:ILE:N	1:B:25:ILE:HD12	2.33	0.44
1:B:324:SER:HA	1:B:336:ILE:O	2.17	0.44
1:C:208:GLY:HA3	1:C:246:PHE:CD2	2.53	0.44
1:C:387:ILE:HD12	1:C:387:ILE:C	2.42	0.44
1:C:441:ASN:CB	1:C:443:PRO:HD3	2.48	0.44
1:D:428:ARG:HH11	1:D:428:ARG:HG2	1.82	0.44
1:A:115:MET:O	1:A:116:GLN:C	2.61	0.44
1:A:115:MET:HE1	1:A:140:ASN:HD21	1.83	0.44
1:A:683:THR:O	1:A:685:LEU:N	2.50	0.44
1:B:213:LYS:HZ2	1:B:264:ASN:HD21	1.66	0.44
1:B:297:SER:O	1:B:299:THR:N	2.48	0.44
1:B:381:VAL:HG12	1:B:382:ILE:N	2.33	0.44
1:B:635:ASN:ND2	1:B:635:ASN:H	2.16	0.44
1:C:19:ILE:CD1	1:C:618:ARG:HG2	2.48	0.44
1:C:213:LYS:HZ2	1:C:264:ASN:HD21	1.64	0.44
1:C:540:ASP:OD2	1:C:541:PRO:HD2	2.17	0.44
1:D:443:PRO:HA	1:D:446:GLU:CG	2.47	0.44
1:A:311:THR:HG22	1:A:538:SER:HA	2.00	0.44
1:A:630:TYR:CD1	1:A:653:LYS:HB3	2.53	0.44
1:A:683:THR:C	1:A:685:LEU:N	2.75	0.44
1:A:688:PHE:N	1:A:688:PHE:CD1	2.86	0.44
1:B:418:THR:CG2	1:B:419:LEU:HG	2.44	0.44
1:B:441:ASN:OD1	1:B:443:PRO:HD3	2.18	0.44
1:B:640:LEU:HD22	1:B:663:HIS:NE2	2.33	0.44
1:B:684:THR:C	1:B:686:PHE:N	2.75	0.44
1:D:204:GLN:OE1	1:D:249:ILE:HD11	2.17	0.44
1:A:427:VAL:O	1:A:430:GLY:N	2.51	0.44
1:A:470:ASP:HB3	1:A:516:VAL:HG12	2.00	0.44
1:B:496:ARG:HA	1:B:496:ARG:NE	2.33	0.44
1:B:627:ARG:HB2	1:B:677:VAL:O	2.18	0.44
1:C:185:GLU:O	1:C:185:GLU:HG2	2.18	0.44
1:C:420:LYS:O	1:C:421:SER:C	2.61	0.44
1:D:154:ASN:CG	1:D:157:SER:H	2.26	0.44
1:D:204:GLN:NE2	1:D:245:GLU:HG2	2.32	0.44
1:A:115:MET:CE	1:A:140:ASN:HD21	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:ARG:HG3	1:A:603:ARG:HH11	1.83	0.43
1:B:427:VAL:HG23	1:B:428:ARG:N	2.32	0.43
1:B:459:LEU:HB2	1:B:473:PHE:CZ	2.52	0.43
1:C:115:MET:CE	1:C:140:ASN:HD21	2.31	0.43
1:D:286:GLU:O	1:D:288:ARG:NE	2.50	0.43
1:D:485:PRO:O	1:D:486:HIS:CB	2.66	0.43
1:A:37:ILE:H	1:A:37:ILE:HG13	1.55	0.43
1:A:163:TYR:HE2	1:A:165:GLU:OE1	2.01	0.43
1:B:77:MET:HE3	1:B:77:MET:CA	2.48	0.43
1:B:80:LEU:HD22	1:B:80:LEU:HA	1.79	0.43
1:B:378:LYS:HD2	1:D:666:ASP:HB2	1.98	0.43
1:C:181:ASN:OD1	1:C:365:VAL:HG21	2.18	0.43
1:C:415:ILE:HD11	1:C:439:PHE:CZ	2.53	0.43
1:C:447:LEU:O	1:C:449:GLU:N	2.51	0.43
1:C:573:LEU:O	1:C:573:LEU:HD22	2.17	0.43
1:D:12:ASP:HA	1:D:40:TYR:C	2.40	0.43
1:D:437:GLU:O	1:D:437:GLU:HG3	2.18	0.43
1:D:441:ASN:OD1	1:D:443:PRO:HD3	2.18	0.43
1:D:625:ALA:HB3	1:D:681:ASN:N	2.32	0.43
1:A:406:CYS:SG	1:A:570:MET:CE	3.06	0.43
1:B:485:PRO:C	1:B:487:LEU:H	2.26	0.43
1:C:37:ILE:H	1:C:37:ILE:HG13	1.60	0.43
1:C:53:ASN:C	1:C:54:LEU:HD12	2.44	0.43
1:C:239:THR:C	1:C:240:ILE:HD13	2.43	0.43
1:C:427:VAL:HG23	1:C:428:ARG:N	2.32	0.43
1:C:542:LEU:O	1:C:546:LEU:HD22	2.18	0.43
1:D:239:THR:C	1:D:240:ILE:HD13	2.43	0.43
1:D:516:VAL:O	1:D:516:VAL:HG12	2.18	0.43
1:A:284:ALA:HB3	1:A:293:THR:C	2.43	0.43
1:A:425:GLU:O	1:A:426:TYR:C	2.61	0.43
1:B:127:PRO:HD2	1:D:73:MET:HG2	2.00	0.43
1:B:185:GLU:HG3	1:B:399:GLU:HG2	2.00	0.43
1:C:182:TYR:O	1:C:183:LEU:C	2.61	0.43
1:C:629:GLU:O	1:C:630:TYR:C	2.60	0.43
1:C:633:PHE:HD2	1:C:634:TYR:N	2.17	0.43
1:D:423:GLN:NE2	1:D:436:ILE:H	2.15	0.43
1:A:185:GLU:HG3	1:A:399:GLU:HG2	1.99	0.43
1:A:488:GLN:OE1	1:A:504:ARG:NH1	2.51	0.43
1:C:12:ASP:HA	1:C:40:TYR:C	2.42	0.43
1:C:405:PHE:O	1:C:408:GLU:HB2	2.17	0.43
1:C:443:PRO:HA	1:C:446:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:624:PHE:CZ	1:D:680:ARG:NH2	2.87	0.43
1:B:197:ARG:HG2	1:B:203:TYR:CE1	2.53	0.43
1:B:469:THR:O	1:B:470:ASP:C	2.61	0.43
1:C:367:LYS:HD3	1:C:367:LYS:C	2.44	0.43
1:C:486:HIS:O	1:C:505:LEU:HA	2.19	0.43
1:C:696:MET:N	1:C:697:PRO:HA	2.23	0.43
1:D:651:THR:HB	1:D:654:GLN:CD	2.43	0.43
1:A:485:PRO:O	1:A:486:HIS:CB	2.66	0.43
1:A:614:LEU:C	1:A:616:ASN:N	2.76	0.43
1:B:185:GLU:O	1:B:185:GLU:HG2	2.17	0.43
1:B:188:ARG:O	1:B:192:ARG:NH1	2.51	0.43
1:B:542:LEU:O	1:B:546:LEU:HD22	2.19	0.43
1:B:560:GLU:O	1:B:561:THR:O	2.36	0.43
1:C:66:ASN:HA	1:C:82:ASN:ND2	2.33	0.43
1:C:287:GLN:HB2	1:C:292:THR:HA	1.99	0.43
1:D:297:SER:O	1:D:299:THR:N	2.50	0.43
1:D:681:ASN:HA	1:D:682:PRO:HD3	1.88	0.43
1:A:213:LYS:HZ2	1:A:264:ASN:HD21	1.66	0.43
1:A:442:LYS:C	1:A:442:LYS:HD3	2.43	0.43
1:A:445:CYS:O	1:A:448:ILE:HG22	2.19	0.43
1:B:132:ILE:HD11	1:B:174:PRO:C	2.43	0.43
1:B:227:GLU:N	1:B:278:ASN:HD21	2.00	0.43
1:B:322:TYR:N	1:B:340:MET:HE2	2.33	0.43
1:B:411:GLN:HG3	1:B:442:LYS:HZ3	1.83	0.43
1:C:163:TYR:HE2	1:C:165:GLU:OE1	2.01	0.43
1:C:431:ILE:HG22	1:C:432:GLU:N	2.34	0.43
1:D:14:VAL:CG1	1:D:621:ARG:HG3	2.48	0.43
1:A:156:ASN:C	5:A:808:HOH:O	2.61	0.43
1:B:210:SER:C	1:B:212:SER:N	2.75	0.43
1:B:488:GLN:OE1	1:B:504:ARG:NH1	2.52	0.43
1:C:59:GLU:O	1:C:63:LYS:HG3	2.18	0.43
1:C:106:GLY:HA2	4:C:891:ADP:O1A	2.18	0.43
1:D:469:THR:O	1:D:470:ASP:C	2.62	0.43
1:A:441:ASN:O	1:A:443:PRO:CD	2.66	0.43
1:B:66:ASN:HD22	1:B:67:GLY:H	1.65	0.43
1:B:249:ILE:O	1:B:253:MET:HG2	2.19	0.43
1:B:542:LEU:HG	1:B:546:LEU:HD21	2.01	0.43
1:C:204:GLN:OE1	1:C:249:ILE:HD11	2.19	0.43
1:C:663:HIS:O	1:C:664:ASN:C	2.62	0.43
1:B:201:ILE:HG23	1:B:202:PHE:N	2.33	0.42
1:C:37:ILE:HG22	1:C:48:THR:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:PHE:N	1:C:407:ASN:OD1	2.51	0.42
1:B:144:GLU:O	1:B:148:ASN:HB2	2.19	0.42
1:C:311:THR:HG22	1:C:538:SER:N	2.35	0.42
1:B:31:ARG:HB3	1:B:31:ARG:NH1	2.23	0.42
1:B:669:GLU:CG	1:B:670:ILE:HD12	2.50	0.42
1:B:682:PRO:C	1:B:684:THR:N	2.77	0.42
1:C:25:ILE:HD12	1:C:25:ILE:N	2.33	0.42
1:C:59:GLU:CD	1:C:59:GLU:N	2.77	0.42
1:C:694:LEU:HD22	1:C:694:LEU:N	2.34	0.42
1:A:59:GLU:CD	1:A:59:GLU:N	2.77	0.42
1:A:496:ARG:NE	1:A:496:ARG:HA	2.35	0.42
1:B:66:ASN:HA	1:B:82:ASN:ND2	2.35	0.42
1:B:132:ILE:HD11	1:B:174:PRO:HB2	2.01	0.42
1:B:192:ARG:CG	1:B:232:SER:HB3	2.49	0.42
1:B:284:ALA:HB3	1:B:293:THR:C	2.45	0.42
1:B:322:TYR:CE2	1:B:339:PRO:HG3	2.54	0.42
1:B:516:VAL:HG12	1:B:516:VAL:O	2.19	0.42
1:D:42:GLY:O	1:D:43:ASP:HB2	2.18	0.42
1:D:103:SER:HA	3:D:895:VO4:O2	2.19	0.42
1:D:166:MET:HE3	1:D:166:MET:HB3	1.97	0.42
1:D:365:VAL:CG2	1:D:366:SER:N	2.83	0.42
1:B:59:GLU:CD	1:B:59:GLU:N	2.78	0.42
1:C:459:LEU:HB2	1:C:473:PHE:CZ	2.55	0.42
1:D:59:GLU:CD	1:D:60:SER:N	2.77	0.42
1:D:408:GLU:OE2	1:D:442:LYS:NZ	2.53	0.42
1:D:460:ASP:CG	1:D:561:THR:HG1	2.28	0.42
1:A:627:ARG:HG3	1:A:627:ARG:HH11	1.83	0.42
1:A:636:ARG:HG3	1:A:637:TYR:CE1	2.53	0.42
1:B:125:GLN:HE21	1:B:125:GLN:HB3	1.67	0.42
1:C:469:THR:O	1:C:470:ASP:C	2.60	0.42
1:C:641:CYS:HB2	1:C:659:ILE:HG12	2.02	0.42
1:D:98:ILE:HD11	1:D:584:TYR:HD2	1.85	0.42
1:D:138:ASP:C	1:D:141:PRO:HD2	2.45	0.42
1:D:470:ASP:HB3	1:D:516:VAL:HG12	2.01	0.42
1:A:125:GLN:HE21	1:C:68:ARG:NH2	2.18	0.42
1:A:125:GLN:CB	1:C:68:ARG:NH2	2.68	0.42
1:A:297:SER:O	1:A:299:THR:HG23	2.19	0.42
1:A:657:GLU:HG2	1:A:661:GLN:OE1	2.20	0.42
1:B:259:LYS:C	1:B:261:SER:N	2.78	0.42
1:B:405:PHE:O	1:B:408:GLU:HB2	2.20	0.42
1:C:692:ARG:O	1:C:695:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:ILE:HD11	1:D:174:PRO:C	2.44	0.42
1:D:223:ALA:N	1:D:224:PRO:CD	2.83	0.42
1:A:58:LYS:O	1:A:61:ASP:N	2.53	0.42
1:A:634:TYR:C	1:A:636:ARG:H	2.27	0.42
1:A:663:HIS:CE1	1:A:687:TYR:HE2	2.38	0.42
1:B:140:ASN:CB	1:B:141:PRO:HD3	2.50	0.42
1:B:600:ASP:O	1:B:601:GLU:C	2.63	0.42
1:C:154:ASN:CG	1:C:157:SER:H	2.28	0.42
1:C:516:VAL:HG12	1:C:516:VAL:O	2.19	0.42
1:C:681:ASN:HA	1:C:682:PRO:HD3	1.75	0.42
1:D:362:ASN:O	1:D:365:VAL:HG22	2.20	0.42
1:D:655:ALA:O	1:D:656:THR:C	2.62	0.42
1:D:659:ILE:O	1:D:659:ILE:HG22	2.20	0.42
1:A:59:GLU:CD	1:A:60:SER:N	2.78	0.42
1:A:182:TYR:O	1:A:183:LEU:C	2.62	0.42
1:A:275:HIS:CE1	1:A:304:ALA:HB1	2.55	0.42
1:A:381:VAL:HG12	1:A:382:ILE:N	2.34	0.42
1:A:429:GLU:OE2	1:A:674:LYS:HB2	2.19	0.42
1:B:213:LYS:HZ1	1:B:264:ASN:HD21	1.67	0.42
1:B:630:TYR:CD2	1:B:677:VAL:HG22	2.54	0.42
1:B:641:CYS:C	1:B:642:LYS:HD2	2.45	0.42
1:C:197:ARG:HG2	1:C:203:TYR:CE1	2.53	0.42
1:D:445:CYS:O	1:D:448:ILE:HG22	2.19	0.42
1:D:670:ILE:HD11	1:D:677:VAL:HG21	2.02	0.42
1:A:66:ASN:HA	1:A:82:ASN:ND2	2.35	0.42
1:A:259:LYS:C	1:A:261:SER:N	2.78	0.42
1:A:397:SER:OG	1:A:398:PHE:N	2.51	0.42
1:B:21:GLU:HB2	1:B:614:LEU:HD22	2.02	0.42
1:B:119:THR:OG1	1:B:133:SER:HB3	2.19	0.42
1:B:323:ARG:HB3	1:B:324:SER:H	1.62	0.42
1:B:413:LEU:HD11	1:B:578:LEU:HD21	2.02	0.42
1:B:639:MET:SD	1:B:639:MET:N	2.83	0.42
1:C:73:MET:HB3	1:C:74:PRO:HD2	2.01	0.42
1:C:88:MET:CG	1:C:380:PRO:HB2	2.49	0.42
1:D:161:GLY:HA3	1:D:182:TYR:HB2	2.02	0.42
1:D:439:PHE:CE2	1:D:612:GLY:CA	3.02	0.42
1:D:542:LEU:O	1:D:546:LEU:HD22	2.20	0.42
1:D:642:LYS:O	1:D:643:LYS:CB	2.68	0.42
1:A:223:ALA:N	1:A:224:PRO:CD	2.82	0.41
1:A:467:LYS:HE2	1:A:467:LYS:HA	2.02	0.41
1:A:469:THR:O	1:A:470:ASP:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:HIS:O	1:A:505:LEU:HA	2.19	0.41
1:A:660:LEU:HD22	1:A:665:ILE:CD1	2.50	0.41
1:C:138:ASP:C	1:C:141:PRO:HD2	2.45	0.41
1:C:496:ARG:HA	1:C:496:ARG:NE	2.35	0.41
1:A:446:GLU:O	1:A:447:LEU:C	2.63	0.41
1:A:668:GLU:O	1:A:680:ARG:NH1	2.53	0.41
1:B:68:ARG:NH1	1:B:68:ARG:HG2	2.34	0.41
1:C:557:LYS:N	1:C:557:LYS:HD3	2.35	0.41
1:C:600:ASP:O	1:C:601:GLU:C	2.63	0.41
1:D:152:LEU:HG	1:D:196:GLU:HG3	2.01	0.41
1:D:616:ASN:O	1:D:617:VAL:C	2.61	0.41
1:A:166:MET:HE3	1:A:166:MET:HB3	1.96	0.41
1:A:614:LEU:HD12	1:A:614:LEU:HA	1.78	0.41
1:B:11:PRO:HA	1:B:31:ARG:NH2	2.25	0.41
1:B:115:MET:O	1:B:116:GLN:C	2.63	0.41
1:B:447:LEU:C	1:B:449:GLU:N	2.78	0.41
1:C:418:THR:HG23	1:C:419:LEU:HG	2.02	0.41
1:D:288:ARG:CZ	1:D:289:THR:H	2.33	0.41
1:D:288:ARG:NE	1:D:288:ARG:N	2.67	0.41
1:A:53:ASN:C	1:A:54:LEU:HD12	2.46	0.41
1:A:73:MET:HB3	1:A:74:PRO:CD	2.51	0.41
1:C:58:LYS:O	1:C:61:ASP:N	2.54	0.41
1:C:557:LYS:HB2	1:C:557:LYS:NZ	2.35	0.41
1:D:156:ASN:ND2	4:D:894:ADP:O3'	2.49	0.41
1:D:279:ILE:CD1	1:D:302:LEU:HD23	2.50	0.41
1:D:459:LEU:HB2	1:D:473:PHE:CZ	2.55	0.41
1:D:481:PHE:CB	1:D:487:LEU:HD23	2.50	0.41
1:D:636:ARG:NH2	1:D:637:TYR:CE2	2.89	0.41
1:A:138:ASP:O	1:A:141:PRO:HD2	2.20	0.41
1:B:620:ARG:HA	1:B:620:ARG:HE	1.78	0.41
1:B:639:MET:O	1:B:640:LEU:CG	2.59	0.41
1:C:323:ARG:HB3	1:C:324:SER:H	1.65	0.41
1:C:438:TYR:C	1:C:439:PHE:O	2.63	0.41
1:C:567:ARG:HG2	1:C:567:ARG:NH1	2.34	0.41
1:D:405:PHE:O	1:D:408:GLU:HB2	2.21	0.41
1:B:373:ASN:HD22	1:B:374:CYS:N	2.19	0.41
1:B:635:ASN:C	1:B:637:TYR:N	2.76	0.41
1:C:109:GLU:O	1:C:113:LYS:HG2	2.21	0.41
1:C:434:LYS:H	1:C:434:LYS:CD	2.33	0.41
1:A:210:SER:C	1:A:212:SER:N	2.74	0.41
1:A:586:ARG:NH1	5:A:793:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:ARG:O	1:A:622:ALA:C	2.63	0.41
1:B:98:ILE:HD11	1:B:584:TYR:HD2	1.86	0.41
1:B:335:VAL:O	1:B:335:VAL:HG22	2.20	0.41
1:C:115:MET:O	1:C:116:GLN:C	2.63	0.41
1:C:152:LEU:HG	1:C:196:GLU:HG3	2.02	0.41
1:C:249:ILE:O	1:C:253:MET:HG2	2.21	0.41
1:C:412:GLN:OE1	1:C:442:LYS:HD3	2.21	0.41
1:D:66:ASN:HA	1:D:82:ASN:ND2	2.35	0.41
1:D:496:ARG:NE	1:D:496:ARG:HA	2.36	0.41
1:D:542:LEU:HG	1:D:546:LEU:HD21	2.02	0.41
1:A:58:LYS:HB3	1:A:59:GLU:OE2	2.20	0.41
1:A:418:THR:CG2	1:A:419:LEU:N	2.82	0.41
1:A:630:TYR:CE2	1:A:677:VAL:CG2	3.04	0.41
1:A:666:ASP:C	1:A:668:GLU:N	2.79	0.41
1:B:293:THR:HG22	1:B:339:PRO:CG	2.50	0.41
1:B:535:MET:HA	1:B:535:MET:HE2	2.03	0.41
1:B:663:HIS:O	1:B:663:HIS:ND1	2.48	0.41
1:B:683:THR:HA	1:B:686:PHE:HD2	1.86	0.41
1:C:66:ASN:HD22	1:C:67:GLY:H	1.66	0.41
1:C:365:VAL:HG23	1:C:366:SER:H	1.84	0.41
1:D:73:MET:HB3	1:D:74:PRO:HD2	2.02	0.41
1:D:232:SER:O	1:D:233:GLY:C	2.64	0.41
1:D:661:GLN:C	1:D:663:HIS:N	2.79	0.41
1:A:201:ILE:HG23	1:A:202:PHE:N	2.36	0.41
1:A:227:GLU:N	1:A:278:ASN:HD21	1.99	0.41
1:A:335:VAL:O	1:A:335:VAL:HG22	2.21	0.41
1:A:373:ASN:HD22	1:A:374:CYS:N	2.19	0.41
1:B:152:LEU:HG	1:B:196:GLU:HG3	2.02	0.41
1:B:214:LEU:HD23	1:B:214:LEU:HA	1.87	0.41
1:B:223:ALA:HB3	1:B:224:PRO:HD3	2.03	0.41
1:B:223:ALA:N	1:B:224:PRO:CD	2.83	0.41
1:B:443:PRO:HD2	1:B:444:ILE:HG13	2.02	0.41
1:B:657:GLU:C	1:B:657:GLU:CD	2.89	0.41
1:C:310:LYS:O	1:C:538:SER:HA	2.21	0.41
1:C:439:PHE:O	1:C:440:ASN:C	2.64	0.41
1:C:542:LEU:HG	1:C:546:LEU:HD21	2.02	0.41
1:C:685:LEU:O	1:C:687:TYR:N	2.52	0.41
1:D:10:VAL:O	1:D:10:VAL:HG12	2.20	0.41
1:D:49:ASN:HA	1:D:50:PRO:HD3	1.87	0.41
1:D:58:LYS:HB3	1:D:59:GLU:OE2	2.20	0.41
1:D:182:TYR:O	1:D:183:LEU:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:ALA:O	1:D:307:SER:HB3	2.21	0.41
1:D:639:MET:C	1:D:640:LEU:HD12	2.46	0.41
1:D:652:ALA:O	1:D:653:LYS:C	2.63	0.41
1:A:302:LEU:HD13	1:A:302:LEU:C	2.46	0.41
1:A:439:PHE:CZ	1:A:612:GLY:CA	3.03	0.41
1:A:629:GLU:CG	1:A:676:LYS:NZ	2.82	0.41
1:B:94:ASN:ND2	1:B:381:VAL:H	2.18	0.41
1:B:428:ARG:HG2	1:B:428:ARG:NH1	2.34	0.41
1:B:685:LEU:HA	1:B:688:PHE:CD1	2.56	0.41
1:C:161:GLY:HA3	1:C:182:TYR:HB2	2.03	0.41
1:C:200:HIS:O	1:C:201:ILE:C	2.62	0.41
1:C:434:LYS:NZ	1:C:622:ALA:HB1	2.35	0.41
1:D:181:ASN:HD21	1:D:362:ASN:HD22	1.63	0.41
1:D:268:ARG:CZ	1:D:310:LYS:HE2	2.50	0.41
1:D:634:TYR:CD2	1:D:634:TYR:O	2.74	0.41
1:D:679:ILE:O	1:D:679:ILE:HG22	2.21	0.41
1:A:98:ILE:O	1:A:98:ILE:HG13	2.20	0.40
1:A:193:THR:O	1:A:196:GLU:HB2	2.22	0.40
1:A:516:VAL:HG12	1:A:516:VAL:O	2.19	0.40
1:A:560:GLU:O	1:A:561:THR:C	2.63	0.40
1:B:193:THR:O	1:B:196:GLU:HB2	2.21	0.40
1:B:397:SER:OG	1:B:398:PHE:N	2.52	0.40
1:C:18:GLN:HG2	1:C:20:THR:HG23	2.03	0.40
1:C:185:GLU:HG3	1:C:399:GLU:HG2	2.01	0.40
1:C:259:LYS:C	1:C:261:SER:N	2.79	0.40
1:C:405:PHE:CE1	1:C:409:LYS:HD3	2.56	0.40
1:D:322:TYR:C	1:D:340:MET:HE2	2.46	0.40
1:A:185:GLU:O	1:A:185:GLU:HG2	2.20	0.40
1:B:652:ALA:C	1:B:654:GLN:N	2.80	0.40
1:B:655:ALA:O	1:B:656:THR:C	2.64	0.40
1:C:439:PHE:CE2	1:C:610:TYR:O	2.74	0.40
1:D:443:PRO:O	1:D:447:LEU:HG	2.21	0.40
1:A:49:ASN:HA	1:A:50:PRO:HD3	1.88	0.40
1:A:80:LEU:CD1	1:A:583:HIS:HB3	2.45	0.40
1:A:269:ILE:HG21	1:A:360:LEU:HD22	2.04	0.40
1:A:610:TYR:CD1	1:A:610:TYR:C	3.00	0.40
1:B:431:ILE:O	1:B:432:GLU:C	2.64	0.40
1:B:662:GLN:O	1:B:664:ASN:N	2.55	0.40
1:C:167:GLN:OE1	1:C:373:ASN:ND2	2.54	0.40
1:C:553:GLU:O	1:C:554:ASP:HB2	2.20	0.40
1:C:637:TYR:CD2	1:C:688:PHE:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:639:MET:CG	1:C:640:LEU:HD12	2.47	0.40
1:C:656:THR:HG21	1:C:677:VAL:HG21	2.03	0.40
1:D:76:HIS:CD2	1:D:77:MET:N	2.89	0.40
1:D:311:THR:HG22	1:D:538:SER:CA	2.52	0.40
1:D:367:LYS:O	1:D:370:THR:HB	2.22	0.40
1:D:610:TYR:CD1	1:D:610:TYR:C	2.99	0.40
1:A:279:ILE:HG23	1:A:296:VAL:HG13	2.03	0.40
1:B:163:TYR:HE2	1:B:165:GLU:OE1	2.05	0.40
1:B:442:LYS:O	1:B:446:GLU:HG2	2.22	0.40
1:B:675:THR:O	1:B:675:THR:CG2	2.69	0.40
1:C:416:GLU:HA	1:C:420:LYS:HB3	2.03	0.40
1:C:450:LYS:CB	1:C:451:LYS:HD2	2.51	0.40
1:C:640:LEU:HD12	1:C:640:LEU:N	2.36	0.40
1:D:628:ILE:O	1:D:676:LYS:HA	2.22	0.40
1:A:67:GLY:N	1:A:82:ASN:ND2	2.62	0.40
1:A:447:LEU:C	1:A:449:GLU:H	2.29	0.40
1:A:607:GLN:HA	1:A:610:TYR:CE2	2.56	0.40
1:B:356:LEU:HD12	1:B:356:LEU:HA	1.91	0.40
1:C:634:TYR:CD1	1:C:635:ASN:N	2.89	0.40
1:D:97:VAL:HG11	1:D:114:ILE:CD1	2.51	0.40
1:D:259:LYS:C	1:D:261:SER:N	2.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	640/697 (92%)	529 (83%)	80 (12%)	31 (5%)	2	11
1	B	640/697 (92%)	541 (84%)	64 (10%)	35 (6%)	1	8
1	C	675/697 (97%)	553 (82%)	80 (12%)	42 (6%)	1	6
1	D	652/697 (94%)	557 (85%)	66 (10%)	29 (4%)	2	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2607/2788 (94%)	2180 (84%)	290 (11%)	137 (5%)	1	9

All (137) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	157	SER
1	A	376	THR
1	A	439	PHE
1	A	442	LYS
1	A	483	LYS
1	A	494	LYS
1	A	561	THR
1	A	664	ASN
1	B	124	ASN
1	B	157	SER
1	B	376	THR
1	B	439	PHE
1	B	442	LYS
1	B	449	GLU
1	B	483	LYS
1	B	494	LYS
1	B	561	THR
1	B	621	ARG
1	B	640	LEU
1	B	653	LYS
1	B	668	GLU
1	C	124	ASN
1	C	157	SER
1	C	376	THR
1	C	439	PHE
1	C	442	LYS
1	C	483	LYS
1	C	494	LYS
1	C	554	ASP
1	C	561	THR
1	C	646	PRO
1	C	695	GLU
1	D	124	ASN
1	D	157	SER
1	D	376	THR
1	D	439	PHE

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Mol	Chain	Res	Type
1	D	442	LYS
1	D	483	LYS
1	D	494	LYS
1	D	561	THR
1	A	120	PHE
1	A	183	LEU
1	A	285	ALA
1	A	453	ILE
1	A	491	VAL
1	A	625	ALA
1	A	663	HIS
1	A	684	THR
1	B	120	PHE
1	B	183	LEU
1	B	285	ALA
1	B	448	ILE
1	B	453	ILE
1	B	491	VAL
1	B	625	ALA
1	B	654	GLN
1	C	12	ASP
1	C	120	PHE
1	C	183	LEU
1	C	285	ALA
1	C	418	THR
1	C	440	ASN
1	C	453	ILE
1	C	491	VAL
1	C	549	PRO
1	C	550	THR
1	C	621	ARG
1	C	666	ASP
1	C	683	THR
1	D	120	PHE
1	D	183	LEU
1	D	285	ALA
1	D	453	ILE
1	D	491	VAL
1	D	694	LEU
1	A	12	ASP
1	A	432	GLU
1	A	621	ARG

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Mol	Chain	Res	Type
1	A	635	ASN
1	A	656	THR
1	B	12	ASP
1	B	222	ASN
1	B	432	GLU
1	B	663	HIS
1	B	669	GLU
1	C	222	ASN
1	C	430	GLY
1	C	634	TYR
1	C	651	THR
1	C	664	ASN
1	C	696	MET
1	D	12	ASP
1	D	42	GLY
1	D	55	ASN
1	D	222	ASN
1	D	664	ASN
1	D	681	ASN
1	A	42	GLY
1	A	222	ASN
1	A	435	ASN
1	A	601	GLU
1	A	634	TYR
1	B	123	SER
1	B	601	GLU
1	B	675	THR
1	C	42	GLY
1	C	55	ASN
1	C	551	ARG
1	C	601	GLU
1	C	681	ASN
1	D	543	VAL
1	D	601	GLU
1	A	55	ASN
1	B	42	GLY
1	B	55	ASN
1	B	680	ARG
1	C	452	PRO
1	C	682	PRO
1	C	692	ARG
1	D	123	SER

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Mol	Chain	Res	Type
1	D	448	ILE
1	D	631	THR
1	A	452	PRO
1	B	452	PRO
1	B	543	VAL
1	C	126	SER
1	C	421	SER
1	C	543	VAL
1	C	636	ARG
1	D	126	SER
1	D	636	ARG
1	A	126	SER
1	B	126	SER
1	D	452	PRO
1	A	543	VAL
1	D	221	PRO

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	575/616 (93%)	521 (91%)	54 (9%)	8	32
1	B	574/616 (93%)	520 (91%)	54 (9%)	8	32
1	C	601/616 (98%)	537 (89%)	64 (11%)	6	27
1	D	583/616 (95%)	525 (90%)	58 (10%)	7	30
All	All	2333/2464 (95%)	2103 (90%)	230 (10%)	7	30

All (230) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
1	A	59	GLU
1	A	80	LEU
1	A	89	ARG
1	A	90	GLN

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Mol	Chain	Res	Type
1	A	109	GLU
1	A	123	SER
1	A	125	GLN
1	A	142	LEU
1	A	144	GLU
1	A	164	MET
1	A	178	LYS
1	A	183	LEU
1	A	184	LEU
1	A	192	ARG
1	A	194	GLN
1	A	206	LEU
1	A	211	GLN
1	A	220	THR
1	A	235	PHE
1	A	265	SER
1	A	316	LEU
1	A	337	SER
1	A	342	CYS
1	A	352	LEU
1	A	356	LEU
1	A	364	LEU
1	A	367	LYS
1	A	378	LYS
1	A	388	TYR
1	A	410	LEU
1	A	418	THR
1	A	435	ASN
1	A	439	PHE
1	A	442	LYS
1	A	444	ILE
1	A	448	ILE
1	A	459	LEU
1	A	460	ASP
1	A	496	ARG
1	A	526	THR
1	A	530	ASP
1	A	567	ARG
1	A	573	LEU
1	A	576	THR
1	A	584	TYR
1	A	639	MET

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Mol	Chain	Res	Type
1	A	640	LEU
1	A	642	LYS
1	A	653	LYS
1	A	663	HIS
1	A	665	ILE
1	A	671	ARG
1	A	692	ARG
1	B	31	ARG
1	B	59	GLU
1	B	80	LEU
1	B	90	GLN
1	B	109	GLU
1	B	123	SER
1	B	125	GLN
1	B	142	LEU
1	B	144	GLU
1	B	164	MET
1	B	178	LYS
1	B	183	LEU
1	B	184	LEU
1	B	192	ARG
1	B	194	GLN
1	B	206	LEU
1	B	211	GLN
1	B	220	THR
1	B	235	PHE
1	B	265	SER
1	B	316	LEU
1	B	337	SER
1	B	342	CYS
1	B	352	LEU
1	B	356	LEU
1	B	364	LEU
1	B	367	LYS
1	B	378	LYS
1	B	388	TYR
1	B	410	LEU
1	B	418	THR
1	B	442	LYS
1	B	448	ILE
1	B	459	LEU
1	B	460	ASP

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Mol	Chain	Res	Type
1	B	496	ARG
1	B	526	THR
1	B	530	ASP
1	B	567	ARG
1	B	573	LEU
1	B	576	THR
1	B	584	TYR
1	B	620	ARG
1	B	621	ARG
1	B	627	ARG
1	B	628	ILE
1	B	634	TYR
1	B	635	ASN
1	B	653	LYS
1	B	657	GLU
1	B	677	VAL
1	B	685	LEU
1	B	691	LYS
1	B	692	ARG
1	C	31	ARG
1	C	59	GLU
1	C	80	LEU
1	C	89	ARG
1	C	90	GLN
1	C	109	GLU
1	C	123	SER
1	C	125	GLN
1	C	142	LEU
1	C	144	GLU
1	C	164	MET
1	C	178	LYS
1	C	183	LEU
1	C	184	LEU
1	C	192	ARG
1	C	194	GLN
1	C	206	LEU
1	C	211	GLN
1	C	220	THR
1	C	235	PHE
1	C	253	MET
1	C	265	SER
1	C	288	ARG

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Mol	Chain	Res	Type
1	C	289	THR
1	C	316	LEU
1	C	337	SER
1	C	342	CYS
1	C	352	LEU
1	C	356	LEU
1	C	364	LEU
1	C	367	LYS
1	C	378	LYS
1	C	388	TYR
1	C	410	LEU
1	C	418	THR
1	C	434	LYS
1	C	442	LYS
1	C	443	PRO
1	C	459	LEU
1	C	460	ASP
1	C	496	ARG
1	C	526	THR
1	C	530	ASP
1	C	551	ARG
1	C	554	ASP
1	C	557	LYS
1	C	567	ARG
1	C	573	LEU
1	C	576	THR
1	C	584	TYR
1	C	614	LEU
1	C	616	ASN
1	C	627	ARG
1	C	629	GLU
1	C	636	ARG
1	C	638	LYS
1	C	642	LYS
1	C	646	PRO
1	C	653	LYS
1	C	654	GLN
1	C	668	GLU
1	C	669	GLU
1	C	677	VAL
1	C	695	GLU
1	D	31	ARG

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Mol	Chain	Res	Type
1	D	59	GLU
1	D	80	LEU
1	D	89	ARG
1	D	90	GLN
1	D	109	GLU
1	D	123	SER
1	D	125	GLN
1	D	142	LEU
1	D	144	GLU
1	D	164	MET
1	D	178	LYS
1	D	183	LEU
1	D	184	LEU
1	D	192	ARG
1	D	194	GLN
1	D	206	LEU
1	D	220	THR
1	D	235	PHE
1	D	265	SER
1	D	288	ARG
1	D	316	LEU
1	D	337	SER
1	D	342	CYS
1	D	352	LEU
1	D	356	LEU
1	D	364	LEU
1	D	367	LYS
1	D	378	LYS
1	D	388	TYR
1	D	410	LEU
1	D	418	THR
1	D	434	LYS
1	D	442	LYS
1	D	446	GLU
1	D	448	ILE
1	D	459	LEU
1	D	460	ASP
1	D	496	ARG
1	D	526	THR
1	D	530	ASP
1	D	567	ARG
1	D	573	LEU

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Mol	Chain	Res	Type
1	D	576	THR
1	D	584	TYR
1	D	620	ARG
1	D	631	THR
1	D	642	LYS
1	D	662	GLN
1	D	663	HIS
1	D	666	ASP
1	D	668	GLU
1	D	671	ARG
1	D	681	ASN
1	D	683	THR
1	D	692	ARG
1	D	693	GLU
1	D	695	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	55	ASN
1	A	66	ASN
1	A	76	HIS
1	A	82	ASN
1	A	90	GLN
1	A	94	ASN
1	A	125	GLN
1	A	140	ASN
1	A	156	ASN
1	A	167	GLN
1	A	211	GLN
1	A	264	ASN
1	A	275	HIS
1	A	278	ASN
1	A	313	GLN
1	A	362	ASN
1	A	373	ASN
1	A	423	GLN
1	A	435	ASN
1	A	440	ASN
1	A	536	GLN
1	A	544	GLN

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Mol	Chain	Res	Type
1	A	565	GLN
1	A	593	ASN
1	A	606	HIS
1	A	607	GLN
1	A	663	HIS
1	A	681	ASN
1	B	27	ASN
1	B	55	ASN
1	B	66	ASN
1	B	76	HIS
1	B	82	ASN
1	B	90	GLN
1	B	94	ASN
1	B	125	GLN
1	B	140	ASN
1	B	156	ASN
1	B	167	GLN
1	B	211	GLN
1	B	264	ASN
1	B	275	HIS
1	B	278	ASN
1	B	313	GLN
1	B	362	ASN
1	B	373	ASN
1	B	411	GLN
1	B	423	GLN
1	B	486	HIS
1	B	536	GLN
1	B	565	GLN
1	B	606	HIS
1	B	607	GLN
1	B	635	ASN
1	B	654	GLN
1	C	27	ASN
1	C	55	ASN
1	C	66	ASN
1	C	76	HIS
1	C	82	ASN
1	C	94	ASN
1	C	124	ASN
1	C	125	GLN
1	C	140	ASN

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Mol	Chain	Res	Type
1	C	156	ASN
1	C	167	GLN
1	C	211	GLN
1	C	264	ASN
1	C	275	HIS
1	C	278	ASN
1	C	313	GLN
1	C	362	ASN
1	C	373	ASN
1	C	423	GLN
1	C	536	GLN
1	C	544	GLN
1	C	565	GLN
1	C	607	GLN
1	C	616	ASN
1	C	662	GLN
1	C	664	ASN
1	C	681	ASN
1	D	27	ASN
1	D	55	ASN
1	D	66	ASN
1	D	76	HIS
1	D	82	ASN
1	D	90	GLN
1	D	94	ASN
1	D	125	GLN
1	D	140	ASN
1	D	167	GLN
1	D	264	ASN
1	D	275	HIS
1	D	278	ASN
1	D	313	GLN
1	D	362	ASN
1	D	373	ASN
1	D	395	ASN
1	D	423	GLN
1	D	440	ASN
1	D	536	GLN
1	D	544	GLN
1	D	565	GLN
1	D	607	GLN
1	D	661	GLN

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Mol	Chain	Res	Type
1	D	662	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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	$\# Z > 2$
3	VO4	C	892	4,2	0,4,4	-	-	-		
4	ADP	C	891	2,3	28,29,29	1.44	4 (14%)	43,45,45	1.02	2 (4%)
4	ADP	D	894	2,3	28,29,29	1.47	4 (14%)	43,45,45	1.07	4 (9%)
3	VO4	D	895	4,2	0,4,4	-	-	-		
3	VO4	B	795	4,2	0,4,4	-	-	-		
4	ADP	B	794	2,3	28,29,29	1.47	4 (14%)	43,45,45	1.11	3 (6%)
3	VO4	A	792	4,2	0,4,4	-	-	-		
4	ADP	A	791	2,3	28,29,29	1.42	4 (14%)	43,45,45	1.15	3 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	D	894	2,3	-	1/16/32/32	0/3/3/3
4	ADP	C	891	2,3	-	2/16/32/32	0/3/3/3
4	ADP	B	794	2,3	-	0/16/32/32	0/3/3/3
4	ADP	A	791	2,3	-	1/16/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	794	ADP	C2-N1	4.74	1.42	1.33
4	D	894	ADP	C2-N1	4.10	1.41	1.33
4	A	791	ADP	C2-N1	4.06	1.41	1.33
4	C	891	ADP	C2-N1	3.88	1.40	1.33
4	A	791	ADP	C4-N3	3.51	1.41	1.34
4	D	894	ADP	C4-N3	3.39	1.40	1.34
4	C	891	ADP	C4-N3	3.26	1.40	1.34
4	B	794	ADP	C4-N3	3.23	1.40	1.34
4	D	894	ADP	PA-O3A	2.58	1.62	1.59
4	C	891	ADP	PB-O2B	-2.52	1.45	1.54
4	D	894	ADP	PB-O2B	-2.38	1.45	1.54
4	C	891	ADP	C6-N1	2.33	1.42	1.35
4	A	791	ADP	PB-O2B	-2.31	1.46	1.54
4	B	794	ADP	PB-O2B	-2.28	1.46	1.54
4	B	794	ADP	C6-N1	2.23	1.42	1.35
4	A	791	ADP	O4'-C4'	-2.16	1.40	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	791	ADP	O3'-C3'-C2'	2.57	120.06	111.82
4	C	891	ADP	O3'-C3'-C2'	2.53	119.93	111.82
4	B	794	ADP	O3'-C3'-C4'	2.53	118.34	111.08
4	C	891	ADP	O3'-C3'-C4'	2.53	118.34	111.08
4	D	894	ADP	O3'-C3'-C2'	2.50	119.84	111.82
4	A	791	ADP	O3'-C3'-C4'	2.47	118.19	111.08
4	B	794	ADP	O3'-C3'-C2'	2.43	119.62	111.82
4	D	894	ADP	O3'-C3'-C4'	2.40	117.96	111.08
4	D	894	ADP	O4'-C4'-C3'	-2.20	100.78	105.15
4	A	791	ADP	O4'-C4'-C5'	-2.19	102.33	109.33
4	D	894	ADP	C2'-C3'-C4'	-2.10	98.55	102.61
4	B	794	ADP	O2'-C2'-C1'	2.10	117.33	110.10

There are no chirality outliers.

All (4) torsion outliers are listed below:

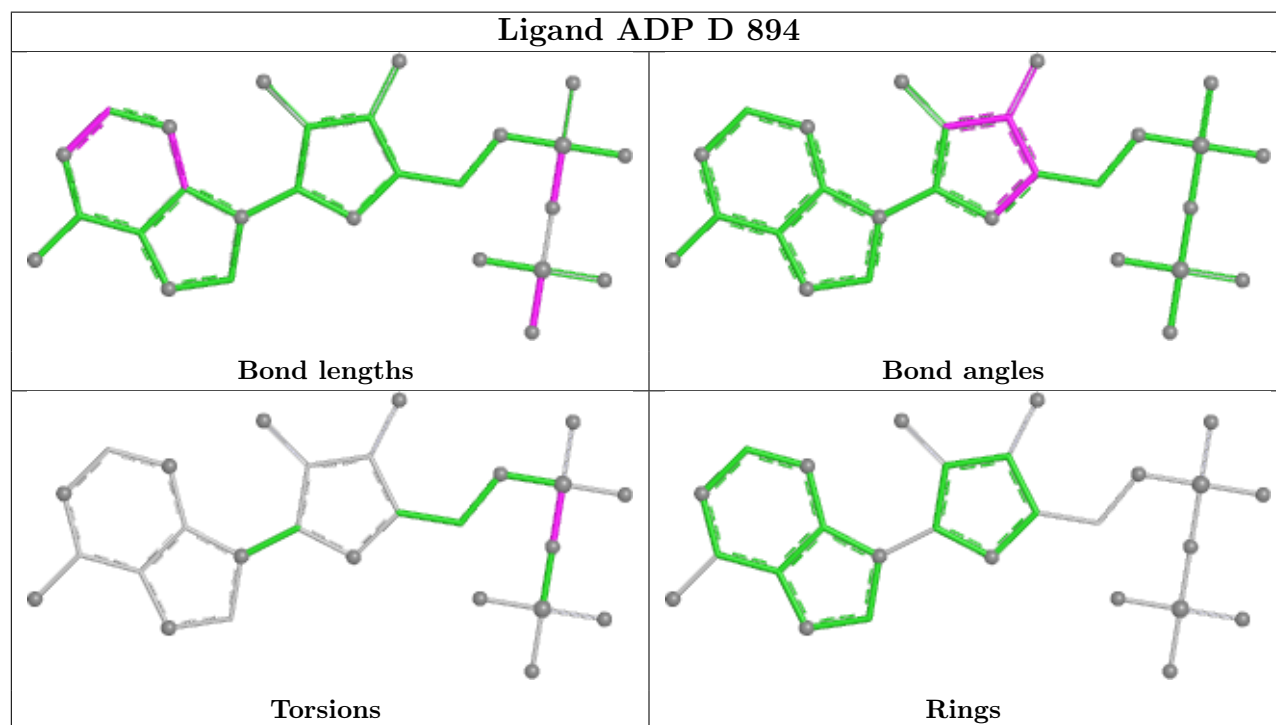
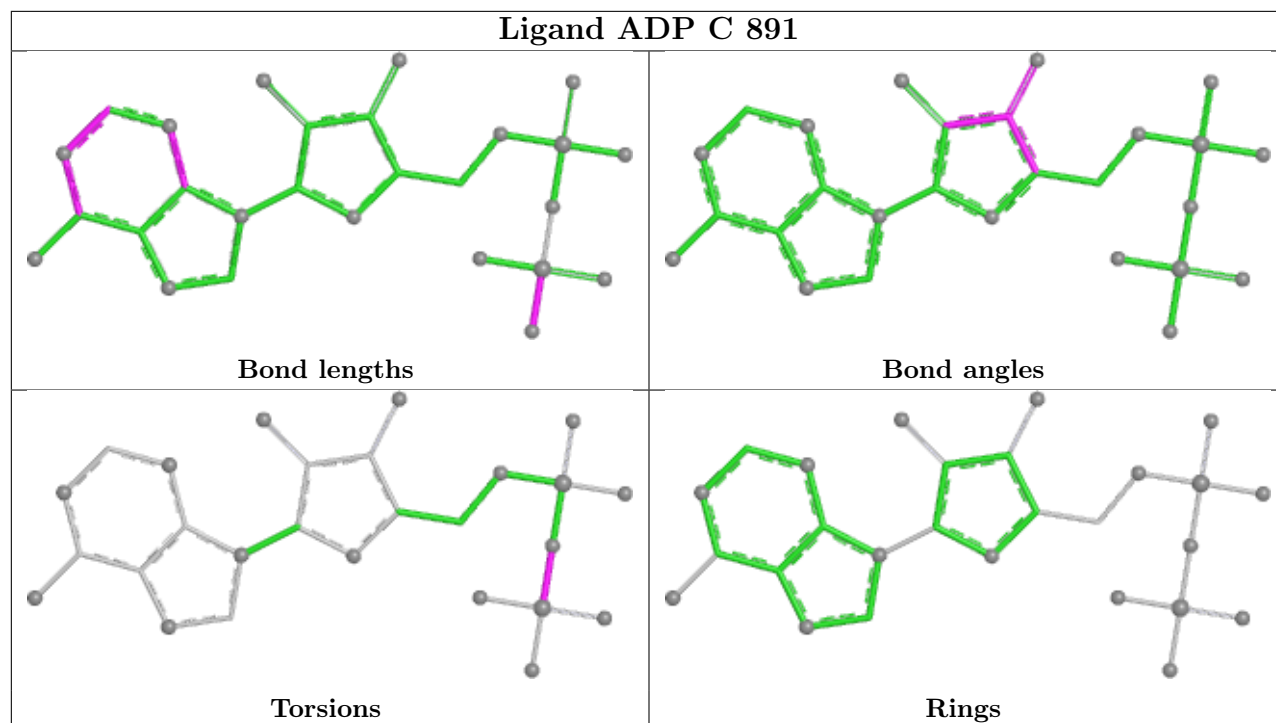
Mol	Chain	Res	Type	Atoms
4	A	791	ADP	PA-O3A-PB-O3B
4	C	891	ADP	PA-O3A-PB-O1B
4	C	891	ADP	PA-O3A-PB-O2B
4	D	894	ADP	PB-O3A-PA-O2A

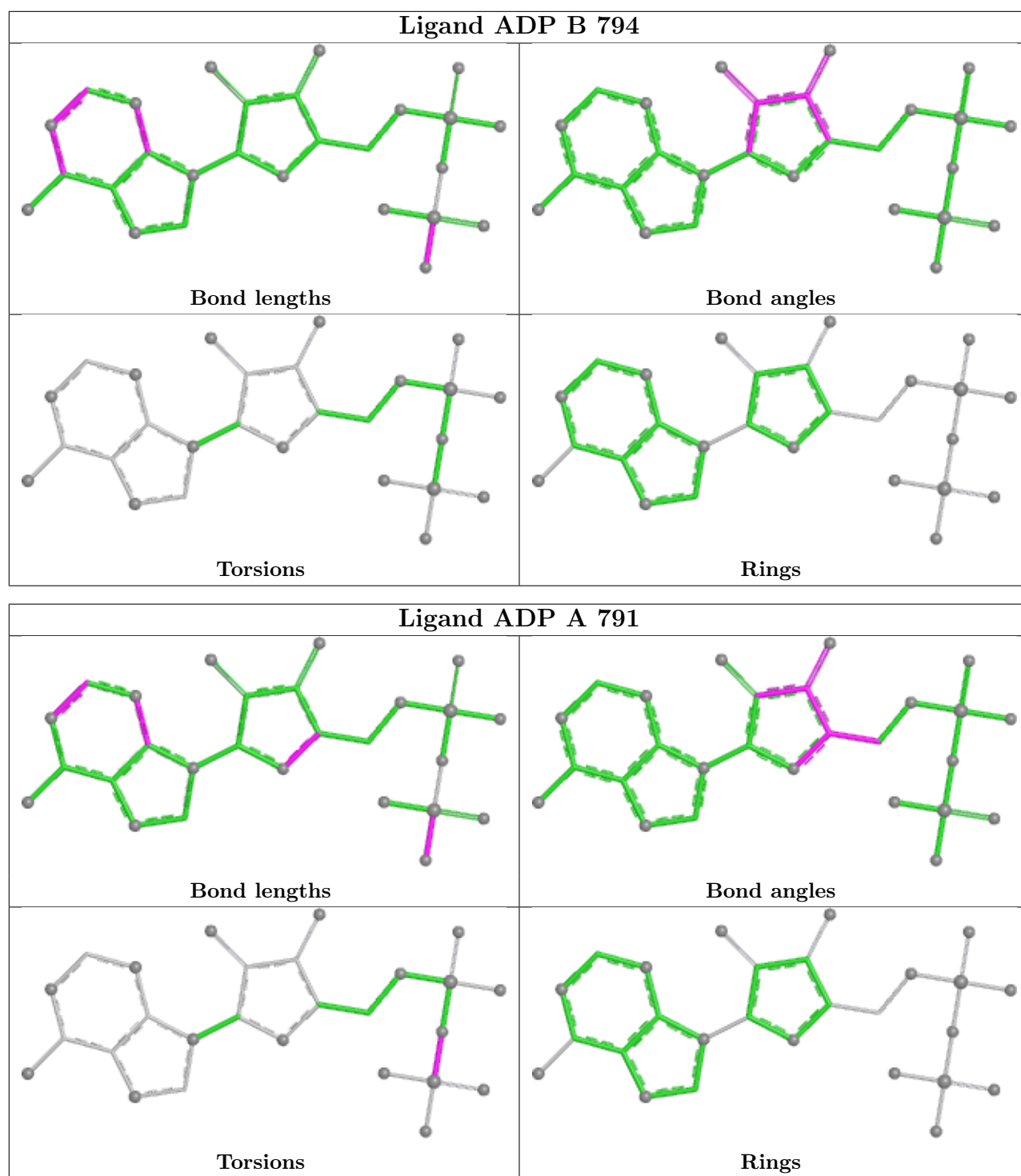
There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	892	VO4	1	0
4	C	891	ADP	2	0
4	D	894	ADP	3	0
3	D	895	VO4	1	0
4	B	794	ADP	2	0
3	A	792	VO4	1	0
4	A	791	ADP	2	0

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.