



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:52 AM UTC

PDB ID : 1KY5 / pdb_00001ky5
Title : D244E mutant S-Adenosylhomocysteine hydrolase refined with noncrystallographic restraints
Authors : Takata, Y.; Takusagawa, F.
Deposited on : 2002-02-03
Resolution : 2.80 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

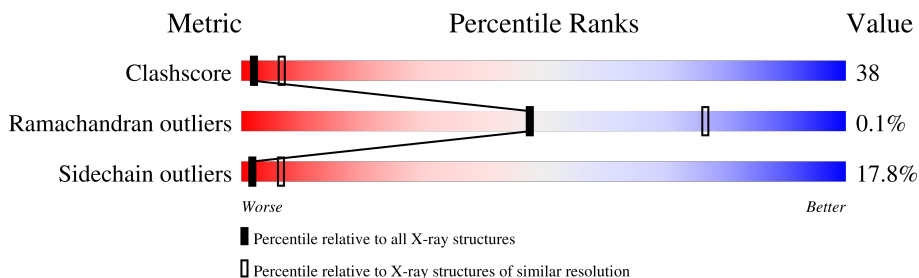
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	431	
1	B	431	
1	C	431	
1	D	431	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13784 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 S-adenosylhomocysteine hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3320	2109	571	615	25			
1	B	430	Total	C	N	O	S	0	0	0
			3320	2109	571	615	25			
1	C	430	Total	C	N	O	S	0	0	0
			3320	2109	571	615	25			
1	D	430	Total	C	N	O	S	0	0	0
			3320	2109	571	615	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	GLU	ASP	engineered mutation	UNP P10760
B	1244	GLU	ASP	engineered mutation	UNP P10760
C	2244	GLU	ASP	engineered mutation	UNP P10760
D	3244	GLU	ASP	engineered mutation	UNP P10760

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	10	5	4		
3	B	1	Total	C	N	O	0	0
			19	10	5	4		
3	C	1	Total	C	N	O	0	0
			19	10	5	4		
3	D	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 4 is water.

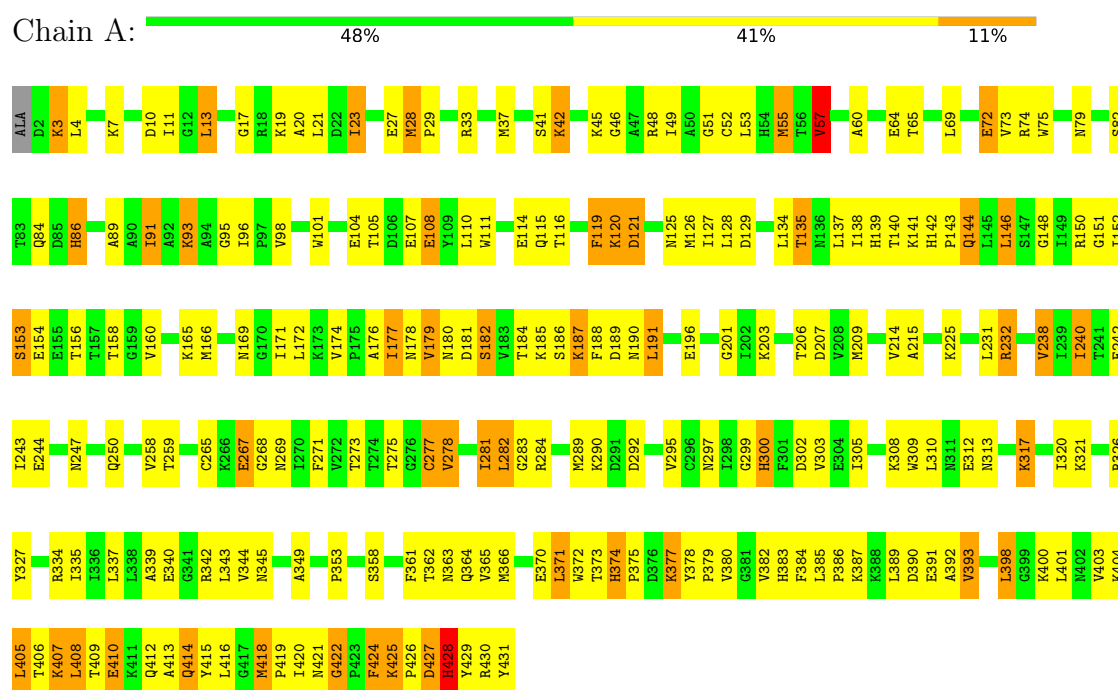
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total	O	0	0
			79	79		
4	B	68	Total	O	0	0
			68	68		
4	C	54	Total	O	0	0
			54	54		
4	D	51	Total	O	0	0
			51	51		

3 Residue-property plots

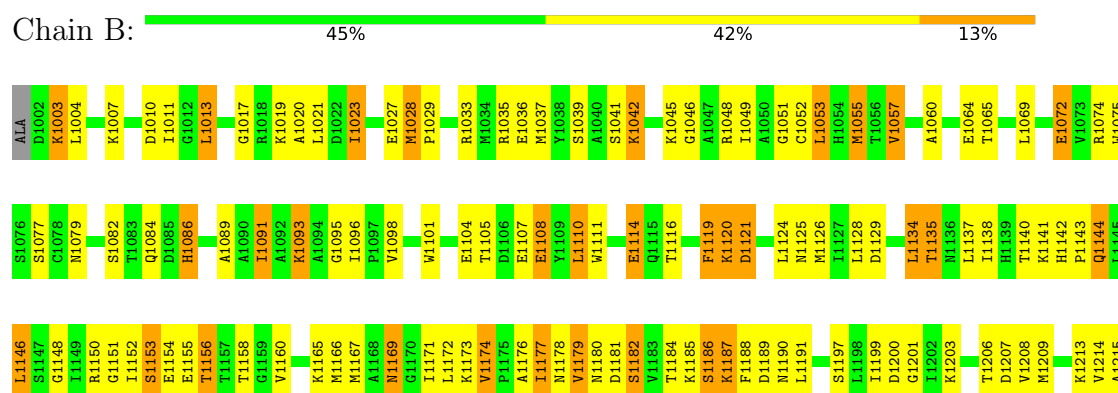
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

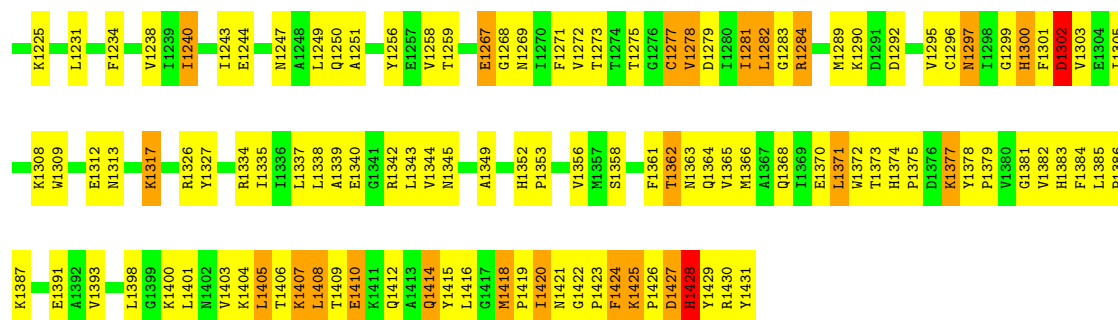
Note EDS was not executed.

• Molecule 1: S-adenosylhomocysteine hydrolase



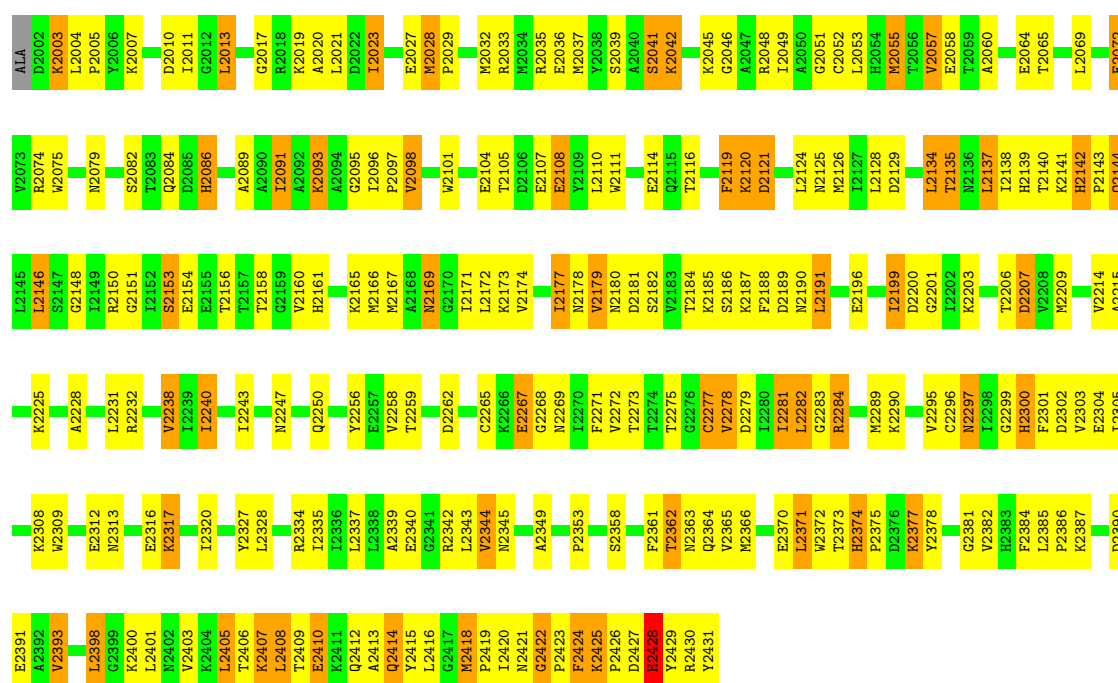
• Molecule 1: S-adenosylhomocysteine hydrolase





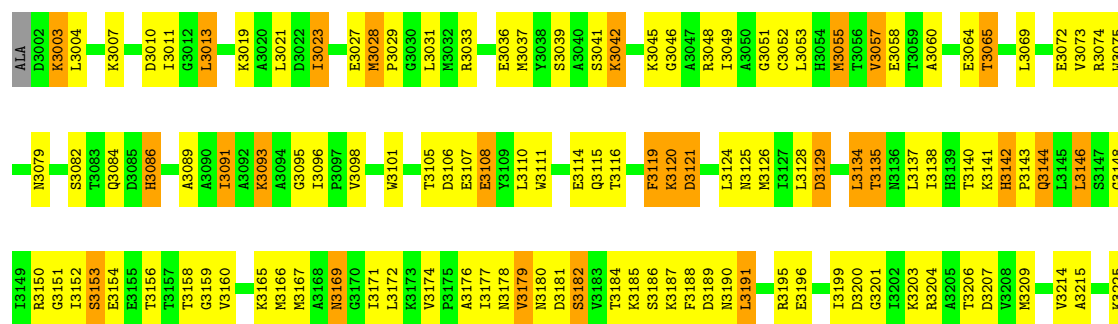
• Molecule 1: S-adenosylhomocysteine hydrolase

Chain C: 46% 41% 13%



• Molecule 1: S-adenosylhomocysteine hydrolase

Chain D: 47% 40% 13%



F3402	N3313		L3231
V3403	K3317		V3238
K3404			I3239
L3405	Y3327		I3240
T3406			
K3407	R3334		I3243
L3408	I3335		E3244
T3409	I3336		P3245
E3410	I3337		I3246
K3411	I3338		N3247
Q3412	I3339		A3248
A3413	E3340		L3249
Q3414	G3341		Q3250
Y3415	R3342		
L3416	L3343		E3257
G3417	K3344		V3258
K3418	N3345		
P3419			D3262
I3420	A3349		
N3421			C3265
G3422	H3352		K3266
F3424	P3353		E3267
K3425			G3268
P3426	M3357		N3269
D3427	S3358		
K3428	F3361		V3272
Y3429	T3362		T3273
R3430	N3363		T3274
Y3431	Q3364		T3275
	V3365		G3276
	M3366		C3277
			V3278
	E3370		D3279
	L3371		I3280
	W3372		I3281
	T3373		L3282
	H3374		G3283
	P3375		R3284
	D3376		H3285
	K3377		
	Y3378		K3290
	P3379		
	V3380		V3295
	G3381		C3296
	V3382		N3297
	H3383		I3298
	P3384		G3299
			H3300
	K3387		F3301
	E3391		D3302
	A3392		V3303
	V3393		E3304
			I3305
	L3398		K3308
	G3399		W3309
	K3400		
	L3401		F3212

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	91.00Å 223.00Å 91.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.215 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13784	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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: NAI, ADY

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	0.52	0/3385	0.98	15/4580 (0.3%)
1	B	0.52	0/3385	0.99	17/4580 (0.4%)
1	C	0.54	0/3385	0.98	17/4580 (0.4%)
1	D	0.53	0/3385	0.98	17/4580 (0.4%)
All	All	0.53	0/13540	0.98	66/18320 (0.4%)

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3278	VAL	N-CA-C	8.15	118.94	110.05
1	A	278	VAL	N-CA-C	8.12	118.90	110.05
1	B	1302	ASP	N-CA-C	7.82	123.36	112.72
1	B	1278	VAL	N-CA-C	7.78	118.53	110.05
1	D	3302	ASP	N-CA-C	7.65	122.65	112.25
1	A	302	ASP	N-CA-C	7.52	122.95	112.72
1	A	156	THR	N-CA-C	7.38	121.57	110.14
1	C	2049	ILE	N-CA-C	7.36	118.61	108.89
1	D	3278	VAL	CB-CA-C	-7.32	103.53	111.59
1	D	3156	THR	N-CA-C	7.20	121.31	110.14
1	B	1268	GLY	N-CA-C	7.07	120.11	112.33
1	B	1156	THR	N-CA-C	7.05	121.07	110.14
1	A	268	GLY	N-CA-C	7.02	120.00	111.93
1	A	300	HIS	N-CA-C	7.00	118.99	111.36
1	B	1300	HIS	N-CA-C	6.86	118.55	111.14
1	C	2278	VAL	N-CA-C	6.83	117.50	110.05
1	C	2302	ASP	N-CA-C	6.82	121.52	112.25
1	C	2268	GLY	N-CA-C	6.71	119.72	112.33
1	C	2075	TRP	N-CA-C	6.69	120.52	110.14
1	D	3268	GLY	N-CA-C	6.66	119.66	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3300	HIS	N-CA-C	6.65	118.61	111.36
1	B	1278	VAL	CB-CA-C	-6.50	104.44	111.59
1	C	2156	THR	N-CA-C	6.44	120.12	110.14
1	D	3075	TRP	N-CA-C	6.43	120.11	110.14
1	B	1238	VAL	N-CA-C	6.41	117.34	107.99
1	D	3344	VAL	N-CA-C	6.40	116.54	110.53
1	D	3238	VAL	N-CA-C	6.31	117.88	108.23
1	A	422	GLY	CA-C-N	6.21	126.12	119.85
1	A	422	GLY	C-N-CA	6.21	126.12	119.85
1	B	1049	ILE	N-CA-C	6.18	117.48	108.58
1	A	344	VAL	N-CA-C	6.17	116.96	110.72
1	A	238	VAL	N-CA-C	6.15	117.15	108.36
1	C	2300	HIS	N-CA-C	6.11	118.02	111.36
1	A	75	TRP	N-CA-C	6.08	119.57	110.14
1	D	3428	HIS	N-CA-C	-6.07	105.70	113.23
1	C	2344	VAL	N-CA-C	6.05	116.83	110.72
1	B	1344	VAL	N-CA-C	6.00	116.78	110.72
1	C	2072	GLU	N-CA-C	-5.99	99.13	108.90
1	C	2238	VAL	N-CA-C	5.99	116.92	108.36
1	D	3073	VAL	N-CA-C	5.98	117.10	108.48
1	D	3049	ILE	N-CA-C	5.94	117.13	108.58
1	B	1428	HIS	N-CA-C	-5.91	105.91	113.23
1	C	2428	HIS	N-CA-C	-5.83	106.00	113.23
1	A	428	HIS	N-CA-C	-5.75	105.77	112.89
1	B	1075	TRP	N-CA-C	5.69	118.84	109.85
1	A	72	GLU	N-CA-C	-5.67	99.66	108.90
1	B	1072	GLU	N-CA-C	-5.58	99.80	108.90
1	D	3376	ASP	CB-CA-C	-5.52	102.21	110.88
1	C	2362	THR	N-CA-C	-5.49	105.21	111.14
1	B	1200	ASP	N-CA-C	-5.48	105.31	111.28
1	B	1197	SER	N-CA-C	5.46	119.78	113.18
1	D	3422	GLY	CA-C-N	5.46	125.36	119.85
1	D	3422	GLY	C-N-CA	5.46	125.36	119.85
1	A	73	VAL	N-CA-C	5.45	116.57	108.46
1	A	49	ILE	N-CA-C	5.42	116.39	108.58
1	C	2278	VAL	CB-CA-C	-5.36	105.70	111.59
1	B	1155	GLU	N-CA-C	5.31	117.88	111.40
1	D	3417	GLY	N-CA-C	-5.28	107.93	115.64
1	B	1362	THR	N-CA-C	-5.25	105.64	111.36
1	B	1338	LEU	N-CA-C	5.23	117.25	108.73
1	D	3129	ASP	N-CA-C	5.12	118.08	110.14
1	C	2207	ASP	N-CA-C	-5.10	107.01	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	VAL	N-CA-C	-5.09	105.54	110.42
1	C	2200	ASP	N-CA-C	-5.05	105.77	111.28
1	C	2422	GLY	CA-C-N	5.02	124.92	119.85
1	C	2422	GLY	C-N-CA	5.02	124.92	119.85

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	3320	0	3343	273	0
1	B	3320	0	3343	275	0
1	C	3320	0	3343	284	0
1	D	3320	0	3343	284	1
2	A	44	0	27	2	0
2	B	44	0	27	2	0
2	C	44	0	27	2	0
2	D	44	0	27	2	0
3	A	19	0	11	0	0
3	B	19	0	11	0	0
3	C	19	0	10	0	0
3	D	19	0	10	0	0
4	A	79	0	0	2	0
4	B	68	0	0	2	0
4	C	54	0	0	1	0
4	D	51	0	0	2	0
All	All	13784	0	13522	1021	1

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 38.

All (1021) 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:2120:LYS:H	1:C:2120:LYS:HD2	1.13	1.10
1:C:2060:ALA:HB1	1:C:2091:ILE:HD11	1.34	1.08
1:D:3420:ILE:HG23	1:D:3421:ASN:OD1	1.56	1.05
1:A:430:ARG:HA	1:B:1430:ARG:HG2	1.38	1.03
1:D:3120:LYS:H	1:D:3120:LYS:HD2	1.20	1.02
1:D:3060:ALA:HB1	1:D:3091:ILE:HD11	1.38	1.02
1:A:120:LYS:H	1:A:120:LYS:HD2	1.21	1.02
1:C:2120:LYS:H	1:C:2120:LYS:CD	1.72	1.01
1:B:1060:ALA:HB1	1:B:1091:ILE:HD11	1.38	1.00
1:B:1120:LYS:H	1:B:1120:LYS:HD2	1.23	1.00
1:A:430:ARG:HG2	1:B:1430:ARG:HA	1.43	1.00
1:A:169:ASN:HB2	1:A:171:ILE:HD11	1.43	0.99
1:C:2277:CYS:HB2	1:D:3416:LEU:HD21	1.42	0.98
1:B:1214:VAL:H	1:B:1269:ASN:HD22	1.01	0.97
1:B:1408:LEU:C	1:B:1420:ILE:HD11	1.90	0.96
1:C:2420:ILE:HG23	1:C:2421:ASN:OD1	1.65	0.96
1:A:60:ALA:HB1	1:A:91:ILE:HD11	1.46	0.96
1:C:2214:VAL:H	1:C:2269:ASN:HD22	0.97	0.96
1:C:2408:LEU:C	1:C:2420:ILE:HD11	1.90	0.95
1:A:408:LEU:C	1:A:420:ILE:HD11	1.92	0.95
1:D:3169:ASN:HB2	1:D:3171:ILE:HD11	1.49	0.94
1:A:308:LYS:H	1:A:308:LYS:HD2	1.28	0.94
1:C:2308:LYS:H	1:C:2308:LYS:HD2	1.32	0.94
1:A:126:MET:HE3	1:A:150:ARG:HB3	1.48	0.93
1:B:1408:LEU:O	1:B:1420:ILE:HD11	1.66	0.93
1:D:3120:LYS:H	1:D:3120:LYS:CD	1.77	0.93
1:D:3409:THR:O	1:D:3420:ILE:CD1	2.17	0.93
1:D:3126:MET:HE3	1:D:3150:ARG:HB3	1.48	0.92
1:D:3308:LYS:H	1:D:3308:LYS:HD2	1.32	0.92
1:B:1169:ASN:HB2	1:B:1171:ILE:HD11	1.51	0.91
1:D:3214:VAL:H	1:D:3269:ASN:HD22	0.96	0.91
1:B:1120:LYS:H	1:B:1120:LYS:CD	1.77	0.91
1:A:120:LYS:H	1:A:120:LYS:CD	1.79	0.90
1:A:408:LEU:O	1:A:420:ILE:HD11	1.70	0.90
1:C:2187:LYS:HD3	1:D:3430:ARG:HH12	1.33	0.90
1:A:420:ILE:HG23	1:A:421:ASN:OD1	1.72	0.89
1:C:2169:ASN:HB2	1:C:2171:ILE:HD11	1.55	0.89
1:A:214:VAL:H	1:A:269:ASN:HD22	0.93	0.89
1:D:3214:VAL:H	1:D:3269:ASN:ND2	1.72	0.88
1:D:3408:LEU:HB3	1:D:3420:ILE:HD12	1.54	0.88
1:B:1420:ILE:HG23	1:B:1421:ASN:OD1	1.72	0.88
1:D:3387:LYS:O	1:D:3391:GLU:HG3	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3408:LEU:C	1:D:3420:ILE:HD11	1.99	0.87
1:C:2214:VAL:H	1:C:2269:ASN:ND2	1.72	0.87
1:B:1308:LYS:H	1:B:1308:LYS:HD2	1.39	0.87
1:C:2120:LYS:HD2	1:C:2120:LYS:N	1.90	0.86
1:D:3413:ALA:HB2	1:D:3420:ILE:CD1	2.05	0.86
1:A:48:ARG:HD3	1:A:121:ASP:OD2	1.76	0.86
1:A:387:LYS:O	1:A:391:GLU:HG3	1.76	0.85
1:D:3413:ALA:HB2	1:D:3420:ILE:HD12	1.57	0.85
1:A:214:VAL:H	1:A:269:ASN:ND2	1.75	0.85
1:C:2428:HIS:HB3	1:D:3384:PHE:HZ	1.39	0.85
1:C:2126:MET:HE3	1:C:2150:ARG:HB3	1.58	0.85
1:D:3409:THR:O	1:D:3420:ILE:HD13	1.78	0.84
1:D:3409:THR:C	1:D:3420:ILE:HD11	2.02	0.83
1:C:2060:ALA:CB	1:C:2091:ILE:HD11	2.08	0.83
1:A:430:ARG:CA	1:B:1430:ARG:HG2	2.07	0.83
1:A:126:MET:CE	1:A:150:ARG:HB3	2.09	0.83
1:C:2428:HIS:HB3	1:D:3384:PHE:CZ	2.13	0.83
1:C:2408:LEU:O	1:C:2420:ILE:HD11	1.78	0.83
1:C:2308:LYS:O	1:C:2312:GLU:HG2	1.77	0.83
1:A:48:ARG:HD3	1:A:121:ASP:CG	2.03	0.83
1:C:2416:LEU:HD21	1:D:3277:CYS:HB2	1.60	0.83
1:D:3048:ARG:HD3	1:D:3121:ASP:CG	2.05	0.82
1:A:169:ASN:HB2	1:A:171:ILE:CD1	2.10	0.82
1:D:3120:LYS:HD2	1:D:3120:LYS:N	1.94	0.82
1:B:1060:ALA:CB	1:B:1091:ILE:HD11	2.09	0.81
1:B:1214:VAL:H	1:B:1269:ASN:ND2	1.77	0.81
1:B:1120:LYS:HD2	1:B:1120:LYS:N	1.95	0.81
1:D:3060:ALA:CB	1:D:3091:ILE:HD11	2.09	0.81
1:C:2007:LYS:HG2	1:C:2101:TRP:CZ3	2.16	0.81
1:A:277:CYS:HB2	1:B:1416:LEU:HD21	1.63	0.80
1:C:2225:LYS:NZ	1:C:2250:GLN:HE22	1.79	0.80
1:B:1387:LYS:O	1:B:1391:GLU:HG3	1.81	0.80
1:C:2430:ARG:HA	1:D:3430:ARG:HG2	1.64	0.79
1:C:2430:ARG:HG2	1:D:3430:ARG:HA	1.61	0.79
1:C:2387:LYS:O	1:C:2391:GLU:HG3	1.81	0.79
1:D:3409:THR:N	1:D:3420:ILE:HD11	1.96	0.79
1:A:7:LYS:HG2	1:A:101:TRP:CZ3	2.18	0.79
1:D:3409:THR:C	1:D:3420:ILE:CD1	2.55	0.79
1:D:3126:MET:CE	1:D:3150:ARG:HB3	2.13	0.79
1:A:430:ARG:CG	1:B:1430:ARG:HG2	2.13	0.78
1:B:1150:ARG:HD2	1:B:1372:TRP:HA	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ARG:HG2	1:B:1430:ARG:CG	2.14	0.78
1:B:1126:MET:HE3	1:B:1150:ARG:HB3	1.64	0.78
1:C:2048:ARG:HD3	1:C:2121:ASP:CG	2.09	0.78
1:A:120:LYS:HD2	1:A:120:LYS:N	1.99	0.78
1:A:225:LYS:NZ	1:A:250:GLN:HE22	1.82	0.78
1:A:430:ARG:HG2	1:B:1430:ARG:HG2	1.64	0.78
1:A:153:SER:HB3	1:A:364:GLN:NE2	1.99	0.78
1:A:398:LEU:HD23	1:A:405:LEU:HD22	1.67	0.77
1:B:1143:PRO:HA	1:B:1146:LEU:HD22	1.67	0.77
1:A:143:PRO:HA	1:A:146:LEU:HD22	1.65	0.76
1:B:1353:PRO:HB2	1:D:3209:MET:HB2	1.66	0.76
1:C:2028:MET:HB3	1:C:2358:SER:HB2	1.67	0.76
1:A:153:SER:HB3	1:A:364:GLN:HE21	1.51	0.76
1:B:1126:MET:CE	1:B:1150:ARG:HB3	2.16	0.76
1:D:3010:ASP:HB3	1:D:3013:LEU:HD22	1.68	0.75
1:D:3150:ARG:HD2	1:D:3372:TRP:HA	1.69	0.75
1:A:225:LYS:HZ1	1:A:250:GLN:HE22	1.32	0.75
1:C:2178:ASN:HD21	1:C:2181:ASP:CG	1.94	0.75
1:A:214:VAL:N	1:A:269:ASN:HD22	1.78	0.74
1:A:430:ARG:HG2	1:B:1430:ARG:CA	2.17	0.74
1:D:3007:LYS:HG2	1:D:3101:TRP:CZ3	2.22	0.74
1:C:2409:THR:OG1	1:C:2412:GLN:HG3	1.87	0.74
1:D:3153:SER:HB3	1:D:3364:GLN:NE2	2.03	0.74
1:A:10:ASP:HB3	1:A:13:LEU:HD22	1.69	0.74
1:C:2143:PRO:HA	1:C:2146:LEU:HD22	1.70	0.74
1:C:2153:SER:HB3	1:C:2364:GLN:NE2	2.02	0.74
1:D:3225:LYS:NZ	1:D:3250:GLN:HE22	1.85	0.74
1:D:3408:LEU:HB3	1:D:3420:ILE:CD1	2.17	0.74
1:B:1048:ARG:HD3	1:B:1121:ASP:CG	2.14	0.73
1:B:1169:ASN:HB2	1:B:1171:ILE:CD1	2.16	0.73
1:C:2153:SER:HB3	1:C:2364:GLN:HE21	1.53	0.73
1:A:140:THR:OG1	1:A:141:LYS:HD2	1.88	0.73
1:D:3048:ARG:HD3	1:D:3121:ASP:OD2	1.89	0.73
1:A:27:GLU:O	1:A:29:PRO:HD3	1.89	0.72
1:C:2409:THR:C	1:C:2420:ILE:HD13	2.14	0.72
1:D:3027:GLU:O	1:D:3029:PRO:HD3	1.89	0.72
1:D:3153:SER:HB3	1:D:3364:GLN:HE21	1.54	0.72
1:D:3178:ASN:HD21	1:D:3181:ASP:CG	1.97	0.72
1:D:3362:THR:O	1:D:3366:MET:HG3	1.90	0.72
1:D:3180:ASN:HA	1:D:3185:LYS:HD2	1.69	0.72
1:A:60:ALA:CB	1:A:91:ILE:HD11	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3409:THR:O	1:D:3420:ILE:HD11	1.88	0.71
1:C:2430:ARG:HH12	1:D:3187:LYS:HD3	1.53	0.71
1:B:1010:ASP:HB3	1:B:1013:LEU:HD22	1.72	0.71
1:C:2140:THR:OG1	1:C:2141:LYS:HD2	1.89	0.71
1:B:1153:SER:HB3	1:B:1364:GLN:NE2	2.06	0.71
1:C:2150:ARG:HD2	1:C:2372:TRP:HA	1.71	0.71
1:B:1153:SER:HB3	1:B:1364:GLN:HE21	1.55	0.71
1:A:339:ALA:O	1:A:342:ARG:HB2	1.91	0.71
1:B:1362:THR:O	1:B:1366:MET:HG3	1.90	0.71
1:C:2126:MET:CE	1:C:2150:ARG:HB3	2.21	0.71
1:B:1408:LEU:C	1:B:1420:ILE:CD1	2.64	0.70
1:C:2010:ASP:HB3	1:C:2013:LEU:HD22	1.73	0.70
1:B:1409:THR:C	1:B:1420:ILE:HD13	2.17	0.70
1:C:2430:ARG:NH1	1:C:2430:ARG:HB2	2.06	0.70
1:A:150:ARG:HD2	1:A:372:TRP:HA	1.72	0.70
1:D:3169:ASN:HB2	1:D:3171:ILE:CD1	2.21	0.70
1:D:3143:PRO:HA	1:D:3146:LEU:HD22	1.72	0.70
1:C:2277:CYS:HB2	1:D:3416:LEU:CD2	2.19	0.70
1:D:3140:THR:OG1	1:D:3141:LYS:HD2	1.92	0.70
1:A:430:ARG:HA	1:B:1430:ARG:CG	2.17	0.70
1:B:1178:ASN:HD21	1:B:1181:ASP:CG	2.00	0.70
1:C:2409:THR:C	1:C:2420:ILE:CD1	2.64	0.70
1:A:3:LYS:HE3	1:A:74:ARG:HH12	1.56	0.69
1:C:2398:LEU:HD23	1:C:2405:LEU:HD22	1.73	0.69
1:B:1072:GLU:OE2	1:B:1120:LYS:HD3	1.93	0.69
1:A:362:THR:O	1:A:366:MET:HG3	1.93	0.69
1:A:320:ILE:HG13	1:C:2023:ILE:HD11	1.75	0.69
1:C:2180:ASN:HA	1:C:2185:LYS:HD2	1.74	0.69
1:C:2418:MET:SD	1:C:2424:PHE:HB3	2.32	0.69
1:B:1409:THR:C	1:B:1420:ILE:CD1	2.65	0.69
1:D:3065:THR:O	1:D:3069:LEU:HD13	1.92	0.69
1:C:2363:ASN:ND2	1:C:2393:VAL:HG21	2.08	0.69
1:D:3409:THR:OG1	1:D:3412:GLN:HG3	1.93	0.69
1:D:3398:LEU:HD23	1:D:3405:LEU:HD22	1.74	0.69
1:A:409:THR:C	1:A:420:ILE:CD1	2.67	0.68
1:C:2339:ALA:O	1:C:2342:ARG:HB2	1.93	0.68
1:C:2021:LEU:HD21	1:C:2060:ALA:HB3	1.74	0.68
1:D:3334:ARG:HD2	4:D:5031:HOH:O	1.92	0.68
1:C:2169:ASN:HB2	1:C:2171:ILE:CD1	2.24	0.68
1:C:2408:LEU:HB3	1:C:2420:ILE:HD12	1.76	0.68
1:A:21:LEU:HD21	1:A:60:ALA:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3430:ARG:NH1	1:D:3430:ARG:HB2	2.08	0.68
1:B:1007:LYS:HG2	1:B:1101:TRP:CZ3	2.28	0.68
1:B:1409:THR:H	1:B:1412:GLN:HE21	1.42	0.67
1:C:2247:ASN:ND2	1:D:3431:TYR:HE2	1.92	0.67
1:D:3363:ASN:ND2	1:D:3393:VAL:HG21	2.09	0.67
1:A:72:GLU:OE2	1:A:120:LYS:HD3	1.94	0.67
1:B:1180:ASN:HA	1:B:1185:LYS:HD2	1.76	0.67
1:B:1409:THR:OG1	1:B:1412:GLN:HG3	1.93	0.67
1:A:178:ASN:HD21	1:A:181:ASP:CG	2.02	0.67
1:A:408:LEU:C	1:A:420:ILE:CD1	2.67	0.67
1:A:23:ILE:HD11	1:C:2320:ILE:HG13	1.75	0.67
1:D:3339:ALA:O	1:D:3342:ARG:HB2	1.95	0.67
1:D:3418:MET:HB2	1:D:3424:PHE:HD1	1.60	0.67
1:A:409:THR:C	1:A:420:ILE:HD13	2.20	0.67
1:C:2011:ILE:HA	1:C:2089:ALA:HB1	1.77	0.67
1:C:2027:GLU:O	1:C:2029:PRO:HD3	1.95	0.67
1:A:430:ARG:NH1	1:A:430:ARG:HB2	2.10	0.66
1:B:1408:LEU:HB3	1:B:1420:ILE:HD12	1.77	0.66
1:A:187:LYS:HD3	1:B:1430:ARG:HH12	1.59	0.66
1:B:1419:PRO:HG2	1:B:1422:GLY:HA3	1.77	0.66
1:A:33:ARG:O	1:A:37:MET:HG3	1.95	0.66
1:A:408:LEU:HB3	1:A:420:ILE:HD12	1.77	0.66
1:A:409:THR:OG1	1:A:412:GLN:HG3	1.96	0.66
1:A:416:LEU:HD21	1:B:1277:CYS:HB2	1.77	0.66
1:A:137:LEU:O	1:A:141:LYS:HB2	1.95	0.66
1:B:1019:LYS:O	1:B:1023:ILE:HG13	1.96	0.66
1:C:2384:PHE:CZ	1:D:3428:HIS:HB3	2.31	0.66
1:A:428:HIS:HB3	1:B:1384:PHE:CZ	2.30	0.66
1:A:430:ARG:CG	1:B:1430:ARG:HA	2.21	0.66
1:B:1225:LYS:NZ	1:B:1250:GLN:HE22	1.93	0.66
1:A:428:HIS:HB3	1:B:1384:PHE:HZ	1.61	0.65
1:D:3072:GLU:OE2	1:D:3120:LYS:HD3	1.95	0.65
1:C:2277:CYS:CB	1:D:3416:LEU:HD21	2.23	0.65
1:A:3:LYS:HE2	1:A:74:ARG:NH2	2.12	0.65
1:A:180:ASN:HA	1:A:185:LYS:HD2	1.78	0.65
1:B:1021:LEU:HD21	1:B:1060:ALA:HB3	1.77	0.65
1:C:2430:ARG:HG2	1:D:3430:ARG:HG2	1.77	0.65
1:C:2418:MET:HB2	1:C:2424:PHE:HD1	1.61	0.65
1:B:1339:ALA:O	1:B:1342:ARG:HB2	1.97	0.65
1:D:3419:PRO:HG2	1:D:3422:GLY:HA3	1.78	0.65
1:B:1137:LEU:O	1:B:1141:LYS:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1398:LEU:HD23	1:B:1405:LEU:HD22	1.77	0.64
1:A:295:VAL:HG12	1:A:305:ILE:HD13	1.79	0.64
1:C:2003:LYS:HE3	1:C:2074:ARG:HH12	1.63	0.64
1:D:3011:ILE:HA	1:D:3089:ALA:HB1	1.79	0.64
1:D:3409:THR:H	1:D:3412:GLN:HE21	1.43	0.64
1:C:2408:LEU:C	1:C:2420:ILE:CD1	2.68	0.64
1:A:11:ILE:HA	1:A:89:ALA:HB1	1.80	0.64
1:B:1387:LYS:HE2	1:B:1425:LYS:O	1.97	0.64
1:A:409:THR:H	1:A:412:GLN:HE21	1.46	0.64
1:B:1140:THR:OG1	1:B:1141:LYS:HD2	1.97	0.64
1:B:1209:MET:HB2	1:D:3353:PRO:HB2	1.78	0.64
1:D:3225:LYS:HZ1	1:D:3250:GLN:HE22	1.44	0.64
1:B:1345:ASN:O	1:B:1349:ALA:HB3	1.98	0.64
1:C:2072:GLU:OE2	1:C:2120:LYS:HD3	1.97	0.63
1:C:2225:LYS:HZ1	1:C:2250:GLN:HE22	1.45	0.63
1:D:3425:LYS:HE2	1:D:3429:TYR:CE1	2.33	0.63
1:D:3003:LYS:HE3	1:D:3074:ARG:HH12	1.62	0.63
1:D:3019:LYS:O	1:D:3023:ILE:HG13	1.98	0.63
1:D:3045:LYS:HD3	1:D:3046:GLY:N	2.13	0.63
1:A:408:LEU:HA	1:A:412:GLN:NE2	2.13	0.63
1:B:1011:ILE:HA	1:B:1089:ALA:HB1	1.80	0.63
1:C:2387:LYS:HE2	1:C:2425:LYS:O	1.98	0.63
1:C:2048:ARG:HD3	1:C:2121:ASP:OD2	1.99	0.63
1:B:1370:GLU:HB3	1:B:1378:TYR:CE1	2.34	0.63
1:C:2384:PHE:HZ	1:D:3428:HIS:HB3	1.64	0.62
1:C:2428:HIS:ND1	1:C:2428:HIS:N	2.47	0.62
1:D:3215:ALA:HB1	1:D:3231:LEU:HD13	1.81	0.62
1:A:418:MET:HB2	1:A:424:PHE:HD1	1.62	0.62
1:D:3240:ILE:O	1:D:3258:VAL:HA	1.98	0.62
1:B:1065:THR:O	1:B:1069:LEU:HD13	1.98	0.62
1:C:2019:LYS:O	1:C:2023:ILE:HG13	1.98	0.62
1:C:2308:LYS:H	1:C:2308:LYS:CD	2.10	0.62
1:C:2151:GLY:HA3	1:C:2371:LEU:HG	1.82	0.62
1:B:1430:ARG:HB2	1:B:1430:ARG:NH1	2.14	0.62
1:D:3137:LEU:O	1:D:3141:LYS:HB2	1.99	0.62
1:A:345:ASN:O	1:A:349:ALA:HB3	2.00	0.62
1:C:2125:ASN:HA	1:C:2148:GLY:O	1.99	0.62
1:C:2419:PRO:HG2	1:C:2422:GLY:HA3	1.81	0.62
1:A:418:MET:SD	1:A:424:PHE:HB3	2.39	0.62
1:A:419:PRO:HG2	1:A:422:GLY:HA3	1.80	0.62
1:A:430:ARG:O	1:B:1430:ARG:HD2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1003:LYS:HG3	1:B:1004:LEU:N	2.15	0.62
1:D:3418:MET:SD	1:D:3424:PHE:HB3	2.40	0.61
1:B:1418:MET:SD	1:B:1424:PHE:HB3	2.40	0.61
1:B:1418:MET:HB2	1:B:1424:PHE:HD1	1.65	0.61
1:B:1308:LYS:O	1:B:1312:GLU:HG2	2.00	0.61
1:D:3003:LYS:HE2	1:D:3074:ARG:NH2	2.15	0.61
1:C:2033:ARG:O	1:C:2037:MET:HG3	2.00	0.61
1:A:3:LYS:HE2	1:A:74:ARG:HH22	1.66	0.61
1:D:3185:LYS:HD3	1:D:3185:LYS:C	2.25	0.61
1:B:1353:PRO:HG2	1:D:3209:MET:SD	2.41	0.61
1:A:259:THR:HA	1:B:1404:LYS:HB2	1.83	0.60
1:B:1225:LYS:HZ1	1:B:1250:GLN:HE22	1.48	0.60
1:B:1240:ILE:O	1:B:1258:VAL:HA	2.01	0.60
1:A:373:THR:C	1:A:375:PRO:HD2	2.26	0.60
1:B:1048:ARG:HD2	1:B:1119:PHE:HB2	1.82	0.60
1:C:2048:ARG:HD2	1:C:2119:PHE:HB2	1.84	0.60
1:D:3033:ARG:O	1:D:3037:MET:HG3	2.00	0.60
1:D:3214:VAL:N	1:D:3269:ASN:HD22	1.82	0.60
1:B:1125:ASN:HA	1:B:1148:GLY:O	2.01	0.60
1:B:1428:HIS:ND1	1:B:1428:HIS:N	2.50	0.60
1:D:3308:LYS:H	1:D:3308:LYS:CD	2.11	0.60
1:A:91:ILE:HD13	1:A:91:ILE:N	2.17	0.60
1:A:185:LYS:C	1:A:185:LYS:HD3	2.27	0.60
1:B:1028:MET:HB3	1:B:1358:SER:HB2	1.84	0.60
1:C:2259:THR:HA	1:D:3404:LYS:HB2	1.83	0.60
1:C:2028:MET:HE2	1:C:2358:SER:HB2	1.83	0.60
1:C:2065:THR:O	1:C:2069:LEU:HD13	2.02	0.60
1:C:2185:LYS:HD3	1:C:2185:LYS:C	2.27	0.59
1:D:3048:ARG:HD2	1:D:3119:PHE:HB2	1.84	0.59
1:B:1021:LEU:CD2	1:B:1060:ALA:HB3	2.31	0.59
1:C:2409:THR:H	1:C:2412:GLN:HE21	1.49	0.59
1:B:1419:PRO:HG2	1:B:1422:GLY:C	2.28	0.59
1:C:2167:MET:SD	1:C:2381:GLY:HA2	2.42	0.59
1:A:154:GLU:O	1:A:179:VAL:HB	2.03	0.59
1:B:1214:VAL:N	1:B:1269:ASN:HD22	1.86	0.59
1:C:2166:MET:HA	1:C:2171:ILE:HD12	1.85	0.59
1:A:428:HIS:ND1	1:A:428:HIS:N	2.50	0.59
1:B:1363:ASN:ND2	1:B:1393:VAL:HG21	2.18	0.59
1:C:2426:PRO:HB2	1:C:2428:HIS:CE1	2.37	0.59
1:D:3387:LYS:HE2	1:D:3425:LYS:O	2.02	0.59
1:D:3169:ASN:HD22	1:D:3171:ILE:CD1	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ARG:CB	1:B:1430:ARG:HG2	2.33	0.58
1:D:3091:ILE:HD13	1:D:3091:ILE:N	2.16	0.58
1:D:3409:THR:CA	1:D:3420:ILE:HD11	2.32	0.58
1:B:1167:MET:SD	1:B:1381:GLY:HA2	2.43	0.58
1:B:1027:GLU:O	1:B:1029:PRO:HD3	2.02	0.58
1:B:1209:MET:SD	1:D:3353:PRO:HG2	2.44	0.58
1:B:1308:LYS:H	1:B:1308:LYS:CD	2.12	0.58
1:B:1418:MET:CG	1:B:1424:PHE:HB3	2.33	0.58
1:C:2187:LYS:HD3	1:D:3430:ARG:NH1	2.12	0.58
1:A:125:ASN:HA	1:A:148:GLY:O	2.04	0.58
1:A:308:LYS:O	1:A:312:GLU:HG2	2.04	0.58
1:B:1409:THR:N	1:B:1412:GLN:HE21	2.01	0.58
1:D:3419:PRO:HG2	1:D:3422:GLY:C	2.28	0.58
1:B:1051:GLY:HA2	1:B:1128:LEU:O	2.03	0.58
1:B:1408:LEU:HA	1:B:1412:GLN:NE2	2.18	0.58
1:C:2225:LYS:NZ	1:C:2250:GLN:NE2	2.50	0.58
1:A:21:LEU:CD2	1:A:60:ALA:HB3	2.33	0.58
1:A:430:ARG:HH12	1:B:1187:LYS:HD3	1.67	0.58
1:C:2408:LEU:HA	1:C:2412:GLN:NE2	2.18	0.57
1:D:3295:VAL:HG12	1:D:3305:ILE:HD13	1.86	0.57
1:C:2021:LEU:CD2	1:C:2060:ALA:HB3	2.34	0.57
1:B:1137:LEU:HD12	1:B:1141:LYS:HD3	1.87	0.57
1:B:1334:ARG:O	1:B:1335:ILE:HD13	2.03	0.57
1:D:3418:MET:CG	1:D:3424:PHE:HB3	2.35	0.57
1:A:51:GLY:HA2	1:A:128:LEU:O	2.04	0.57
1:B:1033:ARG:HD2	1:B:1037:MET:HG3	1.86	0.57
1:C:2247:ASN:HD21	1:D:3431:TYR:HE2	1.52	0.57
1:D:3177:ILE:HG13	1:D:3371:LEU:HD21	1.87	0.57
1:D:3178:ASN:ND2	1:D:3181:ASP:HB2	2.20	0.57
1:C:2137:LEU:O	1:C:2141:LYS:HB2	2.05	0.57
1:C:2430:ARG:HG2	1:D:3430:ARG:CG	2.34	0.57
1:C:2430:ARG:HB2	1:C:2430:ARG:CZ	2.34	0.57
1:D:3424:PHE:N	1:D:3424:PHE:CD2	2.73	0.57
1:C:2091:ILE:HD13	1:C:2091:ILE:N	2.19	0.57
1:C:2362:THR:O	1:C:2366:MET:HG3	2.05	0.57
1:D:3419:PRO:HG2	1:D:3422:GLY:CA	2.35	0.57
1:A:93:LYS:NZ	4:A:5155:HOH:O	2.37	0.57
1:B:1247:ASN:O	1:B:1250:GLN:HB2	2.05	0.57
1:C:2003:LYS:HE2	1:C:2074:ARG:NH2	2.19	0.57
1:C:2240:ILE:O	1:C:2258:VAL:HA	2.05	0.57
1:C:2418:MET:CG	1:C:2424:PHE:HB3	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3408:LEU:HA	1:D:3412:GLN:NE2	2.20	0.57
1:B:1178:ASN:ND2	1:B:1181:ASP:HB2	2.21	0.56
1:B:1419:PRO:HG2	1:B:1422:GLY:CA	2.35	0.56
1:B:1278:VAL:HG12	1:B:1303:VAL:CG2	2.34	0.56
1:C:2169:ASN:HD22	1:C:2171:ILE:CD1	2.18	0.56
1:D:3138:ILE:HG22	1:D:3146:LEU:HD13	1.86	0.56
1:D:3428:HIS:ND1	1:D:3428:HIS:N	2.53	0.56
1:A:278:VAL:HG12	1:A:303:VAL:CG2	2.36	0.56
1:A:387:LYS:HE2	1:A:425:LYS:O	2.05	0.56
1:A:419:PRO:HG2	1:A:422:GLY:C	2.30	0.56
1:B:1299:GLY:O	1:B:1343:LEU:HD11	2.05	0.56
1:D:3278:VAL:HG12	1:D:3303:VAL:CG2	2.36	0.56
1:A:308:LYS:H	1:A:308:LYS:CD	2.09	0.56
1:B:1033:ARG:O	1:B:1037:MET:HG3	2.06	0.56
1:C:2409:THR:N	1:C:2420:ILE:HD11	2.20	0.56
1:C:2430:ARG:CG	1:D:3430:ARG:HG2	2.35	0.56
1:C:2431:TYR:HE2	1:D:3247:ASN:HD21	1.52	0.56
1:A:138:ILE:HG22	1:A:146:LEU:HD13	1.87	0.56
1:A:258:VAL:HB	1:B:1403:VAL:HG13	1.88	0.56
1:B:1424:PHE:CD2	1:B:1424:PHE:N	2.73	0.56
1:C:2278:VAL:HG12	1:C:2303:VAL:CG2	2.36	0.56
1:C:2409:THR:CA	1:C:2420:ILE:HD11	2.36	0.56
1:C:2424:PHE:N	1:C:2424:PHE:CD2	2.73	0.56
1:D:3003:LYS:HG3	1:D:3004:LEU:N	2.21	0.56
1:D:3137:LEU:HA	1:D:3141:LYS:HD3	1.87	0.56
1:B:1003:LYS:HE2	1:B:1074:ARG:NH2	2.21	0.56
1:C:2186:SER:O	1:C:2190:ASN:HB2	2.06	0.56
1:C:2419:PRO:HB2	1:C:2422:GLY:H	1.71	0.56
1:C:2430:ARG:HG2	1:D:3430:ARG:CA	2.34	0.56
1:A:142:HIS:HA	1:A:144:GLN:OE1	2.06	0.56
1:B:1091:ILE:HD13	1:B:1091:ILE:N	2.21	0.56
1:B:1119:PHE:CD1	1:B:1119:PHE:N	2.74	0.55
1:C:2430:ARG:CA	1:D:3430:ARG:HG2	2.34	0.55
1:D:3003:LYS:HE2	1:D:3074:ARG:HH22	1.70	0.55
1:B:1048:ARG:HD3	1:B:1121:ASP:OD2	2.05	0.55
1:A:48:ARG:HD2	1:A:119:PHE:HB2	1.88	0.55
1:D:3151:GLY:HA3	1:D:3371:LEU:HG	1.88	0.55
1:D:3409:THR:C	1:D:3420:ILE:HD13	2.28	0.55
1:A:419:PRO:HB2	1:A:422:GLY:H	1.71	0.55
1:D:3119:PHE:N	1:D:3119:PHE:CD1	2.74	0.55
1:B:1091:ILE:HB	1:B:1098:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2409:THR:N	1:C:2412:GLN:HE21	2.04	0.55
1:D:3125:ASN:HA	1:D:3148:GLY:O	2.06	0.55
1:D:3373:THR:C	1:D:3375:PRO:HD2	2.32	0.55
1:A:320:ILE:HG13	1:C:2023:ILE:CD1	2.37	0.55
1:D:3406:THR:HG22	1:D:3407:LYS:N	2.22	0.55
1:A:370:GLU:HB3	1:A:378:TYR:CE1	2.42	0.55
1:B:1154:GLU:O	1:B:1179:VAL:HB	2.07	0.55
1:D:3028:MET:HB3	1:D:3358:SER:HB2	1.89	0.55
1:A:425:LYS:HE2	1:A:429:TYR:CE1	2.41	0.54
1:A:299:GLY:O	1:A:343:LEU:HD11	2.07	0.54
1:A:398:LEU:CD2	1:A:405:LEU:HD22	2.36	0.54
1:A:419:PRO:HG2	1:A:422:GLY:CA	2.37	0.54
1:B:1273:THR:OG1	1:B:1297:ASN:HB2	2.06	0.54
1:A:151:GLY:HA3	1:A:371:LEU:HG	1.88	0.54
1:A:374:HIS:N	1:A:375:PRO:CD	2.70	0.54
1:A:409:THR:N	1:A:412:GLN:HE21	2.05	0.54
1:A:3:LYS:HE3	1:A:74:ARG:NH1	2.22	0.54
1:A:17:GLY:O	1:A:20:ALA:HB3	2.08	0.54
1:D:3257:GLU:HB3	4:D:5184:HOH:O	2.06	0.54
1:A:45:LYS:HD3	1:A:46:GLY:N	2.22	0.54
1:C:2273:THR:OG1	1:C:2297:ASN:HB2	2.07	0.54
1:D:3021:LEU:HD21	1:D:3060:ALA:HB3	1.88	0.54
1:D:3154:GLU:HG3	1:D:3160:VAL:HG23	1.88	0.54
1:D:3374:HIS:HB3	1:D:3377:LYS:HD3	1.88	0.54
1:D:3413:ALA:CB	1:D:3420:ILE:CD1	2.83	0.54
1:A:406:THR:HG22	1:A:407:LYS:N	2.22	0.54
1:A:409:THR:CA	1:A:420:ILE:HD11	2.38	0.54
1:B:1317:LYS:HD2	1:B:1327:TYR:CZ	2.42	0.54
1:A:91:ILE:HB	1:A:98:VAL:HG21	1.89	0.54
1:B:1003:LYS:HE3	1:B:1074:ARG:HH12	1.73	0.54
1:C:2431:TYR:HE2	1:D:3247:ASN:ND2	2.06	0.54
1:B:1138:ILE:HG22	1:B:1146:LEU:HD13	1.88	0.54
1:B:1409:THR:CA	1:B:1420:ILE:HD11	2.38	0.54
1:B:1091:ILE:HG22	1:B:1096:ILE:HB	1.88	0.54
1:A:225:LYS:NZ	1:A:250:GLN:NE2	2.54	0.53
1:C:2178:ASN:ND2	1:C:2181:ASP:HB2	2.24	0.53
1:B:1425:LYS:HE2	1:B:1429:TYR:CE1	2.43	0.53
1:D:3060:ALA:O	1:D:3064:GLU:HG3	2.08	0.53
1:C:2334:ARG:O	1:C:2335:ILE:HD13	2.08	0.53
1:D:3091:ILE:HB	1:D:3098:VAL:HG21	1.90	0.53
1:D:3374:HIS:N	1:D:3375:PRO:CD	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:THR:HB	1:B:1243:ILE:HG22	1.90	0.53
1:B:1295:VAL:HG12	1:B:1305:ILE:HD13	1.91	0.53
1:C:2374:HIS:N	1:C:2375:PRO:CD	2.72	0.53
1:B:1426:PRO:HB2	1:B:1428:HIS:CE1	2.43	0.53
1:C:2003:LYS:HG3	1:C:2004:LEU:N	2.23	0.53
1:D:3055:MET:HE2	1:D:3055:MET:HA	1.90	0.53
1:A:154:GLU:HG3	1:A:160:VAL:HG23	1.90	0.53
1:A:215:ALA:HB1	1:A:231:LEU:HD13	1.90	0.53
1:B:1374:HIS:O	1:B:1377:LYS:HG3	2.09	0.53
1:D:3093:LYS:C	1:D:3095:GLY:H	2.17	0.53
1:A:384:PHE:CZ	1:B:1428:HIS:HB3	2.43	0.53
1:C:2051:GLY:HA2	1:C:2128:LEU:O	2.09	0.53
1:D:3091:ILE:HG22	1:D:3096:ILE:HB	1.91	0.53
1:D:3308:LYS:O	1:D:3312:GLU:HG2	2.08	0.53
1:C:2119:PHE:N	1:C:2119:PHE:CD1	2.77	0.53
1:C:2373:THR:C	1:C:2375:PRO:HD2	2.34	0.53
1:C:2401:LEU:HD12	1:D:3249:LEU:HD12	1.91	0.53
1:C:2406:THR:HB	1:D:3243:ILE:HG22	1.91	0.53
1:D:3021:LEU:CD2	1:D:3060:ALA:HB3	2.39	0.53
1:D:3093:LYS:C	1:D:3095:GLY:N	2.64	0.53
1:A:240:ILE:O	1:A:258:VAL:HA	2.09	0.53
1:C:2273:THR:CG2	1:C:2281:ILE:HD12	2.38	0.53
1:A:19:LYS:O	1:A:23:ILE:HG13	2.09	0.52
1:B:1312:GLU:HG3	1:B:1313:ASN:ND2	2.24	0.52
1:D:3374:HIS:O	1:D:3377:LYS:HG3	2.09	0.52
1:A:3:LYS:HG3	1:A:4:LEU:N	2.24	0.52
1:D:3185:LYS:O	1:D:3189:ASP:HB3	2.08	0.52
1:B:1374:HIS:N	1:B:1375:PRO:CD	2.71	0.52
1:D:3418:MET:HB3	1:D:3424:PHE:HB3	1.90	0.52
1:A:121:ASP:OD1	1:A:121:ASP:N	2.33	0.52
1:A:169:ASN:HD22	1:A:171:ILE:CD1	2.23	0.52
1:A:209:MET:HB2	1:C:2353:PRO:HB2	1.90	0.52
1:A:424:PHE:N	1:A:424:PHE:CD2	2.77	0.52
1:B:1185:LYS:HD3	1:B:1185:LYS:C	2.34	0.52
1:C:2299:GLY:HA3	1:C:2304:GLU:OE2	2.09	0.52
1:C:2299:GLY:O	1:C:2343:LEU:HD11	2.09	0.52
1:D:3408:LEU:C	1:D:3420:ILE:CD1	2.79	0.52
1:D:3419:PRO:HB2	1:D:3422:GLY:H	1.74	0.52
1:A:10:ASP:HB3	1:A:13:LEU:CD2	2.39	0.52
1:C:2039:SER:O	1:C:2042:LYS:HG2	2.10	0.52
1:D:3105:THR:H	1:D:3108:GLU:HG3	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3121:ASP:OD1	1:D:3121:ASP:N	2.34	0.52
1:D:3177:ILE:HG13	1:D:3371:LEU:CD2	2.38	0.52
1:D:3299:GLY:O	1:D:3343:LEU:HD11	2.09	0.52
1:D:3345:ASN:O	1:D:3349:ALA:HB3	2.10	0.52
1:D:3033:ARG:HD2	1:D:3037:MET:SD	2.50	0.52
1:A:317:LYS:HD2	1:A:327:TYR:CZ	2.44	0.52
1:A:379:PRO:HD2	1:A:383:HIS:NE2	2.25	0.52
1:B:1125:ASN:C	1:B:1125:ASN:OD1	2.52	0.52
1:B:1409:THR:O	1:B:1420:ILE:CD1	2.58	0.52
1:A:65:THR:O	1:A:69:LEU:HD13	2.09	0.52
1:D:3137:LEU:HD12	1:D:3141:LYS:HB2	1.90	0.52
1:D:3179:VAL:O	1:D:3182:SER:HB2	2.09	0.52
1:D:3184:THR:HA	1:D:3188:PHE:CD1	2.44	0.52
1:B:1184:THR:HA	1:B:1188:PHE:CD1	2.45	0.52
1:C:2033:ARG:HD2	1:C:2037:MET:HG3	1.91	0.52
1:D:3370:GLU:HB3	1:D:3378:TYR:CE1	2.45	0.52
1:D:3334:ARG:O	1:D:3335:ILE:HD13	2.11	0.51
1:D:3409:THR:N	1:D:3412:GLN:HE21	2.07	0.51
1:A:119:PHE:CD1	1:A:119:PHE:N	2.77	0.51
1:B:1137:LEU:HA	1:B:1141:LYS:HD3	1.92	0.51
1:C:2004:LEU:HD12	1:C:2111:TRP:HZ2	1.75	0.51
1:A:166:MET:HA	1:A:171:ILE:HD12	1.92	0.51
1:C:2363:ASN:HD21	1:C:2393:VAL:HG21	1.75	0.51
1:A:283:GLY:HA3	1:A:309:TRP:CE2	2.45	0.51
1:A:408:LEU:HA	1:A:412:GLN:HE21	1.76	0.51
1:B:1129:ASP:OD2	1:B:1135:THR:HG23	2.09	0.51
1:B:1283:GLY:HA3	1:B:1309:TRP:CE2	2.46	0.51
1:C:2091:ILE:HB	1:C:2098:VAL:HG21	1.92	0.51
1:C:2312:GLU:HG3	1:C:2313:ASN:ND2	2.25	0.51
1:A:23:ILE:CD1	1:C:2320:ILE:HG13	2.40	0.51
1:A:166:MET:O	1:A:171:ILE:HD12	2.11	0.51
1:A:374:HIS:O	1:A:377:LYS:HG3	2.11	0.51
1:B:1169:ASN:HD22	1:B:1171:ILE:CD1	2.24	0.51
1:B:1419:PRO:HB2	1:B:1422:GLY:H	1.75	0.51
1:B:1215:ALA:HB1	1:B:1231:LEU:HD13	1.91	0.51
1:A:418:MET:CG	1:A:424:PHE:HB3	2.41	0.51
1:D:3166:MET:HA	1:D:3171:ILE:HD12	1.93	0.51
1:C:2074:ARG:HB3	1:C:2116:THR:HB	1.92	0.51
1:C:2247:ASN:O	1:C:2250:GLN:HB2	2.11	0.51
1:C:2374:HIS:O	1:C:2377:LYS:HG3	2.10	0.51
1:C:2398:LEU:CD2	1:C:2405:LEU:HD22	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3010:ASP:HB3	1:D:3013:LEU:CD2	2.37	0.51
1:A:166:MET:HA	1:A:171:ILE:CD1	2.40	0.51
1:B:1373:THR:C	1:B:1375:PRO:HD2	2.35	0.51
1:C:2401:LEU:HD12	1:D:3249:LEU:CD1	2.41	0.51
1:B:1409:THR:N	1:B:1420:ILE:HD11	2.26	0.50
1:C:2154:GLU:HG3	1:C:2160:VAL:HG23	1.93	0.50
1:D:3021:LEU:HD23	1:D:3057:VAL:HG13	1.92	0.50
1:D:3166:MET:HA	1:D:3171:ILE:CD1	2.40	0.50
1:D:3186:SER:O	1:D:3190:ASN:HB2	2.11	0.50
1:D:3418:MET:CB	1:D:3424:PHE:HB3	2.41	0.50
1:A:426:PRO:HB2	1:A:428:HIS:CE1	2.46	0.50
1:C:2258:VAL:HB	1:D:3403:VAL:HG13	1.92	0.50
1:D:3267:GLU:O	1:D:3290:LYS:HE3	2.11	0.50
1:A:107:GLU:CD	1:A:107:GLU:H	2.20	0.50
1:A:129:ASP:OD2	1:A:135:THR:HG23	2.12	0.50
1:B:1203:LYS:HZ1	1:D:3196:GLU:HB3	1.76	0.50
1:B:1039:SER:O	1:B:1042:LYS:HG2	2.12	0.50
1:C:2003:LYS:HE3	1:C:2074:ARG:NH1	2.25	0.50
1:C:2295:VAL:HG12	1:C:2305:ILE:HD13	1.92	0.50
1:D:3051:GLY:HA2	1:D:3128:LEU:O	2.11	0.50
1:D:3398:LEU:CD2	1:D:3405:LEU:HD22	2.41	0.50
1:C:2003:LYS:HE2	1:C:2074:ARG:HH22	1.75	0.50
1:C:2279:ASP:HB3	1:C:2282:LEU:HD11	1.93	0.50
1:D:3317:LYS:HD2	1:D:3327:TYR:CZ	2.46	0.50
1:D:3352:HIS:HB2	1:D:3357:MET:SD	2.52	0.50
1:A:153:SER:CB	1:A:364:GLN:HE21	2.21	0.50
1:C:2137:LEU:HD12	1:C:2141:LYS:HB2	1.92	0.50
1:C:2225:LYS:HZ2	1:C:2250:GLN:NE2	2.08	0.50
1:D:3279:ASP:HB3	1:D:3282:LEU:HD11	1.94	0.50
1:A:125:ASN:OD1	1:A:125:ASN:C	2.54	0.50
1:A:206:THR:O	1:A:207:ASP:HB2	2.11	0.50
1:B:1003:LYS:HE2	1:B:1074:ARG:HH22	1.77	0.50
1:B:1055:MET:HE2	1:B:1055:MET:HA	1.93	0.50
1:C:2142:HIS:C	1:C:2144:GLN:OE1	2.55	0.50
1:C:2283:GLY:HA3	1:C:2309:TRP:CE2	2.46	0.50
1:D:3154:GLU:O	1:D:3179:VAL:HB	2.11	0.50
1:A:430:ARG:HG2	1:B:1430:ARG:CB	2.42	0.50
1:C:2093:LYS:C	1:C:2095:GLY:N	2.70	0.50
1:B:1004:LEU:HD12	1:B:1111:TRP:HZ2	1.76	0.50
1:B:1048:ARG:HD2	1:B:1119:PHE:CB	2.42	0.50
1:C:2055:MET:HE2	1:C:2055:MET:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2166:MET:HA	1:C:2171:ILE:CD1	2.42	0.50
1:D:3126:MET:HE1	1:D:3151:GLY:N	2.26	0.50
1:A:184:THR:HA	1:A:188:PHE:CD1	2.47	0.49
1:A:409:THR:O	1:A:410:GLU:C	2.55	0.49
1:C:2185:LYS:O	1:C:2189:ASP:HB3	2.12	0.49
1:D:3126:MET:CE	1:D:3151:GLY:N	2.75	0.49
1:A:404:LYS:HB2	1:B:1259:THR:HA	1.95	0.49
1:A:430:ARG:HD2	1:B:1430:ARG:O	2.13	0.49
1:B:1093:LYS:C	1:B:1095:GLY:N	2.67	0.49
1:B:1408:LEU:O	1:B:1420:ILE:CD1	2.51	0.49
1:C:2385:LEU:HG	1:C:2386:PRO:HD2	1.93	0.49
1:C:2419:PRO:HG2	1:C:2422:GLY:CA	2.42	0.49
1:A:247:ASN:O	1:A:250:GLN:HB2	2.12	0.49
1:C:2121:ASP:OD1	1:C:2121:ASP:N	2.33	0.49
1:C:2154:GLU:O	1:C:2179:VAL:HB	2.12	0.49
1:C:2184:THR:HA	1:C:2188:PHE:CD1	2.47	0.49
1:A:409:THR:N	1:A:420:ILE:HD11	2.25	0.49
1:B:1142:HIS:HA	1:B:1144:GLN:OE1	2.12	0.49
1:B:1398:LEU:CD2	1:B:1405:LEU:HD22	2.41	0.49
1:C:2138:ILE:HG22	1:C:2146:LEU:HD13	1.94	0.49
1:D:3363:ASN:HD21	1:D:3393:VAL:HG21	1.78	0.49
1:A:203:LYS:NZ	1:C:2196:GLU:HB3	2.28	0.49
1:C:2169:ASN:HD22	1:C:2171:ILE:HD11	1.78	0.49
1:C:2425:LYS:HE2	1:C:2429:TYR:CE1	2.47	0.49
1:B:1178:ASN:CG	1:B:1181:ASP:HB2	2.38	0.49
1:C:2409:THR:O	1:C:2420:ILE:CD1	2.61	0.49
1:D:3052:CYS:HB3	1:D:3129:ASP:OD1	2.13	0.49
1:D:3166:MET:O	1:D:3171:ILE:HD12	2.12	0.49
1:A:267:GLU:O	1:A:290:LYS:HE3	2.13	0.49
1:A:425:LYS:HZ3	1:B:1244:GLU:HG3	1.78	0.49
1:B:1401:LEU:HB2	1:B:1403:VAL:HG23	1.95	0.49
1:C:2045:LYS:HD3	1:C:2046:GLY:N	2.28	0.49
1:C:2048:ARG:HD2	1:C:2119:PHE:CB	2.43	0.49
1:A:126:MET:CE	1:A:151:GLY:N	2.76	0.49
1:B:1409:THR:O	1:B:1420:ILE:HD13	2.12	0.49
1:C:2215:ALA:HB1	1:C:2231:LEU:HD13	1.95	0.49
1:D:3225:LYS:NZ	1:D:3250:GLN:NE2	2.56	0.49
1:B:1093:LYS:C	1:B:1095:GLY:H	2.21	0.48
1:B:1385:LEU:HG	1:B:1386:PRO:HD2	1.94	0.48
1:D:3142:HIS:C	1:D:3144:GLN:OE1	2.56	0.48
1:D:3167:MET:SD	1:D:3381:GLY:HA2	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3430:ARG:HB2	1:D:3430:ARG:CZ	2.43	0.48
1:C:2430:ARG:NH1	1:C:2430:ARG:CB	2.76	0.48
1:D:3105:THR:N	1:D:3108:GLU:HG3	2.28	0.48
1:D:3272:VAL:HG22	1:D:3296:CYS:SG	2.53	0.48
1:A:127:ILE:HD11	1:A:138:ILE:HD13	1.96	0.48
1:A:247:ASN:ND2	1:B:1431:TYR:HE2	2.11	0.48
1:A:384:PHE:HZ	1:B:1428:HIS:HB3	1.78	0.48
1:C:2345:ASN:O	1:C:2349:ALA:HB3	2.13	0.48
1:C:2409:THR:O	1:C:2420:ILE:HD13	2.13	0.48
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.29	0.48
1:B:1045:LYS:HD3	1:B:1046:GLY:N	2.28	0.48
1:B:1362:THR:HB	1:B:1393:VAL:HG13	1.96	0.48
1:A:105:THR:H	1:A:108:GLU:HG3	1.78	0.48
1:C:2267:GLU:O	1:C:2290:LYS:HE3	2.14	0.48
1:C:2327:TYR:O	1:C:2334:ARG:HA	2.13	0.48
1:C:2344:VAL:HG13	1:C:2345:ASN:N	2.27	0.48
1:C:2398:LEU:HD21	1:D:3245:PRO:HA	1.96	0.48
1:D:3074:ARG:HB3	1:D:3116:THR:HB	1.96	0.48
1:D:3410:GLU:OE1	1:D:3410:GLU:HA	2.13	0.48
1:A:353:PRO:HB2	1:C:2209:MET:HB2	1.94	0.48
1:D:3039:SER:O	1:D:3042:LYS:HG2	2.12	0.48
1:D:3413:ALA:CB	1:D:3420:ILE:HD13	2.43	0.48
1:B:1013:LEU:HB3	1:B:1086:HIS:HA	1.96	0.48
1:B:1137:LEU:HD11	1:B:1142:HIS:NE2	2.29	0.48
1:B:1185:LYS:O	1:B:1189:ASP:HB3	2.14	0.48
1:B:1301:PHE:HB2	4:B:5172:HOH:O	2.13	0.48
1:C:2153:SER:CB	1:C:2364:GLN:HE21	2.24	0.48
1:A:74:ARG:HB3	1:A:116:THR:HB	1.94	0.48
1:B:1151:GLY:HA3	1:B:1371:LEU:HG	1.94	0.48
1:A:179:VAL:O	1:A:182:SER:HB2	2.13	0.48
1:A:353:PRO:HG2	1:C:2209:MET:SD	2.54	0.48
1:C:2052:CYS:HB3	1:C:2129:ASP:OD1	2.14	0.48
1:C:2142:HIS:HA	1:C:2144:GLN:OE1	2.13	0.48
1:C:2317:LYS:HD2	1:C:2327:TYR:CZ	2.49	0.48
1:D:3003:LYS:HE3	1:D:3074:ARG:NH1	2.27	0.48
1:D:3283:GLY:HA3	1:D:3309:TRP:CE2	2.49	0.48
1:C:2137:LEU:HA	1:C:2141:LYS:HD3	1.96	0.48
1:A:312:GLU:HG3	1:A:313:ASN:ND2	2.30	0.47
1:A:320:ILE:N	1:A:320:ILE:HD13	2.29	0.47
1:B:1126:MET:CE	1:B:1151:GLY:N	2.77	0.47
1:D:3418:MET:CB	1:D:3424:PHE:HD1	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:CYS:HB3	1:A:129:ASP:OD1	2.14	0.47
1:B:1418:MET:HB3	1:B:1424:PHE:HB3	1.96	0.47
1:B:1418:MET:CB	1:B:1424:PHE:HB3	2.44	0.47
1:C:2057:VAL:H	1:C:2084:GLN:NE2	2.11	0.47
1:B:1126:MET:HE1	1:B:1151:GLY:N	2.30	0.47
1:A:430:ARG:HB2	1:A:430:ARG:CZ	2.44	0.47
1:B:1206:THR:O	1:B:1207:ASP:HB2	2.12	0.47
1:B:1272:VAL:HG22	1:B:1296:CYS:SG	2.54	0.47
1:A:27:GLU:C	1:A:29:PRO:HD3	2.39	0.47
1:C:2370:GLU:HB3	1:C:2378:TYR:CE1	2.50	0.47
1:C:2419:PRO:HG2	1:C:2422:GLY:C	2.40	0.47
1:D:3129:ASP:OD2	1:D:3135:THR:HG23	2.15	0.47
1:B:1251:ALA:O	1:B:1256:TYR:HB2	2.14	0.47
1:B:1363:ASN:HD21	1:B:1393:VAL:HG21	1.80	0.47
1:A:91:ILE:HG22	1:A:96:ILE:HB	1.95	0.47
1:A:137:LEU:HD11	1:A:142:HIS:NE2	2.28	0.47
1:A:142:HIS:C	1:A:144:GLN:OE1	2.58	0.47
1:B:1121:ASP:OD1	1:B:1121:ASP:N	2.34	0.47
1:B:1137:LEU:HD12	1:B:1141:LYS:HB2	1.96	0.47
1:C:2177:ILE:HG13	1:C:2371:LEU:CD2	2.45	0.47
1:C:2418:MET:CB	1:C:2424:PHE:HB3	2.45	0.47
1:D:3058:GLU:H	1:D:3058:GLU:CD	2.22	0.47
1:D:3154:GLU:CD	1:D:3159:GLY:HA3	2.39	0.47
1:D:3178:ASN:CG	1:D:3181:ASP:HB2	2.40	0.47
1:D:3344:VAL:HG13	1:D:3345:ASN:N	2.29	0.47
1:D:3401:LEU:HB2	1:D:3403:VAL:HG23	1.95	0.47
1:B:1267:GLU:O	1:B:1290:LYS:HE3	2.14	0.47
1:C:2079:ASN:HB3	1:C:2082:SER:OG	2.14	0.47
1:D:3137:LEU:HD12	1:D:3141:LYS:HD3	1.97	0.47
1:D:3137:LEU:HD11	1:D:3142:HIS:NE2	2.29	0.47
1:B:1154:GLU:HG3	1:B:1160:VAL:HG23	1.97	0.47
1:B:1186:SER:O	1:B:1190:ASN:HB2	2.15	0.47
1:B:1299:GLY:O	1:B:1343:LEU:CD1	2.62	0.47
1:D:3169:ASN:HD22	1:D:3171:ILE:HD11	1.80	0.47
1:A:13:LEU:HB3	1:A:86:HIS:HA	1.96	0.47
1:B:1010:ASP:HB3	1:B:1013:LEU:CD2	2.44	0.47
1:C:2206:THR:O	1:C:2207:ASP:HB2	2.14	0.47
1:D:3033:ARG:HD2	1:D:3037:MET:HG3	1.97	0.47
1:D:3379:PRO:O	1:D:3380:VAL:C	2.58	0.47
1:D:3414:GLN:O	1:D:3415:TYR:C	2.58	0.47
1:D:3425:LYS:HD3	1:D:3429:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2146:LEU:HG	1:C:2173:LYS:HB2	1.96	0.46
1:C:2387:LYS:CE	1:C:2425:LYS:O	2.62	0.46
1:A:33:ARG:HD2	1:A:37:MET:SD	2.55	0.46
1:C:2232:ARG:NH1	1:C:2232:ARG:HG3	2.30	0.46
1:C:2428:HIS:CB	1:D:3384:PHE:HZ	2.18	0.46
1:D:3048:ARG:HD2	1:D:3119:PHE:CB	2.44	0.46
1:D:3281:ILE:C	1:D:3282:LEU:HD13	2.39	0.46
1:A:389:LEU:O	1:A:392:ALA:HB3	2.14	0.46
1:B:1327:TYR:O	1:B:1334:ARG:HA	2.15	0.46
1:C:2430:ARG:O	1:D:3430:ARG:HD2	2.14	0.46
1:B:1060:ALA:O	1:B:1064:GLU:HG3	2.16	0.46
1:B:1361:PHE:O	1:B:1365:VAL:HG23	2.15	0.46
1:C:2361:PHE:O	1:C:2365:VAL:HG23	2.16	0.46
1:C:2406:THR:HG22	1:C:2407:LYS:N	2.31	0.46
1:C:2430:ARG:O	1:C:2431:TYR:HB2	2.15	0.46
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.80	0.46
1:A:308:LYS:HD2	1:A:308:LYS:N	2.12	0.46
1:A:363:ASN:ND2	1:A:393:VAL:HG21	2.31	0.46
1:A:401:LEU:HB2	1:A:403:VAL:HG23	1.98	0.46
1:D:3107:GLU:CD	1:D:3107:GLU:H	2.23	0.46
1:A:201:GLY:HA2	1:A:349:ALA:HB2	1.97	0.46
1:A:387:LYS:NZ	1:A:425:LYS:O	2.49	0.46
1:B:1107:GLU:CD	1:B:1107:GLU:H	2.24	0.46
1:B:1120:LYS:H	1:B:1120:LYS:CE	2.29	0.46
1:C:2105:THR:H	1:C:2108:GLU:HG3	1.80	0.46
1:C:2137:LEU:HD11	1:C:2142:HIS:NE2	2.30	0.46
1:C:2409:THR:O	1:C:2410:GLU:C	2.57	0.46
1:D:3027:GLU:C	1:D:3029:PRO:HD3	2.39	0.46
1:D:3033:ARG:NH1	1:D:3036:GLU:OE1	2.49	0.46
1:A:379:PRO:O	1:A:380:VAL:C	2.59	0.46
1:D:3278:VAL:HG12	1:D:3303:VAL:HB	1.96	0.46
1:D:3426:PRO:HB2	1:D:3428:HIS:CE1	2.50	0.46
1:B:1048:ARG:HD2	1:B:1119:PHE:CG	2.51	0.46
1:B:1177:ILE:HG13	1:B:1371:LEU:HD21	1.98	0.46
1:C:2191:LEU:HD12	1:C:2191:LEU:C	2.41	0.46
1:A:4:LEU:HD12	1:A:111:TRP:HZ2	1.81	0.46
1:A:300:HIS:HA	1:A:343:LEU:HD11	1.97	0.46
1:A:321:LYS:HA	4:A:5052:HOH:O	2.16	0.46
1:D:3373:THR:C	1:D:3374:HIS:ND1	2.74	0.46
1:B:1153:SER:CB	1:B:1364:GLN:HE21	2.27	0.46
1:C:2134:LEU:HD22	1:C:2138:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2401:LEU:HB2	1:C:2403:VAL:HG23	1.97	0.46
1:D:3300:HIS:HA	1:D:3343:LEU:HD11	1.98	0.46
1:D:3408:LEU:HA	1:D:3412:GLN:HE21	1.80	0.46
1:D:3409:THR:O	1:D:3410:GLU:C	2.58	0.46
1:D:3430:ARG:O	1:D:3431:TYR:HB2	2.16	0.46
1:A:57:VAL:H	1:A:84:GLN:NE2	2.14	0.45
1:A:271:PHE:CE1	1:A:289:MET:HG2	2.50	0.45
1:B:1033:ARG:NH1	1:B:1036:GLU:OE1	2.49	0.45
1:B:1142:HIS:C	1:B:1144:GLN:OE1	2.59	0.45
1:D:3201:GLY:HA2	1:D:3349:ALA:HB2	1.98	0.45
1:D:3247:ASN:O	1:D:3250:GLN:HB2	2.16	0.45
1:A:425:LYS:NZ	1:B:1244:GLU:HG3	2.31	0.45
1:B:1187:LYS:HA	1:B:1187:LYS:HD2	1.82	0.45
1:B:1203:LYS:NZ	1:D:3196:GLU:HB3	2.31	0.45
1:C:2048:ARG:HD2	1:C:2119:PHE:CG	2.52	0.45
1:C:2409:THR:C	1:C:2420:ILE:HD11	2.40	0.45
1:C:2418:MET:HB3	1:C:2424:PHE:HB3	1.99	0.45
1:D:3074:ARG:NH1	1:D:3115:GLN:O	2.50	0.45
1:A:390:ASP:O	1:A:393:VAL:HG23	2.15	0.45
1:B:1119:PHE:N	1:B:1119:PHE:HD1	2.15	0.45
1:C:2033:ARG:NH1	1:C:2036:GLU:OE1	2.49	0.45
1:C:2126:MET:CE	1:C:2151:GLY:N	2.79	0.45
1:D:3153:SER:CB	1:D:3364:GLN:HE21	2.27	0.45
1:A:190:ASN:CG	2:A:432:NAI:H5N	2.42	0.45
1:B:1300:HIS:HA	1:B:1343:LEU:HD11	1.98	0.45
1:B:1374:HIS:HB3	1:B:1377:LYS:HG3	1.99	0.45
1:C:2300:HIS:HA	1:C:2343:LEU:HD11	1.99	0.45
1:D:3299:GLY:O	1:D:3343:LEU:CD1	2.65	0.45
1:B:1201:GLY:HA2	1:B:1349:ALA:HB2	1.99	0.45
1:C:2028:MET:HE2	1:C:2358:SER:CB	2.47	0.45
1:C:2301:PHE:HB2	4:C:5067:HOH:O	2.16	0.45
1:D:3284:ARG:O	1:D:3284:ARG:HG3	2.16	0.45
1:A:3:LYS:CE	1:A:74:ARG:NH1	2.79	0.45
1:A:33:ARG:HD2	1:A:37:MET:HG3	1.97	0.45
1:C:2048:ARG:HD3	1:C:2121:ASP:OD1	2.14	0.45
1:C:2129:ASP:OD2	1:C:2135:THR:HG23	2.17	0.45
1:A:137:LEU:HD12	1:A:141:LYS:HB2	1.99	0.45
1:A:412:GLN:C	1:A:414:GLN:N	2.73	0.45
1:A:416:LEU:HB2	1:A:418:MET:HG2	1.99	0.45
1:B:1079:ASN:HB3	1:B:1082:SER:CB	2.47	0.45
1:B:1119:PHE:HB3	1:B:1120:LYS:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1169:ASN:HB3	4:B:5169:HOH:O	2.16	0.45
1:A:185:LYS:O	1:A:189:ASP:HB3	2.17	0.45
1:A:299:GLY:O	1:A:343:LEU:CD1	2.65	0.45
1:A:385:LEU:HG	1:A:386:PRO:HD2	1.99	0.45
1:B:1057:VAL:H	1:B:1084:GLN:NE2	2.15	0.45
1:D:3119:PHE:N	1:D:3119:PHE:HD1	2.15	0.45
1:A:419:PRO:HB2	1:A:422:GLY:N	2.31	0.45
1:B:1177:ILE:HG13	1:B:1371:LEU:CD2	2.46	0.45
1:B:1179:VAL:O	1:B:1182:SER:HB2	2.17	0.45
1:B:1379:PRO:HD2	1:B:1383:HIS:NE2	2.32	0.45
1:C:2035:ARG:NH2	1:C:2064:GLU:HB2	2.32	0.45
1:D:3048:ARG:HD3	1:D:3121:ASP:OD1	2.16	0.45
1:D:3079:ASN:HB3	1:D:3082:SER:OG	2.17	0.45
1:A:21:LEU:HD21	1:A:60:ALA:CB	2.45	0.45
1:A:137:LEU:HA	1:A:141:LYS:HD3	1.99	0.45
1:C:2091:ILE:HG22	1:C:2096:ILE:HB	1.99	0.45
1:C:2178:ASN:CG	1:C:2181:ASP:HB2	2.42	0.45
1:D:3203:LYS:O	1:D:3207:ASP:N	2.50	0.45
1:D:3262:ASP:OD1	1:D:3284:ARG:NH1	2.50	0.45
1:D:3374:HIS:HB3	1:D:3377:LYS:CG	2.46	0.45
1:C:2079:ASN:HB3	1:C:2082:SER:CB	2.47	0.44
1:C:2272:VAL:HG22	1:C:2296:CYS:SG	2.56	0.44
1:D:3045:LYS:HD3	1:D:3045:LYS:C	2.42	0.44
1:A:196:GLU:HB3	1:C:2203:LYS:NZ	2.33	0.44
1:A:403:VAL:HG13	1:B:1258:VAL:HB	1.98	0.44
1:A:427:ASP:OD2	1:A:427:ASP:N	2.49	0.44
1:B:1037:MET:HE2	1:B:1037:MET:HB3	1.86	0.44
1:C:2419:PRO:CD	1:C:2423:PRO:O	2.65	0.44
1:A:48:ARG:HD2	1:A:119:PHE:CB	2.46	0.44
1:B:1134:LEU:HD22	1:B:1138:ILE:HD12	2.00	0.44
1:C:2093:LYS:C	1:C:2095:GLY:H	2.25	0.44
1:D:3003:LYS:CE	1:D:3074:ARG:HH12	2.30	0.44
1:D:3004:LEU:HD12	1:D:3111:TRP:HZ2	1.82	0.44
1:D:3042:LYS:O	1:D:3045:LYS:HB2	2.17	0.44
1:D:3142:HIS:HA	1:D:3144:GLN:OE1	2.16	0.44
1:A:142:HIS:CA	1:A:144:GLN:OE1	2.65	0.44
1:A:273:THR:CG2	1:A:281:ILE:HD12	2.48	0.44
1:B:1074:ARG:HB3	1:B:1116:THR:HB	1.99	0.44
1:B:1408:LEU:HA	1:B:1412:GLN:HE21	1.82	0.44
1:B:1430:ARG:HB2	1:B:1430:ARG:CZ	2.47	0.44
1:C:2161:HIS:CE1	1:D:3416:LEU:O	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2199:ILE:H	1:C:2199:ILE:HG12	1.60	0.44
1:C:2316:GLU:HG2	1:C:2328:LEU:HB3	1.99	0.44
1:D:3419:PRO:HB2	1:D:3422:GLY:N	2.32	0.44
1:A:244:GLU:HG3	1:B:1425:LYS:NZ	2.32	0.44
1:B:1153:SER:HB2	1:B:1368:GLN:HE21	1.82	0.44
1:B:1418:MET:CB	1:B:1424:PHE:HD1	2.30	0.44
1:B:1419:PRO:CD	1:B:1423:PRO:O	2.65	0.44
1:C:2060:ALA:O	1:C:2064:GLU:HG3	2.17	0.44
1:C:2119:PHE:HB3	1:C:2120:LYS:HD2	1.99	0.44
1:A:48:ARG:HD2	1:A:119:PHE:CG	2.53	0.44
1:A:126:MET:HE2	1:A:151:GLY:N	2.32	0.44
1:C:2142:HIS:CA	1:C:2144:GLN:OE1	2.66	0.44
1:D:3013:LEU:HB3	1:D:3086:HIS:HA	1.98	0.44
1:D:3327:TYR:O	1:D:3334:ARG:HA	2.17	0.44
1:A:425:LYS:HD3	1:A:429:TYR:CE2	2.53	0.44
1:C:2299:GLY:O	1:C:2343:LEU:CD1	2.65	0.44
1:D:3003:LYS:CE	1:D:3074:ARG:NH1	2.81	0.44
1:A:362:THR:HB	1:A:393:VAL:HG13	2.00	0.44
1:B:1027:GLU:C	1:B:1029:PRO:HD3	2.43	0.44
1:B:1203:LYS:O	1:B:1207:ASP:N	2.50	0.44
1:B:1419:PRO:HB2	1:B:1422:GLY:HA3	2.00	0.44
1:C:2137:LEU:HD12	1:C:2141:LYS:HD3	1.99	0.44
1:C:2178:ASN:ND2	1:C:2181:ASP:CG	2.69	0.44
1:C:2271:PHE:CE1	1:C:2289:MET:HG2	2.53	0.44
1:C:2362:THR:HB	1:C:2393:VAL:HG13	1.99	0.44
1:D:3200:ASP:OD2	1:D:3204:ARG:NH2	2.49	0.44
1:D:3387:LYS:CE	1:D:3425:LYS:O	2.65	0.44
1:A:177:ILE:HG13	1:A:371:LEU:CD2	2.48	0.44
1:B:1284:ARG:O	1:B:1284:ARG:HG3	2.18	0.44
1:C:2013:LEU:HB3	1:C:2086:HIS:HA	1.99	0.44
1:C:2105:THR:N	1:C:2108:GLU:HG3	2.32	0.44
1:C:2141:LYS:HD2	1:C:2141:LYS:N	2.32	0.44
1:C:2408:LEU:HA	1:C:2412:GLN:HE21	1.82	0.44
1:D:3105:THR:O	1:D:3106:ASP:C	2.60	0.44
1:D:3273:THR:OG1	1:D:3297:ASN:HB2	2.18	0.44
1:D:3419:PRO:HB2	1:D:3422:GLY:HA3	2.00	0.44
1:B:1190:ASN:CG	2:B:1432:NAI:H5N	2.43	0.43
1:B:1419:PRO:O	1:B:1420:ILE:C	2.59	0.43
1:C:2005:PRO:O	1:C:2097:PRO:HB3	2.18	0.43
1:C:2124:LEU:H	1:C:2124:LEU:HD23	1.83	0.43
1:D:3190:ASN:CG	2:D:3432:NAI:H5N	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LYS:CE	1:A:74:ARG:HH12	2.29	0.43
1:A:418:MET:CB	1:A:424:PHE:HD1	2.30	0.43
1:B:1225:LYS:NZ	1:B:1250:GLN:NE2	2.64	0.43
1:B:1387:LYS:CE	1:B:1425:LYS:O	2.63	0.43
1:D:3125:ASN:C	1:D:3125:ASN:OD1	2.61	0.43
1:A:21:LEU:HD23	1:A:57:VAL:HG13	1.99	0.43
1:A:178:ASN:ND2	1:A:181:ASP:OD2	2.50	0.43
1:A:203:LYS:HZ1	1:C:2196:GLU:HB3	1.83	0.43
1:A:278:VAL:HG12	1:A:303:VAL:HG23	2.00	0.43
1:A:430:ARG:O	1:B:1430:ARG:HB3	2.18	0.43
1:C:2017:GLY:O	1:C:2020:ALA:HB3	2.18	0.43
1:C:2028:MET:O	1:C:2032:MET:HG2	2.17	0.43
1:C:2107:GLU:CD	1:C:2107:GLU:H	2.27	0.43
1:C:2190:ASN:CG	2:C:2432:NAI:H5N	2.43	0.43
1:C:2215:ALA:O	1:C:2238:VAL:HA	2.19	0.43
1:C:2262:ASP:OD1	1:C:2284:ARG:NH1	2.52	0.43
1:C:2281:ILE:C	1:C:2282:LEU:HD13	2.43	0.43
1:A:178:ASN:ND2	1:A:181:ASP:HB2	2.34	0.43
1:A:373:THR:C	1:A:374:HIS:ND1	2.76	0.43
1:B:1208:VAL:HG22	1:B:1209:MET:N	2.34	0.43
1:B:1406:THR:HG22	1:B:1407:LYS:N	2.33	0.43
1:C:2138:ILE:HG23	1:C:2142:HIS:O	2.18	0.43
1:C:2374:HIS:HB3	1:C:2377:LYS:CG	2.49	0.43
1:C:2430:ARG:HD2	1:D:3430:ARG:O	2.19	0.43
1:D:3057:VAL:H	1:D:3084:GLN:NE2	2.17	0.43
1:C:2028:MET:HE2	1:C:2358:SER:CA	2.49	0.43
1:C:2124:LEU:HD23	1:C:2124:LEU:N	2.34	0.43
1:C:2126:MET:HE1	1:C:2151:GLY:N	2.33	0.43
1:A:144:GLN:CD	1:A:144:GLN:H	2.23	0.43
1:A:387:LYS:CE	1:A:425:LYS:O	2.66	0.43
1:B:1003:LYS:HE3	1:B:1074:ARG:NH1	2.34	0.43
1:D:3007:LYS:NZ	1:D:3101:TRP:CH2	2.86	0.43
1:A:28:MET:HB3	1:A:358:SER:HB2	2.00	0.43
1:A:42:LYS:O	1:A:45:LYS:HB2	2.19	0.43
1:A:139:HIS:CD2	1:A:166:MET:HE2	2.54	0.43
1:B:1353:PRO:CG	1:D:3209:MET:SD	3.06	0.43
1:C:2120:LYS:CD	1:C:2120:LYS:N	2.54	0.43
1:C:2137:LEU:O	1:C:2137:LEU:HD12	2.19	0.43
1:C:2177:ILE:HG13	1:C:2371:LEU:HD21	2.00	0.43
1:C:2420:ILE:HG23	1:C:2421:ASN:N	2.33	0.43
1:D:3206:THR:O	1:D:3207:ASP:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3387:LYS:NZ	1:D:3425:LYS:O	2.51	0.43
1:D:3425:LYS:HD3	1:D:3429:TYR:CZ	2.53	0.43
1:A:93:LYS:C	1:A:95:GLY:N	2.75	0.43
1:B:1142:HIS:CA	1:B:1144:GLN:OE1	2.67	0.43
1:B:1278:VAL:HG12	1:B:1303:VAL:HB	1.99	0.43
1:C:2178:ASN:ND2	1:C:2181:ASP:OD2	2.51	0.43
1:C:2265:CYS:HA	1:C:2271:PHE:CZ	2.54	0.43
1:C:2419:PRO:HB2	1:C:2422:GLY:N	2.32	0.43
1:B:1042:LYS:O	1:B:1045:LYS:HB2	2.18	0.43
1:B:1105:THR:OG1	1:B:1108:GLU:HG3	2.19	0.43
1:C:2041:SER:O	1:C:2042:LYS:C	2.61	0.43
1:D:3214:VAL:N	1:D:3269:ASN:ND2	2.54	0.43
1:D:3265:CYS:SG	1:D:3285:HIS:HD2	2.42	0.43
1:D:3427:ASP:OD2	1:D:3427:ASP:N	2.51	0.43
1:A:265:CYS:HA	1:A:271:PHE:CZ	2.54	0.43
1:A:408:LEU:O	1:A:420:ILE:CD1	2.56	0.42
1:A:418:MET:HB3	1:A:424:PHE:HB3	2.01	0.42
1:B:1052:CYS:HB3	1:B:1129:ASP:OD1	2.18	0.42
1:B:1166:MET:HA	1:B:1171:ILE:HD12	2.00	0.42
1:B:1234:PHE:HE1	1:D:3195:ARG:O	2.02	0.42
1:C:2387:LYS:NZ	1:C:2425:LYS:O	2.51	0.42
1:D:3312:GLU:HG3	1:D:3313:ASN:ND2	2.34	0.42
1:D:3361:PHE:O	1:D:3365:VAL:HG23	2.19	0.42
1:A:242:GLU:OE1	2:A:432:NAI:H1B	2.18	0.42
1:C:2187:LYS:HA	1:C:2187:LYS:HD2	1.79	0.42
1:D:3215:ALA:CB	1:D:3231:LEU:HD13	2.47	0.42
1:A:177:ILE:HG13	1:A:371:LEU:HD21	2.01	0.42
1:B:1152:ILE:HG13	1:B:1174:VAL:CG2	2.50	0.42
1:C:2277:CYS:HB2	1:D:3416:LEU:CG	2.48	0.42
1:D:3142:HIS:CA	1:D:3144:GLN:OE1	2.67	0.42
1:C:2201:GLY:HA2	1:C:2349:ALA:HB2	2.01	0.42
1:C:2374:HIS:HB3	1:C:2377:LYS:HG3	2.00	0.42
1:A:374:HIS:HB3	1:A:377:LYS:HG3	2.01	0.42
1:B:1048:ARG:HD3	1:B:1121:ASP:OD1	2.19	0.42
1:B:1152:ILE:HB	1:B:1176:ALA:HB2	2.01	0.42
1:B:1352:HIS:HB3	1:B:1356:VAL:CG1	2.49	0.42
1:D:3374:HIS:HB3	1:D:3377:LYS:CD	2.50	0.42
1:D:3419:PRO:CG	1:D:3422:GLY:HA3	2.48	0.42
1:A:137:LEU:O	1:A:137:LEU:HD12	2.18	0.42
1:A:141:LYS:C	1:A:143:PRO:HD3	2.45	0.42
1:A:186:SER:O	1:A:190:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:TYR:O	1:A:334:ARG:HA	2.20	0.42
1:A:414:GLN:O	1:A:415:TYR:C	2.62	0.42
1:A:418:MET:CB	1:A:424:PHE:HB3	2.50	0.42
1:B:1146:LEU:HG	1:B:1173:LYS:HB2	2.01	0.42
1:C:2144:GLN:CD	1:C:2144:GLN:H	2.21	0.42
1:C:2300:HIS:HB2	2:C:2432:NAI:O2D	2.19	0.42
1:A:55:MET:HA	1:A:55:MET:HE2	2.02	0.42
1:A:277:CYS:CB	1:B:1416:LEU:HD21	2.42	0.42
1:B:1419:PRO:O	1:B:1422:GLY:N	2.53	0.42
1:C:2278:VAL:HG13	1:D:3415:TYR:CZ	2.55	0.42
1:C:2410:GLU:OE1	1:C:2410:GLU:HA	2.19	0.42
1:A:60:ALA:O	1:A:64:GLU:HG3	2.19	0.42
1:A:105:THR:N	1:A:108:GLU:HG3	2.35	0.42
1:A:152:ILE:HB	1:A:176:ALA:HB2	2.02	0.42
1:B:1419:PRO:HB2	1:B:1422:GLY:N	2.34	0.42
1:A:425:LYS:HD3	1:A:429:TYR:CZ	2.55	0.42
1:B:1409:THR:C	1:B:1420:ILE:HD11	2.42	0.42
1:C:2373:THR:C	1:C:2374:HIS:ND1	2.78	0.42
1:D:3055:MET:HA	1:D:3055:MET:CE	2.49	0.42
1:D:3416:LEU:CB	1:D:3418:MET:HG2	2.50	0.42
1:A:7:LYS:NZ	1:A:101:TRP:CH2	2.88	0.42
1:A:93:LYS:C	1:A:95:GLY:H	2.28	0.42
1:B:1273:THR:CG2	1:B:1281:ILE:HD12	2.49	0.42
1:C:2390:ASP:O	1:C:2393:VAL:HG23	2.20	0.42
1:D:3337:LEU:HD13	1:D:3340:GLU:HA	2.02	0.42
1:A:45:LYS:HD3	1:A:45:LYS:C	2.45	0.41
1:A:334:ARG:O	1:A:335:ILE:HD13	2.20	0.41
1:A:91:ILE:N	1:A:91:ILE:CD1	2.83	0.41
1:A:430:ARG:HA	1:B:1430:ARG:CD	2.50	0.41
1:B:1079:ASN:HB3	1:B:1082:SER:OG	2.20	0.41
1:B:1156:THR:HG1	2:B:1432:NAI:HO2N	1.66	0.41
1:C:2010:ASP:HB3	1:C:2013:LEU:CD2	2.46	0.41
1:A:374:HIS:HB3	1:A:377:LYS:CG	2.50	0.41
1:A:431:TYR:HE2	1:B:1247:ASN:ND2	2.18	0.41
1:B:1271:PHE:CE1	1:B:1289:MET:HG2	2.54	0.41
1:C:2228:ALA:HB1	1:C:2256:TYR:CZ	2.55	0.41
1:C:2232:ARG:HG3	1:C:2232:ARG:HH11	1.85	0.41
1:C:2412:GLN:O	1:C:2413:ALA:C	2.63	0.41
1:D:3187:LYS:HA	1:D:3187:LYS:HD2	1.87	0.41
1:D:3419:PRO:O	1:D:3422:GLY:N	2.53	0.41
1:A:244:GLU:HG3	1:B:1425:LYS:HZ2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ILE:C	1:A:282:LEU:HD13	2.46	0.41
1:A:413:ALA:HB2	1:A:420:ILE:HD12	2.01	0.41
1:A:430:ARG:HB3	1:B:1430:ARG:O	2.20	0.41
1:B:1302:ASP:O	1:B:1302:ASP:CG	2.63	0.41
1:B:1373:THR:C	1:B:1374:HIS:ND1	2.78	0.41
1:C:2139:HIS:ND1	1:C:2146:LEU:HD11	2.35	0.41
1:C:2203:LYS:O	1:C:2207:ASP:N	2.53	0.41
1:C:2416:LEU:CD2	1:D:3277:CYS:HB2	2.40	0.41
1:D:3308:LYS:HD2	1:D:3308:LYS:N	2.16	0.41
1:A:191:LEU:C	1:A:191:LEU:HD12	2.46	0.41
1:A:401:LEU:HD12	1:B:1249:LEU:HD12	2.03	0.41
1:B:1035:ARG:NH2	1:B:1064:GLU:HB2	2.35	0.41
1:C:2027:GLU:C	1:C:2029:PRO:HD3	2.45	0.41
1:C:2125:ASN:C	1:C:2125:ASN:OD1	2.63	0.41
1:C:2243:ILE:HG21	1:D:3408:LEU:HD13	2.01	0.41
1:C:2401:LEU:CD1	1:D:3249:LEU:CD1	2.98	0.41
1:D:3152:ILE:HB	1:D:3176:ALA:HB2	2.01	0.41
1:A:243:ILE:HG21	1:B:1408:LEU:HD13	2.02	0.41
1:A:309:TRP:O	1:A:310:LEU:C	2.62	0.41
1:A:409:THR:O	1:A:420:ILE:CD1	2.68	0.41
1:B:1017:GLY:O	1:B:1020:ALA:HB3	2.21	0.41
1:B:1374:HIS:HB3	1:B:1377:LYS:CG	2.50	0.41
1:D:3031:LEU:HD23	1:D:3031:LEU:HA	1.92	0.41
1:D:3134:LEU:HD22	1:D:3138:ILE:HD12	2.02	0.41
1:C:2374:HIS:HB3	1:C:2377:LYS:HD3	2.03	0.41
1:A:412:GLN:O	1:A:413:ALA:C	2.63	0.41
1:B:1387:LYS:HZ3	1:B:1425:LYS:C	2.29	0.41
1:B:1427:ASP:OD2	1:B:1427:ASP:N	2.54	0.41
1:D:3191:LEU:HD12	1:D:3191:LEU:C	2.46	0.41
1:A:119:PHE:HB3	1:A:120:LYS:HD2	2.03	0.41
1:A:361:PHE:O	1:A:365:VAL:HG23	2.21	0.41
1:B:1137:LEU:O	1:B:1137:LEU:HD12	2.21	0.41
1:B:1144:GLN:H	1:B:1144:GLN:CD	2.23	0.41
1:B:1292:ASP:CG	1:B:1326:ARG:HH21	2.29	0.41
1:C:2033:ARG:HD2	1:C:2037:MET:CG	2.51	0.41
1:C:2045:LYS:HD3	1:C:2045:LYS:C	2.46	0.41
1:C:2278:VAL:HG12	1:C:2303:VAL:HG23	2.02	0.41
1:C:2413:ALA:HB2	1:C:2420:ILE:HD12	2.01	0.41
1:C:2414:GLN:O	1:C:2415:TYR:C	2.63	0.41
1:D:3119:PHE:HB3	1:D:3120:LYS:HD2	2.03	0.41
1:D:3300:HIS:HB2	2:D:3432:NAI:O2D	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:THR:C	1:A:375:PRO:CD	2.93	0.41
1:A:410:GLU:HA	1:A:410:GLU:OE1	2.20	0.41
1:B:1033:ARG:HD2	1:B:1037:MET:CG	2.50	0.41
1:B:1153:SER:HB2	1:B:1368:GLN:NE2	2.36	0.41
1:B:1181:ASP:HB3	1:B:1384:PHE:HE1	1.85	0.41
1:C:2007:LYS:NZ	1:C:2101:TRP:CH2	2.89	0.41
1:C:2058:GLU:CD	1:C:2058:GLU:H	2.29	0.41
1:C:2243:ILE:HD12	1:D:3424:PHE:CZ	2.56	0.41
1:A:79:ASN:HB3	1:A:82:SER:CB	2.51	0.40
1:A:137:LEU:HD12	1:A:141:LYS:HD3	2.02	0.40
1:A:292:ASP:CG	1:A:326:ARG:HH21	2.29	0.40
1:B:1021:LEU:HD21	1:B:1060:ALA:CB	2.49	0.40
1:B:1124:LEU:H	1:B:1124:LEU:HD23	1.86	0.40
1:D:3058:GLU:CD	1:D:3058:GLU:N	2.80	0.40
1:A:187:LYS:HA	1:A:187:LYS:HD2	1.83	0.40
1:B:1079:ASN:HB3	1:B:1082:SER:HB3	2.03	0.40
1:B:1110:LEU:HD12	1:B:1114:GLU:CG	2.52	0.40
1:B:1208:VAL:HG22	1:B:1213:LYS:HE2	2.01	0.40
1:B:1409:THR:O	1:B:1410:GLU:C	2.60	0.40
1:D:3141:LYS:HD2	1:D:3141:LYS:N	2.35	0.40
1:D:3299:GLY:HA3	1:D:3304:GLU:OE2	2.20	0.40
1:B:1053:LEU:O	1:B:1077:SER:HA	2.20	0.40
1:B:1178:ASN:ND2	1:B:1181:ASP:CG	2.75	0.40
1:D:3048:ARG:HD2	1:D:3119:PHE:CG	2.57	0.40
1:D:3124:LEU:HD23	1:D:3124:LEU:N	2.36	0.40
1:A:74:ARG:NH1	1:A:115:GLN:O	2.54	0.40
1:A:419:PRO:HB2	1:A:422:GLY:HA3	2.04	0.40
1:B:1302:ASP:OD2	1:B:1302:ASP:C	2.64	0.40
1:B:1414:GLN:O	1:B:1415:TYR:C	2.64	0.40
1:B:1419:PRO:CG	1:B:1422:GLY:HA3	2.48	0.40
1:A:215:ALA:O	1:A:238:VAL:HA	2.21	0.40
1:A:387:LYS:NZ	1:A:425:LYS:HB3	2.36	0.40
1:A:412:GLN:O	1:A:414:GLN:N	2.54	0.40
1:B:1048:ARG:HH11	1:B:1048:ARG:HG3	1.86	0.40
1:B:1279:ASP:HB3	1:B:1282:LEU:HD11	2.02	0.40
1:C:2278:VAL:HG22	1:D:3415:TYR:CG	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3317:LYS:O	1:D:3317:LYS:O[2_555]	2.12	0.08

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	428/431 (99%)	398 (93%)	30 (7%)	0	100	100
1	B	428/431 (99%)	401 (94%)	26 (6%)	1 (0%)	43	72
1	C	428/431 (99%)	396 (92%)	32 (8%)	0	100	100
1	D	428/431 (99%)	400 (94%)	28 (6%)	0	100	100
All	All	1712/1724 (99%)	1595 (93%)	116 (7%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1420	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	353/353 (100%)	291 (82%)	62 (18%)	2	7
1	B	353/353 (100%)	291 (82%)	62 (18%)	2	7
1	C	353/353 (100%)	288 (82%)	65 (18%)	1	6
1	D	353/353 (100%)	291 (82%)	62 (18%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1412/1412 (100%)	1161 (82%)	251 (18%)	2 6

All (251) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	13	LEU
1	A	23	ILE
1	A	28	MET
1	A	41	SER
1	A	42	LYS
1	A	53	LEU
1	A	55	MET
1	A	57	VAL
1	A	86	HIS
1	A	91	ILE
1	A	93	LYS
1	A	104	GLU
1	A	108	GLU
1	A	110	LEU
1	A	114	GLU
1	A	119	PHE
1	A	120	LYS
1	A	121	ASP
1	A	134	LEU
1	A	135	THR
1	A	144	GLN
1	A	146	LEU
1	A	153	SER
1	A	158	THR
1	A	165	LYS
1	A	172	LEU
1	A	174	VAL
1	A	177	ILE
1	A	179	VAL
1	A	182	SER
1	A	187	LYS
1	A	191	LEU
1	A	232	ARG
1	A	240	ILE
1	A	267	GLU
1	A	275	THR

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Mol	Chain	Res	Type
1	A	277	CYS
1	A	281	ILE
1	A	282	LEU
1	A	284	ARG
1	A	297	ASN
1	A	317	LYS
1	A	337	LEU
1	A	340	GLU
1	A	371	LEU
1	A	374	HIS
1	A	377	LYS
1	A	382	VAL
1	A	393	VAL
1	A	398	LEU
1	A	400	LYS
1	A	405	LEU
1	A	407	LYS
1	A	408	LEU
1	A	410	GLU
1	A	414	GLN
1	A	418	MET
1	A	424	PHE
1	A	425	LYS
1	A	427	ASP
1	A	428	HIS
1	B	1003	LYS
1	B	1013	LEU
1	B	1023	ILE
1	B	1028	MET
1	B	1041	SER
1	B	1042	LYS
1	B	1053	LEU
1	B	1055	MET
1	B	1057	VAL
1	B	1086	HIS
1	B	1091	ILE
1	B	1093	LYS
1	B	1104	GLU
1	B	1108	GLU
1	B	1110	LEU
1	B	1114	GLU
1	B	1119	PHE

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Mol	Chain	Res	Type
1	B	1120	LYS
1	B	1121	ASP
1	B	1134	LEU
1	B	1135	THR
1	B	1144	GLN
1	B	1146	LEU
1	B	1153	SER
1	B	1158	THR
1	B	1165	LYS
1	B	1169	ASN
1	B	1172	LEU
1	B	1174	VAL
1	B	1177	ILE
1	B	1179	VAL
1	B	1182	SER
1	B	1186	SER
1	B	1187	LYS
1	B	1191	LEU
1	B	1199	ILE
1	B	1240	ILE
1	B	1267	GLU
1	B	1275	THR
1	B	1277	CYS
1	B	1281	ILE
1	B	1282	LEU
1	B	1284	ARG
1	B	1297	ASN
1	B	1302	ASP
1	B	1317	LYS
1	B	1337	LEU
1	B	1340	GLU
1	B	1371	LEU
1	B	1377	LYS
1	B	1382	VAL
1	B	1400	LYS
1	B	1405	LEU
1	B	1407	LYS
1	B	1408	LEU
1	B	1410	GLU
1	B	1414	GLN
1	B	1418	MET
1	B	1424	PHE

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Mol	Chain	Res	Type
1	B	1425	LYS
1	B	1427	ASP
1	B	1428	HIS
1	C	2003	LYS
1	C	2013	LEU
1	C	2023	ILE
1	C	2028	MET
1	C	2041	SER
1	C	2042	LYS
1	C	2053	LEU
1	C	2055	MET
1	C	2057	VAL
1	C	2086	HIS
1	C	2091	ILE
1	C	2093	LYS
1	C	2098	VAL
1	C	2104	GLU
1	C	2108	GLU
1	C	2110	LEU
1	C	2114	GLU
1	C	2119	PHE
1	C	2120	LYS
1	C	2121	ASP
1	C	2134	LEU
1	C	2135	THR
1	C	2137	LEU
1	C	2142	HIS
1	C	2144	GLN
1	C	2146	LEU
1	C	2153	SER
1	C	2158	THR
1	C	2165	LYS
1	C	2169	ASN
1	C	2172	LEU
1	C	2174	VAL
1	C	2177	ILE
1	C	2179	VAL
1	C	2182	SER
1	C	2191	LEU
1	C	2199	ILE
1	C	2240	ILE
1	C	2267	GLU

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Mol	Chain	Res	Type
1	C	2275	THR
1	C	2277	CYS
1	C	2281	ILE
1	C	2282	LEU
1	C	2284	ARG
1	C	2297	ASN
1	C	2317	LYS
1	C	2337	LEU
1	C	2340	GLU
1	C	2371	LEU
1	C	2374	HIS
1	C	2377	LYS
1	C	2382	VAL
1	C	2393	VAL
1	C	2398	LEU
1	C	2400	LYS
1	C	2405	LEU
1	C	2407	LYS
1	C	2408	LEU
1	C	2410	GLU
1	C	2414	GLN
1	C	2418	MET
1	C	2424	PHE
1	C	2425	LYS
1	C	2427	ASP
1	C	2428	HIS
1	D	3003	LYS
1	D	3013	LEU
1	D	3023	ILE
1	D	3028	MET
1	D	3041	SER
1	D	3042	LYS
1	D	3053	LEU
1	D	3055	MET
1	D	3057	VAL
1	D	3065	THR
1	D	3086	HIS
1	D	3091	ILE
1	D	3093	LYS
1	D	3108	GLU
1	D	3110	LEU
1	D	3114	GLU

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Mol	Chain	Res	Type
1	D	3119	PHE
1	D	3120	LYS
1	D	3121	ASP
1	D	3134	LEU
1	D	3135	THR
1	D	3142	HIS
1	D	3144	GLN
1	D	3146	LEU
1	D	3153	SER
1	D	3158	THR
1	D	3165	LYS
1	D	3169	ASN
1	D	3172	LEU
1	D	3174	VAL
1	D	3179	VAL
1	D	3182	SER
1	D	3191	LEU
1	D	3199	ILE
1	D	3240	ILE
1	D	3267	GLU
1	D	3275	THR
1	D	3277	CYS
1	D	3281	ILE
1	D	3282	LEU
1	D	3284	ARG
1	D	3297	ASN
1	D	3317	LYS
1	D	3337	LEU
1	D	3340	GLU
1	D	3371	LEU
1	D	3374	HIS
1	D	3377	LYS
1	D	3382	VAL
1	D	3393	VAL
1	D	3398	LEU
1	D	3400	LYS
1	D	3405	LEU
1	D	3407	LYS
1	D	3408	LEU
1	D	3410	GLU
1	D	3414	GLN
1	D	3418	MET

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Mol	Chain	Res	Type
1	D	3424	PHE
1	D	3425	LYS
1	D	3427	ASP
1	D	3428	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	84	GLN
1	A	169	ASN
1	A	247	ASN
1	A	250	GLN
1	A	269	ASN
1	A	313	ASN
1	A	364	GLN
1	A	368	GLN
1	A	412	GLN
1	A	414	GLN
1	B	1026	ASN
1	B	1084	GLN
1	B	1136	ASN
1	B	1169	ASN
1	B	1247	ASN
1	B	1250	GLN
1	B	1269	ASN
1	B	1364	GLN
1	B	1368	GLN
1	B	1402	ASN
1	B	1412	GLN
1	B	1414	GLN
1	C	2026	ASN
1	C	2084	GLN
1	C	2169	ASN
1	C	2247	ASN
1	C	2250	GLN
1	C	2269	ASN
1	C	2313	ASN
1	C	2364	GLN
1	C	2368	GLN
1	C	2412	GLN
1	C	2414	GLN

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Mol	Chain	Res	Type
1	D	3026	ASN
1	D	3084	GLN
1	D	3136	ASN
1	D	3169	ASN
1	D	3247	ASN
1	D	3250	GLN
1	D	3269	ASN
1	D	3313	ASN
1	D	3364	GLN
1	D	3368	GLN
1	D	3412	GLN
1	D	3414	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](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAI	D	3432	-	47,48,48	1.19	4 (8%)	64,73,73	1.16	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAI	C	2432	-	47,48,48	1.16	4 (8%)	64,73,73	1.13	6 (9%)
3	ADY	C	2433	-	19,21,21	1.99	2 (10%)	22,31,31	1.21	3 (13%)
3	ADY	A	433	-	19,21,21	1.05	1 (5%)	22,31,31	1.30	4 (18%)
2	NAI	A	432	-	47,48,48	1.30	4 (8%)	64,73,73	1.23	7 (10%)
3	ADY	B	1433	-	19,21,21	1.20	2 (10%)	22,31,31	1.35	4 (18%)
3	ADY	D	3433	-	19,21,21	1.78	3 (15%)	22,31,31	1.32	3 (13%)
2	NAI	B	1432	-	47,48,48	1.19	4 (8%)	64,73,73	1.14	5 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAI	D	3432	-	-	8/29/72/72	0/5/5/5
2	NAI	C	2432	-	-	8/29/72/72	0/5/5/5
3	ADY	C	2433	-	-	0/6/22/22	0/3/3/3
3	ADY	A	433	-	-	0/6/22/22	0/3/3/3
2	NAI	A	432	-	-	8/29/72/72	0/5/5/5
3	ADY	B	1433	-	-	0/6/22/22	0/3/3/3
3	ADY	D	3433	-	-	0/6/22/22	0/3/3/3
2	NAI	B	1432	-	-	9/29/72/72	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2433	ADY	O3'-C3'	7.05	1.32	1.21
3	D	3433	ADY	O3'-C3'	5.61	1.30	1.21
2	A	432	NAI	PN-O3	4.51	1.64	1.59
2	A	432	NAI	C2N-C3N	4.19	1.46	1.35
2	D	3432	NAI	C2N-C3N	3.97	1.46	1.35
2	B	1432	NAI	C2N-C3N	3.85	1.45	1.35
2	C	2432	NAI	C2N-C3N	3.68	1.45	1.35
2	A	432	NAI	C6N-N1N	3.50	1.45	1.37
2	D	3432	NAI	PN-O3	3.33	1.63	1.59
3	C	2433	ADY	C4'-C3'	-3.23	1.45	1.52
2	B	1432	NAI	PN-O3	3.22	1.63	1.59
2	C	2432	NAI	C6N-N1N	3.17	1.45	1.37
2	B	1432	NAI	C6N-N1N	3.14	1.44	1.37
2	D	3432	NAI	C6N-N1N	3.11	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	433	ADY	C8-N9	2.92	1.42	1.37
3	D	3433	ADY	C4'-C3'	-2.86	1.46	1.52
3	D	3433	ADY	C8-N9	2.85	1.42	1.37
2	C	2432	NAI	O4B-C1B	-2.79	1.35	1.42
3	B	1433	ADY	C8-N9	2.60	1.42	1.37
2	D	3432	NAI	O4B-C1B	-2.43	1.36	1.42
3	B	1433	ADY	O3'-C3'	2.39	1.25	1.21
2	A	432	NAI	C2A-N1A	2.26	1.38	1.33
2	B	1432	NAI	O4B-C1B	-2.11	1.37	1.42
2	C	2432	NAI	C2A-N1A	2.07	1.37	1.33

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1432	NAI	O7N-C7N-C3N	-4.30	112.79	120.90
3	D	3433	ADY	O5'-C5'-C4'	-4.18	101.11	111.73
2	D	3432	NAI	O7N-C7N-C3N	-4.14	113.11	120.90
2	A	432	NAI	O7N-C7N-C3N	-4.05	113.28	120.90
2	A	432	NAI	C3N-C7N-N7N	3.92	124.63	117.67
2	B	1432	NAI	C3N-C7N-N7N	3.88	124.55	117.67
2	D	3432	NAI	C3N-C7N-N7N	3.85	124.50	117.67
2	C	2432	NAI	O7N-C7N-C3N	-3.72	113.89	120.90
3	B	1433	ADY	O5'-C5'-C4'	-3.63	102.51	111.73
2	A	432	NAI	O1N-PN-O3	3.56	116.89	107.27
2	C	2432	NAI	C3N-C7N-N7N	3.51	123.89	117.67
3	C	2433	ADY	O5'-C5'-C4'	-3.50	102.83	111.73
2	C	2432	NAI	O1N-PN-O3	3.39	116.43	107.27
3	A	433	ADY	O5'-C5'-C4'	-3.23	103.53	111.73
2	D	3432	NAI	O1N-PN-O3	3.05	115.52	107.27
2	A	432	NAI	O5B-C5B-C4B	-3.03	98.69	108.99
2	C	2432	NAI	O4B-C1B-C2B	-2.93	100.34	106.62
2	B	1432	NAI	O1N-PN-O3	2.80	114.85	107.27
2	D	3432	NAI	O5B-C5B-C4B	-2.80	99.47	108.99
2	B	1432	NAI	O4B-C1B-C2B	-2.77	100.68	106.62
3	B	1433	ADY	O4'-C1'-N9	2.75	113.37	108.09
3	B	1433	ADY	C1'-O4'-C4'	-2.72	101.89	108.29
3	A	433	ADY	C1'-O4'-C4'	-2.68	101.97	108.29
3	D	3433	ADY	C1'-O4'-C4'	-2.68	101.98	108.29
3	C	2433	ADY	C1'-O4'-C4'	-2.55	102.28	108.29
2	B	1432	NAI	O5B-C5B-C4B	-2.47	100.57	108.99
3	A	433	ADY	O4'-C1'-N9	2.46	112.82	108.09
2	C	2432	NAI	O5B-C5B-C4B	-2.40	100.82	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	432	NAI	O4B-C1B-C2B	-2.40	101.49	106.62
3	A	433	ADY	O3'-C3'-C2'	2.34	129.43	124.17
3	D	3433	ADY	O4'-C1'-N9	2.27	112.44	108.09
3	C	2433	ADY	O4'-C1'-N9	2.22	112.35	108.09
2	D	3432	NAI	O4B-C1B-C2B	-2.21	101.89	106.62
2	D	3432	NAI	O5D-PN-O2N	2.10	117.26	108.94
2	A	432	NAI	O5D-PN-O2N	2.09	117.21	108.94
3	B	1433	ADY	O3'-C3'-C2'	2.07	128.81	124.17
2	C	2432	NAI	C1D-N1N-C2N	-2.06	117.75	121.14
2	A	432	NAI	O4B-C1B-N9A	-2.03	104.18	108.09
2	D	3432	NAI	C1D-N1N-C2N	-2.00	117.84	121.14

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1432	NAI	C2B-C1B-N9A-C8A
2	A	432	NAI	C2D-C1D-N1N-C2N
2	A	432	NAI	C2D-C1D-N1N-C6N
2	B	1432	NAI	C2D-C1D-N1N-C2N
2	D	3432	NAI	C2D-C1D-N1N-C2N
2	A	432	NAI	C2B-C1B-N9A-C8A
2	C	2432	NAI	C2D-C1D-N1N-C2N
2	D	3432	NAI	C2D-C1D-N1N-C6N
2	A	432	NAI	C5D-O5D-PN-O2N
2	B	1432	NAI	C5D-O5D-PN-O2N
2	C	2432	NAI	C5D-O5D-PN-O2N
2	D	3432	NAI	C5D-O5D-PN-O2N
2	D	3432	NAI	O4D-C1D-N1N-C2N
2	A	432	NAI	O4D-C1D-N1N-C2N
2	B	1432	NAI	O4D-C1D-N1N-C2N
2	C	2432	NAI	O4D-C1D-N1N-C2N
2	B	1432	NAI	C2D-C1D-N1N-C6N
2	D	3432	NAI	O4D-C1D-N1N-C6N
2	C	2432	NAI	C2B-C1B-N9A-C8A
2	C	2432	NAI	C2D-C1D-N1N-C6N
2	C	2432	NAI	O4D-C1D-N1N-C6N
2	D	3432	NAI	C2B-C1B-N9A-C8A
2	A	432	NAI	O4D-C1D-N1N-C6N
2	A	432	NAI	C2N-C3N-C7N-N7N
2	B	1432	NAI	O4D-C1D-N1N-C6N
2	B	1432	NAI	C2N-C3N-C7N-N7N

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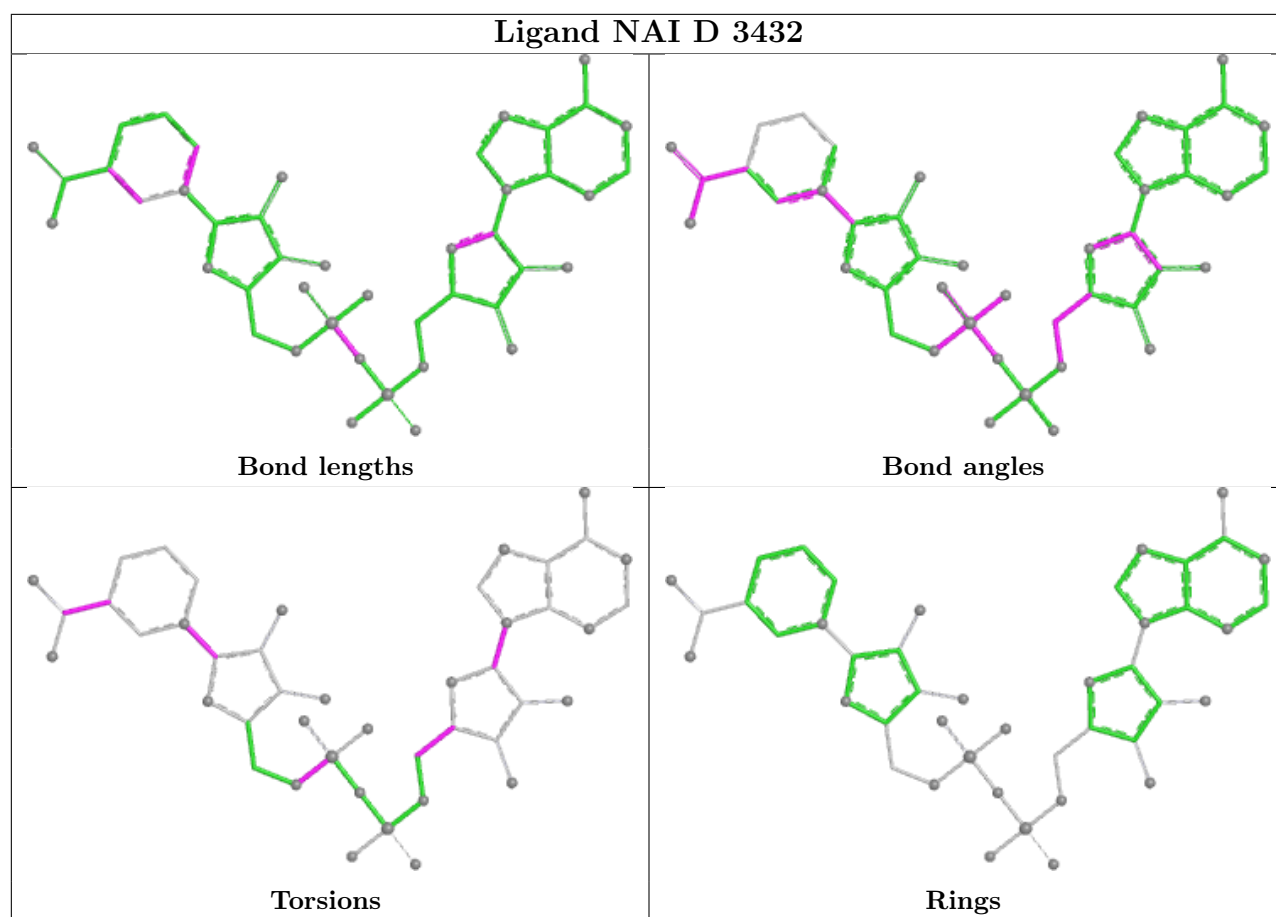
Mol	Chain	Res	Type	Atoms
2	C	2432	NAI	C2N-C3N-C7N-N7N
2	D	3432	NAI	C2N-C3N-C7N-N7N
2	B	1432	NAI	PN-O3-PA-O1A
2	A	432	NAI	O4B-C4B-C5B-O5B
2	B	1432	NAI	O4B-C4B-C5B-O5B
2	C	2432	NAI	O4B-C4B-C5B-O5B
2	D	3432	NAI	O4B-C4B-C5B-O5B

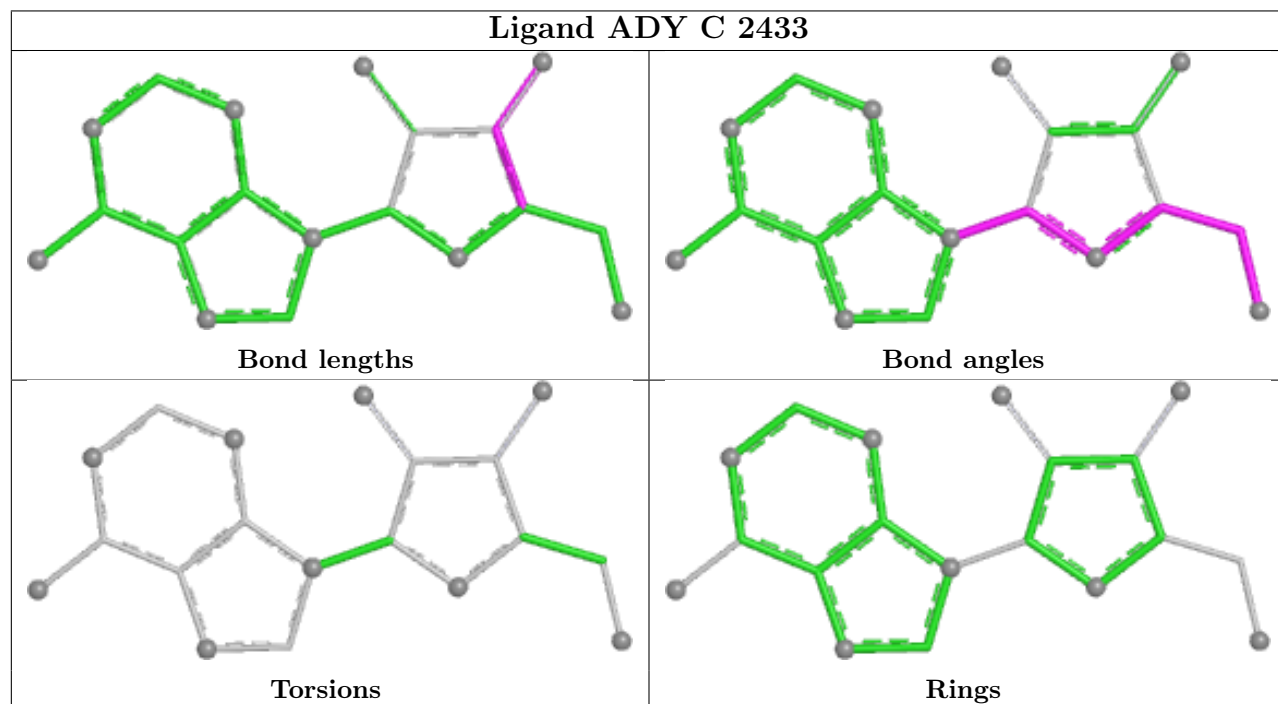
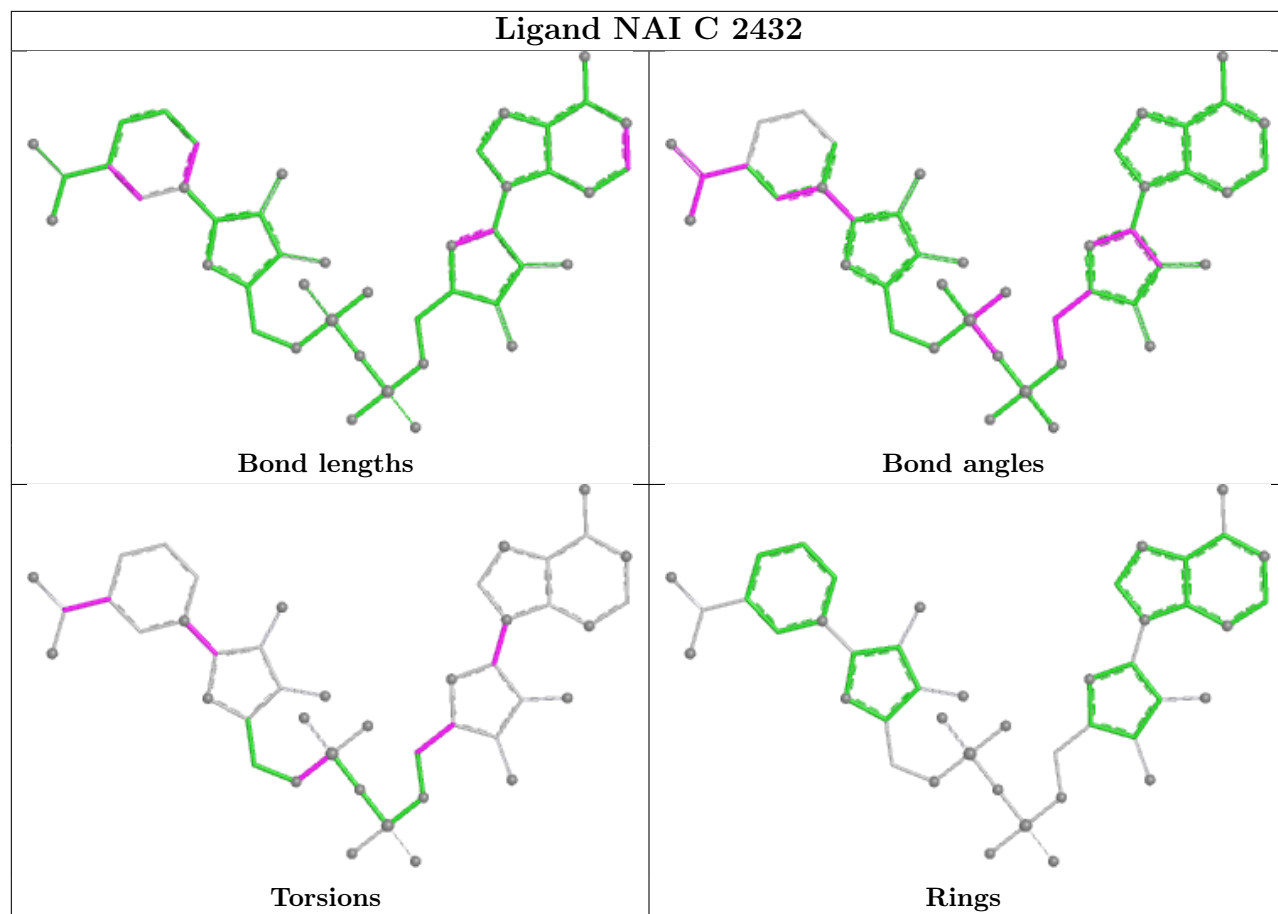
There are no ring outliers.

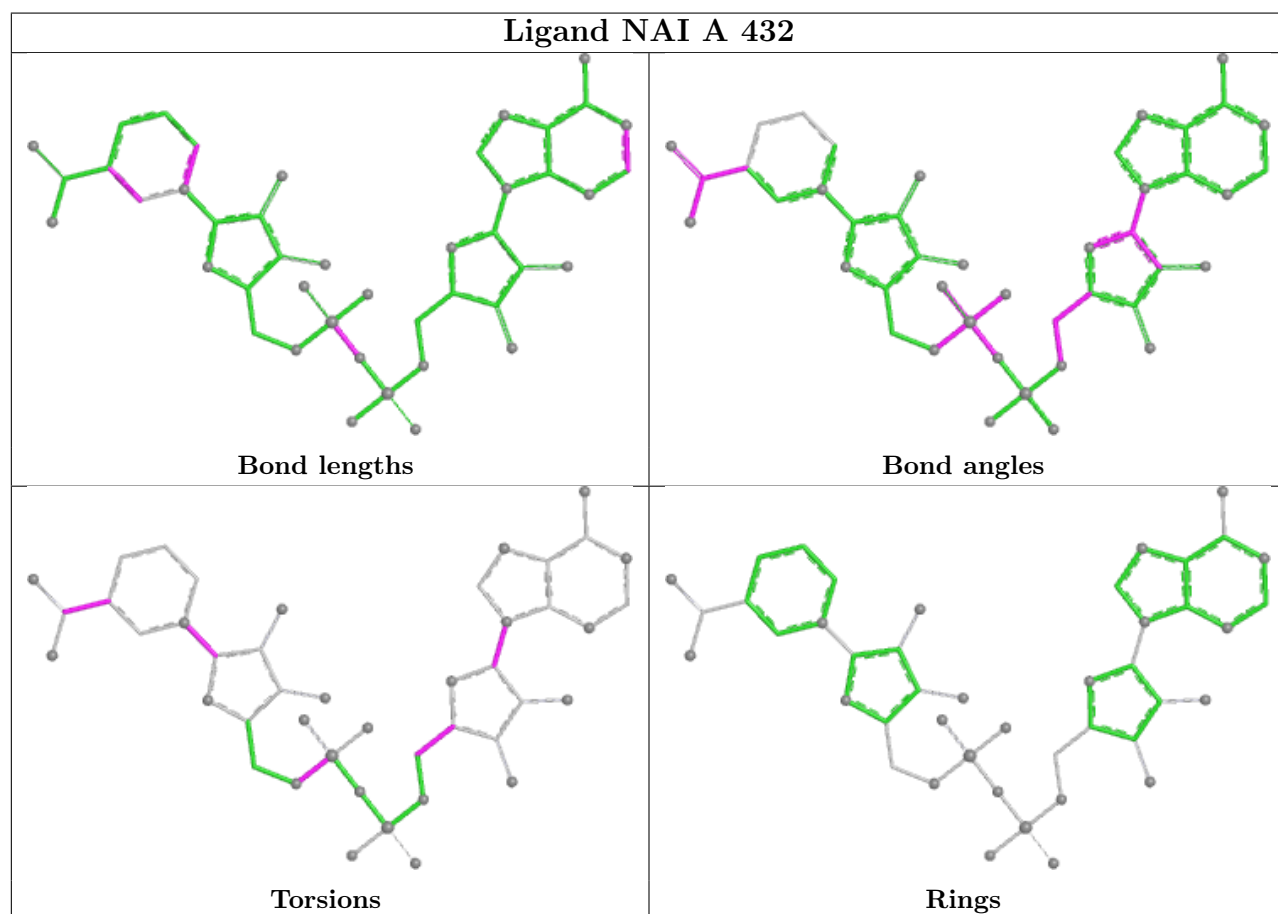
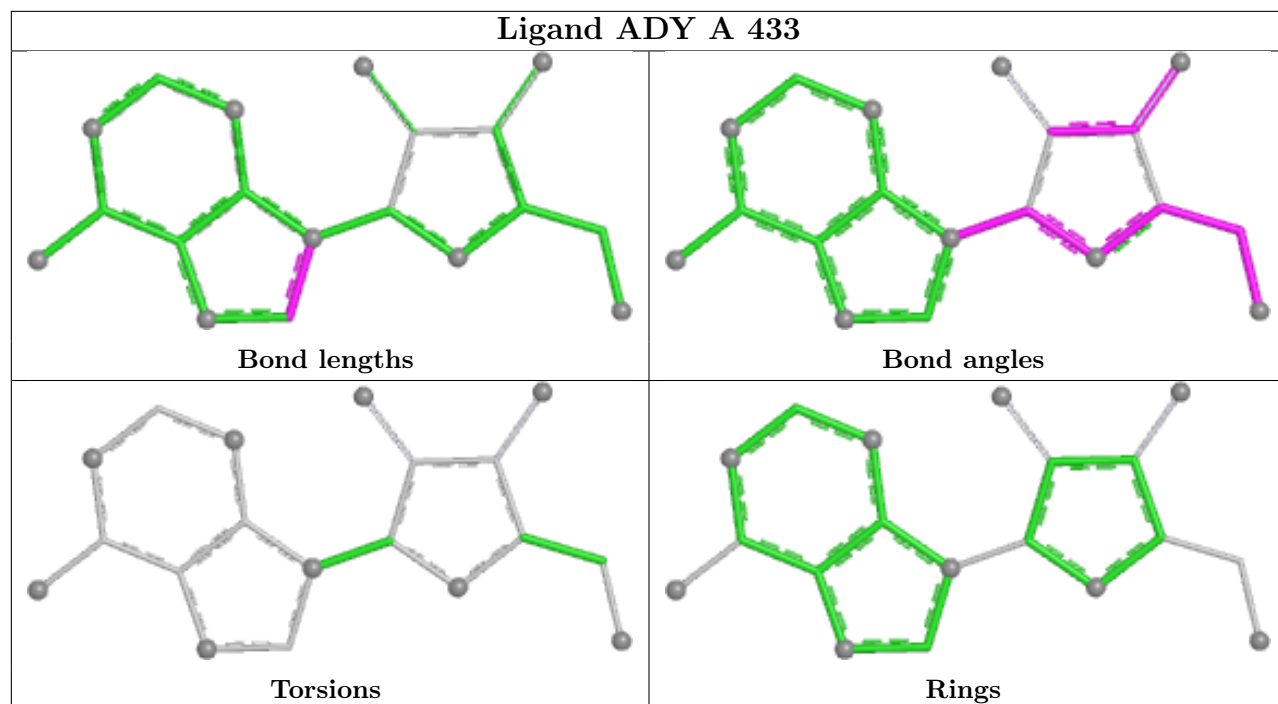
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3432	NAI	2	0
2	C	2432	NAI	2	0
2	A	432	NAI	2	0
2	B	1432	NAI	2	0

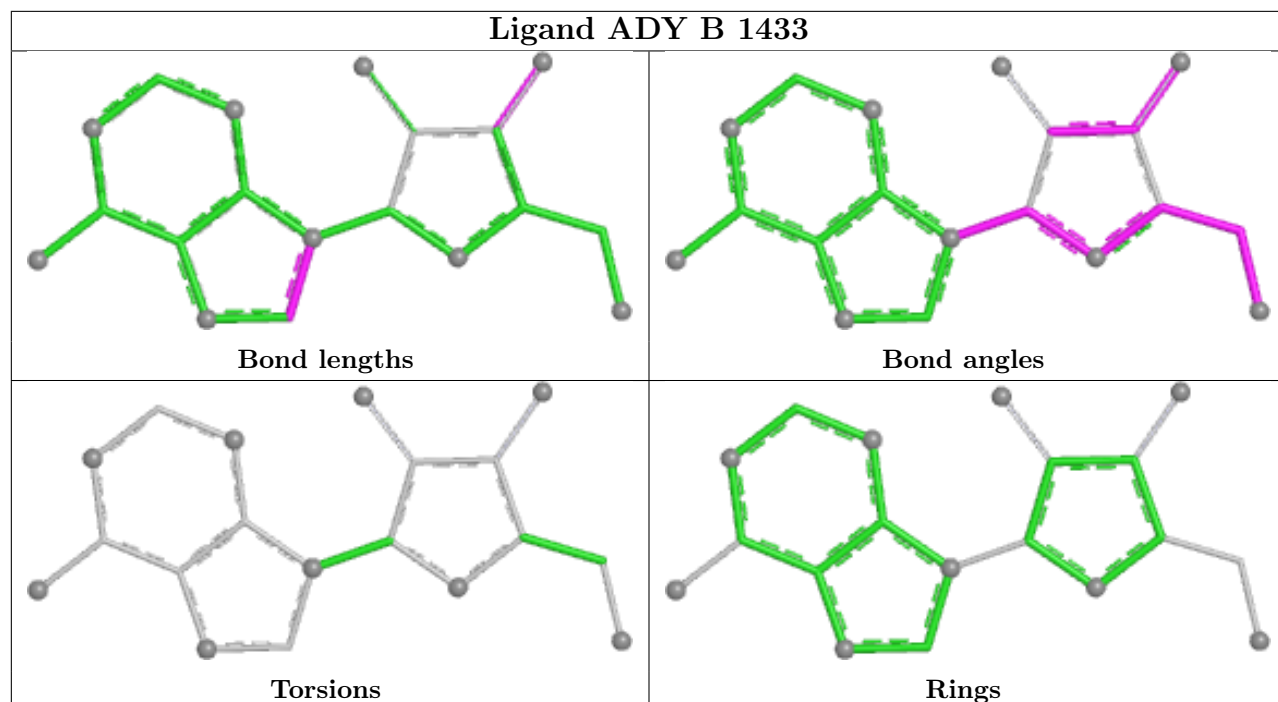
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



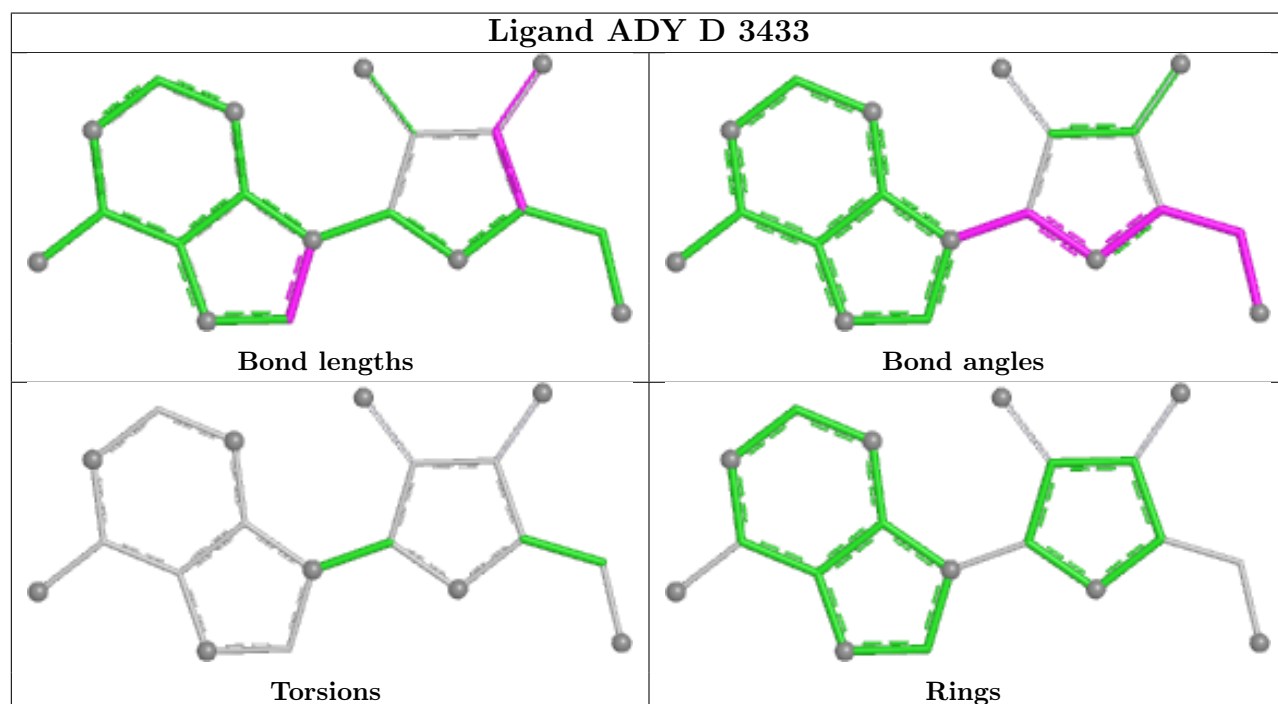


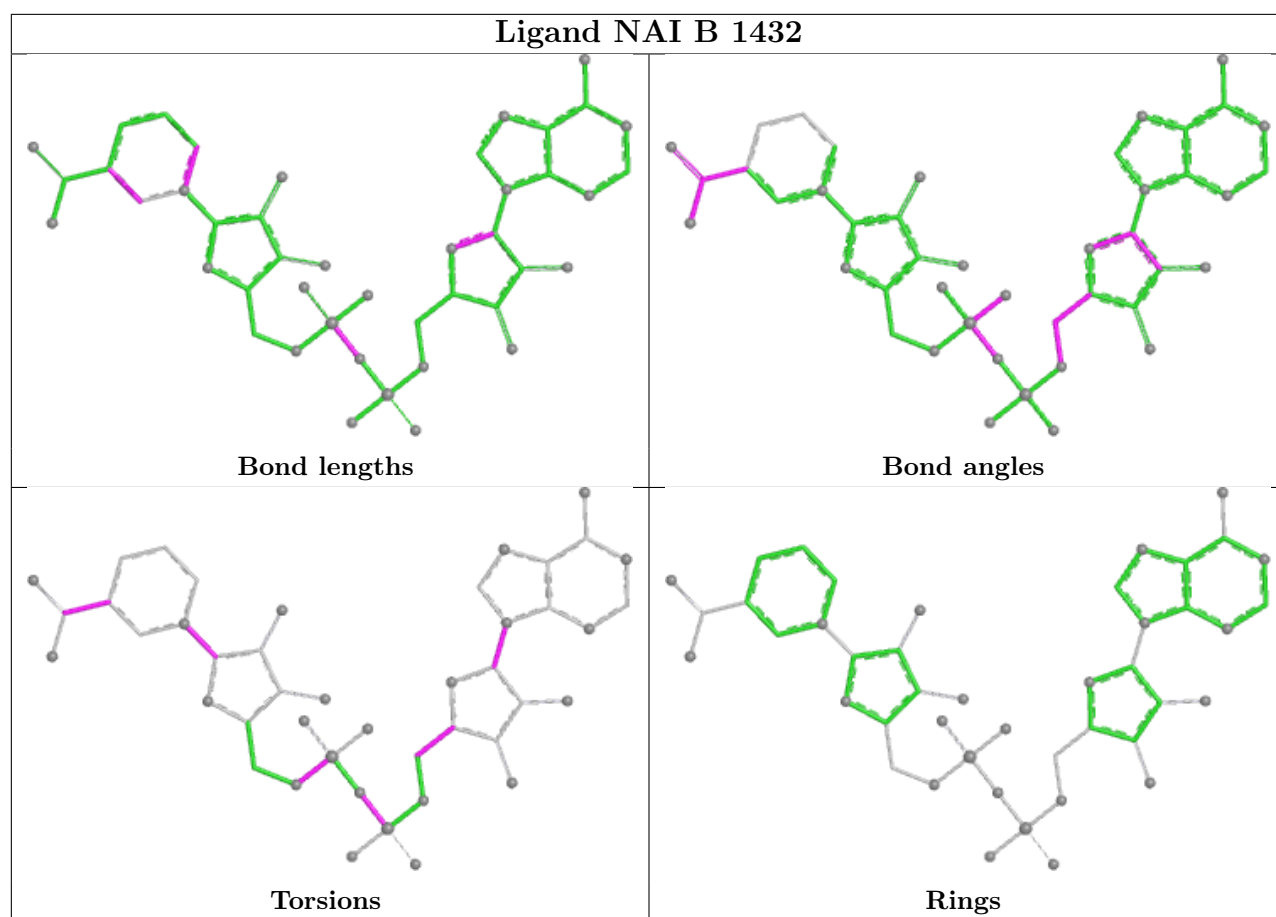


Ligand ADY B 1433



Ligand ADY D 3433





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.