Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:34 PM GMT

PDB ID	:	1KY5
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

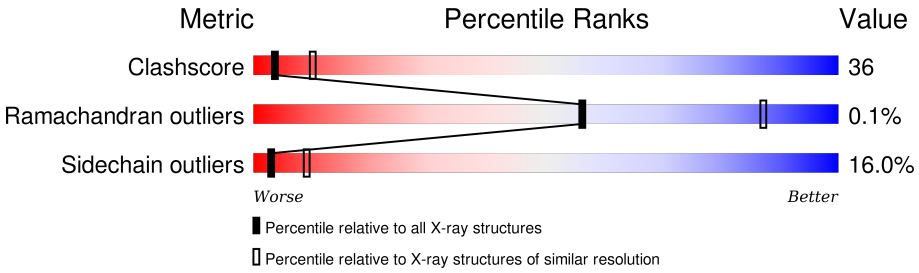
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	431	51% 41% 9%
1	B	431	48% 42% 10%
1	C	431	47% 44% 9%
1	D	431	48% 42% 10%

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.

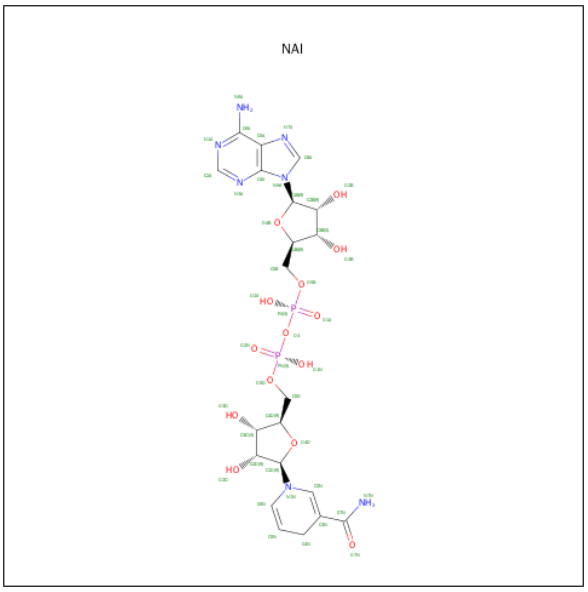
- Molecule 1 is a protein called S-adenosylhomocysteine hydrolase.

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:

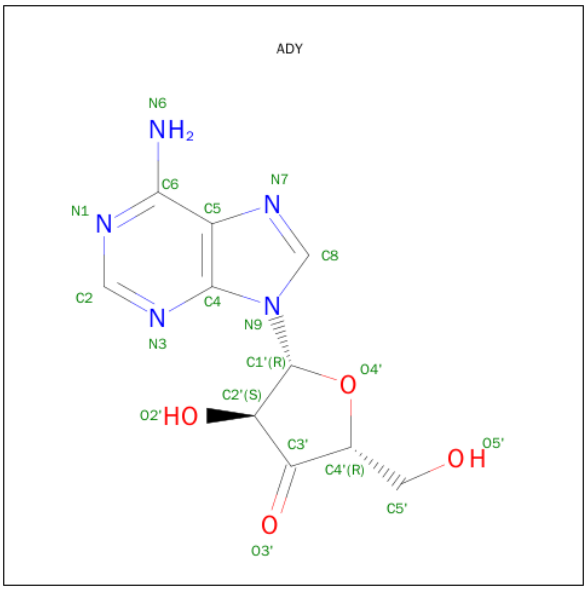
Chain	Residue	Modelled	Actual	Comment	Reference
A	244	GLU	ASP	ENGINEERED	UNP P10760
B	1244	GLU	ASP	ENGINEERED	UNP P10760
C	2244	GLU	ASP	ENGINEERED	UNP P10760
D	3244	GLU	ASP	ENGINEERED	UNP P10760

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 3'-OXO-ADENOSINE (three-letter code: ADY) (formula: $C_{10}H_{11}N_5O_4$).



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		

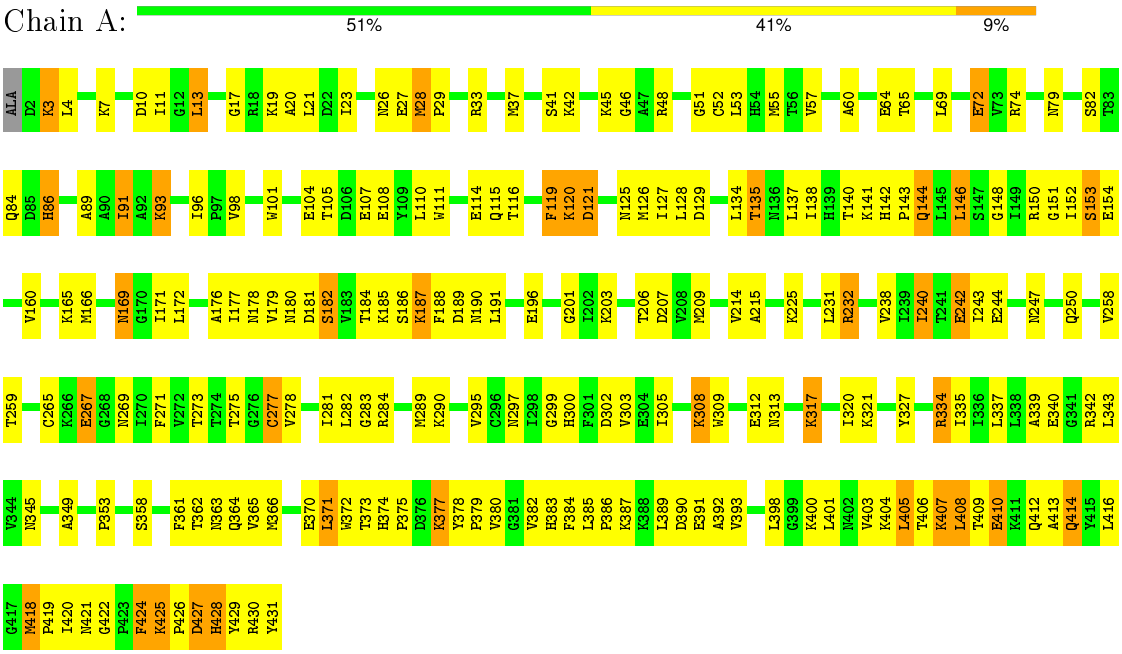
3 Residue-property plots (i)

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

Note EDS was not executed.

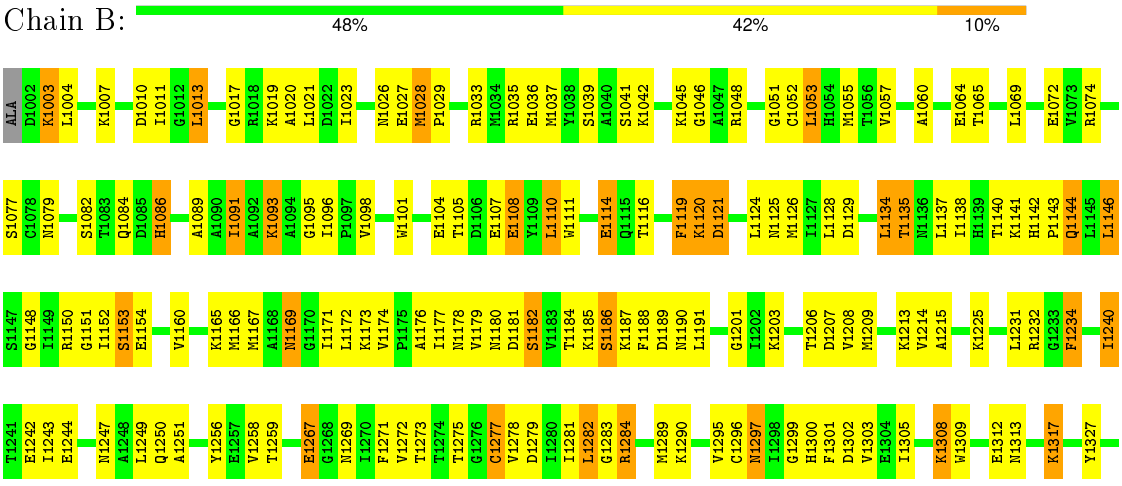
- Molecule 1: S-adenosylhomocysteine hydrolase

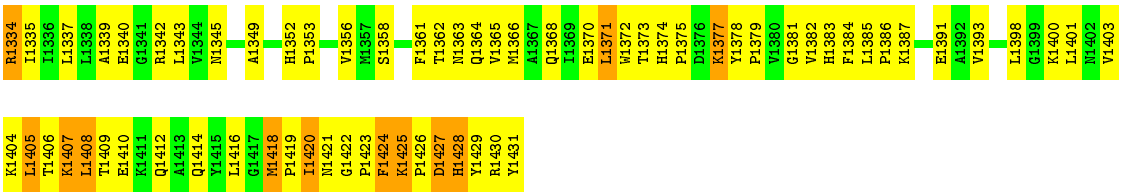
Chain A:



- Molecule 1: S-adenosylhomocysteine hydrolase

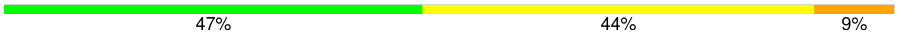
Chain B:

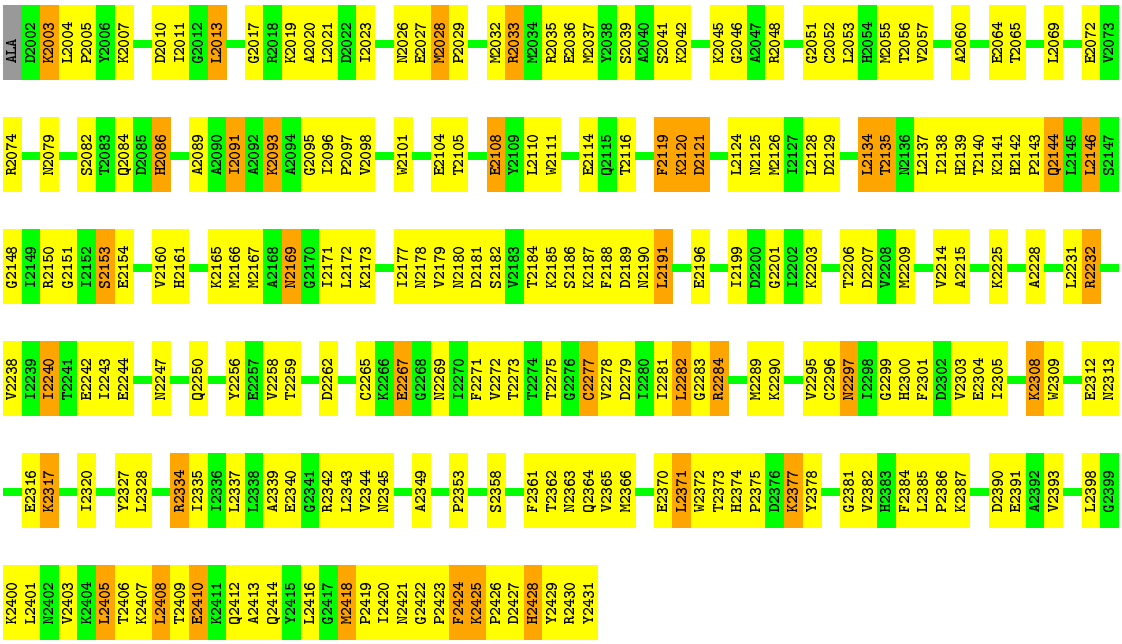




- Molecule 1: S-adenosylhomocysteine hydrolase

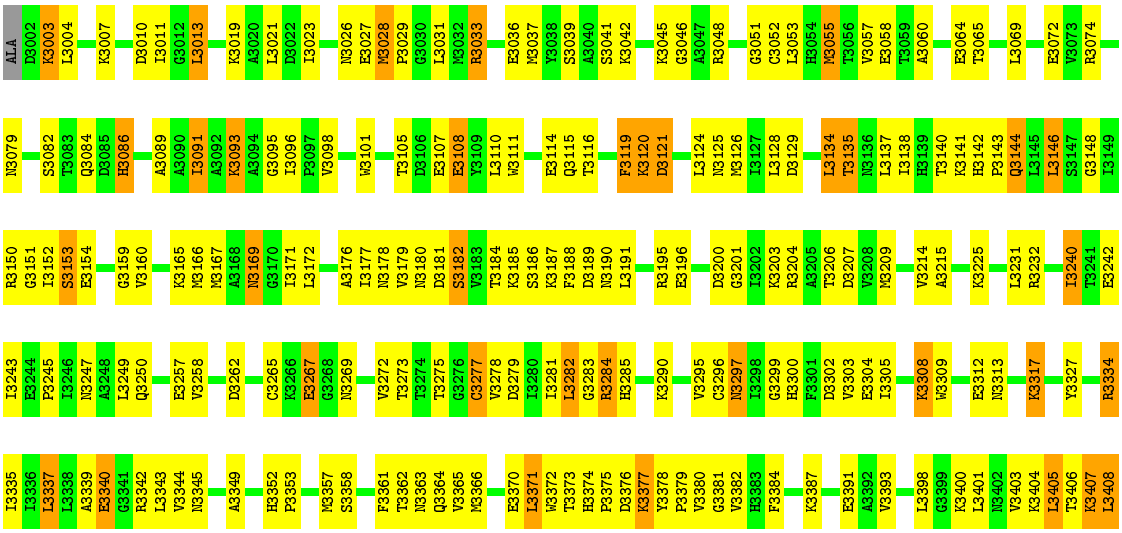
Chain C:





- Molecule 1: S-adenosylhomocysteine hydrolase

Chain D:




T3409
E3410
K3411
Q3412
A3413
Q3414
Y3415
L3416
G3417
M3418
P3419
I3420
N3421
G3422
P3423
F3424
K3425
P3426
D3427
H3428
Y3429
R3430
Y3431

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	0.41	0/3385	0.63	0/4580
1	B	0.41	0/3385	0.63	0/4580
1	C	0.44	0/3385	0.63	0/4580
1	D	0.42	0/3385	0.66	1/4580 (0.0%)
All	All	0.42	0/13540	0.64	1/18320 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	3376	ASP	CB-CG-OD1	-10.07	109.24	118.30

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	257	0
1	B	3320	0	3343	255	0
1	C	3320	0	3343	268	0
1	D	3320	0	3343	278	1
2	A	44	0	27	2	0
2	B	44	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	44	0	27	1	0
2	D	44	0	27	1	0
3	A	19	0	11	0	0
3	B	19	0	11	0	0
3	C	19	0	10	1	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	965	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 36.

All (965) 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:HD2	1:C:2120:LYS:H	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:HD2	1:D:3120:LYS:H	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:CD	1:C:2120:LYS:H	1.72	1.01
1:B:1060:ALA:HB1	1:B:1091:ILE:HD11	1.38	1.00
1:B:1120:LYS:HD2	1:B:1120:LYS:H	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: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:D:3169:ASN:HB2	1:D:3171:ILE:HD11	1.49	0.94
1:A:308:LYS:HD2	1:A:308:LYS:H	1.28	0.94
1:C:2308:LYS:HD2	1:C:2308:LYS:H	1.32	0.94
1:B:1408:LEU:O	1:B:1420:ILE:HD11	1.66	0.93
1:A:126:MET:HE3	1:A:150:ARG:HB3	1.49	0.93
1:D:3120:LYS:CD	1:D:3120:LYS:H	1.77	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3126:MET:HE3	1:D:3150:ARG:HB3	1.50	0.93
1:D:3409:THR:O	1:D:3420:ILE:CD1	2.17	0.93
1:D:3308:LYS:HD2	1:D:3308:LYS:H	1.32	0.92
1:B:1408:LEU:C	1:B:1420:ILE:HD11	1.90	0.92
1:D:3225:LYS:HZ1	1:D:3250:GLN:HE22	1.17	0.91
1:D:3214:VAL:H	1:D:3269:ASN:HD22	0.96	0.91
1:B:1169:ASN:HB2	1:B:1171:ILE:HD11	1.51	0.91
1:C:2408:LEU:C	1:C:2420:ILE:HD11	1.90	0.91
1:B:1120:LYS:CD	1:B:1120:LYS:H	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:A:408:LEU:C	1:A:420:ILE:HD11	1.92	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:3408:LEU:HB3	1:D:3420:ILE:HD12	1.54	0.88
1:D:3214:VAL:H	1:D:3269:ASN:ND2	1.72	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
1:C:2214:VAL:H	1:C:2269:ASN:ND2	1.72	0.87
1:C:2126:MET:HE3	1:C:2150:ARG:HB3	1.57	0.87
1:B:1308:LYS:H	1:B:1308:LYS:HD2	1.39	0.87
1:C:2120:LYS:N	1:C:2120:LYS:HD2	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:D:3409:THR:O	1:D:3420:ILE:HD13	1.78	0.84
1:B:1126:MET:HE3	1:B:1150:ARG:HB3	1.60	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:C:2416:LEU:HD21	1:D:3277:CYS:HB2	1.60	0.83
1:D:3408:LEU:C	1:D:3420:ILE:HD11	1.99	0.82
1:D:3120:LYS:N	1:D:3120:LYS:HD2	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ASN:HB2	1:A:171:ILE:CD1	2.10	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:D:3060:ALA:CB	1:D:3091:ILE:HD11	2.09	0.81
1:B:1120:LYS:N	1:B:1120:LYS:HD2	1.95	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:HG2	1:D:3430:ARG:HA	1.61	0.79
1:C:2430:ARG:HA	1:D:3430:ARG:HG2	1.64	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:HD11	2.02	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
1:A:430:ARG:HG2	1:B:1430:ARG:CG	2.14	0.78
1:A:48:ARG:HD3	1:A:121:ASP:CG	2.03	0.78
1:A:430:ARG:HG2	1:B:1430:ARG:HG2	1.64	0.78
1:A:120:LYS:N	1:A:120:LYS:HD2	1.99	0.78
1:A:225:LYS:NZ	1:A:250:GLN:HE22	1.82	0.78
1:A:153:SER:HB3	1:A:364:GLN:NE2	1.99	0.78
1:D:3048:ARG:HD3	1:D:3121:ASP:CG	2.05	0.77
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: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:A:430:ARG:HG2	1:B:1430:ARG:CA	2.17	0.74
1:A:214:VAL:N	1:A:269:ASN:HD22	1.78	0.74
1:B:1126:MET:CE	1:B:1150:ARG:HB3	2.16	0.74
1:D:3007:LYS:HG2	1:D:3101:TRP:CZ3	2.22	0.74
1:D:3409:THR:C	1:D:3420:ILE:CD1	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ASP:HB3	1:A:13:LEU:HD22	1.69	0.74
1:C:2153:SER:HB3	1:C:2364:GLN:NE2	2.02	0.74
1:C:2143:PRO:HA	1:C:2146:LEU:HD22	1.70	0.74
1:D:3408:LEU:HB3	1:D:3420:ILE:CD1	2.17	0.74
1:D:3225:LYS:NZ	1:D:3250:GLN:HE22	1.85	0.73
1:C:2048:ARG:HD3	1:C:2121:ASP:CG	2.09	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:D:3048:ARG:HD3	1:D:3121:ASP:OD2	1.89	0.73
1:A:140:THR:OG1	1:A:141:LYS:HD2	1.88	0.73
1:D:3153:SER:HB3	1:D:3364:GLN:HE21	1.54	0.72
1:A:27:GLU:O	1:A:29:PRO:HD3	1.89	0.72
1:D:3027:GLU:O	1:D:3029:PRO:HD3	1.89	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
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:C:2150:ARG:HD2	1:C:2372:TRP:HA	1.71	0.71
1:B:1153:SER:HB3	1:B:1364:GLN:NE2	2.06	0.71
1:B:1153:SER:HB3	1:B:1364:GLN:HE21	1.55	0.71
1:C:2126:MET:CE	1:C:2150:ARG:HB3	2.21	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:2010:ASP:HB3	1:C:2013:LEU:HD22	1.73	0.70
1:C:2430:ARG:NH1	1:C:2430:ARG:HB2	2.06	0.70
1:D:3169:ASN:HB2	1:D:3171:ILE:CD1	2.21	0.70
1:A:150:ARG:HD2	1:A:372:TRP:HA	1.72	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:C:2178:ASN:HD21	1:C:2181:ASP:CG	1.94	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: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:C:2225:LYS:HZ1	1:C:2250:GLN:HE22	1.40	0.69
1:C:2180:ASN:HA	1:C:2185:LYS:HD2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ILE:HG13	1:C:2023:ILE:HD11	1.75	0.69
1:C:2418:MET:SD	1:C:2424:PHE:HB3	2.32	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:B:1048:ARG:HD3	1:B:1121:ASP:CG	2.14	0.69
1:D:3398:LEU:HD23	1:D:3405:LEU:HD22	1.74	0.69
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:2408:LEU:HB3	1:C:2420:ILE:HD12	1.76	0.68
1:C:2409:THR:C	1:C:2420:ILE:HD13	2.14	0.68
1:C:2169:ASN:HB2	1:C:2171:ILE:CD1	2.24	0.68
1:A:21:LEU:HD21	1:A:60:ALA:HB3	1.76	0.68
1:D:3430:ARG:HB2	1:D:3430:ARG:NH1	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:D:3178:ASN:HD21	1:D:3181:ASP:CG	1.97	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:23:ILE:HD11	1:C:2320:ILE:HG13	1.75	0.67
1:D:3418:MET:HB2	1:D:3424:PHE:HD1	1.60	0.67
1:D:3339:ALA:O	1:D:3342:ARG:HB2	1.95	0.67
1:C:2027:GLU:O	1:C:2029:PRO:HD3	1.95	0.67
1:C:2011:ILE:HA	1:C:2089:ALA:HB1	1.77	0.67
1:A:430:ARG:HB2	1:A:430:ARG:NH1	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:409:THR:OG1	1:A:412:GLN:HG3	1.96	0.66
1:A:408:LEU:HB3	1:A:420:ILE:HD12	1.77	0.66
1:A:33:ARG:O	1:A:37:MET:HG3	1.95	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:1408:LEU:C	1:B:1420:ILE:CD1	2.64	0.66
1:B:1019:LYS:O	1:B:1023:ILE:HG13	1.96	0.66
1:B:1409:THR:C	1:B:1420:ILE:HD13	2.17	0.66
1:C:2384:PHE:CZ	1:D:3428:HIS:HB3	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1225:LYS:NZ	1:B:1250:GLN:HE22	1.93	0.66
1:A:430:ARG:CG	1:B:1430:ARG:HA	2.21	0.66
1:A:428:HIS:HB3	1:B:1384:PHE:CZ	2.30	0.66
1:D:3072:GLU:OE2	1:D:3120:LYS:HD3	1.95	0.65
1:A:428:HIS:HB3	1:B:1384:PHE:HZ	1.61	0.65
1:C:2277:CYS:CB	1:D:3416:LEU:HD21	2.23	0.65
1:C:2409:THR:C	1:C:2420:ILE:CD1	2.64	0.65
1:A:3:LYS:HE2	1:A:74:ARG:NH2	2.12	0.65
1:B:1178:ASN:HD21	1:B:1181:ASP:CG	2.00	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:B:1409:THR:C	1:B:1420:ILE:CD1	2.65	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
1:B:1398:LEU:HD23	1:B:1405:LEU:HD22	1.77	0.64
1:D:3011:ILE:HA	1:D:3089:ALA:HB1	1.79	0.64
1:C:2003:LYS:HE3	1:C:2074:ARG:HH12	1.63	0.64
1:A:295:VAL:HG12	1:A:305:ILE:HD13	1.79	0.64
1:D:3409:THR:H	1:D:3412:GLN:HE21	1.43	0.64
1:B:1387:LYS:HE2	1:B:1425:LYS:O	1.97	0.64
1:A:11:ILE:HA	1:A:89:ALA:HB1	1.80	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:A:409:THR:C	1:A:420:ILE:CD1	2.67	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: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:C:2387:LYS:HE2	1:C:2425:LYS:O	1.98	0.63
1:B:1011:ILE:HA	1:B:1089:ALA:HB1	1.80	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:2428:HIS:N	1:C:2428:HIS:ND1	2.47	0.62
1:C:2384:PHE:HZ	1:D:3428:HIS:HB3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:2308:LYS:CD	1:C:2308:LYS:H	2.10	0.62
1:A:408:LEU:C	1:A:420:ILE:CD1	2.67	0.62
1:C:2019:LYS:O	1:C:2023:ILE:HG13	1.98	0.62
1:B:1065:THR:O	1:B:1069:LEU:HD13	1.98	0.62
1:A:178:ASN:HD21	1:A:181:ASP:CG	2.02	0.62
1:C:2151:GLY:HA3	1:C:2371:LEU:HG	1.82	0.62
1:B:1430:ARG:NH1	1:B:1430:ARG:HB2	2.14	0.62
1:A:409:THR:C	1:A:420:ILE:HD13	2.20	0.62
1:D:3137:LEU:O	1:D:3141:LYS:HB2	1.99	0.62
1:C:2125:ASN:HA	1:C:2148:GLY:O	1.99	0.62
1:A:345:ASN:O	1:A:349:ALA:HB3	2.00	0.62
1:C:2419:PRO:HG2	1:C:2422:GLY:HA3	1.81	0.62
1:A:430:ARG:O	1:B:1430:ARG:HD2	2.00	0.62
1:A:418:MET:SD	1:A:424:PHE:HB3	2.39	0.62
1:B:1003:LYS:HG3	1:B:1004:LEU:N	2.15	0.62
1:A:419:PRO:HG2	1:A:422:GLY:HA3	1.80	0.62
1:D:3418:MET:SD	1:D:3424:PHE:HB3	2.40	0.61
1:B:1418:MET:HB2	1:B:1424:PHE:HD1	1.65	0.61
1:B:1418:MET:SD	1:B:1424:PHE:HB3	2.40	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: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:1240:ILE:O	1:B:1258:VAL:HA	2.01	0.60
1:C:2048:ARG:HD2	1:C:2119:PHE:HB2	1.84	0.60
1:B:1048:ARG:HD2	1:B:1119:PHE:HB2	1.82	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:D:3308:LYS:CD	1:D:3308:LYS:H	2.11	0.60
1:B:1428:HIS:ND1	1:B:1428:HIS:N	2.50	0.60
1:B:1125:ASN:HA	1:B:1148:GLY:O	2.01	0.60
1:A:91:ILE:N	1:A:91:ILE:HD13	2.17	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:2065:THR:O	1:C:2069:LEU:HD13	2.02	0.60
1:C:2408:LEU:C	1:C:2420:ILE:CD1	2.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:3387:LYS:HE2	1:D:3425:LYS:O	2.02	0.59
1:C:2426:PRO:HB2	1:C:2428:HIS:CE1	2.37	0.59
1:B:1363:ASN:ND2	1:B:1393:VAL:HG21	2.18	0.59
1:A:428:HIS:N	1:A:428:HIS:ND1	2.50	0.59
1:D:3169:ASN:HD22	1:D:3171:ILE:CD1	2.16	0.59
1:D:3409:THR:CA	1:D:3420:ILE:HD11	2.32	0.58
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:B:1167:MET:SD	1:B:1381:GLY:HA2	2.43	0.58
1:B:1209:MET:SD	1:D:3353:PRO:HG2	2.44	0.58
1:B:1027:GLU:O	1:B:1029:PRO:HD3	2.02	0.58
1:B:1308:LYS:H	1:B:1308:LYS:CD	2.12	0.58
1:C:2187:LYS:HD3	1:D:3430:ARG:NH1	2.12	0.58
1:B:1418:MET:CG	1:B:1424:PHE:HB3	2.33	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:A:125:ASN:HA	1:A:148:GLY:O	2.04	0.58
1:B:1408:LEU:HA	1:B:1412:GLN:NE2	2.18	0.58
1:D:3126:MET:HE2	1:D:3151:GLY:N	2.19	0.58
1:C:2225:LYS:NZ	1:C:2250:GLN:NE2	2.50	0.58
1:B:1051:GLY:HA2	1:B:1128:LEU:O	2.03	0.58
1:A:430:ARG:HH12	1:B:1187:LYS:HD3	1.67	0.58
1:A:21:LEU:CD2	1:A:60:ALA:HB3	2.33	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:D:3418:MET:CG	1:D:3424:PHE:HB3	2.35	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:3177:ILE:HG13	1:D:3371:LEU:HD21	1.87	0.57
1:C:2247:ASN:HD21	1:D:3431:TYR:HE2	1.52	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:D:3178:ASN:ND2	1:D:3181:ASP:HB2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3424:PHE:N	1:D:3424:PHE:CD2	2.73	0.57
1:C:2430:ARG:CZ	1:C:2430:ARG:HB2	2.34	0.57
1:C:2430:ARG:HG2	1:D:3430:ARG:CG	2.34	0.57
1:C:2137:LEU:O	1:C:2141:LYS:HB2	2.05	0.57
1:D:3185:LYS:HD3	1:D:3185:LYS:C	2.25	0.57
1:C:2091:ILE:N	1:C:2091:ILE:HD13	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:B:1247:ASN:O	1:B:1250:GLN:HB2	2.05	0.57
1:C:2418:MET:CG	1:C:2424:PHE:HB3	2.35	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:A:93:LYS:NZ	4:A:5155:HOH:O	2.37	0.57
1:D:3408:LEU:HA	1:D:3412:GLN:NE2	2.20	0.57
1:B:1419:PRO:HG2	1:B:1422:GLY:CA	2.35	0.56
1:B:1178:ASN:ND2	1:B:1181:ASP:HB2	2.21	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:N	1:D:3428:HIS:ND1	2.53	0.56
1:B:1278:VAL:HG12	1:B:1303:VAL:CG2	2.34	0.56
1:A:387:LYS:HE2	1:A:425:LYS:O	2.05	0.56
1:B:1299:GLY:O	1:B:1343:LEU:HD11	2.05	0.56
1:A:278:VAL:HG12	1:A:303:VAL:CG2	2.36	0.56
1:D:3278:VAL:HG12	1:D:3303:VAL:CG2	2.36	0.56
1:C:2409:THR:N	1:C:2420:ILE:HD11	2.20	0.56
1:A:308:LYS:CD	1:A:308:LYS:H	2.09	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:B:1033:ARG:O	1:B:1037:MET:HG3	2.06	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:C:2409:THR:CA	1:C:2420:ILE:HD11	2.36	0.56
1:D:3137:LEU:HA	1:D:3141:LYS:HD3	1.87	0.56
1:C:2424:PHE:CD2	1:C:2424:PHE:N	2.73	0.56
1:D:3003:LYS:HG3	1:D:3004:LEU:N	2.21	0.56
1:B:1424:PHE:N	1:B:1424:PHE:CD2	2.73	0.56
1:C:2278:VAL:HG12	1:C:2303:VAL:CG2	2.36	0.56
1:C:2430:ARG:HG2	1:D:3430:ARG:CA	2.34	0.56
1:C:2419:PRO:HB2	1:C:2422:GLY:H	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:THR:C	1:A:375:PRO:HD2	2.26	0.56
1:B:1091:ILE:N	1:B:1091:ILE:HD13	2.21	0.56
1:A:142:HIS:HA	1:A:144:GLN:OE1	2.06	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:3119:PHE:N	1:D:3119:PHE:CD1	2.74	0.55
1:A:419:PRO:HB2	1:A:422:GLY:H	1.71	0.55
1:B:1091:ILE:HB	1:B:1098:VAL:HG21	1.88	0.55
1:C:2409:THR:N	1:C:2412:GLN:HE21	2.04	0.55
1:C:2185:LYS:HD3	1:C:2185:LYS:C	2.27	0.55
1:A:185:LYS:HD3	1:A:185:LYS:C	2.27	0.55
1:D:3125:ASN:HA	1:D:3148:GLY:O	2.06	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:B:1154:GLU:O	1:B:1179:VAL:HB	2.07	0.55
1:A:370:GLU:HB3	1:A:378:TYR:CE1	2.42	0.55
1:D:3028:MET:HB3	1:D:3358:SER:HB2	1.89	0.55
1:B:1419:PRO:HG2	1:B:1422:GLY:C	2.28	0.55
1:A:425:LYS:HE2	1:A:429:TYR:CE1	2.41	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:A:299:GLY:O	1:A:343:LEU:HD11	2.07	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:409:THR:N	1:A:412:GLN:HE21	2.05	0.54
1:A:374:HIS:N	1:A:375:PRO:CD	2.70	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:D:3413:ALA:CB	1:D:3420:ILE:CD1	2.83	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:THR:HG22	1:A:407:LYS:N	2.22	0.54
1:A:91:ILE:HB	1:A:98:VAL:HG21	1.89	0.54
1:C:2431:TYR:HE2	1:D:3247:ASN:ND2	2.06	0.54
1:B:1003:LYS:HE3	1:B:1074:ARG:HH12	1.73	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:D:3060:ALA:O	1:D:3064:GLU:HG3	2.08	0.53
1:B:1425:LYS:HE2	1:B:1429:TYR:CE1	2.43	0.53
1:D:3419:PRO:HG2	1:D:3422:GLY:C	2.28	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
1:C:2334:ARG:O	1:C:2335:ILE:HD13	2.08	0.53
1:A:406:THR:HB	1:B:1243:ILE:HG22	1.90	0.53
1:C:2374:HIS:N	1:C:2375:PRO:CD	2.72	0.53
1:B:1295:VAL:HG12	1:B:1305:ILE:HD13	1.91	0.53
1:C:2003:LYS:HG3	1:C:2004:LEU:N	2.23	0.53
1:B:1426:PRO:HB2	1:B:1428:HIS:CE1	2.43	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: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: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:C:2119:PHE:N	1:C:2119:PHE:CD1	2.77	0.53
1:D:3021:LEU:CD2	1:D:3060:ALA:HB3	2.39	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: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:B:1312:GLU:HG3	1:B:1313:ASN:ND2	2.24	0.52
1:B:1126:MET:HE2	1:B:1151:GLY:N	2.24	0.52
1:A:19:LYS:O	1:A:23:ILE:HG13	2.09	0.52
1:D:3374:HIS:O	1:D:3377:LYS:HG3	2.09	0.52
1:C:2244:GLU:HG3	1:D:3425:LYS:HZ2	1.75	0.52
1:D:3185:LYS:O	1:D:3189:ASP:HB3	2.08	0.52
1:A:3:LYS:HG3	1:A:4:LEU:N	2.24	0.52
1:D:3418:MET:HB3	1:D:3424:PHE:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1374:HIS:N	1:B:1375:PRO:CD	2.71	0.52
1:A:121:ASP:N	1:A:121:ASP:OD1	2.33	0.52
1:A:169:ASN:HD22	1:A:171:ILE:CD1	2.23	0.52
1:A:424:PHE:CD2	1:A:424:PHE:N	2.77	0.52
1:D:3419:PRO:HB2	1:D:3422:GLY:H	1.74	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:A:209:MET:HB2	1:C:2353:PRO:HB2	1.90	0.52
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:A:10:ASP:HB3	1:A:13:LEU:CD2	2.39	0.52
1:D:3105:THR:H	1:D:3108:GLU:HG3	1.73	0.52
1:C:2039:SER:O	1:C:2042:LYS:HG2	2.10	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:B:1409:THR:O	1:B:1420:ILE:CD1	2.58	0.52
1:A:379:PRO:HD2	1:A:383:HIS:NE2	2.25	0.52
1:A:317:LYS:HD2	1:A:327:TYR:CZ	2.44	0.52
1:D:3137:LEU:HD12	1:D:3141:LYS:HB2	1.90	0.52
1:A:419:PRO:HG2	1:A:422:GLY:C	2.30	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:A:65:THR:O	1:A:69:LEU:HD13	2.09	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:B:1184:THR:HA	1:B:1188:PHE:CD1	2.45	0.52
1:D:3409:THR:N	1:D:3412:GLN:HE21	2.07	0.51
1:D:3334:ARG:O	1:D:3335:ILE:HD13	2.11	0.51
1:A:119:PHE:N	1:A:119:PHE:CD1	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: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:408:LEU:HA	1:A:412:GLN:HE21	1.76	0.51
1:A:283:GLY:HA3	1:A:309:TRP:CE2	2.45	0.51
1:B:1283:GLY:HA3	1:B:1309:TRP:CE2	2.46	0.51
1:B:1129:ASP:OD2	1:B:1135:THR:HG23	2.09	0.51
1:A:166:MET:O	1:A:171:ILE:HD12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1169:ASN:HD22	1:B:1171:ILE:CD1	2.24	0.51
1:A:23:ILE:CD1	1:C:2320:ILE:HG13	2.40	0.51
1:B:1419:PRO:HB2	1:B:1422:GLY:H	1.75	0.51
1:A:374:HIS:O	1:A:377:LYS:HG3	2.11	0.51
1:B:1215:ALA:HB1	1:B:1231:LEU:HD13	1.91	0.51
1:D:3166:MET:HA	1:D:3171:ILE:HD12	1.93	0.51
1:A:418:MET:CG	1:A:424:PHE:HB3	2.41	0.51
1:C:2247:ASN:O	1:C:2250:GLN:HB2	2.11	0.51
1:D:3010:ASP:HB3	1:D:3013:LEU:CD2	2.37	0.51
1:C:2398:LEU:CD2	1:C:2405:LEU:HD22	2.41	0.51
1:C:2074:ARG:HB3	1:C:2116:THR:HB	1.92	0.51
1:C:2374:HIS:O	1:C:2377:LYS:HG3	2.10	0.51
1:A:166:MET:HA	1:A:171:ILE:CD1	2.40	0.51
1:A:409:THR:N	1:A:420:ILE:HD11	2.25	0.51
1:C:2401:LEU:HD12	1:D:3249:LEU:CD1	2.41	0.51
1:D:3409:THR:C	1:D:3420:ILE:HD13	2.28	0.50
1:D:3418:MET:CB	1:D:3424:PHE:HB3	2.41	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:B:1409:THR:N	1:B:1420:ILE:HD11	2.26	0.50
1:D:3093:LYS:C	1:D:3095:GLY:N	2.64	0.50
1:C:2154:GLU:HG3	1:C:2160:VAL:HG23	1.93	0.50
1:D:3186:SER:O	1:D:3190:ASN:HB2	2.11	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:129:ASP:OD2	1:A:135:THR:HG23	2.12	0.50
1:D:3398:LEU:CD2	1:D:3405:LEU:HD22	2.41	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:B:1039:SER:O	1:B:1042:LYS:HG2	2.12	0.50
1:D:3317:LYS:HD2	1:D:3327:TYR:CZ	2.46	0.50
1:C:2003:LYS:HE2	1:C:2074:ARG:HH22	1.75	0.50
1:D:3352:HIS:HB2	1:D:3357:MET:SD	2.52	0.50
1:C:2279:ASP:HB3	1:C:2282:LEU:HD11	1.93	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:D:3279:ASP:HB3	1:D:3282:LEU:HD11	1.94	0.50
1:B:1003:LYS:HE2	1:B:1074:ARG:HH22	1.77	0.50
1:D:3154:GLU:O	1:D:3179:VAL:HB	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2283:GLY:HA3	1:C:2309:TRP:CE2	2.46	0.50
1:A:206:THR:O	1:A:207:ASP:HB2	2.11	0.50
1:A:430:ARG:HG2	1:B:1430:ARG:CB	2.42	0.50
1:B:1048:ARG:HD2	1:B:1119:PHE:CB	2.42	0.50
1:C:2166:MET:HA	1:C:2171:ILE:CD1	2.42	0.50
1:B:1004:LEU:HD12	1:B:1111:TRP:HZ2	1.76	0.50
1:A:184:THR:HA	1:A:188:PHE:CD1	2.47	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:D:3373:THR:C	1:D:3375:PRO:HD2	2.32	0.49
1:B:1206:THR:O	1:B:1207:ASP:HB2	2.12	0.49
1:A:430:ARG:HD2	1:B:1430:ARG:O	2.13	0.49
1:B:1408:LEU:O	1:B:1420:ILE:CD1	2.51	0.49
1:C:2419:PRO:HG2	1:C:2422:GLY:CA	2.42	0.49
1:A:404:LYS:HB2	1:B:1259:THR:HA	1.95	0.49
1:C:2385:LEU:HG	1:C:2386:PRO:HD2	1.93	0.49
1:C:2121:ASP:OD1	1:C:2121:ASP:N	2.33	0.49
1:A:247:ASN:O	1:A:250:GLN:HB2	2.12	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: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: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: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:A:203:LYS:NZ	1:C:2196:GLU:HB3	2.28	0.49
1:C:2409:THR:O	1:C:2420:ILE:CD1	2.61	0.49
1:D:3166:MET:O	1:D:3171:ILE:HD12	2.12	0.49
1:D:3126:MET:HE2	1:D:3151:GLY:H	1.78	0.49
1:D:3052:CYS:HB3	1:D:3129:ASP:OD1	2.13	0.49
1:C:2048:ARG:HD2	1:C:2119:PHE:CB	2.43	0.49
1:B:1401:LEU:HB2	1:B:1403:VAL:HG23	1.95	0.49
1:A:267:GLU:O	1:A:290:LYS:HE3	2.13	0.49
1:C:2045:LYS:HD3	1:C:2046:GLY:N	2.28	0.49
1:B:1409:THR:O	1:B:1420:ILE:HD13	2.12	0.49
1:A:126:MET:CE	1:A:151:GLY:N	2.76	0.49
1:D:3225:LYS:NZ	1:D:3250:GLN:NE2	2.56	0.49
1:C:2215:ALA:HB1	1:C:2231:LEU:HD13	1.95	0.49
1:D:3430:ARG:CZ	1:D:3430:ARG:HB2	2.43	0.48
1:B:1385:LEU:HG	1:B:1386:PRO:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3167:MET:SD	1:D:3381:GLY:HA2	2.53	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:C:2409:THR:O	1:C:2420:ILE:HD13	2.13	0.48
1:A:247:ASN:ND2	1:B:1431:TYR:HE2	2.11	0.48
1:A:127:ILE:HD11	1:A:138:ILE:HD13	1.96	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:B:1362:THR:HB	1:B:1393:VAL:HG13	1.96	0.48
1:B:1045:LYS:HD3	1:B:1046:GLY:N	2.28	0.48
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.29	0.48
1:D:3410:GLU:OE1	1:D:3410:GLU:HA	2.13	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:C:2327:TYR:O	1:C:2334:ARG:HA	2.13	0.48
1:D:3093:LYS:C	1:D:3095:GLY:H	2.17	0.48
1:C:2344:VAL:HG13	1:C:2345:ASN:N	2.27	0.48
1:C:2267:GLU:O	1:C:2290:LYS:HE3	2.14	0.48
1:A:105:THR:H	1:A:108:GLU:HG3	1.78	0.48
1:D:3413:ALA:CB	1:D:3420:ILE:HD13	2.43	0.48
1:D:3039:SER:O	1:D:3042:LYS:HG2	2.12	0.48
1:A:353:PRO:HB2	1:C:2209:MET:HB2	1.94	0.48
1:C:2153:SER:CB	1:C:2364:GLN:HE21	2.24	0.48
1:B:1013:LEU:HB3	1:B:1086:HIS:HA	1.96	0.48
1:B:1185:LYS:O	1:B:1189:ASP:HB3	2.14	0.48
1:B:1137:LEU:HD11	1:B:1142:HIS:NE2	2.29	0.48
1:C:2373:THR:C	1:C:2375:PRO:HD2	2.34	0.48
1:B:1301:PHE:HB2	4:B:5172:HOH:O	2.13	0.48
1:B:1151:GLY:HA3	1:B:1371:LEU:HG	1.94	0.48
1:A:74:ARG:HB3	1:A:116:THR:HB	1.94	0.48
1:B:1093:LYS:C	1:B:1095:GLY:N	2.67	0.48
1:C:2142:HIS:HA	1:C:2144:GLN:OE1	2.13	0.48
1:D:3003:LYS:HE3	1:D:3074:ARG:NH1	2.27	0.48
1:A:179:VAL:O	1:A:182:SER:HB2	2.13	0.48
1:C:2317:LYS:HD2	1:C:2327:TYR:CZ	2.49	0.48
1:A:353:PRO:HG2	1:C:2209:MET:SD	2.54	0.48
1:D:3283:GLY:HA3	1:D:3309:TRP:CE2	2.49	0.48
1:C:2052:CYS:HB3	1:C:2129:ASP:OD1	2.14	0.48
1:D:3408:LEU:C	1:D:3420:ILE:CD1	2.79	0.48
1:C:2137:LEU:HA	1:C:2141:LYS:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3418:MET:CB	1:D:3424:PHE:HD1	2.27	0.47
1:A:312:GLU:HG3	1:A:313:ASN:ND2	2.30	0.47
1:B:1126:MET:CE	1:B:1151:GLY:N	2.77	0.47
1:A:320:ILE:N	1:A:320:ILE:HD13	2.29	0.47
1:B:1185:LYS:C	1:B:1185:LYS:HD3	2.34	0.47
1:D:3225:LYS:HZ1	1:D:3250:GLN:NE2	1.97	0.47
1:B:1418:MET:CB	1:B:1424:PHE:HB3	2.44	0.47
1:B:1418:MET:HB3	1:B:1424:PHE:HB3	1.96	0.47
1:A:52:CYS:HB3	1:A:129:ASP:OD1	2.14	0.47
1:C:2057:VAL:H	1:C:2084:GLN:NE2	2.11	0.47
1:A:430:ARG:HB2	1:A:430:ARG:CZ	2.44	0.47
1:B:1272:VAL:HG22	1:B:1296:CYS:SG	2.54	0.47
1:D:3129:ASP:OD2	1:D:3135:THR:HG23	2.15	0.47
1:C:2370:GLU:HB3	1:C:2378:TYR:CE1	2.50	0.47
1:C:2048:ARG:HD3	1:C:2121:ASP:OD1	2.14	0.47
1:B:1363:ASN:HD21	1:B:1393:VAL:HG21	1.80	0.47
1:B:1125:ASN:OD1	1:B:1125:ASN:C	2.52	0.47
1:B:1251:ALA:O	1:B:1256:TYR:HB2	2.14	0.47
1:B:1121:ASP:N	1:B:1121:ASP:OD1	2.34	0.47
1:A:91:ILE:HG22	1:A:96:ILE:HB	1.95	0.47
1:C:2177:ILE:HG13	1:C:2371:LEU:CD2	2.45	0.47
1:A:137:LEU:HD11	1:A:142:HIS:NE2	2.28	0.47
1:C:2418:MET:CB	1:C:2424:PHE:HB3	2.45	0.47
1:B:1137:LEU:HD12	1:B:1141:LYS:HB2	1.96	0.47
1:D:3401:LEU:HB2	1:D:3403:VAL:HG23	1.95	0.47
1:D:3344:VAL:HG13	1:D:3345:ASN:N	2.29	0.47
1:D:3137:LEU:HD11	1:D:3142:HIS:NE2	2.29	0.47
1:D:3137:LEU:HD12	1:D:3141:LYS:HD3	1.97	0.47
1:C:2079:ASN:HB3	1:C:2082:SER:OG	2.14	0.47
1:C:2206:THR:O	1:C:2207:ASP:HB2	2.14	0.47
1:B:1267:GLU:O	1:B:1290:LYS:HE3	2.14	0.47
1:B:1225:LYS:HZ2	1:B:1250:GLN:NE2	2.13	0.47
1:D:3169:ASN:HD22	1:D:3171:ILE:HD11	1.80	0.47
1:B:1299:GLY:O	1:B:1343:LEU:CD1	2.62	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:D:3425:LYS:HD3	1:D:3429:TYR:CE2	2.50	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:D:3033:ARG:HD2	1:D:3037:MET:HG3	1.97	0.47
1:C:2387:LYS:CE	1:C:2425:LYS:O	2.62	0.46

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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:D:3048:ARG:HD2	1:D:3119:PHE:CB	2.44	0.46
1:C:2428:HIS:CB	1:D:3384:PHE:HZ	2.18	0.46
1:A:33:ARG:HD2	1:A:37:MET:SD	2.55	0.46
1:C:2232:ARG:HG3	1:C:2232:ARG:NH1	2.30	0.46
1:C:2430:ARG:O	1:D:3430:ARG:HD2	2.14	0.46
1:B:1327:TYR:O	1:B:1334:ARG:HA	2.15	0.46
1:A:389:LEU:O	1:A:392:ALA:HB3	2.14	0.46
1:B:1060:ALA:O	1:B:1064:GLU:HG3	2.16	0.46
1:C:2430:ARG:O	1:C:2431:TYR:HB2	2.15	0.46
1:C:2406:THR:HG22	1:C:2407:LYS:N	2.31	0.46
1:C:2361:PHE:O	1:C:2365:VAL:HG23	2.16	0.46
1:B:1361:PHE:O	1:B:1365:VAL:HG23	2.15	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:A:232:ARG:HG3	1:A:232:ARG:HH11	1.80	0.46
1:B:1120:LYS:H	1:B:1120:LYS:CE	2.29	0.46
1:A:387:LYS:NZ	1:A:425:LYS:O	2.49	0.46
1:C:2137:LEU:HD11	1:C:2142:HIS:NE2	2.30	0.46
1:A:201:GLY:HA2	1:A:349:ALA:HB2	1.97	0.46
1:D:3033:ARG:NH1	1:D:3036:GLU:OE1	2.49	0.46
1:C:2105:THR:H	1:C:2108:GLU:HG3	1.80	0.46
1:D:3426:PRO:HB2	1:D:3428:HIS:CE1	2.50	0.46
1:D:3278:VAL:HG12	1:D:3303:VAL:HB	1.96	0.46
1:B:1373:THR:C	1:B:1375:PRO:HD2	2.35	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: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:3408:LEU:HA	1:D:3412:GLN:HE21	1.80	0.46
1:D:3430:ARG:O	1:D:3431:TYR:HB2	2.16	0.46
1:C:2134:LEU:HD22	1:C:2138:ILE:HD12	1.98	0.46
1:B:1153:SER:CB	1:B:1364:GLN:HE21	2.27	0.46
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:A:107:GLU:H	1:A:107:GLU:CD	2.20	0.46
1:A:57:VAL:H	1:A:84:GLN:NE2	2.14	0.45
1:D:3247:ASN:O	1:D:3250:GLN:HB2	2.16	0.45
1:B:1033:ARG:NH1	1:B:1036:GLU:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3201:GLY:HA2	1:D:3349:ALA:HB2	1.98	0.45
1:A:271:PHE:CE1	1:A:289:MET:HG2	2.50	0.45
1:C:2048:ARG:HD2	1:C:2119:PHE:CG	2.52	0.45
1:B:1187:LYS:HD2	1:B:1187:LYS:HA	1.82	0.45
1:A:425:LYS:NZ	1:B:1244:GLU:HG3	2.31	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:B:1203:LYS:NZ	1:D:3196:GLU:HB3	2.31	0.45
1:B:1119:PHE:HD1	1:B:1119:PHE:N	2.15	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:390:ASP:O	1:A:393:VAL:HG23	2.15	0.45
1:C:2033:ARG:NH1	1:C:2036:GLU:OE1	2.49	0.45
1:C:2142:HIS:C	1:C:2144:GLN:OE1	2.55	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:A:125:ASN:C	1:A:125:ASN:OD1	2.54	0.45
1:D:3284:ARG:O	1:D:3284:ARG:HG3	2.16	0.45
1:C:2301:PHE:HB2	4:C:5067:HOH:O	2.16	0.45
1:C:2093:LYS:C	1:C:2095:GLY:N	2.70	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:2129:ASP:OD2	1:C:2135:THR:HG23	2.17	0.45
1:B:1119:PHE:HB3	1:B:1120:LYS:HD2	1.98	0.45
1:B:1169:ASN:HB3	4:B:5169:HOH:O	2.16	0.45
1:A:409:THR:O	1:A:410:GLU:C	2.55	0.45
1:A:137:LEU:HD12	1:A:141:LYS:HB2	1.99	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:D:3119:PHE:HD1	1:D:3119:PHE:N	2.15	0.45
1:C:2225:LYS:HZ2	1:C:2250:GLN:NE2	2.14	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:B:1057:VAL:H	1:B:1084:GLN:NE2	2.15	0.45
1:A:385:LEU:HG	1:A:386:PRO:HD2	1.99	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:B:1177:ILE:HG13	1:B:1371:LEU:CD2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:PRO:HB2	1:A:422:GLY:N	2.31	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:D:3079:ASN:HB3	1:D:3082:SER:OG	2.17	0.45
1:C:2091:ILE:HG22	1:C:2096:ILE:HB	1.99	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:D:3142:HIS:C	1:D:3144:GLN:OE1	2.56	0.45
1:D:3374:HIS:HB3	1:D:3377:LYS:CG	2.46	0.45
1:D:3262:ASP:OD1	1:D:3284:ARG:NH1	2.50	0.45
1:D:3203:LYS:O	1:D:3207:ASP:N	2.50	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:C:2419:PRO:CD	1:C:2423:PRO:O	2.65	0.44
1:A:403:VAL:HG13	1:B:1258:VAL:HB	1.98	0.44
1:A:196:GLU:HB3	1:C:2203:LYS:NZ	2.33	0.44
1:A:427:ASP:OD2	1:A:427:ASP:N	2.49	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:D:3142:HIS:HA	1:D:3144:GLN:OE1	2.16	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:C:2161:HIS:CE1	1:D:3416:LEU:O	2.70	0.44
1:B:1430:ARG:CZ	1:B:1430:ARG:HB2	2.47	0.44
1:B:1408:LEU:HA	1:B:1412:GLN:HE21	1.82	0.44
1:A:142:HIS:CA	1:A:144:GLN:OE1	2.65	0.44
1:B:1178:ASN:CG	1:B:1181:ASP:HB2	2.38	0.44
1:D:3419:PRO:HB2	1:D:3422:GLY:N	2.32	0.44
1:B:1074:ARG:HB3	1:B:1116:THR:HB	1.99	0.44
1:A:273:THR:CG2	1:A:281:ILE:HD12	2.48	0.44
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:C:2119:PHE:HB3	1:C:2120:LYS:HD2	1.99	0.44
1:C:2060:ALA:O	1:C:2064:GLU:HG3	2.17	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:1419:PRO:CD	1:B:1423:PRO:O	2.65	0.44
1:B:1418:MET:CB	1:B:1424:PHE:HD1	2.30	0.44
1:A:48:ARG:HD2	1:A:119:PHE:CG	2.53	0.44
1:D:3013:LEU:HB3	1:D:3086:HIS:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2142:HIS:CA	1:C:2144:GLN:OE1	2.66	0.44
1:D:3327:TYR:O	1:D:3334:ARG:HA	2.17	0.44
1:B:1093:LYS:C	1:B:1095:GLY:H	2.21	0.44
1:A:425:LYS:HD3	1:A:429:TYR:CE2	2.53	0.44
1:D:3003:LYS:CE	1:D:3074:ARG:NH1	2.81	0.44
1:C:2299:GLY:O	1:C:2343:LEU:CD1	2.65	0.44
1:D:3387:LYS:CE	1:D:3425:LYS:O	2.65	0.44
1:C:2137:LEU:HD12	1:C:2141:LYS:HD3	1.99	0.44
1:A:362:THR:HB	1:A:393:VAL:HG13	2.00	0.44
1:C:2362:THR:HB	1:C:2393:VAL:HG13	1.99	0.44
1:B:1419:PRO:HB2	1:B:1422:GLY:HA3	2.00	0.44
1:B:1203:LYS:O	1:B:1207:ASP:N	2.50	0.44
1:C:2271:PHE:CE1	1:C:2289:MET:HG2	2.53	0.44
1:D:3200:ASP:OD2	1:D:3204:ARG:NH2	2.49	0.44
1:C:2408:LEU:HA	1:C:2412:GLN:HE21	1.82	0.44
1:A:177:ILE:HG13	1:A:371:LEU:CD2	2.48	0.44
1:C:2141:LYS:N	1:C:2141:LYS:HD2	2.32	0.44
1:C:2013:LEU:HB3	1:C:2086:HIS:HA	1.99	0.44
1:D:3419:PRO:HB2	1:D:3422:GLY:HA3	2.00	0.44
1:C:2105:THR:N	1:C:2108:GLU:HG3	2.32	0.44
1:D:3273:THR:OG1	1:D:3297:ASN:HB2	2.18	0.44
1:B:1284:ARG:O	1:B:1284:ARG:HG3	2.18	0.44
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:B:1387:LYS:CE	1:B:1425:LYS:O	2.63	0.43
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:A:430:ARG:O	1:B:1430:ARG:HB3	2.18	0.43
1:A:21:LEU:HD23	1:A:57:VAL:HG13	1.99	0.43
1:C:2028:MET:O	1:C:2032:MET:HG2	2.17	0.43
1:A:178:ASN:ND2	1:A:181:ASP:OD2	2.50	0.43
1:A:278:VAL:HG12	1:A:303:VAL:HG23	2.00	0.43
1:A:203:LYS:HZ1	1:C:2196:GLU:HB3	1.83	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:2017:GLY:O	1:C:2020:ALA:HB3	2.18	0.43
1:D:3057:VAL:H	1:D:3084:GLN:NE2	2.17	0.43
1:C:2430:ARG:HD2	1:D:3430:ARG:O	2.19	0.43
1:C:2138:ILE:HG23	1:C:2142:HIS:O	2.18	0.43
1:B:1208:VAL:HG22	1:B:1209:MET:N	2.34	0.43
1:A:178:ASN:ND2	1:A:181:ASP:HB2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2374:HIS:HB3	1:C:2377:LYS:CG	2.49	0.43
1:B:1406:THR:HG22	1:B:1407:LYS:N	2.33	0.43
1:C:2124:LEU:N	1:C:2124:LEU:HD23	2.34	0.43
1:D:3058:GLU:H	1:D:3058:GLU:CD	2.22	0.43
1:C:2126:MET:HE2	1:C:2151:GLY:N	2.34	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:C:2120:LYS:N	1:C:2120:LYS:CD	2.54	0.43
1:C:2420:ILE:HG23	1:C:2421:ASN:N	2.33	0.43
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:C:2177:ILE:HG13	1:C:2371:LEU:HD21	2.00	0.43
1:B:1353:PRO:CG	1:D:3209:MET:SD	3.06	0.43
1:C:2137:LEU:O	1:C:2137:LEU:HD12	2.19	0.43
1:A:42:LYS:O	1:A:45:LYS:HB2	2.19	0.43
1:D:3206:THR:O	1:D:3207:ASP:HB2	2.17	0.43
1:A:28:MET:HB3	1:A:358:SER:HB2	2.00	0.43
1:C:2178:ASN:ND2	1:C:2181:ASP:OD2	2.51	0.43
1:B:1142:HIS:CA	1:B:1144:GLN:OE1	2.67	0.43
1:C:2419:PRO:HB2	1:C:2422:GLY:N	2.32	0.43
1:B:1278:VAL:HG12	1:B:1303:VAL:HB	1.99	0.43
1:C:2265:CYS:HA	1:C:2271:PHE:CZ	2.54	0.43
1:D:3214:VAL:N	1:D:3269:ASN:ND2	2.54	0.43
1:B:1042:LYS:O	1:B:1045:LYS:HB2	2.18	0.43
1:D:3265:CYS:SG	1:D:3285:HIS:HD2	2.42	0.43
1:D:3427:ASP:N	1:D:3427:ASP:OD2	2.51	0.43
1:B:1105:THR:OG1	1:B:1108:GLU:HG3	2.19	0.43
1:A:126:MET:HE2	1:A:151:GLY:N	2.33	0.43
1:A:265:CYS:HA	1:A:271:PHE:CZ	2.54	0.43
1:D:3312:GLU:HG3	1:D:3313:ASN:ND2	2.34	0.42
1:B:1166:MET:HA	1:B:1171:ILE:HD12	2.00	0.42
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:D:3361:PHE:O	1:D:3365:VAL:HG23	2.19	0.42
1:B:1234:PHE:HE1	1:D:3195:ARG:O	2.02	0.42
1:C:2187:LYS:HD2	1:C:2187:LYS:HA	1.79	0.42
1:A:27:GLU:C	1:A:29:PRO:HD3	2.39	0.42
1:D:3215:ALA:CB	1:D:3231:LEU:HD13	2.47	0.42
1:C:2419:PRO:HG2	1:C:2422:GLY:C	2.40	0.42
1:A:242:GLU:OE1	2:A:432:NAI:H1B	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3055:MET:HA	1:D:3055:MET:CE	2.49	0.42
1:C:2277:CYS:HB2	1:D:3416:LEU:CG	2.48	0.42
1:A:177:ILE:HG13	1:A:371:LEU:HD21	2.01	0.42
1:D:3142:HIS:CA	1:D:3144:GLN:OE1	2.67	0.42
1:B:1152:ILE:HG13	1:B:1174:VAL:CG2	2.50	0.42
1:B:1048:ARG:HD3	1:B:1121:ASP:OD1	2.19	0.42
1:D:3178:ASN:CG	1:D:3181:ASP:HB2	2.40	0.42
1:C:2374:HIS:HB3	1:C:2377:LYS:HG3	2.00	0.42
1:C:2201:GLY:HA2	1:C:2349:ALA:HB2	2.01	0.42
1:A:142:HIS:C	1:A:144:GLN:OE1	2.58	0.42
1:D:3419:PRO:CG	1:D:3422:GLY:HA3	2.48	0.42
1:A:374:HIS:HB3	1:A:377:LYS:HG3	2.01	0.42
1:D:3154:GLU:CD	1:D:3159:GLY:HA3	2.39	0.42
1:D:3374:HIS:HB3	1:D:3377:LYS:CD	2.50	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:B:1146:LEU:HG	1:B:1173:LYS:HB2	2.01	0.42
1:A:137:LEU:HD12	1:A:137:LEU:O	2.18	0.42
1:A:418:MET:CB	1:A:424:PHE:HB3	2.50	0.42
1:C:2300:HIS:HB2	2:C:2432:NAI:O2D	2.19	0.42
1:A:327:TYR:O	1:A:334:ARG:HA	2.20	0.42
1:A:186:SER:O	1:A:190:ASN:HB2	2.19	0.42
1:C:2410:GLU:HA	1:C:2410:GLU:OE1	2.19	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:D:3107:GLU:CD	1:D:3107:GLU:H	2.23	0.42
1:A:60:ALA:O	1:A:64:GLU:HG3	2.19	0.42
1:C:2387:LYS:NZ	1:C:2425:LYS:O	2.51	0.42
1:B:1419:PRO:HB2	1:B:1422:GLY:N	2.34	0.42
1:D:3414:GLN:O	1:D:3415:TYR:C	2.58	0.42
1:A:105:THR:N	1:A:108:GLU:HG3	2.35	0.42
1:D:3379:PRO:O	1:D:3380:VAL:C	2.58	0.42
1:A:152:ILE:HB	1:A:176:ALA:HB2	2.02	0.42
1:D:3416:LEU:CB	1:D:3418:MET:HG2	2.50	0.42
1:A:425:LYS:HD3	1:A:429:TYR:CZ	2.55	0.42
1:C:2390:ASP:O	1:C:2393:VAL:HG23	2.20	0.42
1:B:1273:THR:CG2	1:B:1281:ILE:HD12	2.49	0.42
1:D:3281:ILE:C	1:D:3282:LEU:HD13	2.39	0.42
1:D:3337:LEU:HD13	1:D:3340:GLU:HA	2.02	0.42
1:A:334:ARG:O	1:A:335:ILE:HD13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ARG:HA	1:B:1430:ARG:CD	2.50	0.41
1:A:91:ILE:N	1:A:91:ILE:CD1	2.83	0.41
1:C:2010:ASP:HB3	1:C:2013:LEU:CD2	2.46	0.41
1:B:1079:ASN:HB3	1:B:1082:SER:OG	2.20	0.41
1:A:431:TYR:HE2	1:B:1247:ASN:ND2	2.18	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:374:HIS:HB3	1:A:377:LYS:CG	2.50	0.41
1:C:2232:ARG:HH11	1:C:2232:ARG:HG3	1.85	0.41
1:C:2228:ALA:HB1	1:C:2256:TYR:CZ	2.55	0.41
1:B:1271:PHE:CE1	1:B:1289:MET:HG2	2.54	0.41
1:A:430:ARG:HB3	1:B:1430:ARG:O	2.20	0.41
1:C:2409:THR:O	1:C:2410:GLU:C	2.57	0.41
1:D:3308:LYS:HD2	1:D:3308:LYS:N	2.16	0.41
1:A:413:ALA:HB2	1:A:420:ILE:HD12	2.01	0.41
1:C:2416:LEU:CD2	1:D:3277:CYS:HB2	2.40	0.41
1:C:2139:HIS:ND1	1:C:2146:LEU:HD11	2.35	0.41
1:A:374:HIS:N	1:A:375:PRO:HD2	2.35	0.41
1:C:2203:LYS:O	1:C:2207:ASP:N	2.53	0.41
1:C:2243:ILE:HG21	1:D:3408:LEU:HD13	2.01	0.41
1:B:1035:ARG:NH2	1:B:1064:GLU:HB2	2.35	0.41
1:C:2409:THR:C	1:C:2420:ILE:HD11	2.40	0.41
1:A:401:LEU:HD12	1:B:1249:LEU:HD12	2.03	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:409:THR:O	1:A:420:ILE:CD1	2.68	0.41
1:D:3134:LEU:HD22	1:D:3138:ILE:HD12	2.02	0.41
1:B:1374:HIS:HB3	1:B:1377:LYS:CG	2.50	0.41
1:A:379:PRO:O	1:A:380:VAL:C	2.59	0.41
1:B:1017:GLY:O	1:B:1020:ALA:HB3	2.21	0.41
1:D:3031:LEU:HA	1:D:3031:LEU:HD23	1.92	0.41
1:C:2374:HIS:HB3	1:C:2377:LYS:HD3	2.03	0.41
1:B:1107:GLU:CD	1:B:1107:GLU:H	2.24	0.41
1:D:3409:THR:O	1:D:3410:GLU:C	2.58	0.41
1:A:430:ARG:O	1:A:431:TYR:HB2	2.21	0.41
1:D:3373:THR:C	1:D:3374:HIS:ND1	2.74	0.41
1:B:1427:ASP:N	1:B:1427:ASP:OD2	2.54	0.41
1:D:3119:PHE:HB3	1:D:3120:LYS:HD2	2.03	0.41
1:A:119:PHE:HB3	1:A:120:LYS:HD2	2.03	0.41
1:C:2413:ALA:HB2	1:C:2420:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3007:LYS:NZ	1:D:3101:TRP:CH2	2.86	0.41
1:B:1137:LEU:HD12	1:B:1137:LEU:O	2.21	0.41
1:B:1142:HIS:C	1:B:1144:GLN:OE1	2.59	0.41
1:C:2033:ARG:HD2	1:C:2037:MET:CG	2.51	0.41
1:C:2278:VAL:HG12	1:C:2303:VAL:HG23	2.02	0.41
1:D:3300:HIS:HB2	2:D:3432:NAI:O2D	2.21	0.41
1:A:361:PHE:O	1:A:365:VAL:HG23	2.21	0.41
1:C:2243:ILE:HD12	1:D:3424:PHE:CZ	2.56	0.41
1:A:410:GLU:HA	1:A:410:GLU:OE1	2.20	0.41
1:C:2007:LYS:NZ	1:C:2101:TRP:CH2	2.89	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:B:1033:ARG:HD2	1:B:1037:MET:CG	2.50	0.41
1:C:2093:LYS:C	1:C:2095:GLY:H	2.25	0.41
1:C:2191:LEU:C	1:C:2191:LEU:HD12	2.41	0.41
1:B:1021:LEU:HD21	1:B:1060:ALA:CB	2.49	0.40
1:A:137:LEU:HD12	1:A:141:LYS:HD3	2.02	0.40
1:A:190:ASN:CG	2:A:432:NAI:H5N	2.42	0.40
1:B:1124:LEU:HD23	1:B:1124:LEU:H	1.86	0.40
1:A:79:ASN:HB3	1:A:82:SER:CB	2.51	0.40
1:A:187:LYS:HA	1:A:187:LYS:HD2	1.83	0.40
1:D:3141:LYS:N	1:D:3141:LYS:HD2	2.35	0.40
1:B:1208:VAL:HG22	1:B:1213:LYS:HE2	2.01	0.40
1:D:3299:GLY:HA3	1:D:3304:GLU:OE2	2.20	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:D:3048:ARG:HD2	1:D:3119:PHE:CG	2.57	0.40
1:A:412:GLN:C	1:A:414:GLN:N	2.73	0.40
1:B:1053:LEU:O	1:B:1077:SER:HA	2.20	0.40
1:D:3124:LEU:N	1:D:3124:LEU:HD23	2.36	0.40
1:A:74:ARG:NH1	1:A:115:GLN:O	2.54	0.40
1:B:1419:PRO:CG	1:B:1422:GLY:HA3	2.48	0.40
1:A:419:PRO:HB2	1:A:422:GLY:HA3	2.04	0.40
1:C:2056:THR:OG1	3:C:2433:ADY:N1	2.51	0.40
1:B:1048:ARG:HG3	1:B:1048:ARG:HH11	1.86	0.40
1:A:412:GLN:O	1:A:414:GLN:N	2.54	0.40
1:A:387:LYS:NZ	1:A:425:LYS:HB3	2.36	0.40
1:C:2278:VAL:HG22	1:D:3415:TYR:CG	2.56	0.40
1:A:215:ALA:O	1:A:238:VAL:HA	2.21	0.40
1:B:1279:ASP:HB3	1:B:1282:LEU:HD11	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry 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

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	428/431 (99%)	398 (93%)	30 (7%)	0	100 100
1	B	428/431 (99%)	401 (94%)	26 (6%)	1 (0%)	52 84
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%)	56 87

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1420	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	353/353 (100%)	296 (84%)	57 (16%)	3 9
1	B	353/353 (100%)	295 (84%)	58 (16%)	3 8
1	C	353/353 (100%)	298 (84%)	55 (16%)	3 9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	353/353 (100%)	297 (84%)	56 (16%)	3 9
All	All	1412/1412 (100%)	1186 (84%)	226 (16%)	3 9

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	13	LEU
1	A	26	ASN
1	A	28	MET
1	A	41	SER
1	A	53	LEU
1	A	55	MET
1	A	72	GLU
1	A	86	HIS
1	A	91	ILE
1	A	93	LYS
1	A	104	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	165	LYS
1	A	169	ASN
1	A	172	LEU
1	A	182	SER
1	A	187	LYS
1	A	191	LEU
1	A	232	ARG
1	A	240	ILE
1	A	242	GLU
1	A	267	GLU
1	A	275	THR
1	A	277	CYS
1	A	282	LEU
1	A	284	ARG

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Mol	Chain	Res	Type
1	A	297	ASN
1	A	302	ASP
1	A	308	LYS
1	A	317	LYS
1	A	334	ARG
1	A	337	LEU
1	A	340	GLU
1	A	371	LEU
1	A	377	LYS
1	A	382	VAL
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	1026	ASN
1	B	1028	MET
1	B	1041	SER
1	B	1053	LEU
1	B	1055	MET
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
1	B	1120	LYS
1	B	1121	ASP
1	B	1134	LEU
1	B	1135	THR
1	B	1144	GLN
1	B	1146	LEU

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Mol	Chain	Res	Type
1	B	1153	SER
1	B	1165	LYS
1	B	1169	ASN
1	B	1172	LEU
1	B	1182	SER
1	B	1186	SER
1	B	1191	LEU
1	B	1232	ARG
1	B	1234	PHE
1	B	1240	ILE
1	B	1242	GLU
1	B	1267	GLU
1	B	1275	THR
1	B	1277	CYS
1	B	1282	LEU
1	B	1284	ARG
1	B	1297	ASN
1	B	1302	ASP
1	B	1308	LYS
1	B	1317	LYS
1	B	1334	ARG
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
1	B	1425	LYS
1	B	1427	ASP
1	B	1428	HIS
1	C	2003	LYS
1	C	2013	LEU
1	C	2026	ASN
1	C	2028	MET
1	C	2033	ARG

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Mol	Chain	Res	Type
1	C	2041	SER
1	C	2053	LEU
1	C	2055	MET
1	C	2086	HIS
1	C	2091	ILE
1	C	2093	LYS
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	2144	GLN
1	C	2146	LEU
1	C	2153	SER
1	C	2165	LYS
1	C	2169	ASN
1	C	2172	LEU
1	C	2182	SER
1	C	2191	LEU
1	C	2232	ARG
1	C	2240	ILE
1	C	2242	GLU
1	C	2267	GLU
1	C	2275	THR
1	C	2277	CYS
1	C	2282	LEU
1	C	2284	ARG
1	C	2297	ASN
1	C	2308	LYS
1	C	2317	LYS
1	C	2334	ARG
1	C	2337	LEU
1	C	2340	GLU
1	C	2371	LEU
1	C	2377	LYS
1	C	2382	VAL
1	C	2400	LYS
1	C	2405	LEU

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Mol	Chain	Res	Type
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	3026	ASN
1	D	3028	MET
1	D	3033	ARG
1	D	3041	SER
1	D	3053	LEU
1	D	3055	MET
1	D	3086	HIS
1	D	3091	ILE
1	D	3093	LYS
1	D	3108	GLU
1	D	3110	LEU
1	D	3114	GLU
1	D	3119	PHE
1	D	3120	LYS
1	D	3121	ASP
1	D	3134	LEU
1	D	3135	THR
1	D	3144	GLN
1	D	3146	LEU
1	D	3153	SER
1	D	3165	LYS
1	D	3169	ASN
1	D	3172	LEU
1	D	3182	SER
1	D	3191	LEU
1	D	3232	ARG
1	D	3240	ILE
1	D	3242	GLU
1	D	3267	GLU
1	D	3275	THR
1	D	3277	CYS
1	D	3282	LEU

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Mol	Chain	Res	Type
1	D	3284	ARG
1	D	3297	ASN
1	D	3302	ASP
1	D	3308	LYS
1	D	3317	LYS
1	D	3334	ARG
1	D	3337	LEU
1	D	3340	GLU
1	D	3371	LEU
1	D	3377	LYS
1	D	3382	VAL
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
1	D	3424	PHE
1	D	3425	LYS
1	D	3427	ASP
1	D	3428	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) 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	359	ASN
1	A	364	GLN
1	A	368	GLN
1	A	402	ASN
1	A	412	GLN
1	A	414	GLN
1	B	1026	ASN
1	B	1084	GLN
1	B	1169	ASN

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Mol	Chain	Res	Type
1	B	1247	ASN
1	B	1250	GLN
1	B	1269	ASN
1	B	1313	ASN
1	B	1359	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	2402	ASN
1	C	2412	GLN
1	C	2414	GLN
1	D	3026	ASN
1	D	3084	GLN
1	D	3169	ASN
1	D	3247	ASN
1	D	3250	GLN
1	D	3269	ASN
1	D	3313	ASN
1	D	3359	ASN
1	D	3364	GLN
1	D	3368	GLN
1	D	3402	ASN
1	D	3412	GLN
1	D	3414	GLN

5.3.3 RNA

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 carbohydrates 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	A	432	-	38,48,48	1.26	4 (10%)	48,73,73	1.20	5 (10%)
3	ADY	A	433	-	16,21,21	0.74	0	9,31,31	1.45	2 (22%)
2	NAI	B	1432	-	38,48,48	1.27	4 (10%)	48,73,73	1.07	5 (10%)
3	ADY	B	1433	-	16,21,21	1.01	1 (6%)	9,31,31	1.47	2 (22%)
2	NAI	C	2432	-	38,48,48	1.34	4 (10%)	48,73,73	1.09	5 (10%)
3	ADY	C	2433	-	16,21,21	1.95	3 (18%)	9,31,31	1.47	3 (33%)
2	NAI	D	3432	-	38,48,48	1.29	3 (7%)	48,73,73	1.12	5 (10%)
3	ADY	D	3433	-	16,21,21	1.65	2 (12%)	9,31,31	1.53	3 (33%)

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	A	432	-	-	0/25/72/72	0/5/5/5
3	ADY	A	433	-	-	0/2/22/22	0/3/3/3
2	NAI	B	1432	-	-	0/25/72/72	0/5/5/5
3	ADY	B	1433	-	-	0/2/22/22	0/3/3/3
2	NAI	C	2432	-	-	0/25/72/72	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADY	C	2433	-	-	0/2/22/22	0/3/3/3
2	NAI	D	3432	-	-	0/25/72/72	0/5/5/5
3	ADY	D	3433	-	-	0/2/22/22	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2432	NAI	O4B-C1B	-4.46	1.35	1.41
2	D	3432	NAI	O4B-C1B	-3.82	1.36	1.41
2	B	1432	NAI	O4B-C1B	-3.23	1.37	1.41
3	C	2433	ADY	C4'-C3'	-3.01	1.45	1.52
3	D	3433	ADY	C4'-C3'	-2.67	1.46	1.52
2	A	432	NAI	O4B-C1B	-2.36	1.38	1.41
2	B	1432	NAI	PN-O1N	-2.00	1.46	1.54
3	C	2433	ADY	C2-N3	2.03	1.35	1.32
2	C	2432	NAI	O3B-C3B	2.04	1.47	1.43
3	B	1433	ADY	O3'-C3'	2.11	1.25	1.21
2	A	432	NAI	C2A-N1A	2.13	1.38	1.33
2	D	3432	NAI	C6N-N1N	2.49	1.44	1.37
2	B	1432	NAI	C6N-N1N	2.51	1.44	1.37
2	C	2432	NAI	C6N-N1N	2.54	1.45	1.37
2	A	432	NAI	C6N-N1N	2.81	1.45	1.37
2	C	2432	NAI	C2N-C3N	4.32	1.45	1.34
2	B	1432	NAI	C2N-C3N	4.52	1.45	1.34
2	D	3432	NAI	C2N-C3N	4.65	1.46	1.34
2	A	432	NAI	C2N-C3N	4.89	1.46	1.34
3	D	3433	ADY	O3'-C3'	4.95	1.30	1.21
3	C	2433	ADY	O3'-C3'	6.23	1.32	1.21

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	432	NAI	O3-PN-O5D	-3.11	94.69	102.94
2	A	432	NAI	O5B-C5B-C4B	-2.83	98.69	109.12
2	C	2432	NAI	O3-PN-O5D	-2.68	95.82	102.94
3	B	1433	ADY	C1'-O4'-C4'	-2.67	101.89	108.54
3	A	433	ADY	C1'-O4'-C4'	-2.64	101.97	108.54
3	D	3433	ADY	C1'-O4'-C4'	-2.63	101.98	108.54
2	D	3432	NAI	O5B-C5B-C4B	-2.62	99.47	109.12
2	B	1432	NAI	O3-PN-O5D	-2.60	96.05	102.94
3	C	2433	ADY	C1'-O4'-C4'	-2.51	102.28	108.54
2	D	3432	NAI	O3-PN-O5D	-2.43	96.48	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1432	NAI	O5B-C5B-C4B	-2.32	100.57	109.12
2	C	2432	NAI	O5B-C5B-C4B	-2.25	100.82	109.12
3	D	3433	ADY	C4-C5-N7	2.02	111.34	109.48
3	C	2433	ADY	C4'-C3'-C2'	2.03	112.45	107.97
3	C	2433	ADY	O4'-C1'-N9	2.03	112.35	108.10
3	D	3433	ADY	O4'-C1'-N9	2.08	112.44	108.10
2	B	1432	NAI	O1N-PN-O3	2.15	114.85	105.09
2	C	2432	NAI	O3-PA-O5B	2.18	108.71	102.94
3	A	433	ADY	O4'-C1'-N9	2.25	112.82	108.10
2	D	3432	NAI	O3-PA-O5B	2.27	108.96	102.94
2	D	3432	NAI	O1N-PN-O3	2.30	115.52	105.09
2	B	1432	NAI	O3-PA-O5B	2.34	109.14	102.94
2	C	2432	NAI	C4A-C5A-N7A	2.36	111.65	109.48
2	A	432	NAI	C4A-C5A-N7A	2.38	111.67	109.48
2	B	1432	NAI	C4A-C5A-N7A	2.38	111.67	109.48
2	C	2432	NAI	O1N-PN-O3	2.50	116.43	105.09
2	D	3432	NAI	C4A-C5A-N7A	2.51	111.79	109.48
3	B	1433	ADY	O4'-C1'-N9	2.52	113.37	108.10
2	A	432	NAI	O1N-PN-O3	2.60	116.89	105.09
2	A	432	NAI	O3-PA-O5B	2.61	109.85	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	432	NAI	2	0
2	C	2432	NAI	1	0
3	C	2433	ADY	1	0
2	D	3432	NAI	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.