Full wwPDB X-ray Structure Validation Report (i)

Feb 4, 2024 – 06:15 AM EST

PDB ID	:	1P7L
Title	:	S-Adenosylmethionine synthetase complexed with AMPPNP and Met.
Authors	:	Takusagawa, F.; Komoto, J.
Deposited on	:	2003-05-02
Resolution	:	2.50 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 (i) 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 (1)) were used in the production of this report:

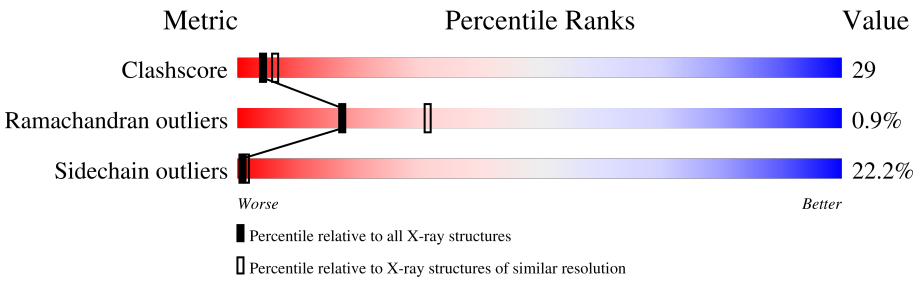
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	383	49% 40% 11%
1	B	383	51% 37% 11%
1	C	383	50% 38% 12% •
1	D	383	50% 38% 11% •

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11960 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-adenosylmethionine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	383	2942	1856	503	570	13	0	0	0
1	B	383	2942	1856	503	570	13	0	0	0
1	C	383	2942	1856	503	570	13	0	0	0
1	D	383	2942	1856	503	570	13	0	0	0

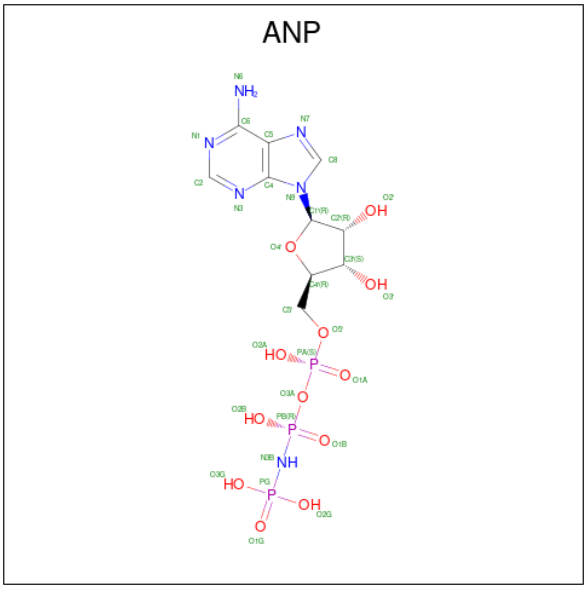
- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

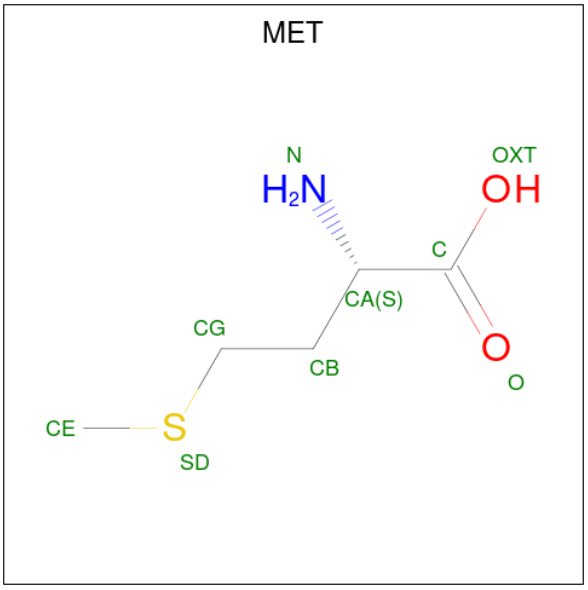
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	2	2	2	0	0
3	B	2	2	2	0	0
3	C	2	2	2	0	0
3	D	2	2	2	0	0

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



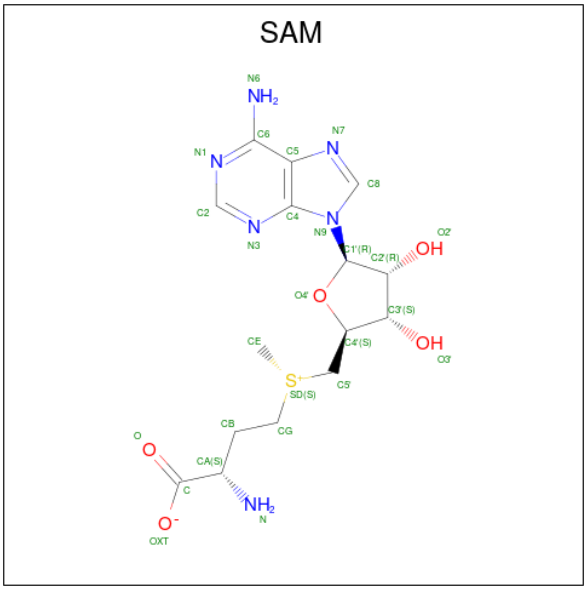
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
4	B	1	31	10	6	12	3	0	0

- Molecule 5 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



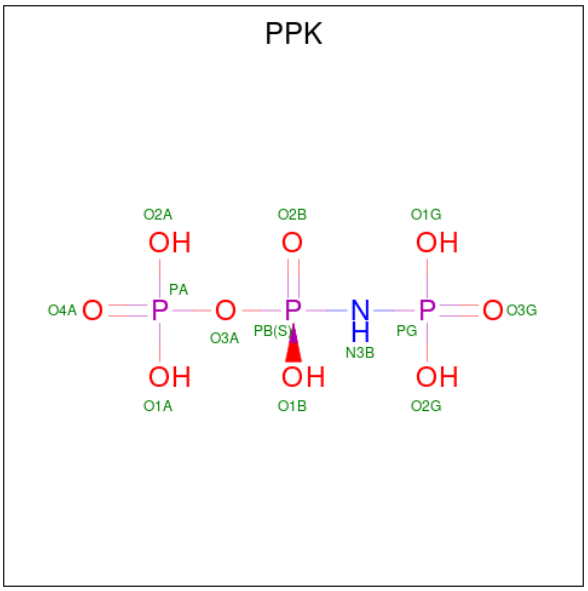
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	A	1	9	5	1	2	1	0	0
			Total	C	N	O	S		
5	B	1	9	5	1	2	1	0	0

- Molecule 6 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	C	1	27	15	6	5	1	0	0
			Total	C	N	O	S		
6	C	1	27	15	6	5	1	0	0

- Molecule 7 is (DIPHOSPHONO)AMINOPHOSPHONIC ACID (three-letter code: PPK) (formula: $H_6NO_9P_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	N	O	P		
7	C	1	13	1	9	3	0	0
			Total	N	O	P		
7	D	1	13	1	9	3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	6	6	6	0	0
			Total	O		
8	B	3	3	3	0	0
			Total	O		
8	C	8	8	8	0	0
			Total	O		
8	D	3	3	3	0	0

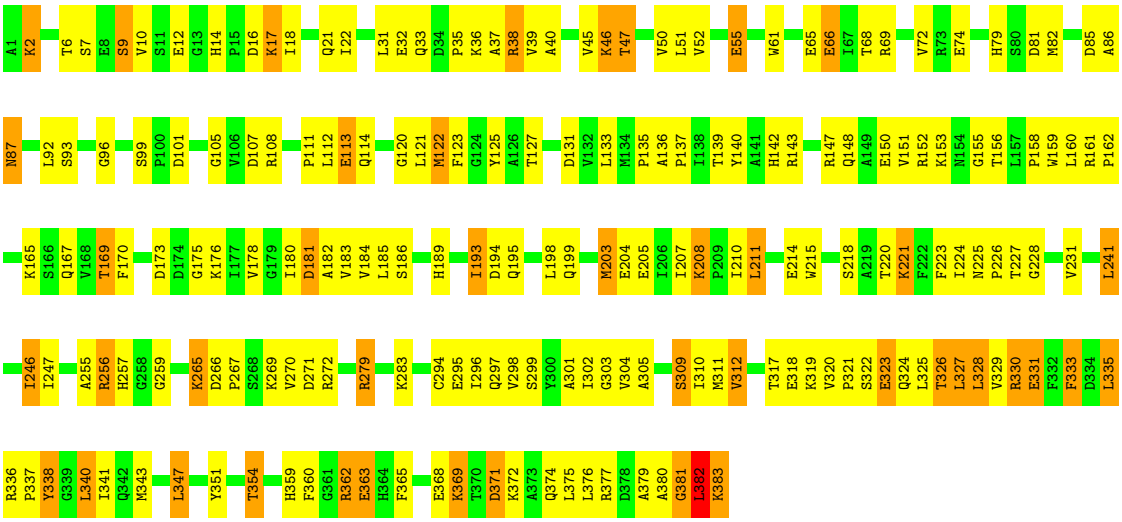
3 Residue-property plots (i)

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.

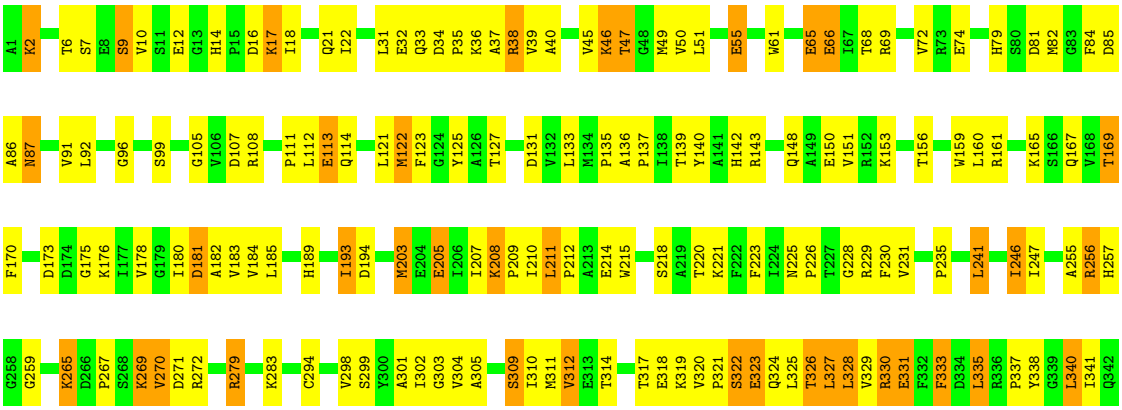
• Molecule 1: S-adenosylmethionine synthetase

Chain A: 49% 40% 11%



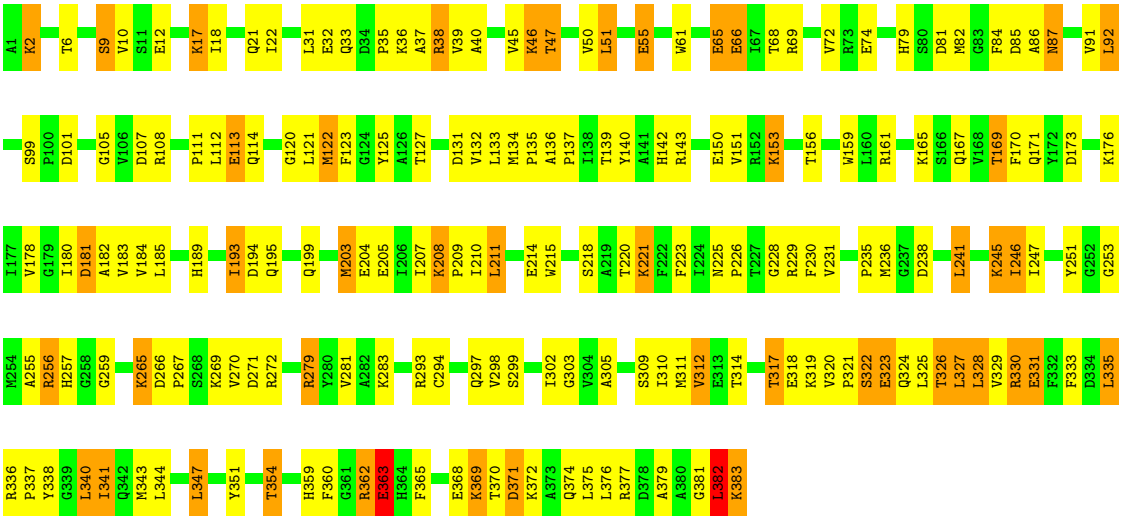
• Molecule 1: S-adenosylmethionine synthetase

Chain B: 51% 37% 11%



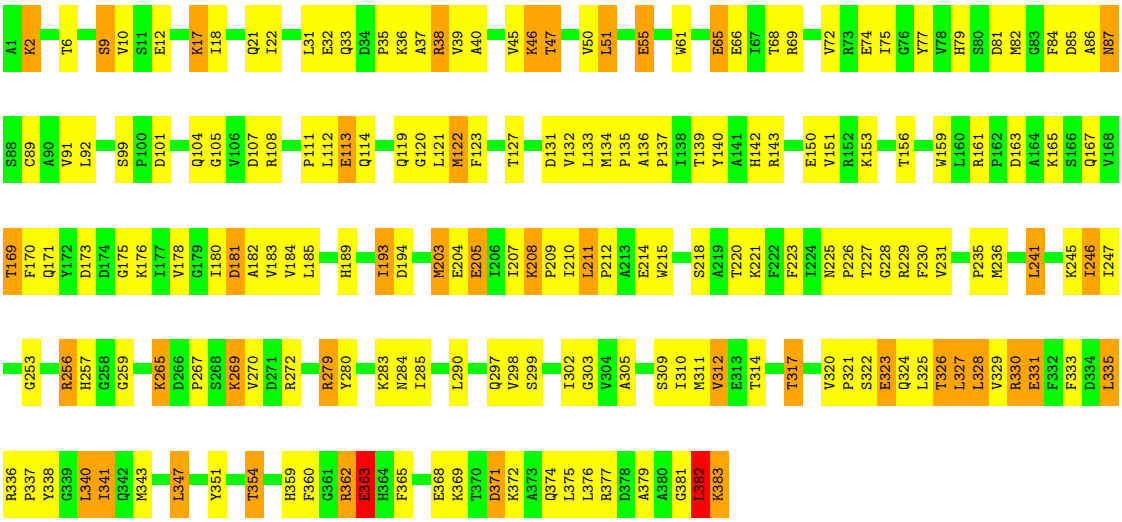
• Molecule 1: S-adenosylmethionine synthetase

Chain C:



• Molecule 1: S-adenosylmethionine synthetase

Chain D:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	225.82Å 69.13Å 118.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.213 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11960	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: K, SAM, ANP, PPK, MG

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	0.43	0/3001	0.65	0/4068
1	B	0.41	0/3001	0.63	0/4068
1	C	0.40	0/3001	0.63	0/4068
1	D	0.39	0/3001	0.63	0/4068
All	All	0.41	0/12004	0.63	0/16272

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	338	TYR	Sidechain

5.2 Too-close contacts (i)

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	2942	0	2908	177	0
1	B	2942	0	2908	181	0
1	C	2942	0	2908	189	0
1	D	2942	0	2908	177	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	31	0	12	1	0
4	B	31	0	12	2	0
5	A	9	0	8	2	0
5	B	9	0	8	1	0
6	C	54	0	44	1	0
7	C	13	0	1	2	0
7	D	13	0	1	1	0
8	A	6	0	0	2	0
8	B	3	0	0	0	0
8	C	8	0	0	1	0
8	D	3	0	0	2	0
All	All	11960	0	11718	696	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (696) 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:241:LEU:HD11	1:D:241:LEU:HD11	1.34	1.05
1:A:10:VAL:HG12	1:A:165:LYS:HG2	1.44	0.98
1:B:10:VAL:HG12	1:B:165:LYS:HG2	1.43	0.97
1:D:10:VAL:HG12	1:D:165:LYS:HG2	1.48	0.95
1:B:122:MET:HG2	1:B:298:VAL:HG23	1.49	0.94
1:B:72:VAL:HG12	1:B:86:ALA:HB2	1.50	0.94
1:D:72:VAL:HG12	1:D:86:ALA:HB2	1.49	0.94
1:A:241:LEU:HD11	1:B:241:LEU:HD11	1.50	0.93
1:B:267:PRO:HB2	1:B:341:ILE:HD13	1.51	0.93
1:B:33:GLN:NE2	1:B:61:TRP:H	1.67	0.92
1:A:33:GLN:NE2	1:A:61:TRP:H	1.69	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:GLN:HB3	1:B:184:VAL:HB	1.53	0.90
1:C:107:ASP:HA	1:C:114:GLN:HE21	1.37	0.89
1:C:10:VAL:HG12	1:C:165:LYS:HG2	1.55	0.89
1:A:122:MET:HG2	1:A:298:VAL:HG23	1.53	0.88
1:D:107:ASP:HA	1:D:114:GLN:HE21	1.38	0.88
1:D:122:MET:HG2	1:D:298:VAL:HG23	1.56	0.87
1:A:33:GLN:HE22	1:A:61:TRP:H	1.22	0.87
1:A:72:VAL:HG12	1:A:86:ALA:HB2	1.55	0.87
1:A:107:ASP:HA	1:A:114:GLN:HE21	1.37	0.87
1:B:79:HIS:HD2	1:B:81:ASP:H	1.19	0.86
1:C:139:THR:O	1:C:143:ARG:HG3	1.76	0.86
1:A:167:GLN:HB3	1:A:184:VAL:HB	1.55	0.86
1:C:122:MET:HG2	1:C:298:VAL:HG23	1.58	0.86
1:D:267:PRO:HB2	1:D:341:ILE:HD13	1.58	0.86
1:B:33:GLN:HE22	1:B:61:TRP:H	1.19	0.85
1:C:72:VAL:HG12	1:C:86:ALA:HB2	1.58	0.85
1:C:167:GLN:HB3	1:C:184:VAL:HB	1.59	0.85
1:B:107:ASP:HA	1:B:114:GLN:HE21	1.40	0.85
1:B:330:ARG:HH21	1:B:331:GLU:HA	1.42	0.85
1:C:267:PRO:HB2	1:C:341:ILE:HD13	1.57	0.85
1:A:330:ARG:HH21	1:A:331:GLU:HA	1.40	0.84
1:C:79:HIS:HD2	1:C:81:ASP:H	1.22	0.84
1:A:267:PRO:HB2	1:A:341:ILE:HD13	1.59	0.83
1:D:330:ARG:HH21	1:D:331:GLU:HA	1.41	0.83
1:C:330:ARG:HH21	1:C:331:GLU:HA	1.41	0.83
1:C:257:HIS:HD2	1:C:259:GLY:H	1.26	0.83
1:D:167:GLN:HB3	1:D:184:VAL:HB	1.61	0.83
1:D:79:HIS:HD2	1:D:81:ASP:H	1.26	0.82
1:A:382:LEU:HG	1:A:383:LYS:N	1.92	0.82
1:D:33:GLN:NE2	1:D:61:TRP:H	1.77	0.82
1:B:79:HIS:CD2	1:B:81:ASP:H	1.97	0.82
1:C:151:VAL:HG23	1:C:156:THR:HB	1.60	0.81
1:C:33:GLN:NE2	1:C:61:TRP:H	1.78	0.81
1:D:12:GLU:HB2	1:D:21:GLN:HE22	1.44	0.81
1:A:257:HIS:HD2	1:A:259:GLY:H	1.27	0.80
1:B:257:HIS:HD2	1:B:259:GLY:H	1.28	0.80
1:C:382:LEU:HG	1:C:383:LYS:N	1.95	0.80
1:D:33:GLN:HE22	1:D:61:TRP:H	1.29	0.79
1:C:33:GLN:HE22	1:C:61:TRP:H	1.26	0.79
1:D:257:HIS:HD2	1:D:259:GLY:H	1.29	0.79
1:A:330:ARG:HE	1:A:331:GLU:N	1.79	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:HIS:HD2	1:A:81:ASP:H	1.29	0.79
1:B:139:THR:O	1:B:143:ARG:HG3	1.83	0.79
1:A:151:VAL:HG23	1:A:156:THR:HB	1.64	0.78
1:B:347:LEU:H	1:B:347:LEU:HD22	1.48	0.78
1:C:79:HIS:CD2	1:C:81:ASP:H	2.00	0.78
1:D:382:LEU:HG	1:D:383:LYS:N	1.97	0.78
1:A:312:VAL:HG13	1:A:326:THR:HG23	1.65	0.77
1:C:12:GLU:HB2	1:C:21:GLN:HE22	1.47	0.77
1:D:139:THR:O	1:D:143:ARG:HG3	1.84	0.77
1:D:330:ARG:HE	1:D:331:GLU:N	1.81	0.77
1:C:351:TYR:O	1:C:354:THR:HG22	1.84	0.77
1:B:12:GLU:HB2	1:B:21:GLN:HE22	1.49	0.77
1:B:151:VAL:HG23	1:B:156:THR:HB	1.65	0.77
1:B:330:ARG:HE	1:B:331:GLU:N	1.83	0.76
1:C:330:ARG:HE	1:C:331:GLU:N	1.82	0.76
1:D:79:HIS:CD2	1:D:81:ASP:H	2.03	0.76
1:B:22:ILE:HD13	1:B:68:THR:HG23	1.66	0.76
1:C:121:LEU:HD13	1:D:6:THR:O	1.86	0.76
1:D:22:ILE:HD13	1:D:68:THR:HG23	1.68	0.76
1:B:6:THR:HG23	1:B:169:THR:HG22	1.67	0.75
1:A:79:HIS:CD2	1:A:81:ASP:H	2.04	0.75
1:A:12:GLU:HB2	1:A:21:GLN:HE22	1.50	0.75
1:B:382:LEU:HG	1:B:383:LYS:N	2.01	0.74
1:B:351:TYR:O	1:B:354:THR:HG22	1.88	0.74
1:A:139:THR:O	1:A:143:ARG:HG3	1.87	0.74
1:A:22:ILE:HD13	1:A:68:THR:HG23	1.69	0.73
1:A:351:TYR:O	1:A:354:THR:HG22	1.87	0.73
1:C:226:PRO:HB2	1:D:302:ILE:O	1.88	0.73
1:D:351:TYR:O	1:D:354:THR:HG22	1.89	0.73
1:D:330:ARG:HH21	1:D:331:GLU:CA	2.01	0.72
1:C:312:VAL:HG13	1:C:326:THR:HG23	1.71	0.72
1:C:302:ILE:O	1:D:226:PRO:HB2	1.90	0.72
1:B:312:VAL:HG13	1:B:326:THR:HG23	1.71	0.72
1:C:6:THR:O	1:D:121:LEU:HD13	1.88	0.72
1:B:330:ARG:HH21	1:B:331:GLU:CA	2.02	0.72
1:B:133:LEU:HD23	1:B:283:LYS:HE2	1.71	0.72
1:C:305:ALA:O	1:C:337:PRO:HD2	1.91	0.71
1:C:22:ILE:HD13	1:C:68:THR:HG23	1.73	0.70
1:C:241:LEU:HG	1:D:241:LEU:HG	1.73	0.70
1:D:151:VAL:HG23	1:D:156:THR:HB	1.73	0.70
1:C:257:HIS:CD2	1:C:259:GLY:H	2.10	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ARG:HH21	1:C:331:GLU:CA	2.04	0.70
1:C:328:LEU:HD23	1:C:376:LEU:HD22	1.73	0.69
1:D:337:PRO:HB2	1:D:338:TYR:CD1	2.28	0.69
1:B:17:LYS:O	1:B:21:GLN:HG3	1.92	0.69
1:D:133:LEU:HD23	1:D:283:LYS:HE2	1.74	0.69
1:D:305:ALA:O	1:D:337:PRO:HD2	1.92	0.69
1:A:330:ARG:HH21	1:A:331:GLU:CA	2.05	0.69
1:D:330:ARG:NH2	1:D:331:GLU:HG3	2.06	0.69
1:A:347:LEU:HD22	1:A:347:LEU:H	1.56	0.69
1:A:6:THR:HG23	1:A:169:THR:HG22	1.75	0.68
1:B:305:ALA:O	1:B:337:PRO:HD2	1.93	0.68
1:A:305:ALA:O	1:A:337:PRO:HD2	1.93	0.68
5:A:485:MET:SD	4:B:484:ANP:H5'1	2.33	0.68
1:C:193:ILE:HG12	1:C:194:ASP:N	2.08	0.68
1:D:257:HIS:CD2	1:D:259:GLY:H	2.13	0.67
7:C:684:PPK:H3B	1:D:265:LYS:NZ	1.93	0.67
1:D:320:VAL:HB	1:D:324:GLN:NE2	2.09	0.67
1:C:279:ARG:HD3	1:C:368:GLU:OE1	1.95	0.66
1:C:328:LEU:HD11	1:C:379:ALA:CB	2.25	0.66
1:B:279:ARG:HD3	1:B:368:GLU:OE1	1.95	0.66
1:A:279:ARG:HD3	1:A:368:GLU:OE1	1.95	0.66
1:B:69:ARG:HD3	1:B:86:ALA:O	1.94	0.66
1:B:362:ARG:HG3	1:B:365:PHE:CE2	2.30	0.66
1:D:312:VAL:HG13	1:D:326:THR:HG23	1.76	0.66
1:A:69:ARG:HD3	1:A:86:ALA:O	1.96	0.66
1:B:257:HIS:CD2	1:B:259:GLY:H	2.11	0.66
1:C:184:VAL:HG22	1:C:223:PHE:HB2	1.79	0.65
1:D:46:LYS:HD3	1:D:47:THR:HG23	1.79	0.65
1:B:337:PRO:HB2	1:B:338:TYR:CD1	2.32	0.65
1:C:328:LEU:HD11	1:C:379:ALA:HB1	1.76	0.65
1:C:133:LEU:HD23	1:C:283:LYS:HE2	1.79	0.65
1:B:246:ILE:HG23	1:B:257:HIS:CE1	2.31	0.65
1:B:328:LEU:HD23	1:B:376:LEU:HD22	1.79	0.65
1:D:225:ASN:N	1:D:226:PRO:HD3	2.12	0.64
1:B:46:LYS:HD3	1:B:47:THR:HG23	1.79	0.64
1:D:363:GLU:HA	1:D:368:GLU:HB3	1.80	0.64
1:D:328:LEU:HD23	1:D:376:LEU:HD22	1.79	0.64
1:A:257:HIS:CD2	1:A:259:GLY:H	2.12	0.64
1:C:225:ASN:N	1:C:226:PRO:HD3	2.12	0.64
1:A:354:THR:HG23	1:A:359:HIS:CE1	2.33	0.64
1:C:241:LEU:HD11	1:D:241:LEU:CD1	2.21	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:LYS:HG3	1:C:173:ASP:HB2	1.80	0.63
1:C:38:ARG:HD2	1:C:38:ARG:N	2.13	0.63
1:D:298:VAL:HG12	1:D:310:ILE:HG12	1.80	0.63
1:D:328:LEU:HD11	1:D:379:ALA:CB	2.28	0.63
1:A:111:PRO:HA	1:A:114:GLN:HG3	1.80	0.63
1:A:321:PRO:HD2	1:A:324:GLN:NE2	2.13	0.63
1:D:2:LYS:HG3	1:D:173:ASP:HB2	1.81	0.63
1:A:337:PRO:HB2	1:A:338:TYR:CD1	2.33	0.63
1:B:225:ASN:N	1:B:226:PRO:HD3	2.14	0.63
1:C:337:PRO:HB2	1:C:338:TYR:CD1	2.34	0.63
1:C:181:ASP:O	1:C:220:THR:HA	1.98	0.63
1:D:328:LEU:HD11	1:D:379:ALA:HB1	1.79	0.62
1:B:354:THR:HG23	1:B:359:HIS:CE1	2.34	0.62
1:D:69:ARG:HD3	1:D:86:ALA:O	1.98	0.62
1:C:17:LYS:O	1:C:21:GLN:HG3	1.98	0.62
1:C:347:LEU:HD22	1:C:347:LEU:H	1.64	0.62
1:A:17:LYS:O	1:A:21:GLN:HG3	1.99	0.62
1:C:151:VAL:CG2	1:C:156:THR:HB	2.28	0.62
1:B:33:GLN:HE22	1:B:61:TRP:N	1.95	0.62
1:C:38:ARG:NH1	1:C:107:ASP:OD1	2.32	0.62
1:D:18:ILE:O	1:D:22:ILE:HG13	2.00	0.62
1:D:184:VAL:HG22	1:D:223:PHE:HB2	1.82	0.62
1:B:111:PRO:HA	1:B:114:GLN:HG3	1.79	0.62
1:B:105:GLY:O	1:B:303:GLY:HA2	1.99	0.62
1:D:347:LEU:H	1:D:347:LEU:HD22	1.64	0.62
1:C:105:GLY:O	1:C:303:GLY:HA2	2.00	0.62
1:D:17:LYS:O	1:D:21:GLN:HG3	1.99	0.62
1:D:135:PRO:O	1:D:139:THR:HG23	2.00	0.62
1:A:121:LEU:HD13	1:B:6:THR:O	2.00	0.62
1:B:38:ARG:N	1:B:38:ARG:HD2	2.14	0.61
1:A:328:LEU:HD23	1:A:376:LEU:HD22	1.82	0.61
1:A:2:LYS:HG3	1:A:173:ASP:HB2	1.83	0.61
1:B:184:VAL:HG22	1:B:223:PHE:HB2	1.80	0.61
1:D:38:ARG:N	1:D:38:ARG:HD2	2.15	0.61
1:C:320:VAL:HB	1:C:324:GLN:NE2	2.15	0.61
1:A:105:GLY:O	1:A:303:GLY:HA2	2.00	0.61
1:A:133:LEU:HD23	1:A:283:LYS:HE2	1.82	0.61
1:A:184:VAL:HG22	1:A:223:PHE:HB2	1.82	0.60
1:B:18:ILE:O	1:B:22:ILE:HG13	2.01	0.60
1:C:324:GLN:O	1:C:328:LEU:HB2	2.02	0.60
1:D:337:PRO:HB2	1:D:338:TYR:HD1	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:THR:HG23	1:C:169:THR:HG22	1.84	0.60
1:A:225:ASN:N	1:A:226:PRO:HD3	2.16	0.60
1:C:39:VAL:O	1:C:265:LYS:HA	2.01	0.60
1:D:193:ILE:HG12	1:D:194:ASP:N	2.16	0.60
1:B:207:ILE:HG23	1:B:211:LEU:HD22	1.83	0.60
1:D:279:ARG:HD3	1:D:368:GLU:OE1	2.02	0.60
1:A:143:ARG:HB3	1:A:210:ILE:HD12	1.82	0.59
1:D:203:MET:O	1:D:208:LYS:HB2	2.02	0.59
1:B:38:ARG:NH1	1:B:107:ASP:OD1	2.35	0.59
1:C:298:VAL:HG12	1:C:310:ILE:HG12	1.84	0.59
1:B:298:VAL:HG12	1:B:310:ILE:HG12	1.84	0.59
1:D:6:THR:HG23	1:D:169:THR:HG22	1.85	0.59
1:A:39:VAL:O	1:A:265:LYS:HA	2.02	0.59
1:B:33:GLN:NE2	1:B:61:TRP:N	2.46	0.59
1:B:324:GLN:O	1:B:328:LEU:HB2	2.02	0.59
1:D:143:ARG:HB3	1:D:210:ILE:HD12	1.85	0.59
1:D:9:SER:OG	1:D:142:HIS:ND1	2.36	0.59
1:D:38:ARG:NH1	1:D:107:ASP:OD1	2.35	0.59
1:A:46:LYS:HD3	1:A:47:THR:HG23	1.84	0.59
1:C:265:LYS:NZ	7:D:884:PPK:H3B	2.01	0.59
1:C:363:GLU:HA	1:C:368:GLU:HB3	1.85	0.59
1:D:323:GLU:HG2	1:D:324:GLN:N	2.17	0.59
1:C:321:PRO:HD2	1:C:324:GLN:NE2	2.17	0.59
1:C:330:ARG:NH2	1:C:331:GLU:HG3	2.17	0.59
1:A:193:ILE:HG12	1:A:194:ASP:N	2.18	0.58
1:D:105:GLY:O	1:D:303:GLY:HA2	2.03	0.58
1:A:324:GLN:O	1:A:328:LEU:HB2	2.03	0.58
1:C:246:ILE:HG22	1:C:247:ILE:N	2.18	0.58
1:C:327:LEU:HA	1:C:330:ARG:HD3	1.85	0.58
1:A:135:PRO:O	1:A:139:THR:HG23	2.03	0.58
1:B:203:MET:O	1:B:208:LYS:HB2	2.03	0.58
1:B:363:GLU:HA	1:B:368:GLU:HB3	1.85	0.58
1:D:111:PRO:HA	1:D:114:GLN:HG3	1.86	0.58
1:D:321:PRO:HD2	1:D:324:GLN:NE2	2.19	0.58
1:D:327:LEU:HA	1:D:330:ARG:HD3	1.85	0.58
1:A:38:ARG:HD2	1:A:38:ARG:N	2.18	0.58
1:A:363:GLU:HA	1:A:368:GLU:HB3	1.86	0.58
1:A:38:ARG:NH1	1:A:107:ASP:OD1	2.37	0.58
1:C:207:ILE:HG23	1:C:211:LEU:HD22	1.84	0.58
1:D:246:ILE:HG22	1:D:247:ILE:N	2.18	0.58
1:A:183:VAL:HG11	1:A:207:ILE:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:VAL:HB	1:A:324:GLN:NE2	2.19	0.58
4:A:384:ANP:H5'1	5:B:385:MET:SD	2.44	0.58
1:B:320:VAL:HB	1:B:324:GLN:NE2	2.18	0.58
1:B:181:ASP:O	1:B:220:THR:HA	2.03	0.57
1:C:111:PRO:HA	1:C:114:GLN:HG3	1.86	0.57
1:A:246:ILE:HG23	1:A:257:HIS:CE1	2.39	0.57
1:B:330:ARG:NH2	1:B:331:GLU:HG3	2.19	0.57
1:D:181:ASP:O	1:D:220:THR:HA	2.04	0.57
1:D:39:VAL:O	1:D:265:LYS:HA	2.04	0.57
1:B:193:ILE:HG12	1:B:194:ASP:N	2.18	0.57
1:A:137:PRO:HA	1:A:170:PHE:CE1	2.40	0.57
1:C:135:PRO:O	1:C:139:THR:HG23	2.05	0.57
1:D:246:ILE:HG22	1:D:247:ILE:HG12	1.85	0.57
1:D:324:GLN:O	1:D:328:LEU:HB2	2.05	0.57
1:A:302:ILE:O	1:B:226:PRO:HB2	2.05	0.57
1:A:330:ARG:NH2	1:A:331:GLU:HG3	2.20	0.57
1:C:253:GLY:O	1:D:256:ARG:HG2	2.04	0.57
1:C:40:ALA:HB3	1:C:55:GLU:HG2	1.85	0.57
1:C:362:ARG:HG3	1:C:365:PHE:CE2	2.39	0.56
1:A:227:THR:HG23	8:A:411:HOH:O	2.05	0.56
1:B:39:VAL:O	1:B:265:LYS:HA	2.05	0.56
1:B:159:TRP:CE2	1:B:193:ILE:HD12	2.41	0.56
1:C:203:MET:O	1:C:208:LYS:HB2	2.05	0.56
1:A:180:ILE:HG13	1:A:215:TRP:HB3	1.88	0.56
1:A:127:THR:O	1:A:133:LEU:HA	2.05	0.56
1:B:2:LYS:HG3	1:B:173:ASP:HB2	1.88	0.56
1:B:347:LEU:HD22	1:B:347:LEU:N	2.17	0.56
1:A:151:VAL:CG2	1:A:156:THR:HB	2.35	0.56
1:B:267:PRO:HB2	1:B:341:ILE:CD1	2.32	0.56
1:B:327:LEU:HA	1:B:330:ARG:HD3	1.88	0.56
1:D:180:ILE:HG13	1:D:215:TRP:HB3	1.86	0.56
1:D:330:ARG:HH21	1:D:331:GLU:HG3	1.67	0.56
1:D:362:ARG:HG3	1:D:365:PHE:CE2	2.41	0.56
1:B:151:VAL:CG2	1:B:156:THR:HB	2.35	0.56
1:C:101:ASP:CG	1:D:229:ARG:HG2	2.25	0.56
1:C:323:GLU:HG2	1:C:324:GLN:N	2.20	0.56
1:A:327:LEU:HA	1:A:330:ARG:HD3	1.89	0.55
1:C:183:VAL:HG11	1:C:207:ILE:HD13	1.89	0.55
1:C:229:ARG:HB3	1:D:104:GLN:NE2	2.21	0.55
1:C:256:ARG:HG2	1:D:253:GLY:O	2.07	0.55
1:A:328:LEU:HD11	1:A:379:ALA:CB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ARG:HG3	1:A:365:PHE:CE2	2.41	0.55
1:C:143:ARG:HB3	1:C:210:ILE:HD12	1.88	0.55
1:B:323:GLU:HG2	1:B:324:GLN:N	2.21	0.55
1:A:328:LEU:HD11	1:A:379:ALA:HB1	1.87	0.54
1:A:272:ARG:HH21	1:A:354:THR:HG21	1.72	0.54
1:B:246:ILE:HG22	1:B:247:ILE:N	2.23	0.54
1:B:328:LEU:HD11	1:B:379:ALA:HB1	1.88	0.54
1:C:51:LEU:HD12	1:D:51:LEU:HD12	1.90	0.54
1:B:337:PRO:HB2	1:B:338:TYR:HD1	1.73	0.54
1:B:127:THR:O	1:B:133:LEU:HA	2.07	0.54
1:B:328:LEU:HD11	1:B:379:ALA:CB	2.37	0.54
1:D:127:THR:O	1:D:133:LEU:HA	2.07	0.54
1:A:347:LEU:HD22	1:A:347:LEU:N	2.23	0.54
1:A:323:GLU:HG2	1:A:324:GLN:N	2.21	0.54
1:B:114:GLN:HB2	1:B:338:TYR:CD1	2.43	0.54
1:B:137:PRO:HA	1:B:170:PHE:CE1	2.44	0.53
1:B:159:TRP:CE3	1:B:193:ILE:HG21	2.43	0.53
1:C:33:GLN:HE22	1:C:61:TRP:N	2.03	0.53
1:C:123:PHE:CD1	1:C:256:ARG:HB3	2.43	0.53
1:C:151:VAL:HG23	1:C:156:THR:CB	2.33	0.53
1:D:338:TYR:CD1	1:D:338:TYR:N	2.76	0.53
1:C:18:ILE:O	1:C:22:ILE:HG13	2.09	0.53
1:A:337:PRO:HB2	1:A:338:TYR:HD1	1.73	0.53
1:A:61:TRP:CE3	1:C:61:TRP:CE3	2.97	0.53
1:A:203:MET:O	1:A:208:LYS:HB2	2.09	0.53
1:C:246:ILE:HG23	1:C:257:HIS:CE1	2.43	0.53
1:A:123:PHE:CD1	1:A:256:ARG:HB3	2.44	0.53
1:B:143:ARG:HB3	1:B:210:ILE:HD12	1.90	0.53
1:B:246:ILE:HG22	1:B:247:ILE:HG12	1.91	0.53
1:D:159:TRP:CE3	1:D:193:ILE:HG21	2.44	0.53
1:D:354:THR:HG23	1:D:359:HIS:CE1	2.43	0.53
1:C:46:LYS:HD3	1:C:47:THR:HG23	1.91	0.53
1:C:337:PRO:HB2	1:C:338:TYR:HD1	1.74	0.53
1:D:207:ILE:HG23	1:D:211:LEU:HD22	1.91	0.53
1:B:210:ILE:HG22	1:B:211:LEU:HD13	1.90	0.52
1:B:301:ALA:O	1:B:304:VAL:HB	2.09	0.52
1:A:40:ALA:HB3	1:A:55:GLU:HG2	1.91	0.52
1:C:37:ALA:C	1:C:38:ARG:HD2	2.28	0.52
1:D:327:LEU:HA	1:D:330:ARG:CD	2.40	0.52
1:A:181:ASP:O	1:A:220:THR:HA	2.09	0.52
1:C:69:ARG:HD3	1:C:86:ALA:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:THR:O	1:C:133:LEU:HA	2.09	0.52
1:D:123:PHE:CD1	1:D:256:ARG:HB3	2.45	0.52
1:B:182:ALA:HB1	1:B:223:PHE:HE2	1.74	0.52
1:D:333:PHE:HZ	1:D:376:LEU:HD11	1.73	0.52
1:C:101:ASP:HB2	8:D:916:HOH:O	2.09	0.52
1:D:122:MET:SD	1:D:122:MET:N	2.82	0.52
1:A:182:ALA:HB1	1:A:223:PHE:HE2	1.74	0.52
1:B:330:ARG:NE	1:B:331:GLU:N	2.57	0.52
1:D:151:VAL:CG2	1:D:156:THR:HB	2.39	0.52
1:B:45:VAL:HG13	1:B:50:VAL:HG22	1.92	0.52
1:A:338:TYR:CD1	1:A:338:TYR:N	2.78	0.52
1:B:212:PRO:HG2	1:B:215:TRP:CZ3	2.45	0.52
1:C:136:ALA:HB3	1:C:137:PRO:HD3	1.91	0.51
1:D:173:ASP:HB3	1:D:178:VAL:HG11	1.91	0.51
1:C:9:SER:OG	1:C:142:HIS:ND1	2.43	0.51
1:C:131:ASP:O	1:C:133:LEU:HD22	2.10	0.51
1:C:180:ILE:HG13	1:C:215:TRP:HB3	1.91	0.51
1:C:182:ALA:HB1	1:C:223:PHE:HE2	1.74	0.51
1:B:338:TYR:CD1	1:B:338:TYR:N	2.78	0.51
1:C:87:ASN:H	1:C:87:ASN:ND2	2.08	0.51
1:A:151:VAL:HG23	1:A:156:THR:CB	2.37	0.51
1:C:338:TYR:CD1	1:C:338:TYR:N	2.79	0.51
1:D:9:SER:HG	1:D:142:HIS:HD1	1.56	0.51
1:B:123:PHE:CD1	1:B:256:ARG:HB3	2.46	0.51
1:B:136:ALA:HB3	1:B:137:PRO:HD3	1.93	0.51
1:B:341:ILE:HG21	1:B:347:LEU:HD11	1.93	0.51
1:B:327:LEU:HA	1:B:330:ARG:CD	2.41	0.51
1:C:328:LEU:CD2	1:C:376:LEU:HD22	2.41	0.51
1:B:298:VAL:HA	1:B:309:SER:O	2.11	0.51
1:D:132:VAL:HG23	1:D:134:MET:HB2	1.93	0.51
1:A:107:ASP:OD2	1:A:114:GLN:NE2	2.44	0.50
1:A:189:HIS:CE1	1:A:231:VAL:HG22	2.46	0.50
1:C:114:GLN:HB2	1:C:338:TYR:CD1	2.46	0.50
1:B:326:THR:O	1:B:330:ARG:HD3	2.12	0.50
1:A:85:ASP:OD1	1:A:87:ASN:ND2	2.36	0.50
1:A:246:ILE:HG22	1:A:247:ILE:HG12	1.93	0.50
1:A:246:ILE:HG22	1:A:247:ILE:N	2.26	0.50
1:C:165:LYS:HE2	1:D:119:GLN:HG2	1.94	0.50
1:A:371:ASP:OD1	1:A:371:ASP:N	2.42	0.50
1:B:378:ASP:OD2	1:B:382:LEU:HD13	2.11	0.50
1:D:40:ALA:HB3	1:D:55:GLU:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:GLU:O	1:D:209:PRO:HG2	2.12	0.50
1:B:87:ASN:ND2	1:B:87:ASN:H	2.08	0.50
1:D:137:PRO:HA	1:D:170:PHE:CE1	2.47	0.50
1:B:72:VAL:CG1	1:B:86:ALA:HB2	2.31	0.50
1:B:85:ASP:OD1	1:B:87:ASN:ND2	2.39	0.50
1:C:330:ARG:HH21	1:C:331:GLU:HG3	1.76	0.50
1:A:107:ASP:CA	1:A:114:GLN:HE21	2.18	0.50
1:B:40:ALA:HB3	1:B:55:GLU:HG2	1.94	0.50
1:B:151:VAL:HG23	1:B:156:THR:CB	2.39	0.50
1:D:183:VAL:HG11	1:D:207:ILE:HD13	1.94	0.50
1:A:159:TRP:CE2	1:A:193:ILE:HD12	2.47	0.50
1:C:173:ASP:HB3	1:C:178:VAL:HG11	1.92	0.50
1:A:136:ALA:HB3	1:A:137:PRO:HD3	1.94	0.50
1:C:33:GLN:NE2	1:C:61:TRP:N	2.56	0.49
1:C:132:VAL:HG23	1:C:134:MET:HB2	1.94	0.49
1:C:382:LEU:HG	1:C:383:LYS:H	1.75	0.49
1:B:107:ASP:CA	1:B:114:GLN:HE21	2.20	0.49
1:C:204:GLU:OE2	1:C:208:LYS:HE2	2.12	0.49
1:A:340:LEU:HA	1:A:343:MET:HB3	1.94	0.49
1:B:87:ASN:H	1:B:87:ASN:HD22	1.60	0.49
1:B:340:LEU:HA	1:B:343:MET:HB3	1.94	0.49
1:C:122:MET:SD	1:C:122:MET:N	2.85	0.49
1:C:123:PHE:CE2	1:C:297:GLN:HB2	2.48	0.49
1:D:87:ASN:ND2	1:D:87:ASN:H	2.10	0.49
1:A:114:GLN:HB2	1:A:338:TYR:CD1	2.47	0.49
1:A:18:ILE:O	1:A:22:ILE:HG13	2.13	0.49
1:A:298:VAL:HG12	1:A:310:ILE:HG12	1.94	0.49
1:B:333:PHE:HZ	1:B:376:LEU:HD11	1.78	0.49
1:A:226:PRO:HB2	1:B:302:ILE:O	2.13	0.49
1:B:159:TRP:CZ2	1:B:193:ILE:HD12	2.47	0.49
1:A:120:GLY:O	1:A:299:SER:HA	2.13	0.48
1:A:226:PRO:C	1:A:228:GLY:N	2.64	0.48
1:C:354:THR:HG23	1:C:359:HIS:CE1	2.47	0.48
1:D:327:LEU:HD12	1:D:330:ARG:HD2	1.94	0.48
1:A:37:ALA:C	1:A:38:ARG:HD2	2.34	0.48
1:B:114:GLN:HB3	1:B:338:TYR:CE1	2.48	0.48
1:B:371:ASP:OD1	1:B:371:ASP:N	2.44	0.48
1:D:114:GLN:HB2	1:D:338:TYR:CD1	2.48	0.48
1:D:159:TRP:CE2	1:D:193:ILE:HD12	2.49	0.48
1:A:159:TRP:CE3	1:A:193:ILE:HG21	2.48	0.48
1:A:17:LYS:O	1:A:21:GLN:CG	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ASP:HB3	1:A:178:VAL:HG11	1.94	0.48
1:A:335:LEU:HA	1:A:340:LEU:HD23	1.95	0.48
1:B:330:ARG:HH21	1:B:331:GLU:HG3	1.78	0.48
1:C:272:ARG:HH21	1:C:354:THR:HG21	1.77	0.48
1:C:314:THR:O	1:C:317:THR:HG23	2.13	0.48
8:A:401:HOH:O	1:B:55:GLU:HG3	2.13	0.48
1:A:131:ASP:O	1:A:133:LEU:HD22	2.14	0.48
1:C:327:LEU:HA	1:C:330:ARG:CD	2.44	0.48
1:A:114:GLN:HB3	1:A:338:TYR:CE1	2.49	0.48
1:A:327:LEU:HA	1:A:330:ARG:CD	2.44	0.48
5:A:485:MET:SD	4:B:484:ANP:C5'	3.02	0.48
1:B:14:HIS:CE1	1:B:16:ASP:HB2	2.49	0.48
1:C:125:TYR:CG	1:C:255:ALA:HB2	2.49	0.48
1:C:321:PRO:O	1:C:322:SER:C	2.52	0.48
1:A:108:ARG:HH11	1:A:108:ARG:HG2	1.78	0.48
1:D:45:VAL:HG13	1:D:50:VAL:HG22	1.96	0.48
1:D:210:ILE:HG22	1:D:211:LEU:HD13	1.95	0.48
1:A:108:ARG:H	1:A:114:GLN:HG2	1.78	0.47
1:C:121:LEU:HA	1:C:299:SER:HA	1.96	0.47
1:B:272:ARG:HH21	1:B:354:THR:HG21	1.79	0.47
1:D:107:ASP:CA	1:D:114:GLN:HE21	2.20	0.47
1:D:330:ARG:NE	1:D:331:GLU:N	2.57	0.47
1:B:46:LYS:HD3	1:B:47:THR:H	1.79	0.47
1:B:173:ASP:HB3	1:B:178:VAL:HG11	1.95	0.47
1:D:31:LEU:HD22	1:D:35:PRO:HA	1.97	0.47
1:D:108:ARG:H	1:D:114:GLN:HG2	1.80	0.47
1:D:246:ILE:CG2	1:D:247:ILE:N	2.77	0.47
1:D:272:ARG:HH21	1:D:354:THR:HG21	1.78	0.47
1:B:169:THR:O	1:B:180:ILE:HG23	2.13	0.47
1:D:225:ASN:N	1:D:226:PRO:CD	2.76	0.47
1:A:6:THR:O	1:B:121:LEU:HD13	2.14	0.47
1:B:335:LEU:HA	1:B:340:LEU:HD23	1.96	0.47
1:D:189:HIS:CE1	1:D:231:VAL:HG22	2.49	0.47
1:B:327:LEU:O	1:B:330:ARG:NE	2.47	0.47
1:A:207:ILE:HG23	1:A:211:LEU:HD22	1.97	0.47
1:B:17:LYS:O	1:B:21:GLN:CG	2.61	0.47
1:B:79:HIS:HD2	1:B:81:ASP:N	2.00	0.47
1:B:189:HIS:CE1	1:B:231:VAL:HG22	2.50	0.47
1:B:321:PRO:HD2	1:B:324:GLN:NE2	2.29	0.47
1:B:325:LEU:O	1:B:329:VAL:HG23	2.14	0.47
1:B:327:LEU:CA	1:B:330:ARG:HD3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ASN:H	1:C:87:ASN:HD22	1.63	0.47
1:C:325:LEU:O	1:C:329:VAL:HG23	2.15	0.47
1:D:37:ALA:C	1:D:38:ARG:HD2	2.34	0.47
1:D:279:ARG:HD2	1:D:360:PHE:CG	2.50	0.47
1:B:9:SER:OG	1:B:142:HIS:ND1	2.47	0.47
1:C:45:VAL:HG13	1:C:50:VAL:HG22	1.96	0.47
1:C:189:HIS:CE1	1:C:231:VAL:HG22	2.50	0.47
1:D:335:LEU:HA	1:D:340:LEU:HD23	1.95	0.47
1:C:226:PRO:C	1:C:228:GLY:N	2.67	0.47
1:C:335:LEU:HA	1:C:340:LEU:HD23	1.96	0.47
1:B:37:ALA:C	1:B:38:ARG:HD2	2.35	0.47
1:C:246:ILE:HG22	1:C:247:ILE:HG12	1.96	0.47
1:C:333:PHE:HZ	1:C:376:LEU:HD11	1.78	0.47
1:B:183:VAL:HG11	1:B:207:ILE:HD13	1.97	0.46
1:C:159:TRP:CE3	1:C:193:ILE:HG21	2.50	0.46
1:C:330:ARG:NE	1:C:331:GLU:N	2.58	0.46
1:C:382:LEU:O	1:C:383:LYS:OXT	2.33	0.46
1:D:326:THR:O	1:D:330:ARG:HD3	2.15	0.46
1:D:327:LEU:CA	1:D:330:ARG:HD3	2.45	0.46
1:A:122:MET:CE	1:A:271:ASP:HA	2.45	0.46
1:A:321:PRO:HD2	1:A:324:GLN:HE22	1.79	0.46
1:C:107:ASP:CA	1:C:114:GLN:HE21	2.20	0.46
1:C:137:PRO:HA	1:C:170:PHE:CE1	2.50	0.46
7:C:684:PPK:H3B	1:D:265:LYS:HZ2	1.63	0.46
1:D:85:ASP:OD1	1:D:87:ASN:ND2	2.39	0.46
1:B:180:ILE:HG13	1:B:215:TRP:HB3	1.98	0.46
1:C:267:PRO:HB2	1:C:341:ILE:CD1	2.40	0.46
1:B:50:VAL:HG23	1:B:84:PHE:HZ	1.81	0.46
1:C:340:LEU:HA	1:C:343:MET:HB3	1.96	0.46
1:D:131:ASP:O	1:D:133:LEU:HD22	2.15	0.46
1:C:293:ARG:O	1:C:293:ARG:HG3	2.15	0.46
1:A:9:SER:OG	1:A:142:HIS:ND1	2.46	0.46
1:A:241:LEU:HG	1:B:241:LEU:HG	1.97	0.46
1:A:325:LEU:O	1:A:329:VAL:HG23	2.15	0.46
1:B:341:ILE:HG23	1:B:346:LEU:HB2	1.97	0.46
1:C:221:LYS:NZ	1:C:221:LYS:HB3	2.31	0.46
1:C:328:LEU:HD11	1:C:379:ALA:HB3	1.97	0.46
1:A:382:LEU:HG	1:A:383:LYS:H	1.76	0.45
1:C:114:GLN:HB3	1:C:338:TYR:CE1	2.51	0.45
1:C:318:GLU:O	1:C:319:LYS:HD3	2.16	0.45
1:A:125:TYR:CD1	1:A:295:GLU:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ARG:H	1:C:114:GLN:HG2	1.82	0.45
1:B:31:LEU:HD22	1:B:35:PRO:HA	1.97	0.45
1:B:279:ARG:HD2	1:B:360:PHE:CG	2.51	0.45
1:D:176:LYS:HD2	1:D:176:LYS:HA	1.64	0.45
1:A:9:SER:HG	1:A:142:HIS:HD1	1.62	0.45
1:A:382:LEU:CG	1:A:383:LYS:N	2.67	0.45
1:C:229:ARG:HG2	1:D:101:ASP:CG	2.36	0.45
1:D:325:LEU:O	1:D:329:VAL:HG23	2.16	0.45
1:C:225:ASN:N	1:C:226:PRO:CD	2.78	0.45
1:C:245:LYS:HA	8:C:731:HOH:O	2.15	0.45
1:C:343:MET:HG2	1:C:344:LEU:HG	1.98	0.45
1:D:341:ILE:HG21	1:D:347:LEU:HD11	1.99	0.45
1:A:122:MET:HG2	1:A:298:VAL:CG2	2.35	0.45
1:D:330:ARG:NE	1:D:330:ARG:C	2.70	0.45
1:A:123:PHE:CE2	1:A:297:GLN:HB2	2.51	0.45
1:A:225:ASN:N	1:A:226:PRO:CD	2.79	0.45
1:D:46:LYS:HD3	1:D:47:THR:H	1.81	0.45
1:A:45:VAL:HG13	1:A:50:VAL:HG22	1.99	0.45
1:A:330:ARG:C	1:A:330:ARG:NE	2.70	0.45
1:C:176:LYS:HD2	1:C:176:LYS:HA	1.64	0.45
1:C:327:LEU:HD12	1:C:330:ARG:HD2	1.99	0.45
1:D:340:LEU:HA	1:D:343:MET:HB3	1.98	0.45
1:A:61:TRP:HE3	1:C:61:TRP:CE3	2.33	0.45
1:A:330:ARG:NE	1:A:331:GLU:N	2.57	0.45
1:B:225:ASN:N	1:B:226:PRO:CD	2.79	0.45
1:C:327:LEU:CA	1:C:330:ARG:HD3	2.47	0.45
1:D:65:GLU:HG3	1:D:69:ARG:HG3	1.99	0.45
1:D:171:GLN:NE2	1:D:181:ASP:OD2	2.50	0.45
1:D:362:ARG:H	1:D:362:ARG:HG2	1.66	0.45
1:A:327:LEU:HD12	1:A:330:ARG:HD2	1.98	0.45
1:B:6:THR:CG2	1:B:169:THR:HG22	2.45	0.45
1:B:140:TYR:CE2	1:B:215:TRP:HZ3	2.34	0.45
1:C:326:THR:O	1:C:330:ARG:HD3	2.17	0.45
1:D:120:GLY:O	1:D:299:SER:HA	2.17	0.45
1:D:327:LEU:HA	1:D:327:LEU:HD12	1.80	0.45
1:D:327:LEU:O	1:D:330:ARG:NE	2.50	0.45
1:D:328:LEU:CD2	1:D:376:LEU:HD22	2.47	0.45
1:B:226:PRO:C	1:B:228:GLY:N	2.68	0.44
1:D:382:LEU:HG	1:D:383:LYS:H	1.80	0.44
1:A:152:ARG:NH1	1:A:162:PRO:HA	2.32	0.44
1:A:327:LEU:CA	1:A:330:ARG:HD3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:MET:HG2	1:B:298:VAL:CG2	2.34	0.44
1:C:120:GLY:O	1:C:299:SER:HA	2.16	0.44
1:C:246:ILE:CG2	1:C:247:ILE:N	2.77	0.44
1:C:279:ARG:HD2	1:C:360:PHE:CG	2.52	0.44
1:D:47:THR:HG22	1:D:236:MET:HA	1.98	0.44
1:D:136:ALA:O	1:D:139:THR:OG1	2.30	0.44
1:A:226:PRO:C	1:A:228:GLY:H	2.20	0.44
1:A:301:ALA:O	1:A:304:VAL:HB	2.17	0.44
1:B:135:PRO:O	1:B:139:THR:HG23	2.17	0.44
1:C:46:LYS:HE2	1:C:235:PRO:O	2.18	0.44
1:C:210:ILE:HG22	1:C:211:LEU:HD13	1.98	0.44
1:C:238:ASP:OD2	6:C:685:SAM:H5'2	2.18	0.44
1:A:14:HIS:CE1	1:A:16:ASP:HB2	2.53	0.44
1:A:33:GLN:NE2	1:A:61:TRP:N	2.51	0.44
1:B:121:LEU:HA	1:B:299:SER:HA	1.98	0.44
1:B:341:ILE:HG22	1:B:347:LEU:CD2	2.48	0.44
1:D:285:ILE:HG23	1:D:290:LEU:HB2	1.99	0.44
1:A:318:GLU:O	1:A:319:LYS:HD3	2.18	0.44
1:C:12:GLU:OE2	1:C:153:LYS:NZ	2.51	0.44
1:C:85:ASP:OD1	1:C:87:ASN:ND2	2.33	0.44
1:C:362:ARG:H	1:C:362:ARG:HG2	1.67	0.44
1:D:69:ARG:NH1	1:D:89:CYS:O	2.42	0.44
1:D:314:THR:O	1:D:317:THR:HG23	2.18	0.44
1:A:330:ARG:HH21	1:A:331:GLU:HG3	1.83	0.44
1:B:17:LYS:HD3	1:B:17:LYS:HA	1.61	0.44
1:D:33:GLN:NE2	1:D:61:TRP:N	2.57	0.44
1:A:333:PHE:HZ	1:A:376:LEU:HD11	1.82	0.44
1:B:328:LEU:CD2	1:B:376:LEU:HD22	2.48	0.44
1:B:351:TYR:O	1:B:352:LYS:C	2.55	0.44
1:C:47:THR:HG22	1:C:236:MET:HA	1.99	0.44
1:D:347:LEU:HD22	1:D:347:LEU:N	2.32	0.44
1:A:121:LEU:HA	1:A:299:SER:HA	1.99	0.43
1:A:175:GLY:O	1:A:176:LYS:HD2	2.18	0.43
1:A:369:LYS:HA	1:A:369:LYS:CE	2.46	0.43
1:B:347:LEU:H	1:B:347:LEU:CD2	2.23	0.43
1:A:66:GLU:OE1	1:A:66:GLU:HA	2.19	0.43
1:C:159:TRP:CE2	1:C:193:ILE:HD12	2.54	0.43
1:A:125:TYR:HD1	1:A:295:GLU:HG3	1.83	0.43
1:C:229:ARG:CZ	1:C:231:VAL:HG21	2.49	0.43
1:C:330:ARG:NE	1:C:330:ARG:C	2.72	0.43
1:D:107:ASP:OD2	1:D:114:GLN:NE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:GLY:O	1:D:176:LYS:HD2	2.17	0.43
1:D:280:TYR:O	1:D:284:ASN:HB2	2.19	0.43
1:A:169:THR:O	1:A:180:ILE:HG23	2.18	0.43
1:A:204:GLU:OE2	1:A:208:LYS:HE2	2.19	0.43
1:A:140:TYR:CE2	1:A:215:TRP:HZ3	2.36	0.43
1:B:107:ASP:OD2	1:B:114:GLN:NE2	2.52	0.43
1:C:120:GLY:N	1:D:167:GLN:OE1	2.52	0.43
1:D:246:ILE:HG23	1:D:257:HIS:CE1	2.53	0.43
1:B:46:LYS:HE2	1:B:235:PRO:O	2.18	0.43
1:A:159:TRP:CZ2	1:A:193:ILE:HD12	2.54	0.43
1:D:123:PHE:CE2	1:D:297:GLN:HB2	2.54	0.43
1:D:204:GLU:OE2	1:D:208:LYS:HE2	2.19	0.43
1:B:108:ARG:HG2	1:B:108:ARG:HH11	1.84	0.43
1:C:50:VAL:HG23	1:C:84:PHE:HZ	1.84	0.43
1:D:72:VAL:O	1:D:75:ILE:HB	2.19	0.43
1:D:151:VAL:HG23	1:D:156:THR:CB	2.44	0.43
1:A:279:ARG:HD2	1:A:360:PHE:CG	2.54	0.43
1:A:362:ARG:H	1:A:362:ARG:HG2	1.66	0.43
1:B:113:GLU:O	1:B:305:ALA:HB2	2.19	0.43
1:C:330:ARG:CZ	1:C:330:ARG:HB2	2.48	0.43
1:D:72:VAL:CG1	1:D:86:ALA:HB2	2.33	0.43
1:D:371:ASP:OD1	1:D:371:ASP:N	2.37	0.43
1:A:72:VAL:CG1	1:A:86:ALA:HB2	2.39	0.42
1:A:199:GLN:HA	1:A:224:ILE:HG21	2.02	0.42
1:A:298:VAL:HA	1:A:309:SER:O	2.19	0.42
1:B:122:MET:SD	1:B:122:MET:N	2.92	0.42
1:C:101:ASP:HB3	1:D:229:ARG:O	2.19	0.42
1:C:369:LYS:CE	1:C:369:LYS:HA	2.47	0.42
1:D:108:ARG:HD3	1:D:113:GLU:HG3	2.00	0.42
1:D:328:LEU:HD11	1:D:379:ALA:HB3	1.99	0.42
1:B:136:ALA:O	1:B:139:THR:OG1	2.27	0.42
1:D:226:PRO:C	1:D:228:GLY:N	2.71	0.42
1:A:31:LEU:HD22	1:A:35:PRO:HA	2.01	0.42
1:A:87:ASN:ND2	1:A:87:ASN:H	2.16	0.42
1:A:101:ASP:CG	1:B:229:ARG:HG2	2.40	0.42
1:A:114:GLN:HB2	1:A:338:TYR:CG	2.54	0.42
1:A:210:ILE:HG22	1:A:211:LEU:HD13	2.01	0.42
1:B:49:MET:SD	1:C:92:LEU:HD21	2.59	0.42
1:B:314:THR:OG1	1:B:318:GLU:HB3	2.19	0.42
1:C:195:GLN:O	1:C:199:GLN:HG3	2.20	0.42
1:C:347:LEU:HD22	1:C:347:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:ASN:H	1:D:87:ASN:HD22	1.68	0.42
1:B:122:MET:CE	1:B:271:ASP:HA	2.49	0.42
1:C:17:LYS:HD3	1:C:17:LYS:HA	1.68	0.42
1:A:148:GLN:HG2	1:A:160:LEU:HD13	2.00	0.42
1:A:186:SER:HA	1:A:225:ASN:OD1	2.19	0.42
1:B:327:LEU:HD12	1:B:330:ARG:HD2	2.00	0.42
1:D:50:VAL:HG23	1:D:84:PHE:HZ	1.85	0.42
1:D:246:ILE:HB	8:D:931:HOH:O	2.18	0.42
1:B:61:TRP:CE3	1:D:61:TRP:CE3	3.07	0.42
1:C:122:MET:CE	1:C:271:ASP:HA	2.50	0.42
1:D:65:GLU:HA	1:D:91:VAL:HG11	2.01	0.42
1:D:121:LEU:HA	1:D:299:SER:HA	2.02	0.42
1:C:121:LEU:C	1:C:122:MET:SD	2.98	0.42
1:D:212:PRO:HG2	1:D:215:TRP:CZ3	2.55	0.42
1:A:55:GLU:HA	1:A:96:GLY:O	2.20	0.42
1:A:380:ALA:O	1:A:381:GLY:C	2.56	0.42
1:A:382:LEU:O	1:A:383:LYS:OXT	2.37	0.42
1:B:114:GLN:HB2	1:B:338:TYR:CG	2.55	0.42
1:B:148:GLN:HG2	1:B:160:LEU:HD13	2.01	0.42
1:C:279:ARG:HD2	1:C:360:PHE:CD1	2.54	0.42
1:A:125:TYR:CG	1:A:255:ALA:HB2	2.55	0.42
1:B:175:GLY:O	1:B:176:LYS:HD2	2.20	0.42
1:B:323:GLU:CG	1:B:324:GLN:N	2.83	0.42
1:A:52:VAL:O	1:A:93:SER:HA	2.19	0.42
1:A:61:TRP:CE3	1:C:61:TRP:HE3	2.38	0.42
1:A:226:PRO:O	1:A:228:GLY:N	2.52	0.42
1:C:38:ARG:HA	1:C:266:ASP:OD2	2.20	0.42
1:C:171:GLN:NE2	1:C:181:ASP:OD2	2.53	0.42
1:A:327:LEU:HA	1:A:327:LEU:HD12	1.79	0.41
1:B:176:LYS:HD2	1:B:176:LYS:HA	1.63	0.41
1:B:341:ILE:HG22	1:B:347:LEU:HD21	2.02	0.41
1:C:31:LEU:HD23	1:C:31:LEU:HA	1.94	0.41
1:C:382:LEU:O	1:C:383:LYS:C	2.59	0.41
1:C:66:GLU:HA	1:C:66:GLU:OE1	2.20	0.41
1:C:336:ARG:O	1:C:337:PRO:C	2.57	0.41
1:D:17:LYS:O	1:D:21:GLN:CG	2.68	0.41
1:A:38:ARG:HA	1:A:266:ASP:OD2	2.20	0.41
1:A:101:ASP:OD1	1:B:229:ARG:HG2	2.20	0.41
1:A:336:ARG:O	1:A:337:PRO:C	2.58	0.41
1:B:122:MET:HE2	1:B:270:VAL:O	2.20	0.41
1:B:205:GLU:O	1:B:209:PRO:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:GLU:HA	1:C:91:VAL:HG11	2.02	0.41
1:C:208:LYS:N	1:C:209:PRO:CD	2.83	0.41
1:C:226:PRO:C	1:C:228:GLY:H	2.24	0.41
1:A:193:ILE:HD13	1:A:198:LEU:HB2	2.03	0.41
1:B:65:GLU:HA	1:B:91:VAL:HG11	2.01	0.41
1:B:330:ARG:NE	1:B:330:ARG:C	2.74	0.41
1:C:108:ARG:HH11	1:C:108:ARG:HG2	1.85	0.41
1:C:335:LEU:HA	1:C:335:LEU:HD12	1.89	0.41
1:D:320:VAL:O	1:D:321:PRO:C	2.57	0.41
1:A:195:GLN:O	1:A:199:GLN:HG3	2.21	0.41
1:C:17:LYS:O	1:C:21:GLN:CG	2.69	0.41
1:D:330:ARG:CZ	1:D:330:ARG:HB2	2.49	0.41
1:A:113:GLU:O	1:A:305:ALA:HB2	2.21	0.41
1:D:279:ARG:HD2	1:D:360:PHE:CD1	2.55	0.41
1:A:330:ARG:HE	1:A:330:ARG:C	2.22	0.41
1:B:31:LEU:HA	1:B:34:ASP:O	2.21	0.41
1:B:131:ASP:O	1:B:133:LEU:HD22	2.21	0.41
1:C:327:LEU:HA	1:C:327:LEU:HD12	1.85	0.41
1:D:46:LYS:HE2	1:D:235:PRO:O	2.21	0.41
1:A:147:ARG:O	1:A:151:VAL:HG12	2.20	0.41
1:A:176:LYS:HD2	1:A:176:LYS:HA	1.63	0.41
1:A:328:LEU:CD2	1:A:376:LEU:HD22	2.51	0.41
1:B:125:TYR:CG	1:B:255:ALA:HB2	2.56	0.41
1:B:246:ILE:HG23	1:B:257:HIS:ND1	2.35	0.41
1:D:77:TYR:OH	1:D:163:ASP:HB2	2.21	0.41
1:D:182:ALA:HB1	1:D:223:PHE:HE2	1.84	0.41
1:A:122:MET:SD	1:A:122:MET:N	2.94	0.41
1:A:320:VAL:O	1:A:321:PRO:C	2.58	0.41
1:B:55:GLU:HA	1:B:96:GLY:O	2.21	0.41
1:B:79:HIS:NE2	1:C:79:HIS:NE2	2.69	0.41
1:B:108:ARG:H	1:B:114:GLN:HG2	1.85	0.41
1:B:114:GLN:O	1:B:337:PRO:HG2	2.20	0.41
1:B:335:LEU:HA	1:B:335:LEU:HD12	1.85	0.41
1:C:31:LEU:HD22	1:C:35:PRO:HA	2.03	0.41
1:A:302:ILE:O	1:A:302:ILE:HG23	2.21	0.41
1:B:212:PRO:HG2	1:B:215:TRP:CE3	2.56	0.41
1:B:321:PRO:O	1:B:322:SER:C	2.59	0.41
1:B:327:LEU:HA	1:B:327:LEU:HD12	1.80	0.41
1:C:38:ARG:HH12	1:C:107:ASP:CG	2.24	0.41
1:C:125:TYR:HB3	1:C:251:TYR:CE1	2.56	0.41
1:A:155:GLY:O	1:A:158:PRO:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:THR:O	1:A:330:ARG:HD3	2.22	0.40
1:C:371:ASP:OD1	1:C:371:ASP:N	2.41	0.40
1:D:65:GLU:O	1:D:69:ARG:HG3	2.21	0.40
1:D:267:PRO:C	1:D:269:LYS:H	2.24	0.40
1:D:333:PHE:CZ	1:D:376:LEU:HD11	2.55	0.40
1:D:363:GLU:HA	1:D:368:GLU:CB	2.49	0.40
1:A:221:LYS:NZ	1:A:221:LYS:HB3	2.35	0.40
1:A:267:PRO:HB2	1:A:341:ILE:CD1	2.39	0.40
1:B:111:PRO:HA	1:B:114:GLN:CG	2.49	0.40
1:B:318:GLU:O	1:B:319:LYS:HD3	2.21	0.40
1:C:79:HIS:CD2	1:C:81:ASP:HB2	2.56	0.40
1:C:113:GLU:O	1:C:305:ALA:HB2	2.20	0.40
1:C:140:TYR:CE2	1:C:215:TRP:HZ3	2.39	0.40
1:B:133:LEU:HD22	1:B:133:LEU:N	2.36	0.40
1:B:210:ILE:HG22	1:B:211:LEU:CD1	2.52	0.40
1:B:362:ARG:H	1:B:362:ARG:HG2	1.71	0.40
1:B:267:PRO:C	1:B:269:LYS:H	2.25	0.40
1:C:123:PHE:CE1	1:C:256:ARG:HB3	2.57	0.40
1:C:281:VAL:HB	1:C:333:PHE:CE2	2.57	0.40
1:D:169:THR:O	1:D:180:ILE:HG23	2.22	0.40
1:D:336:ARG:O	1:D:337:PRO:C	2.59	0.40
1:A:296:ILE:CG2	1:A:297:GLN:N	2.85	0.40
1:A:335:LEU:HA	1:A:335:LEU:HD12	1.87	0.40
1:B:66:GLU:HA	1:B:66:GLU:OE1	2.22	0.40
1:B:69:ARG:O	1:B:86:ALA:HB1	2.22	0.40
1:C:101:ASP:OD1	1:D:229:ARG:HG2	2.20	0.40
1:D:9:SER:HG	1:D:142:HIS:CE1	2.39	0.40
1:D:17:LYS:HA	1:D:17:LYS:HD3	1.67	0.40
1:D:140:TYR:CE2	1:D:215:TRP:HZ3	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	381/383 (100%)	350 (92%)	28 (7%)	3 (1%)	19	35
1	B	381/383 (100%)	352 (92%)	26 (7%)	3 (1%)	19	35
1	C	381/383 (100%)	349 (92%)	28 (7%)	4 (1%)	15	28
1	D	381/383 (100%)	346 (91%)	31 (8%)	4 (1%)	15	28
All	All	1524/1532 (100%)	1397 (92%)	113 (7%)	14 (1%)	17	31

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	THR
1	B	47	THR
1	C	47	THR
1	D	47	THR
1	A	382	LEU
1	B	382	LEU
1	C	382	LEU
1	D	382	LEU
1	D	363	GLU
1	C	363	GLU
1	A	381	GLY
1	D	381	GLY
1	B	381	GLY
1	C	381	GLY

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	311/311 (100%)	243 (78%)	68 (22%)	1	1
1	B	311/311 (100%)	242 (78%)	69 (22%)	1	1
1	C	311/311 (100%)	241 (78%)	70 (22%)	1	1
1	D	311/311 (100%)	242 (78%)	69 (22%)	1	1
All	All	1244/1244 (100%)	968 (78%)	276 (22%)	1	1

All (276) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	7	SER
1	A	9	SER
1	A	17	LYS
1	A	32	GLU
1	A	36	LYS
1	A	38	ARG
1	A	46	LYS
1	A	51	LEU
1	A	55	GLU
1	A	65	GLU
1	A	66	GLU
1	A	74	GLU
1	A	82	MET
1	A	87	ASN
1	A	92	LEU
1	A	99	SER
1	A	112	LEU
1	A	113	GLU
1	A	122	MET
1	A	150	GLU
1	A	153	LYS
1	A	161	ARG
1	A	169	THR
1	A	181	ASP
1	A	185	LEU
1	A	193	ILE
1	A	203	MET
1	A	205	GLU
1	A	208	LYS
1	A	211	LEU
1	A	214	GLU
1	A	218	SER
1	A	221	LYS
1	A	241	LEU
1	A	246	ILE
1	A	256	ARG
1	A	265	LYS
1	A	269	LYS
1	A	270	VAL
1	A	279	ARG
1	A	294	CYS

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Mol	Chain	Res	Type
1	A	309	SER
1	A	311	MET
1	A	312	VAL
1	A	317	THR
1	A	322	SER
1	A	323	GLU
1	A	326	THR
1	A	327	LEU
1	A	328	LEU
1	A	330	ARG
1	A	331	GLU
1	A	333	PHE
1	A	335	LEU
1	A	340	LEU
1	A	347	LEU
1	A	354	THR
1	A	362	ARG
1	A	363	GLU
1	A	369	LYS
1	A	371	ASP
1	A	372	LYS
1	A	374	GLN
1	A	375	LEU
1	A	377	ARG
1	A	382	LEU
1	A	383	LYS
1	B	2	LYS
1	B	7	SER
1	B	9	SER
1	B	17	LYS
1	B	32	GLU
1	B	36	LYS
1	B	38	ARG
1	B	46	LYS
1	B	51	LEU
1	B	55	GLU
1	B	65	GLU
1	B	66	GLU
1	B	74	GLU
1	B	82	MET
1	B	87	ASN
1	B	92	LEU

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Mol	Chain	Res	Type
1	B	99	SER
1	B	112	LEU
1	B	113	GLU
1	B	122	MET
1	B	150	GLU
1	B	153	LYS
1	B	161	ARG
1	B	169	THR
1	B	181	ASP
1	B	185	LEU
1	B	193	ILE
1	B	203	MET
1	B	205	GLU
1	B	208	LYS
1	B	211	LEU
1	B	214	GLU
1	B	218	SER
1	B	221	LYS
1	B	230	PHE
1	B	241	LEU
1	B	246	ILE
1	B	256	ARG
1	B	265	LYS
1	B	269	LYS
1	B	270	VAL
1	B	279	ARG
1	B	294	CYS
1	B	309	SER
1	B	311	MET
1	B	312	VAL
1	B	317	THR
1	B	322	SER
1	B	323	GLU
1	B	326	THR
1	B	327	LEU
1	B	328	LEU
1	B	330	ARG
1	B	331	GLU
1	B	333	PHE
1	B	335	LEU
1	B	340	LEU
1	B	347	LEU

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Mol	Chain	Res	Type
1	B	354	THR
1	B	362	ARG
1	B	363	GLU
1	B	369	LYS
1	B	371	ASP
1	B	372	LYS
1	B	374	GLN
1	B	375	LEU
1	B	377	ARG
1	B	382	LEU
1	B	383	LYS
1	C	2	LYS
1	C	9	SER
1	C	17	LYS
1	C	32	GLU
1	C	36	LYS
1	C	38	ARG
1	C	46	LYS
1	C	51	LEU
1	C	55	GLU
1	C	65	GLU
1	C	66	GLU
1	C	74	GLU
1	C	82	MET
1	C	87	ASN
1	C	92	LEU
1	C	99	SER
1	C	112	LEU
1	C	113	GLU
1	C	122	MET
1	C	150	GLU
1	C	153	LYS
1	C	161	ARG
1	C	169	THR
1	C	181	ASP
1	C	185	LEU
1	C	193	ILE
1	C	203	MET
1	C	205	GLU
1	C	208	LYS
1	C	211	LEU
1	C	214	GLU

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Mol	Chain	Res	Type
1	C	218	SER
1	C	221	LYS
1	C	230	PHE
1	C	241	LEU
1	C	245	LYS
1	C	246	ILE
1	C	256	ARG
1	C	265	LYS
1	C	269	LYS
1	C	270	VAL
1	C	279	ARG
1	C	294	CYS
1	C	309	SER
1	C	311	MET
1	C	312	VAL
1	C	317	THR
1	C	322	SER
1	C	323	GLU
1	C	326	THR
1	C	327	LEU
1	C	328	LEU
1	C	330	ARG
1	C	331	GLU
1	C	335	LEU
1	C	340	LEU
1	C	341	ILE
1	C	347	LEU
1	C	354	THR
1	C	362	ARG
1	C	363	GLU
1	C	369	LYS
1	C	370	THR
1	C	371	ASP
1	C	372	LYS
1	C	374	GLN
1	C	375	LEU
1	C	377	ARG
1	C	382	LEU
1	C	383	LYS
1	D	2	LYS
1	D	9	SER
1	D	17	LYS

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Mol	Chain	Res	Type
1	D	32	GLU
1	D	36	LYS
1	D	38	ARG
1	D	46	LYS
1	D	51	LEU
1	D	55	GLU
1	D	65	GLU
1	D	66	GLU
1	D	74	GLU
1	D	82	MET
1	D	87	ASN
1	D	92	LEU
1	D	99	SER
1	D	112	LEU
1	D	113	GLU
1	D	122	MET
1	D	150	GLU
1	D	153	LYS
1	D	161	ARG
1	D	169	THR
1	D	181	ASP
1	D	185	LEU
1	D	193	ILE
1	D	203	MET
1	D	205	GLU
1	D	208	LYS
1	D	211	LEU
1	D	214	GLU
1	D	218	SER
1	D	221	LYS
1	D	227	THR
1	D	230	PHE
1	D	241	LEU
1	D	245	LYS
1	D	246	ILE
1	D	256	ARG
1	D	265	LYS
1	D	269	LYS
1	D	270	VAL
1	D	279	ARG
1	D	309	SER
1	D	311	MET

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Mol	Chain	Res	Type
1	D	312	VAL
1	D	317	THR
1	D	322	SER
1	D	323	GLU
1	D	326	THR
1	D	327	LEU
1	D	328	LEU
1	D	330	ARG
1	D	331	GLU
1	D	335	LEU
1	D	340	LEU
1	D	341	ILE
1	D	347	LEU
1	D	354	THR
1	D	362	ARG
1	D	363	GLU
1	D	369	LYS
1	D	371	ASP
1	D	372	LYS
1	D	374	GLN
1	D	375	LEU
1	D	377	ARG
1	D	382	LEU
1	D	383	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	21	GLN
1	A	33	GLN
1	A	79	HIS
1	A	114	GLN
1	A	119	GLN
1	A	146	GLN
1	A	257	HIS
1	A	297	GLN
1	A	324	GLN
1	B	3	HIS
1	B	21	GLN
1	B	33	GLN
1	B	79	HIS

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Mol	Chain	Res	Type
1	B	114	GLN
1	B	119	GLN
1	B	146	GLN
1	B	257	HIS
1	B	297	GLN
1	B	324	GLN
1	C	3	HIS
1	C	21	GLN
1	C	33	GLN
1	C	79	HIS
1	C	114	GLN
1	C	119	GLN
1	C	146	GLN
1	C	257	HIS
1	C	324	GLN
1	D	3	HIS
1	D	21	GLN
1	D	33	GLN
1	D	79	HIS
1	D	104	GLN
1	D	114	GLN
1	D	119	GLN
1	D	146	GLN
1	D	257	HIS
1	D	324	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	MET	A	485	-	7,8,8	0.99	0	7,9,9	1.29	2 (28%)
4	ANP	B	484	3,2	29,33,33	3.14	11 (37%)	31,52,52	2.49	15 (48%)
7	PPK	C	684	3,2	11,12,12	2.49	6 (54%)	15,20,20	3.90	6 (40%)
6	SAM	C	885	-	24,29,29	1.04	3 (12%)	23,42,42	0.99	1 (4%)
6	SAM	C	685	-	24,29,29	1.06	2 (8%)	23,42,42	0.99	2 (8%)
4	ANP	A	384	3,2	29,33,33	3.14	11 (37%)	31,52,52	2.49	15 (48%)
5	MET	B	385	-	7,8,8	1.01	0	7,9,9	1.22	1 (14%)
7	PPK	D	884	3,2	11,12,12	2.49	5 (45%)	15,20,20	3.55	4 (26%)

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
5	MET	A	485	-	-	4/8/8/8	-
4	ANP	B	484	3,2	-	8/14/38/38	0/3/3/3
7	PPK	C	684	3,2	-	2/8/12/12	-
6	SAM	C	885	-	-	5/12/33/33	0/3/3/3
6	SAM	C	685	-	-	6/12/33/33	0/3/3/3
4	ANP	A	384	3,2	-	8/14/38/38	0/3/3/3
5	MET	B	385	-	-	4/8/8/8	-
7	PPK	D	884	3,2	-	2/8/12/12	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	484	ANP	C5'-C4'	-7.34	1.28	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	384	ANP	C5'-C4'	-7.33	1.28	1.51
4	B	484	ANP	C4-N3	7.18	1.45	1.35
4	A	384	ANP	C4-N3	7.16	1.45	1.35
4	B	484	ANP	PB-O2B	-5.37	1.42	1.56
4	A	384	ANP	PB-O2B	-5.33	1.42	1.56
4	B	484	ANP	PG-O2G	-5.30	1.42	1.56
4	A	384	ANP	PG-O2G	-5.29	1.42	1.56
4	A	384	ANP	O2'-C2'	5.16	1.55	1.43
4	B	484	ANP	O2'-C2'	5.14	1.55	1.43
4	A	384	ANP	C2-N1	4.89	1.43	1.33
4	B	484	ANP	C2-N1	4.89	1.43	1.33
4	B	484	ANP	C8-N7	-4.55	1.26	1.34
4	A	384	ANP	C8-N7	-4.53	1.26	1.34
7	C	684	PPK	PG-O2G	-4.40	1.44	1.56
7	D	884	PPK	PG-O2G	-3.99	1.46	1.56
7	D	884	PPK	PB-N3B	-3.64	1.53	1.63
7	D	884	PPK	PG-O1G	-3.61	1.47	1.56
7	D	884	PPK	PB-O1B	-3.51	1.47	1.56
7	C	684	PPK	PG-O3G	3.48	1.51	1.46
7	C	684	PPK	PB-N3B	-3.30	1.54	1.63
4	A	384	ANP	C2-N3	3.28	1.37	1.32
4	B	484	ANP	C2-N3	3.25	1.37	1.32
4	B	484	ANP	C2'-C3'	3.07	1.61	1.53
4	A	384	ANP	C2'-C3'	3.07	1.61	1.53
7	C	684	PPK	PG-O1G	-3.00	1.48	1.56
7	C	684	PPK	PB-O1B	-2.88	1.49	1.56
6	C	885	SAM	C2-N3	2.86	1.36	1.32
4	A	384	ANP	PB-N3B	-2.84	1.55	1.63
4	B	484	ANP	PB-N3B	-2.83	1.56	1.63
7	D	884	PPK	PG-O3G	2.75	1.50	1.46
6	C	685	SAM	C2-N3	2.61	1.36	1.32
6	C	685	SAM	C4-N3	2.60	1.39	1.35
4	A	384	ANP	O3'-C3'	-2.22	1.37	1.43
4	B	484	ANP	O3'-C3'	-2.22	1.37	1.43
6	C	885	SAM	C4-N3	2.07	1.38	1.35
7	C	684	PPK	PB-O3A	2.06	1.61	1.59
6	C	885	SAM	C8-N7	-2.05	1.31	1.34

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	684	PPK	O3G-PG-N3B	-13.12	92.45	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	884	PPK	O3G-PG-N3B	-11.98	94.13	111.77
4	B	484	ANP	C5-C6-N6	6.02	129.50	120.35
4	A	384	ANP	C5-C6-N6	6.01	129.48	120.35
4	A	384	ANP	C2'-C3'-C4'	-4.51	93.87	102.64
4	B	484	ANP	C2'-C3'-C4'	-4.50	93.90	102.64
7	C	684	PPK	O2B-PB-N3B	-4.20	105.59	111.77
7	C	684	PPK	O1B-PB-O2B	4.01	118.33	109.92
4	B	484	ANP	O3'-C3'-C4'	3.93	122.42	111.05
4	A	384	ANP	O3'-C3'-C4'	3.93	122.41	111.05
7	D	884	PPK	O2B-PB-N3B	-3.77	106.22	111.77
4	A	384	ANP	C3'-C2'-C1'	3.62	106.43	100.98
4	B	484	ANP	C3'-C2'-C1'	3.61	106.42	100.98
7	D	884	PPK	O1B-PB-O2B	3.52	117.31	109.92
4	A	384	ANP	C4-C5-N7	3.31	112.85	109.40
4	B	484	ANP	O2B-PB-O1B	3.27	116.77	109.92
4	A	384	ANP	O2B-PB-O1B	3.26	116.75	109.92
4	B	484	ANP	C4-C5-N7	3.25	112.79	109.40
4	B	484	ANP	O2G-PG-O1G	-3.17	105.49	113.45
4	A	384	ANP	O2G-PG-O1G	-3.17	105.49	113.45
4	A	384	ANP	O4'-C1'-C2'	-2.87	102.74	106.93
4	B	484	ANP	O4'-C1'-C2'	-2.86	102.75	106.93
4	A	384	ANP	O3'-C3'-C2'	2.82	120.94	111.82
4	B	484	ANP	O3'-C3'-C2'	2.81	120.93	111.82
4	B	484	ANP	O4'-C4'-C3'	-2.77	99.63	105.11
4	A	384	ANP	O4'-C4'-C3'	-2.77	99.64	105.11
4	A	384	ANP	N6-C6-N1	-2.71	112.95	118.57
4	B	484	ANP	N6-C6-N1	-2.71	112.96	118.57
4	B	484	ANP	O2'-C2'-C3'	-2.68	103.17	111.82
4	A	384	ANP	O2'-C2'-C3'	-2.67	103.17	111.82
4	B	484	ANP	PB-O3A-PA	-2.67	123.22	132.62
4	A	384	ANP	PB-O3A-PA	-2.66	123.24	132.62
4	B	484	ANP	O1B-PB-N3B	-2.60	107.94	111.77
4	A	384	ANP	O1B-PB-N3B	-2.57	107.99	111.77
6	C	885	SAM	O2'-C2'-C3'	2.50	119.90	111.82
5	A	485	MET	OXT-C-CA	2.43	121.66	113.38
5	B	385	MET	OXT-C-CA	2.37	121.46	113.38
6	C	685	SAM	O2'-C2'-C3'	2.33	119.35	111.82
4	A	384	ANP	O4'-C4'-C5'	-2.25	101.97	109.37
4	B	484	ANP	O4'-C4'-C5'	-2.25	101.98	109.37
7	C	684	PPK	PB-O3A-PA	-2.23	124.78	132.62
7	D	884	PPK	O3A-PB-N3B	2.16	112.58	106.59
7	C	684	PPK	O1B-PB-O3A	2.13	111.75	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	485	MET	OXT-C-O	-2.11	119.30	124.09
6	C	685	SAM	C1'-N9-C4	-2.04	123.06	126.64
7	C	684	PPK	O3A-PB-N3B	2.00	112.15	106.59

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	384	ANP	PB-N3B-PG-O1G
4	A	384	ANP	PG-N3B-PB-O1B
4	A	384	ANP	C5'-O5'-PA-O3A
4	B	484	ANP	PB-N3B-PG-O1G
4	B	484	ANP	PG-N3B-PB-O1B
4	B	484	ANP	C5'-O5'-PA-O3A
7	C	684	PPK	PB-N3B-PG-O3G
7	C	684	PPK	PG-N3B-PB-O2B
7	D	884	PPK	PB-N3B-PG-O3G
7	D	884	PPK	PG-N3B-PB-O2B
4	A	384	ANP	C3'-C4'-C5'-O5'
4	B	484	ANP	C3'-C4'-C5'-O5'
5	B	385	MET	OXT-C-CA-N
5	A	485	MET	O-C-CA-N
5	B	385	MET	O-C-CA-N
6	C	685	SAM	O-C-CA-N
6	C	885	SAM	O-C-CA-N
4	A	384	ANP	O4'-C4'-C5'-O5'
4	B	484	ANP	O4'-C4'-C5'-O5'
4	A	384	ANP	C5'-O5'-PA-O1A
4	A	384	ANP	C5'-O5'-PA-O2A
4	B	484	ANP	C5'-O5'-PA-O1A
4	B	484	ANP	C5'-O5'-PA-O2A
6	C	685	SAM	CA-CB-CG-SD
6	C	885	SAM	CA-CB-CG-SD
5	B	385	MET	O-C-CA-CB
6	C	885	SAM	O-C-CA-CB
5	A	485	MET	OXT-C-CA-N
6	C	685	SAM	OXT-C-CA-N
6	C	885	SAM	OXT-C-CA-N
5	A	485	MET	O-C-CA-CB
6	C	685	SAM	O-C-CA-CB
5	B	385	MET	OXT-C-CA-CB
5	A	485	MET	OXT-C-CA-CB

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Mol	Chain	Res	Type	Atoms
6	C	685	SAM	OXT-C-CA-CB
6	C	885	SAM	OXT-C-CA-CB
4	A	384	ANP	PG-N3B-PB-O3A
4	B	484	ANP	PG-N3B-PB-O3A
6	C	685	SAM	O4'-C4'-C5'-SD

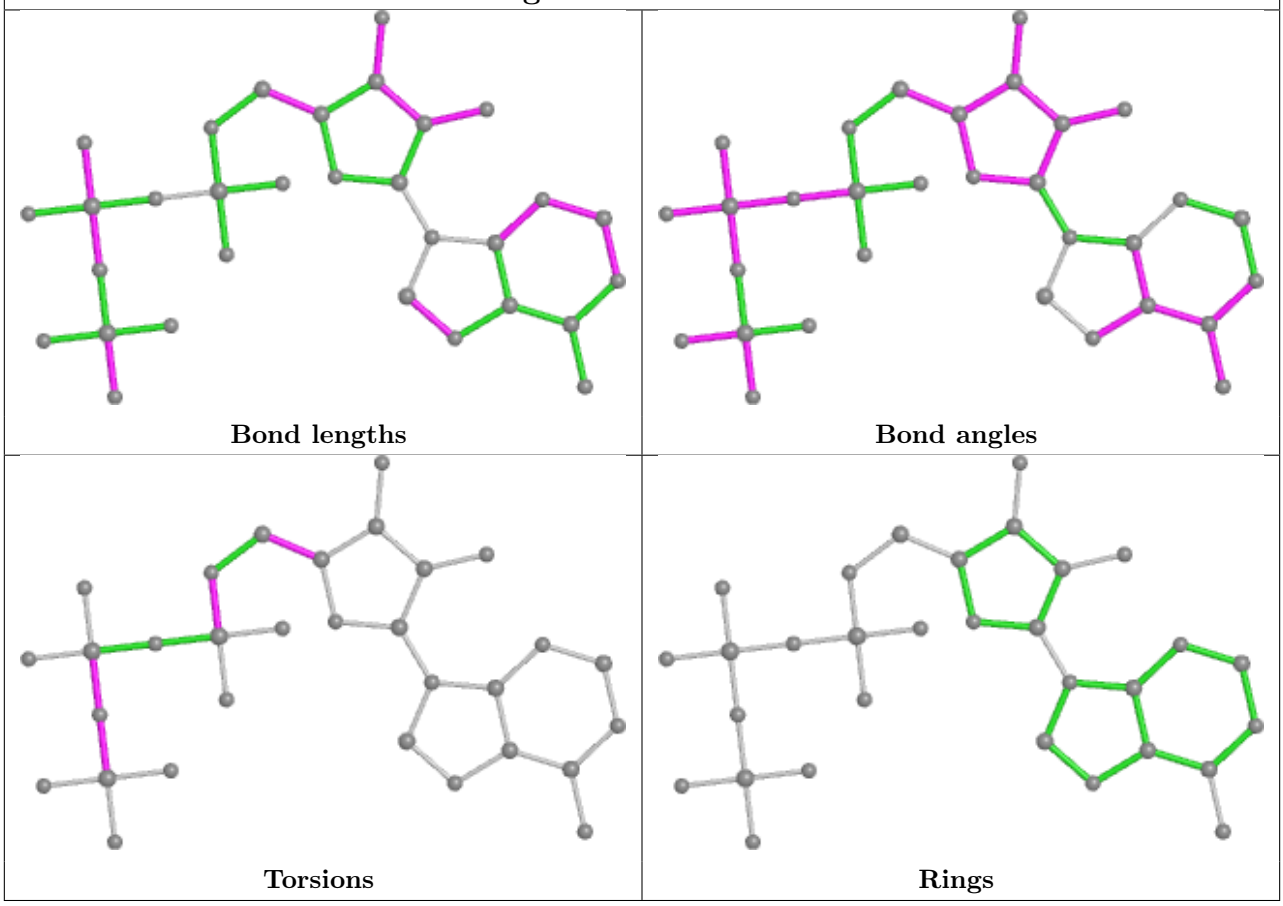
There are no ring outliers.

7 monomers are involved in 7 short contacts:

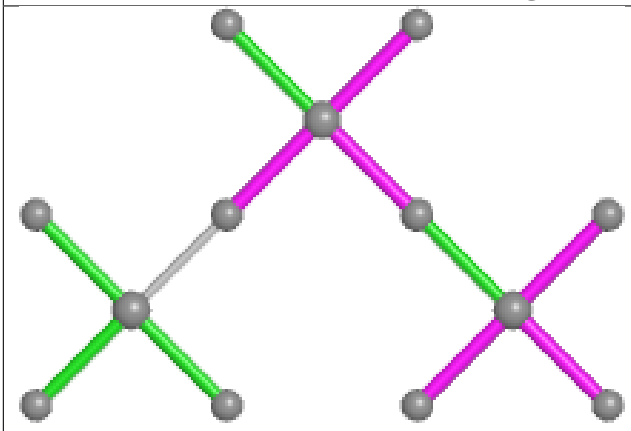
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	485	MET	2	0
4	B	484	ANP	2	0
7	C	684	PPK	2	0
6	C	685	SAM	1	0
4	A	384	ANP	1	0
5	B	385	MET	1	0
7	D	884	PPK	1	0

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 then 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.

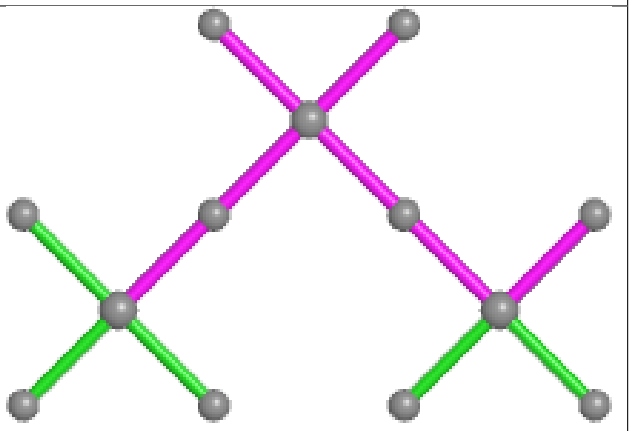
Ligand ANP B 484



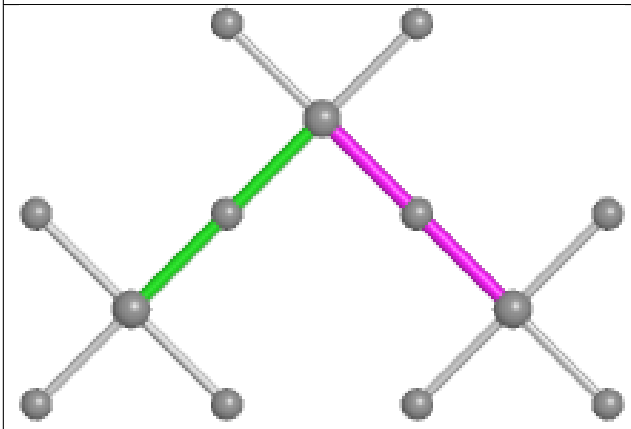
Ligand PPK C 684



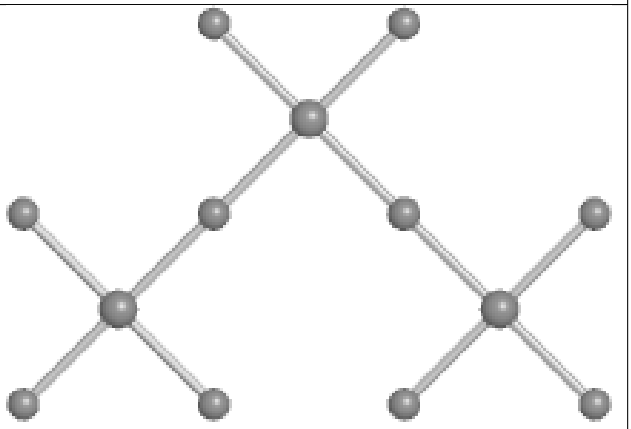
Bond lengths



Bond angles

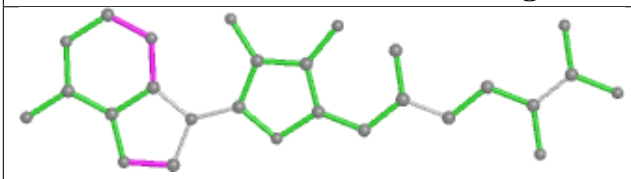


Torsions

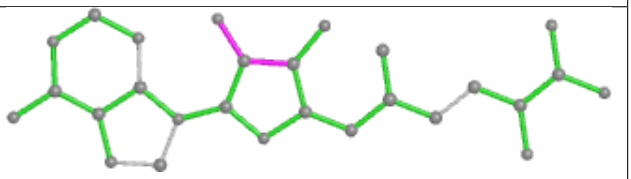


Rings

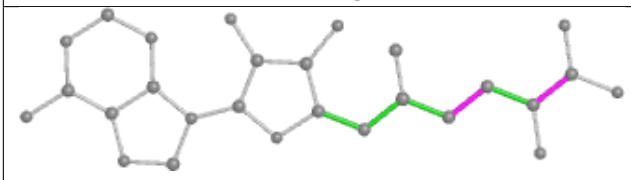
Ligand SAM C 885



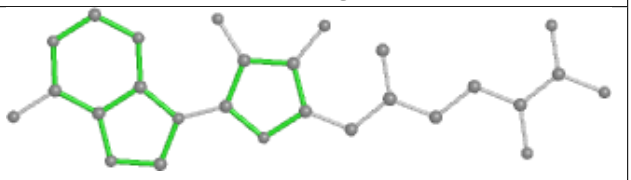
Bond lengths



Bond angles

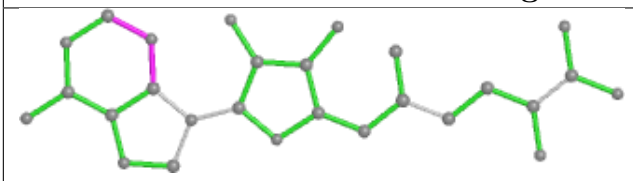


Torsions

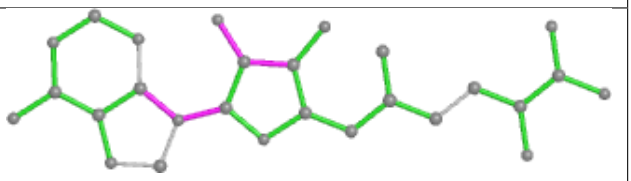


Rings

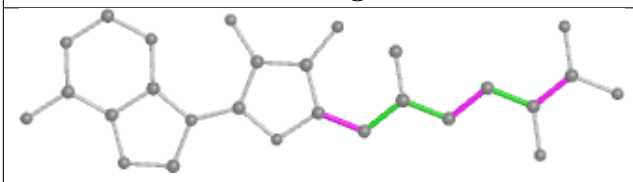
Ligand SAM C 685



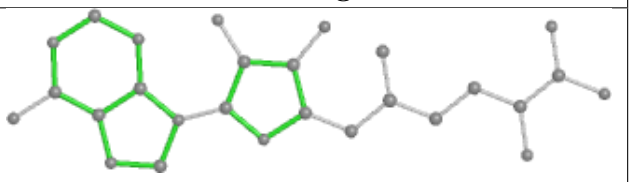
Bond lengths



Bond angles

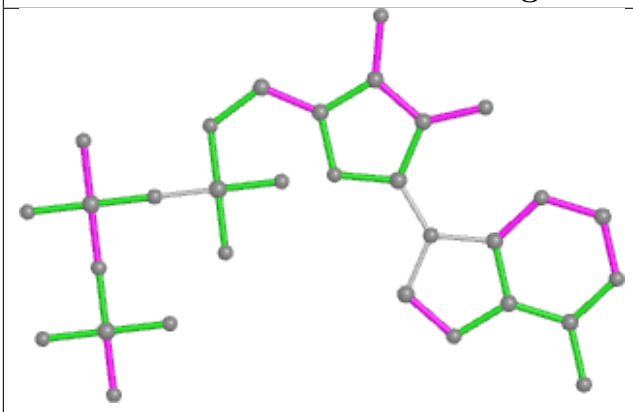


Torsions

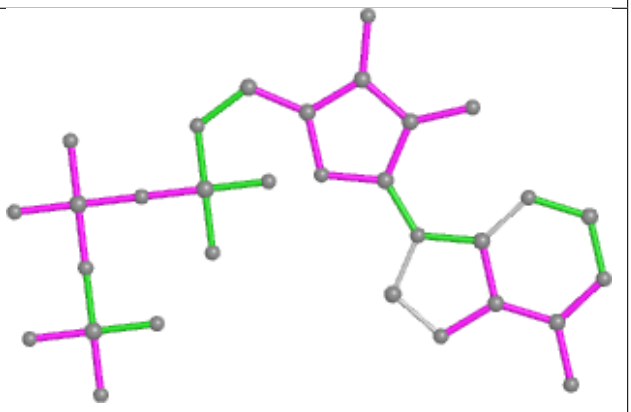


Rings

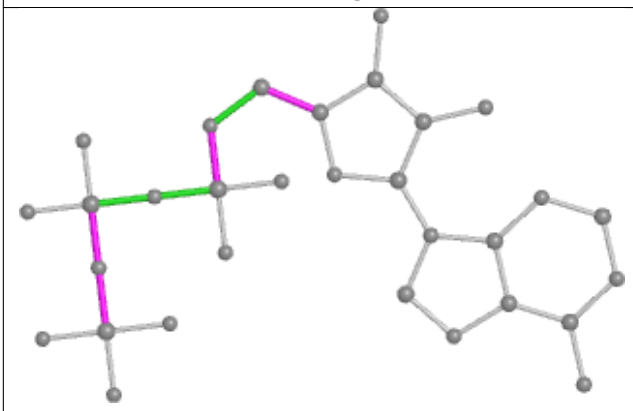
Ligand ANP A 384



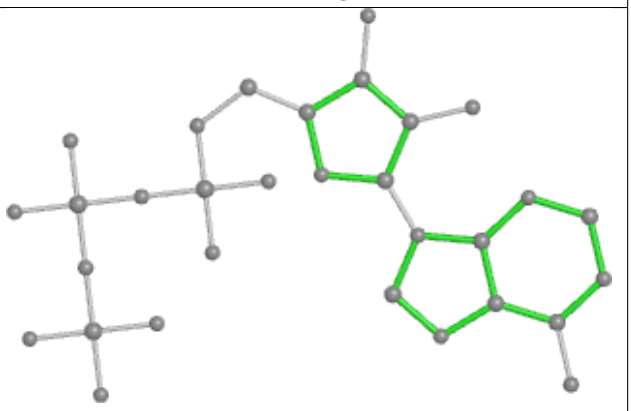
Bond lengths



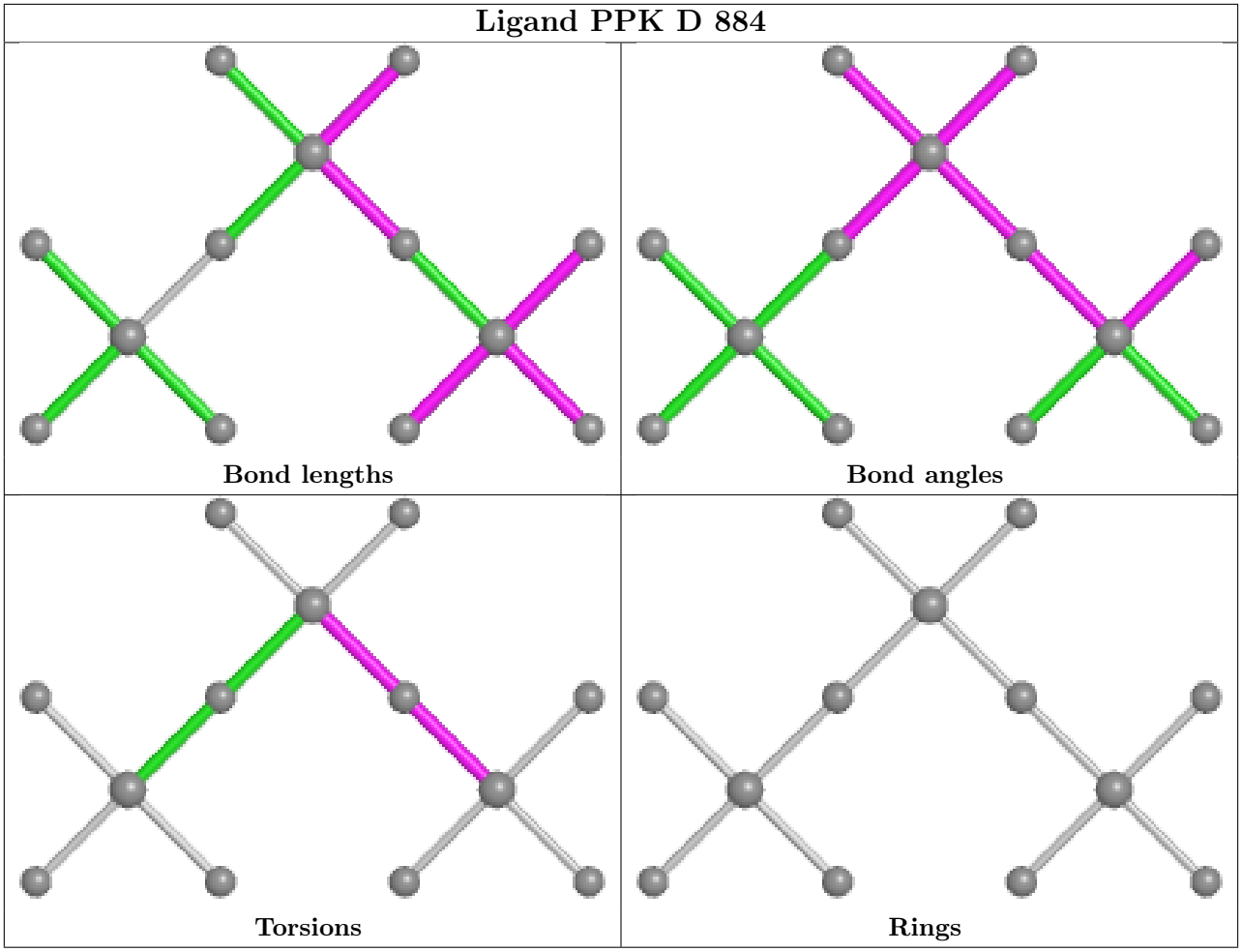
Bond angles



Torsions



Rings



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.