



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:48 PM UTC

PDB ID : 1B6S / pdb_00001b6s
Title : STRUCTURE OF N5-CARBOXYAMINOIMIDAZOLE RIBONUCLEOTIDE SYNTHETASE
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Deposited on : 1999-01-18
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

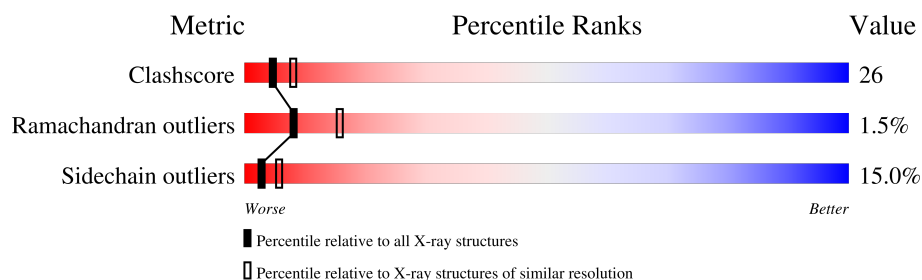
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	355	 45% 44% 10% .
1	B	355	 48% 43% 8% .
1	C	355	 44% 40% 13% ..
1	D	355	 50% 38% 10% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11632 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 PROTEIN (N5-CARBOXYAMINOIMIDAZOLE RIBONUCLEOTIDE SYNTHETASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	0	0
			2751	1752	487	501	11			
1	B	355	Total	C	N	O	S	0	0	0
			2784	1772	493	508	11			
1	C	350	Total	C	N	O	S	0	0	0
			2747	1750	486	500	11			
1	D	350	Total	C	N	O	S	0	0	0
			2747	1750	486	500	11			

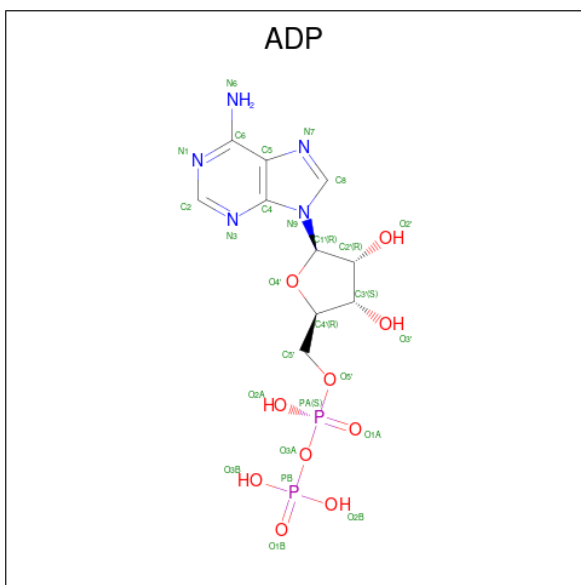
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	ARG	GLN	conflict	UNP P09029
B	205	ARG	GLN	conflict	UNP P09029
C	205	ARG	GLN	conflict	UNP P09029
D	205	ARG	GLN	conflict	UNP P09029

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

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 4 is water.

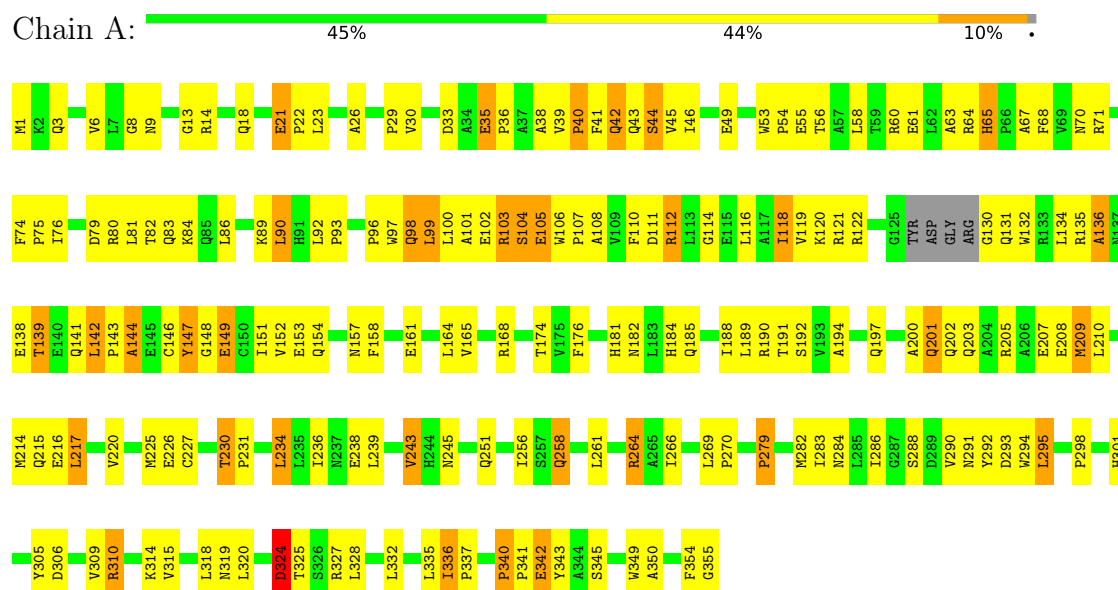
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	107	Total O 107 107	0	0
4	B	121	Total O 121 121	0	0
4	C	136	Total O 136 136	0	0
4	D	127	Total O 127 127	0	0

3 Residue-property plots

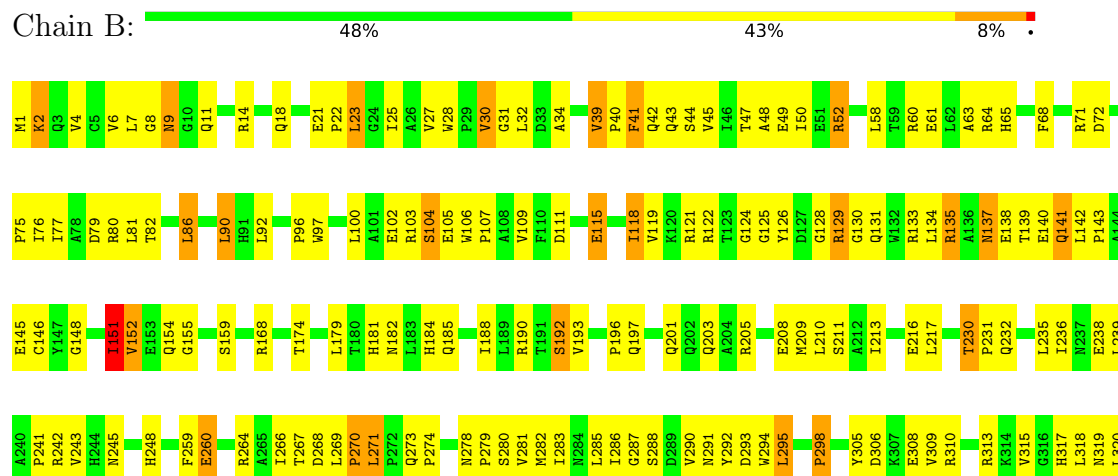
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

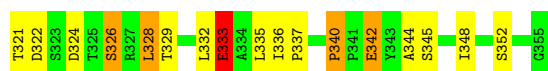
Note EDS was not executed.

- Molecule 1: PROTEIN (N5-CARBOXYAMINOIMIDAZOLE RIBONUCLEOTIDE SYNTHETASE)



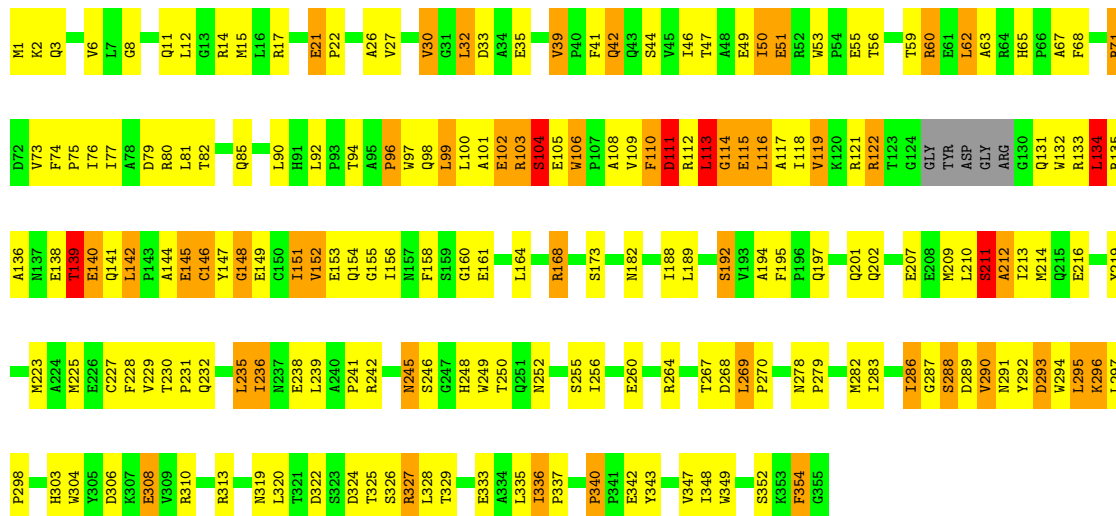
- Molecule 1: PROTEIN (N5-CARBOXYAMINOIMIDAZOLE RIBONUCLEOTIDE SYNTHETASE)





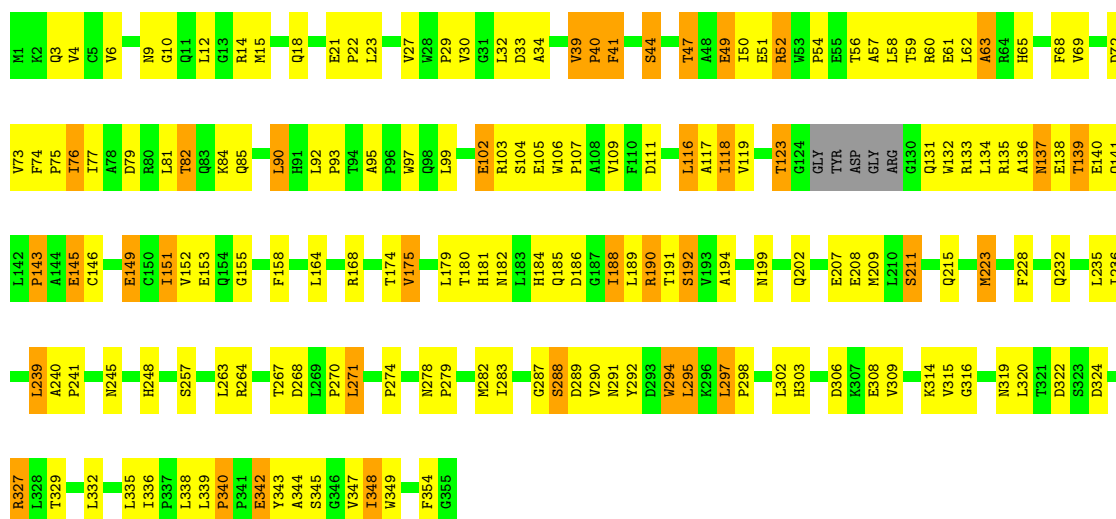
- Molecule 1: PROTEIN (N5-CARBOXYAMINOIMIDAZOLE RIBONUCLEOTIDE SYNTHETASE)

Chain C: 44% 40% 13% ..



- Molecule 1: PROTEIN (N5-CARBOXYAMINOIMIDAZOLE RIBONUCLEOTIDE SYNTHETASE)

Chain D: 50% 38% 10% .



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.60 Å 92.10 Å 102.60 Å 66.10° 82.70° 81.80°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	95.7 (30.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.72	Depositor
Refinement program	TNT 5D	Depositor
R, R_{free}	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11632	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.24	5/2819 (0.2%)	1.61	34/3841 (0.9%)
1	B	1.16	3/2853 (0.1%)	1.59	26/3888 (0.7%)
1	C	1.17	0/2815	1.63	30/3836 (0.8%)
1	D	1.13	4/2815 (0.1%)	1.62	36/3836 (0.9%)
All	All	1.18	12/11302 (0.1%)	1.61	126/15401 (0.8%)

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	324	ASP	CA-C	15.98	1.72	1.52
1	A	324	ASP	C-O	-15.46	1.04	1.24
1	B	65	HIS	CG-CD2	-13.83	1.20	1.35
1	A	324	ASP	CG-OD1	12.26	1.48	1.25
1	A	324	ASP	C-N	7.16	1.43	1.34
1	B	65	HIS	CG-ND1	-6.43	1.31	1.38
1	B	260	GLU	CD-OE1	5.65	1.36	1.25
1	A	264	ARG	C-O	-5.63	1.17	1.24
1	D	316	GLY	N-CA	-5.60	1.39	1.45
1	D	102	GLU	CD-OE1	5.44	1.35	1.25
1	D	175	VAL	CA-C	-5.37	1.46	1.52
1	D	268	ASP	CG-OD1	5.00	1.34	1.25

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	PRO	O-C-N	12.04	126.85	121.31
1	B	65	HIS	ND1-CG-CD2	11.81	117.91	106.10
1	A	103	ARG	N-CA-C	-9.09	101.62	112.89
1	B	290	VAL	N-CA-CB	8.86	120.19	110.53
1	A	324	ASP	O-C-N	8.72	133.16	123.13
1	A	354	PHE	CA-CB-CG	-8.50	105.30	113.80
1	C	354	PHE	CA-CB-CG	-8.29	105.51	113.80
1	C	114	GLY	O-C-N	-8.20	112.03	122.70
1	D	354	PHE	CA-CB-CG	-7.62	106.19	113.80
1	B	340	PRO	N-CA-CB	7.35	107.04	103.22
1	D	340	PRO	CB-CA-C	7.34	118.29	111.39
1	D	30	VAL	N-CA-C	7.33	118.36	108.11
1	A	279	PRO	N-CA-CB	7.29	110.11	103.33
1	A	310	ARG	N-CA-CB	7.14	120.70	110.77
1	D	340	PRO	O-C-N	7.13	124.59	121.31
1	C	148	GLY	N-CA-C	-7.11	103.96	114.90
1	C	245	ASN	CA-CB-CG	6.97	119.58	112.60
1	A	340	PRO	CA-C-N	6.89	127.47	119.47
1	A	340	PRO	C-N-CA	6.89	127.47	119.47
1	A	181	HIS	CA-CB-CG	-6.84	106.96	113.80
1	B	135	ARG	N-CA-CB	6.63	121.95	111.20
1	D	274	PRO	N-CA-CB	6.58	109.08	103.35
1	C	192	SER	N-CA-CB	6.49	122.12	110.83
1	C	106	TRP	N-CA-C	6.45	121.64	113.25
1	B	151	ILE	CB-CA-C	-6.45	102.36	111.19
1	D	72	ASP	CA-CB-CG	-6.43	106.17	112.60
1	B	266	ILE	N-CA-C	6.43	119.09	111.05
1	B	268	ASP	CA-CB-CG	6.42	119.02	112.60
1	B	41	PHE	N-CA-C	6.32	118.98	111.33
1	D	340	PRO	CA-C-N	6.31	126.52	119.32
1	D	340	PRO	C-N-CA	6.31	126.52	119.32
1	D	340	PRO	N-CA-CB	6.31	106.72	103.19
1	D	149	GLU	N-CA-C	-6.30	105.52	113.72
1	B	181	HIS	CA-CB-CG	-6.17	107.63	113.80
1	D	51	GLU	N-CA-C	5.90	117.51	111.14
1	A	147	TYR	CG-CD1-CE1	5.89	130.04	121.20
1	B	274	PRO	N-CA-CB	5.88	108.47	103.35
1	A	270	PRO	N-CA-CB	5.87	108.54	103.31
1	A	251	GLN	N-CA-CB	5.87	120.13	110.39
1	D	339	LEU	O-C-N	5.84	126.31	121.35
1	A	144	ALA	N-CA-C	-5.79	106.18	113.18
1	C	212	ALA	N-CA-CB	-5.79	101.32	109.94
1	A	40	PRO	CA-C-N	5.78	128.61	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	PRO	C-N-CA	5.78	128.61	120.28
1	D	181	HIS	CA-CB-CG	-5.75	108.05	113.80
1	C	236	ILE	N-CA-CB	5.74	116.79	110.53
1	D	76	ILE	N-CA-C	5.73	115.92	110.42
1	B	236	ILE	N-CA-CB	5.72	117.35	110.31
1	C	110	PHE	CA-CB-CG	-5.72	108.08	113.80
1	B	31	GLY	N-CA-C	-5.70	104.79	112.14
1	A	114	GLY	N-CA-C	5.69	118.45	111.45
1	D	41	PHE	N-CA-C	5.66	118.99	111.75
1	A	99	LEU	N-CA-CB	5.65	119.38	110.23
1	A	149	GLU	CA-C-O	5.63	124.72	118.52
1	B	208	GLU	CB-CA-C	-5.63	101.80	110.81
1	A	258	GLN	CA-C-N	5.62	128.85	120.31
1	A	258	GLN	C-N-CA	5.62	128.85	120.31
1	D	63	ALA	N-CA-C	5.60	118.31	111.82
1	A	266	ILE	CA-C-N	-5.59	113.73	122.73
1	A	266	ILE	C-N-CA	-5.59	113.73	122.73
1	C	270	PRO	N-CA-CB	5.58	108.53	103.34
1	C	114	GLY	CA-C-N	-5.57	111.21	120.68
1	C	114	GLY	C-N-CA	-5.57	111.21	120.68
1	A	29	PRO	CA-C-N	-5.57	113.51	122.25
1	A	29	PRO	C-N-CA	-5.57	113.51	122.25
1	C	340	PRO	CA-C-N	5.56	126.79	119.84
1	C	340	PRO	C-N-CA	5.56	126.79	119.84
1	C	260	GLU	CB-CA-C	-5.56	101.56	110.79
1	B	340	PRO	CB-CA-C	5.55	116.38	111.17
1	D	29	PRO	CA-C-N	-5.54	115.88	123.14
1	D	29	PRO	C-N-CA	-5.54	115.88	123.14
1	B	259	PHE	CA-CB-CG	-5.52	108.28	113.80
1	C	113	LEU	CB-CA-C	5.52	121.40	110.42
1	D	223	MET	CG-SD-CE	-5.47	88.86	100.90
1	C	96	PRO	N-CA-CB	5.46	108.11	103.19
1	D	208	GLU	CA-C-N	5.46	127.54	120.44
1	D	208	GLU	C-N-CA	5.46	127.54	120.44
1	D	143	PRO	N-CA-CB	5.46	107.90	103.32
1	C	156	ILE	N-CA-C	5.43	116.39	108.58
1	D	297	LEU	CB-CA-C	5.41	115.52	110.17
1	B	30	VAL	N-CA-C	5.36	115.68	108.17
1	C	290	VAL	CB-CA-C	-5.36	103.34	111.33
1	C	122	ARG	N-CA-C	5.35	117.19	111.36
1	B	143	PRO	N-CA-CB	5.35	107.96	103.25
1	A	65	HIS	O-C-N	5.34	127.29	121.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111	ASP	N-CA-C	-5.34	105.58	112.68
1	C	303	HIS	CA-CB-CG	-5.34	108.46	113.80
1	D	270	PRO	N-CA-CB	5.34	108.30	103.33
1	C	21	GLU	CA-C-O	5.29	123.50	118.63
1	D	315	VAL	CA-C-O	5.27	124.26	119.20
1	C	211	SER	CA-CB-OG	-5.27	100.56	111.10
1	B	333	GLU	O-C-N	5.26	127.56	122.09
1	C	145	GLU	N-CA-C	-5.25	105.15	112.45
1	B	8	GLY	CA-C-N	5.24	131.80	121.58
1	B	8	GLY	C-N-CA	5.24	131.80	121.58
1	D	152	VAL	O-C-N	5.23	128.69	123.10
1	A	208	GLU	CB-CA-C	-5.22	102.45	110.81
1	A	14	ARG	O-C-N	5.22	127.44	122.07
1	A	142	LEU	N-CA-C	5.18	117.81	110.40
1	A	258	GLN	O-C-N	5.17	127.59	122.12
1	A	13	GLY	N-CA-C	-5.15	106.18	112.77
1	B	65	HIS	CB-CG-CD2	-5.15	124.51	131.20
1	D	294	TRP	CA-C-O	5.13	125.70	119.49
1	A	305	TYR	CA-C-N	-5.13	114.96	122.40
1	A	305	TYR	C-N-CA	-5.13	114.96	122.40
1	A	200	ALA	N-CA-C	5.11	117.25	111.11
1	B	270	PRO	CA-C-N	5.08	129.30	123.15
1	B	270	PRO	C-N-CA	5.08	129.30	123.15
1	D	290	VAL	N-CA-CB	5.08	116.56	110.31
1	D	39	VAL	CA-C-O	5.07	122.58	119.94
1	D	57	ALA	N-CA-C	-5.06	105.89	111.71
1	B	96	PRO	N-CA-CB	5.06	107.82	103.27
1	C	164	LEU	CA-C-N	-5.05	116.56	122.93
1	C	164	LEU	C-N-CA	-5.05	116.56	122.93
1	D	15	MET	CA-C-N	-5.05	112.09	120.68
1	D	15	MET	C-N-CA	-5.05	112.09	120.68
1	A	310	ARG	CB-CA-C	5.05	116.78	109.92
1	C	119	VAL	N-CA-C	5.05	115.58	108.36
1	D	327	ARG	CA-C-O	5.04	125.77	120.42
1	D	49	GLU	N-CA-C	-5.04	107.13	113.28
1	C	53	TRP	N-CA-C	5.02	114.08	108.25
1	D	63	ALA	N-CA-CB	5.02	118.06	110.28
1	D	65	HIS	CA-CB-CG	-5.01	108.79	113.80
1	B	45	VAL	CA-C-N	-5.00	116.64	123.10
1	B	45	VAL	C-N-CA	-5.00	116.64	123.10
1	C	134	LEU	N-CA-C	5.00	117.16	109.95

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	324	ASP	Mainchain

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	2751	0	2732	166	0
1	B	2784	0	2759	115	0
1	C	2747	0	2729	171	0
1	D	2747	0	2729	133	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	27	0	12	0	0
3	B	27	0	12	1	0
3	C	27	0	12	1	0
3	D	27	0	12	0	0
4	A	107	0	0	4	1
4	B	121	0	0	5	0
4	C	136	0	0	4	0
4	D	127	0	0	5	1
All	All	11632	0	10997	570	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 26.

All (570) 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:D:93:PRO:HB2	1:D:235:LEU:HD23	1.46	0.96
1:B:119:VAL:HG22	1:B:152:VAL:HG13	1.47	0.94
1:C:8:GLY:HA3	1:C:49:GLU:HG2	1.54	0.90
1:A:42:GLN:NE2	1:A:42:GLN:H	1.73	0.87
1:A:209:MET:HE2	1:A:236:ILE:CD1	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLN:H	1:A:42:GLN:HE21	1.26	0.83
1:A:81:LEU:HD23	1:A:122:ARG:HH21	1.43	0.82
1:A:355:GLY:HA3	1:C:133:ARG:HH11	1.44	0.82
1:C:99:LEU:HD11	1:C:148:GLY:HA2	1.62	0.80
1:C:144:ALA:HA	1:C:147:TYR:HE1	1.47	0.79
1:A:142:LEU:CD1	1:A:143:PRO:HD2	2.13	0.79
1:A:93:PRO:HD2	1:A:209:MET:HE3	1.64	0.78
1:A:40:PRO:HA	1:A:42:GLN:HE22	1.47	0.78
1:A:119:VAL:CG2	1:A:132:TRP:HB2	2.14	0.78
1:A:81:LEU:HD12	1:A:97:TRP:HZ3	1.48	0.78
1:A:99:LEU:HD21	1:A:148:GLY:HA2	1.66	0.77
1:D:319:ASN:C	1:D:320:LEU:HD12	2.08	0.77
1:D:185:GLN:HE21	1:D:190:ARG:HD2	1.49	0.77
1:A:168:ARG:HG3	1:A:174:THR:HG22	1.65	0.77
1:D:49:GLU:HG3	1:D:50:ILE:HG23	1.67	0.76
1:B:340:PRO:HB2	1:B:342:GLU:OE2	1.85	0.76
1:A:144:ALA:HA	1:A:147:TYR:CE2	2.21	0.76
1:B:6:VAL:HG22	1:B:47:THR:CG2	2.15	0.76
1:A:81:LEU:HD12	1:A:97:TRP:CZ3	2.21	0.76
1:A:142:LEU:HD12	1:A:143:PRO:HD2	1.68	0.75
1:D:209:MET:HE3	1:D:236:ILE:CD1	2.16	0.75
1:C:99:LEU:HD12	1:C:100:LEU:N	2.02	0.75
1:C:96:PRO:HG2	1:C:154:GLN:OE1	1.86	0.75
1:D:79:ASP:HB3	1:D:82:THR:OG1	1.87	0.75
1:D:116:LEU:HG	1:D:117:ALA:N	2.01	0.74
1:B:86:LEU:HD11	1:B:90:LEU:HD22	1.69	0.74
1:D:137:ASN:ND2	1:D:137:ASN:H	1.83	0.74
1:A:65:HIS:CE1	1:A:67:ALA:HB3	2.23	0.74
1:C:144:ALA:HA	1:C:147:TYR:CE1	2.22	0.73
1:A:144:ALA:HA	1:A:147:TYR:CD2	2.22	0.73
1:A:309:VAL:HG22	1:A:315:VAL:HG11	1.70	0.73
1:D:137:ASN:H	1:D:137:ASN:HD22	1.34	0.73
1:B:2:LYS:HG2	1:B:25:ILE:HG12	1.71	0.73
1:B:102:GLU:O	1:B:105:GLU:HB2	1.89	0.73
1:B:278:ASN:HB3	1:B:279:PRO:HD2	1.70	0.72
1:D:118:ILE:HD13	1:D:155:GLY:HA2	1.71	0.72
1:A:355:GLY:HA3	1:C:133:ARG:NH1	2.05	0.72
1:C:115:GLU:O	1:C:135:ARG:HG2	1.89	0.72
1:A:157:ASN:HB3	1:C:232:GLN:HA	1.71	0.71
1:A:96:PRO:HG2	1:A:154:GLN:OE1	1.91	0.71
1:C:209:MET:O	1:C:212:ALA:HB3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LEU:HG	1:A:143:PRO:HD2	1.73	0.70
1:D:143:PRO:HB2	1:D:145:GLU:HG3	1.74	0.70
1:D:3:GLN:HB3	1:D:44:SER:HB3	1.73	0.70
1:C:81:LEU:HD22	1:C:122:ARG:HH21	1.57	0.70
1:A:119:VAL:HG22	1:A:132:TRP:O	1.93	0.69
1:A:36:PRO:HA	1:A:58:LEU:HD13	1.75	0.69
1:B:230:THR:HB	1:B:231:PRO:HD2	1.74	0.69
1:C:340:PRO:HG2	1:C:343:TYR:CE1	2.28	0.69
1:A:142:LEU:CG	1:A:143:PRO:HD2	2.23	0.69
1:D:81:LEU:O	1:D:85:GLN:HG3	1.93	0.69
1:C:139:THR:HG22	1:C:140:GLU:N	2.08	0.68
1:D:102:GLU:O	1:D:105:GLU:HB2	1.93	0.68
1:D:58:LEU:HD12	1:D:62:LEU:HD13	1.76	0.68
1:D:52:ARG:NH2	1:D:123:THR:HG23	2.08	0.68
1:D:93:PRO:CB	1:D:235:LEU:HD23	2.24	0.68
1:B:118:ILE:CD1	1:B:155:GLY:HA2	2.23	0.67
1:B:190:ARG:NH2	4:B:2464:HOH:O	2.27	0.67
1:C:30:VAL:HG11	1:C:39:VAL:HG11	1.75	0.67
1:A:108:ALA:HB1	1:A:112:ARG:NH1	2.09	0.67
1:C:182:ASN:HD21	1:C:246:SER:HB2	1.57	0.67
1:C:278:ASN:HB3	1:C:279:PRO:HD2	1.76	0.67
1:A:209:MET:HE2	1:A:236:ILE:HD11	1.75	0.67
1:D:291:ASN:HB3	1:D:294:TRP:CE2	2.30	0.66
1:A:209:MET:HE2	1:A:236:ILE:HD12	1.78	0.66
1:D:289:ASP:OD1	1:D:309:VAL:HG21	1.95	0.66
1:D:106:TRP:O	1:D:109:VAL:HB	1.96	0.66
1:A:230:THR:HB	1:A:231:PRO:HD2	1.78	0.66
1:C:81:LEU:O	1:C:85:GLN:HG3	1.95	0.66
1:D:56:THR:O	1:D:60:ARG:HG3	1.96	0.65
1:B:86:LEU:CD1	1:B:90:LEU:HD22	2.25	0.65
1:B:168:ARG:HG3	1:B:174:THR:HG22	1.77	0.65
1:D:84:LYS:NZ	1:D:153:GLU:OE2	2.30	0.65
1:A:191:THR:HG22	1:A:349:TRP:CZ3	2.32	0.65
1:B:242:ARG:HG3	1:B:243:VAL:O	1.96	0.65
1:A:337:PRO:HA	1:C:348:ILE:CD1	2.27	0.65
1:C:252:ASN:HB2	4:C:2310:HOH:O	1.96	0.65
1:C:51:GLU:N	1:C:51:GLU:OE1	2.29	0.65
1:D:3:GLN:CB	1:D:44:SER:HB3	2.27	0.65
1:D:135:ARG:N	1:D:138:GLU:OE1	2.30	0.64
1:B:138:GLU:O	1:B:141:GLN:HB2	1.97	0.64
1:C:182:ASN:HB3	1:C:189:LEU:CD1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ARG:N	1:B:138:GLU:OE1	2.30	0.64
1:D:84:LYS:HB3	1:D:97:TRP:CE2	2.32	0.64
1:C:308:GLU:O	1:C:313:ARG:NH1	2.31	0.63
1:D:209:MET:CE	1:D:236:ILE:HG13	2.28	0.63
1:C:65:HIS:HE1	1:C:67:ALA:HB3	1.64	0.63
1:A:227:CYS:HB3	1:A:234:LEU:HD23	1.79	0.63
1:D:106:TRP:NE1	1:D:139:THR:HG23	2.13	0.63
1:C:99:LEU:CD1	1:C:148:GLY:HA2	2.27	0.63
1:B:115:GLU:H	1:B:115:GLU:CD	2.06	0.63
1:B:333:GLU:HA	1:B:336:ILE:HD12	1.80	0.63
1:D:191:THR:HG22	1:D:349:TRP:HZ3	1.62	0.63
1:B:34:ALA:HB3	1:B:58:LEU:HD22	1.80	0.62
1:A:210:LEU:HG	1:A:214:MET:HE2	1.81	0.62
1:B:6:VAL:HG22	1:B:47:THR:HG23	1.81	0.62
1:A:191:THR:HG22	1:A:349:TRP:HZ3	1.63	0.62
1:B:216:GLU:O	1:B:216:GLU:HG3	1.99	0.62
1:C:98:GLN:HG2	1:C:152:VAL:HG23	1.82	0.62
1:C:118:ILE:CD1	1:C:155:GLY:HA2	2.29	0.62
1:D:322:ASP:CG	1:D:327:ARG:HH21	2.06	0.62
1:B:119:VAL:HG22	1:B:152:VAL:CG1	2.25	0.62
1:B:205:ARG:O	1:B:209:MET:HG3	2.00	0.62
1:A:35:GLU:OE1	1:A:38:ALA:HB2	2.00	0.62
1:A:291:ASN:HB3	1:A:294:TRP:CE2	2.35	0.62
1:C:56:THR:O	1:C:60:ARG:HB2	2.00	0.62
1:A:3:GLN:HB3	1:A:44:SER:HB3	1.82	0.62
1:D:185:GLN:HB2	1:D:190:ARG:HD2	1.80	0.62
1:B:72:ASP:O	1:B:75:PRO:HD2	2.00	0.62
1:C:80:ARG:HH12	1:C:238:GLU:HG3	1.65	0.61
1:D:21:GLU:HB3	1:D:22:PRO:HD3	1.82	0.61
1:A:119:VAL:O	1:A:131:GLN:HA	2.00	0.61
1:C:8:GLY:HA3	1:C:49:GLU:CG	2.30	0.61
1:B:264:ARG:O	1:B:269:LEU:N	2.30	0.61
1:B:118:ILE:HD13	1:B:155:GLY:HA2	1.83	0.60
1:A:319:ASN:C	1:A:320:LEU:HD12	2.27	0.60
1:C:138:GLU:HB3	1:C:141:GLN:OE1	2.02	0.59
1:B:90:LEU:HB3	1:B:92:LEU:HG	1.83	0.59
1:B:182:ASN:ND2	1:B:192:SER:HB3	2.17	0.59
1:C:340:PRO:HG2	1:C:343:TYR:HE1	1.66	0.59
1:D:340:PRO:HB2	1:D:342:GLU:OE2	2.02	0.59
1:C:290:VAL:HG22	1:C:304:TRP:CE3	2.37	0.59
1:D:282:MET:HG2	1:D:283:ILE:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:PHE:CE1	1:A:161:GLU:HG3	2.37	0.59
1:B:4:VAL:O	1:B:27:VAL:HA	2.03	0.59
1:B:193:VAL:HG22	1:B:281:VAL:HG22	1.84	0.59
1:D:302:LEU:HD12	1:D:303:HIS:N	2.18	0.59
1:C:81:LEU:HD22	1:C:122:ARG:NH2	2.17	0.59
1:A:70:ASN:ND2	1:A:220:VAL:O	2.30	0.58
1:B:77:ILE:HD13	1:B:77:ILE:N	2.19	0.58
1:A:81:LEU:CD2	1:A:122:ARG:HH21	2.16	0.58
1:B:285:LEU:HD11	1:B:318:LEU:HD21	1.84	0.58
1:C:322:ASP:OD2	1:C:327:ARG:HD2	2.04	0.57
1:A:102:GLU:HB3	1:A:104:SER:OG	2.03	0.57
1:B:76:ILE:HG22	1:B:77:ILE:HD13	1.86	0.57
1:C:96:PRO:O	1:C:153:GLU:HA	2.03	0.57
1:A:99:LEU:HG	1:A:100:LEU:N	2.19	0.57
1:A:106:TRP:N	1:A:107:PRO:HD2	2.20	0.57
1:A:108:ALA:O	1:A:112:ARG:NH1	2.38	0.57
1:B:50:ILE:HD12	1:B:52:ARG:O	2.05	0.57
1:D:209:MET:HE3	1:D:236:ILE:HG13	1.86	0.57
1:B:21:GLU:HB3	1:B:22:PRO:HD3	1.87	0.57
1:C:92:LEU:HB3	1:C:236:ILE:HD12	1.87	0.57
1:A:81:LEU:CD1	1:A:97:TRP:HZ3	2.18	0.57
1:B:287:GLY:HA2	1:B:310:ARG:O	2.04	0.57
1:D:278:ASN:HB3	1:D:279:PRO:HD2	1.87	0.57
1:A:55:GLU:O	1:A:55:GLU:HG2	2.03	0.56
1:C:213:ILE:HG21	1:C:239:LEU:HD21	1.86	0.56
1:D:6:VAL:HG22	1:D:47:THR:CG2	2.35	0.56
1:A:97:TRP:HA	1:A:152:VAL:O	2.06	0.56
1:B:309:VAL:HG22	1:B:315:VAL:HG11	1.87	0.56
1:C:225:MET:HE3	1:C:227:CYS:SG	2.45	0.56
1:D:56:THR:OG1	1:D:59:THR:HG23	2.06	0.56
1:D:185:GLN:NE2	1:D:190:ARG:HD2	2.19	0.56
1:D:292:TYR:O	1:D:295:LEU:HB2	2.05	0.56
1:A:56:THR:O	1:A:60:ARG:HB2	2.06	0.56
1:B:129:ARG:HG3	1:B:130:GLY:N	2.20	0.56
1:D:302:LEU:HD12	1:D:303:HIS:H	1.69	0.56
1:B:190:ARG:NE	1:B:286:ILE:HD13	2.20	0.56
1:C:292:TYR:HD1	1:C:295:LEU:HD22	1.71	0.56
1:A:45:VAL:O	1:A:46:ILE:HD13	2.06	0.56
1:D:118:ILE:CD1	1:D:155:GLY:HA2	2.36	0.55
1:A:92:LEU:HD22	1:A:209:MET:HG2	1.88	0.55
1:C:55:GLU:HG3	1:C:60:ARG:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:VAL:HG22	1:D:47:THR:HG22	1.88	0.55
1:A:243:VAL:HG22	4:A:2006:HOH:O	2.06	0.55
1:C:99:LEU:HD11	1:C:148:GLY:CA	2.34	0.55
1:C:106:TRP:NE1	1:C:139:THR:HG23	2.21	0.55
1:C:110:PHE:HD2	1:C:114:GLY:O	1.89	0.55
1:D:4:VAL:O	1:D:27:VAL:HA	2.06	0.55
1:D:320:LEU:HD12	1:D:320:LEU:N	2.21	0.55
1:B:282:MET:HG2	1:B:283:ILE:N	2.22	0.55
1:A:108:ALA:O	1:A:111:ASP:HB3	2.07	0.55
1:A:89:LYS:HG2	1:A:90:LEU:CD1	2.36	0.54
1:D:191:THR:HG22	1:D:349:TRP:CZ3	2.41	0.54
1:D:103:ARG:NH2	4:D:2425:HOH:O	2.29	0.54
1:A:65:HIS:HE1	1:A:67:ALA:HB3	1.70	0.54
1:C:68:PHE:CD2	1:C:71:ARG:HG3	2.43	0.54
1:C:286:ILE:HA	1:C:313:ARG:O	2.08	0.54
1:D:184:HIS:HA	1:D:188:ILE:O	2.07	0.54
1:A:45:VAL:C	1:A:46:ILE:HD13	2.33	0.54
1:A:184:HIS:HA	1:A:188:ILE:O	2.08	0.54
1:A:201:GLN:HA	1:A:201:GLN:OE1	2.07	0.54
1:B:81:LEU:HD23	1:B:122:ARG:NH2	2.23	0.54
1:B:168:ARG:HG3	1:B:174:THR:CG2	2.38	0.54
1:A:35:GLU:CD	1:A:35:GLU:H	2.14	0.54
1:A:144:ALA:HA	1:A:147:TYR:HE2	1.70	0.54
1:B:21:GLU:HB3	1:B:22:PRO:CD	2.37	0.53
1:C:278:ASN:HB3	1:C:279:PRO:CD	2.39	0.53
1:A:74:PHE:HB2	1:A:75:PRO:HD3	1.89	0.53
1:A:332:LEU:O	1:A:335:LEU:HB2	2.08	0.53
1:C:219:TYR:CE2	1:C:223:MET:HB2	2.44	0.53
1:C:238:GLU:HG2	4:C:2170:HOH:O	2.07	0.53
1:C:292:TYR:O	1:C:295:LEU:HB2	2.08	0.53
1:C:99:LEU:HD12	1:C:100:LEU:C	2.34	0.53
1:D:185:GLN:O	1:D:186:ASP:HB2	2.09	0.53
1:D:209:MET:HE3	1:D:236:ILE:HD11	1.91	0.53
1:C:291:ASN:HB3	1:C:294:TRP:CE2	2.44	0.53
1:A:138:GLU:HG2	1:A:141:GLN:OE1	2.09	0.52
1:A:298:PRO:HD2	4:A:2027:HOH:O	2.10	0.52
1:C:134:LEU:HG	1:C:138:GLU:O	2.09	0.52
1:C:116:LEU:HD23	1:C:117:ALA:N	2.23	0.52
1:D:137:ASN:ND2	1:D:137:ASN:N	2.56	0.52
1:A:226:GLU:HB3	4:A:2155:HOH:O	2.09	0.52
1:C:11:GLN:HG2	1:C:12:LEU:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:LEU:HA	1:D:151:ILE:HG22	1.91	0.52
1:D:209:MET:HE3	1:D:236:ILE:CG1	2.39	0.52
1:B:64:ARG:NH1	4:B:2088:HOH:O	2.42	0.52
1:B:103:ARG:C	1:B:105:GLU:H	2.17	0.52
1:C:96:PRO:HD2	1:C:154:GLN:HB3	1.92	0.51
1:C:108:ALA:O	1:C:111:ASP:N	2.30	0.51
1:B:184:HIS:HA	1:B:188:ILE:O	2.10	0.51
1:D:39:VAL:C	1:D:41:PHE:H	2.17	0.51
1:A:105:GLU:C	1:A:107:PRO:HD2	2.35	0.51
1:A:182:ASN:HB3	1:A:189:LEU:CD1	2.39	0.51
1:C:94:THR:C	1:C:235:LEU:HD23	2.36	0.51
1:C:230:THR:HB	1:C:231:PRO:HD2	1.92	0.51
1:C:210:LEU:HG	1:C:214:MET:HE2	1.91	0.51
1:D:245:ASN:HA	1:D:248:HIS:CE1	2.45	0.51
1:A:336:ILE:N	1:A:337:PRO:HD2	2.26	0.51
1:C:3:GLN:HG2	1:C:26:ALA:HB3	1.92	0.51
1:D:182:ASN:HB3	1:D:189:LEU:CD1	2.40	0.51
1:B:128:GLY:N	3:B:1200:ADP:O1B	2.39	0.51
1:C:74:PHE:N	1:C:75:PRO:HD2	2.26	0.51
1:C:73:VAL:C	1:C:75:PRO:HD2	2.36	0.51
1:C:145:GLU:C	1:C:147:TYR:H	2.17	0.51
1:B:190:ARG:CZ	1:B:286:ILE:HD13	2.41	0.51
1:B:317:HIS:C	1:B:318:LEU:HD23	2.36	0.51
1:C:336:ILE:HB	1:C:337:PRO:HD3	1.93	0.51
1:A:144:ALA:O	1:A:147:TYR:HD2	1.93	0.51
1:A:40:PRO:CA	1:A:42:GLN:HE22	2.22	0.50
1:A:284:ASN:HB3	1:A:286:ILE:HD11	1.92	0.50
1:B:137:ASN:OD1	1:B:137:ASN:N	2.44	0.50
1:C:109:VAL:HG13	1:C:113:LEU:HD12	1.93	0.50
1:D:58:LEU:CD1	1:D:62:LEU:HD13	2.40	0.50
1:A:337:PRO:HA	1:C:348:ILE:HD13	1.92	0.50
1:C:132:TRP:CE3	1:C:142:LEU:HD11	2.46	0.50
1:C:139:THR:O	1:C:141:GLN:N	2.44	0.50
1:C:286:ILE:HG22	1:C:286:ILE:O	2.10	0.50
1:D:76:ILE:HG22	1:D:77:ILE:HD13	1.93	0.50
1:D:288:SER:OG	1:D:343:TYR:OH	2.29	0.50
1:B:230:THR:CB	1:B:231:PRO:HD2	2.37	0.50
1:B:336:ILE:N	1:B:337:PRO:HD2	2.27	0.49
1:C:90:LEU:HD11	1:C:216:GLU:HG2	1.93	0.49
1:C:102:GLU:HB3	1:C:104:SER:OG	2.13	0.49
1:B:14:ARG:O	1:B:18:GLN:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:TYR:OH	1:B:129:ARG:NH1	2.45	0.49
1:D:106:TRP:N	1:D:107:PRO:HD2	2.28	0.49
1:C:160:GLY:O	1:C:229:VAL:HB	2.12	0.49
1:A:110:PHE:CE1	1:A:136:ALA:N	2.81	0.49
1:C:290:VAL:HG22	1:C:304:TRP:CZ3	2.47	0.49
1:A:76:ILE:O	1:A:82:THR:OG1	2.30	0.49
1:A:355:GLY:C	1:C:133:ARG:HD3	2.36	0.49
1:C:106:TRP:O	1:C:110:PHE:HD1	1.95	0.49
1:A:191:THR:HG21	1:A:350:ALA:HB2	1.94	0.49
1:C:182:ASN:HB3	1:C:189:LEU:HD11	1.95	0.49
1:A:119:VAL:HG23	1:A:132:TRP:HB2	1.92	0.49
1:D:106:TRP:HA	1:D:106:TRP:CE3	2.47	0.49
1:B:80:ARG:HH12	1:B:238:GLU:CG	2.26	0.49
1:B:324:ASP:OD1	1:B:326:SER:OG	2.30	0.48
1:C:77:ILE:CD1	1:C:239:LEU:HD23	2.42	0.48
1:C:139:THR:C	1:C:141:GLN:H	2.21	0.48
1:D:73:VAL:C	1:D:75:PRO:HD2	2.38	0.48
1:D:245:ASN:HB2	4:D:2411:HOH:O	2.13	0.48
1:A:225:MET:HE3	1:A:227:CYS:SG	2.53	0.48
1:A:245:ASN:OD1	1:A:314:LYS:NZ	2.39	0.48
1:B:118:ILE:HG13	1:B:133:ARG:HG2	1.95	0.48
1:B:336:ILE:HB	1:B:337:PRO:HD3	1.94	0.48
1:D:105:GLU:C	1:D:107:PRO:HD2	2.38	0.48
1:B:105:GLU:HG2	4:B:2459:HOH:O	2.12	0.48
1:C:295:LEU:HG	1:D:264:ARG:NH2	2.28	0.48
1:D:199:ASN:OD1	1:D:202:GLN:HB2	2.13	0.48
1:A:89:LYS:HG2	1:A:90:LEU:HD13	1.95	0.48
1:A:176:PHE:HE1	1:A:210:LEU:HD23	1.78	0.48
1:C:14:ARG:NH2	1:C:304:TRP:O	2.46	0.48
1:C:100:LEU:HD12	1:C:100:LEU:HA	1.69	0.48
1:C:119:VAL:O	1:C:131:GLN:HB2	2.13	0.48
1:D:322:ASP:OD2	1:D:324:ASP:HB3	2.14	0.48
1:A:138:GLU:O	1:A:141:GLN:HB2	2.12	0.48
1:A:138:GLU:O	1:A:141:GLN:N	2.30	0.48
1:B:285:LEU:HD21	1:B:318:LEU:HG	1.94	0.48
1:C:194:ALA:O	1:C:279:PRO:HA	2.14	0.48
1:C:65:HIS:CE1	1:C:67:ALA:HB3	2.45	0.48
1:C:121:ARG:NH2	1:C:132:TRP:CH2	2.82	0.48
1:A:142:LEU:HG	1:A:143:PRO:CD	2.43	0.47
1:B:39:VAL:C	1:B:41:PHE:H	2.22	0.47
1:B:179:LEU:HD11	1:B:203:GLN:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:TYR:O	1:B:295:LEU:HB2	2.14	0.47
1:D:116:LEU:HG	1:D:117:ALA:H	1.77	0.47
1:C:161:GLU:OE2	3:C:1300:ADP:O3'	2.30	0.47
1:C:325:THR:O	1:C:329:THR:HG23	2.14	0.47
1:D:264:ARG:HB3	1:D:271:LEU:HD13	1.96	0.47
1:A:79:ASP:OD1	1:A:81:LEU:HB3	2.15	0.47
1:B:269:LEU:HB3	1:B:270:PRO:HD2	1.96	0.47
1:D:79:ASP:OD1	1:D:81:LEU:HB3	2.14	0.47
1:A:291:ASN:C	1:A:293:ASP:H	2.22	0.47
1:C:207:GLU:O	1:C:211:SER:OG	2.30	0.47
1:D:95:ALA:CB	1:D:153:GLU:HG2	2.44	0.47
1:B:100:LEU:O	1:B:148:GLY:N	2.39	0.47
1:C:92:LEU:HB3	1:C:236:ILE:CD1	2.45	0.47
1:D:344:ALA:O	1:D:348:ILE:HD12	2.14	0.47
1:C:97:TRP:HA	1:C:152:VAL:O	2.15	0.47
1:C:99:LEU:HB2	1:C:151:ILE:HG22	1.97	0.47
1:C:101:ALA:O	1:C:147:TYR:HD2	1.98	0.47
1:D:322:ASP:OD1	1:D:327:ARG:NH2	2.47	0.47
1:A:80:ARG:HH12	1:A:238:GLU:HG3	1.79	0.47
1:B:328:LEU:HA	1:B:328:LEU:HD12	1.51	0.47
1:C:119:VAL:HG12	1:C:132:TRP:CE3	2.49	0.47
1:C:289:ASP:HB2	4:C:2292:HOH:O	2.14	0.47
1:D:95:ALA:HB3	1:D:153:GLU:HG2	1.96	0.47
1:A:108:ALA:C	1:A:112:ARG:HH11	2.23	0.47
1:B:291:ASN:ND2	1:B:293:ASP:HB2	2.30	0.47
1:B:298:PRO:HD2	4:B:2109:HOH:O	2.14	0.47
1:C:109:VAL:O	1:C:113:LEU:N	2.48	0.46
1:D:137:ASN:ND2	4:D:2424:HOH:O	2.48	0.46
1:B:285:LEU:O	1:B:315:VAL:HG22	2.16	0.46
1:D:84:LYS:HZ1	1:D:153:GLU:CD	2.23	0.46
1:D:168:ARG:HG3	1:D:174:THR:HG22	1.96	0.46
1:D:335:LEU:O	1:D:338:LEU:HB2	2.14	0.46
1:A:98:GLN:HE21	1:A:98:GLN:HB2	1.51	0.46
1:A:203:GLN:O	1:A:207:GLU:HG3	2.16	0.46
1:A:202:GLN:HG2	1:A:234:LEU:HD11	1.96	0.46
1:A:355:GLY:CA	1:C:133:ARG:HD3	2.44	0.46
1:C:336:ILE:CB	1:C:337:PRO:HD3	2.46	0.46
1:D:12:LEU:HB2	1:D:49:GLU:OE1	2.15	0.46
1:D:90:LEU:HD23	1:D:92:LEU:HD11	1.96	0.46
1:A:324:ASP:O	1:A:328:LEU:HB2	2.16	0.46
1:C:267:THR:O	1:C:268:ASP:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:ASP:O	1:D:82:THR:OG1	2.30	0.46
1:D:194:ALA:O	1:D:279:PRO:HA	2.15	0.46
1:C:30:VAL:CG1	1:C:39:VAL:HG11	2.45	0.46
1:C:121:ARG:NH2	1:C:132:TRP:CZ2	2.84	0.46
1:D:99:LEU:HB3	4:D:2183:HOH:O	2.15	0.46
1:A:84:LYS:HE3	1:A:97:TRP:CD1	2.50	0.46
1:A:119:VAL:HG21	1:A:132:TRP:HB2	1.95	0.46
1:A:264:ARG:HA	1:A:269:LEU:HB2	1.96	0.46
1:C:21:GLU:HG2	1:D:18:GLN:NE2	2.31	0.46
1:D:309:VAL:HG23	4:D:2384:HOH:O	2.14	0.46
1:A:142:LEU:HD12	1:A:143:PRO:CD	2.42	0.46
1:B:79:ASP:HB3	1:B:82:THR:OG1	2.16	0.46
1:B:90:LEU:HD12	1:B:90:LEU:HA	1.44	0.46
1:B:285:LEU:HD11	1:B:318:LEU:CD2	2.46	0.46
1:C:100:LEU:HD21	1:C:106:TRP:CZ2	2.51	0.46
1:A:256:ILE:HG21	1:A:261:LEU:HD13	1.97	0.45
1:C:241:PRO:O	1:C:242:ARG:HB3	2.15	0.45
1:C:264:ARG:HA	1:C:269:LEU:HB2	1.98	0.45
1:C:328:LEU:HA	1:C:328:LEU:HD12	1.74	0.45
1:D:68:PHE:HD1	1:D:69:VAL:N	2.14	0.45
1:D:158:PHE:HB3	1:D:228:PHE:HB3	1.97	0.45
1:D:263:LEU:O	1:D:267:THR:HG23	2.16	0.45
1:A:139:THR:HB	4:A:2011:HOH:O	2.16	0.45
1:B:9:ASN:HD22	1:B:9:ASN:HA	1.45	0.45
1:C:131:GLN:O	1:C:131:GLN:HG3	2.15	0.45
1:C:145:GLU:O	1:C:147:TYR:N	2.41	0.45
1:C:249:TRP:CH2	1:C:250:THR:HG22	2.51	0.45
1:D:245:ASN:OD1	1:D:314:LYS:HE2	2.15	0.45
1:A:243:VAL:CG1	1:A:258:GLN:HG3	2.47	0.45
1:C:132:TRP:CE3	1:C:142:LEU:CD1	3.00	0.45
1:D:106:TRP:N	1:D:107:PRO:CD	2.80	0.45
1:A:21:GLU:CB	1:A:22:PRO:HD3	2.47	0.45
1:D:32:LEU:HD13	1:D:54:PRO:HD2	1.97	0.45
1:D:119:VAL:O	1:D:131:GLN:HB2	2.16	0.45
1:A:60:ARG:O	1:A:63:ALA:HB3	2.15	0.45
1:B:245:ASN:HA	1:B:248:HIS:CE1	2.52	0.45
1:C:132:TRP:CD2	1:C:142:LEU:CD1	3.00	0.45
1:C:182:ASN:ND2	1:C:246:SER:HB2	2.28	0.45
1:A:288:SER:HG	1:A:343:TYR:HH	1.62	0.45
1:B:321:THR:O	1:B:322:ASP:HB2	2.17	0.45
1:C:106:TRP:NE1	1:C:139:THR:CG2	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:TRP:HB3	1:D:134:LEU:HD13	1.99	0.45
1:D:240:ALA:HA	1:D:241:PRO:HD3	1.73	0.45
1:A:261:LEU:HD12	1:A:261:LEU:HA	1.71	0.45
1:A:74:PHE:N	1:A:75:PRO:CD	2.80	0.45
1:A:108:ALA:CA	1:A:112:ARG:NH1	2.80	0.45
1:A:355:GLY:HA3	1:C:133:ARG:HD3	1.98	0.45
1:B:264:ARG:HD3	1:B:270:PRO:O	2.17	0.45
1:D:245:ASN:ND2	1:D:248:HIS:CD2	2.85	0.45
1:A:101:ALA:O	1:A:147:TYR:HD1	2.00	0.44
1:A:106:TRP:N	1:A:107:PRO:CD	2.80	0.44
1:A:157:ASN:HB3	1:C:232:GLN:CA	2.44	0.44
1:B:308:GLU:O	1:B:313:ARG:NH1	2.39	0.44
1:C:74:PHE:N	1:C:75:PRO:CD	2.80	0.44
1:C:349:TRP:O	1:C:352:SER:OG	2.34	0.44
1:D:145:GLU:H	1:D:145:GLU:HG2	1.43	0.44
1:D:336:ILE:HG13	1:D:347:VAL:HG11	1.99	0.44
1:A:68:PHE:O	1:A:71:ARG:HB2	2.17	0.44
1:B:210:LEU:O	1:B:213:ILE:HB	2.17	0.44
1:A:295:LEU:HA	1:A:295:LEU:HD12	1.72	0.44
1:C:32:LEU:H	1:C:32:LEU:HG	1.49	0.44
1:D:74:PHE:N	1:D:75:PRO:CD	2.80	0.44
1:D:207:GLU:O	1:D:211:SER:OG	2.35	0.44
1:A:6:VAL:O	1:A:30:VAL:N	2.49	0.44
1:A:342:GLU:H	1:A:342:GLU:HG3	1.24	0.44
1:B:182:ASN:ND2	1:B:192:SER:CB	2.80	0.44
1:C:210:LEU:O	1:C:214:MET:HG3	2.17	0.44
1:D:239:LEU:HD12	1:D:239:LEU:HA	1.60	0.44
1:A:18:GLN:NE2	1:B:21:GLU:OE2	2.35	0.44
1:D:295:LEU:HD12	1:D:295:LEU:HA	1.42	0.44
1:A:55:GLU:HG3	1:A:60:ARG:HG3	2.00	0.44
1:A:21:GLU:HG2	1:B:18:GLN:NE2	2.32	0.44
1:A:320:LEU:HD12	1:A:320:LEU:N	2.33	0.44
1:A:336:ILE:N	1:A:337:PRO:CD	2.81	0.44
1:C:335:LEU:HA	1:C:335:LEU:HD23	1.82	0.44
1:D:106:TRP:CE2	1:D:139:THR:HG23	2.52	0.44
1:B:185:GLN:N	1:B:188:ILE:O	2.40	0.44
1:D:59:THR:O	1:D:63:ALA:N	2.41	0.44
1:A:61:GLU:OE1	1:A:64:ARG:NH2	2.50	0.44
1:A:81:LEU:HD23	1:A:122:ARG:NH2	2.22	0.44
1:A:84:LYS:HE3	1:A:97:TRP:CG	2.52	0.44
1:A:103:ARG:HG2	1:A:147:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LEU:HD23	1:A:118:ILE:HD12	2.00	0.44
1:C:21:GLU:HG2	1:D:18:GLN:HE21	1.83	0.44
1:C:101:ALA:O	1:C:147:TYR:HB3	2.17	0.44
1:A:8:GLY:HA3	1:A:49:GLU:CG	2.47	0.43
1:B:72:ASP:C	1:B:75:PRO:HD2	2.43	0.43
1:B:291:ASN:HD21	1:B:293:ASP:HB2	1.83	0.43
1:C:255:SER:C	1:C:256:ILE:HG13	2.43	0.43
1:C:319:ASN:HB3	4:C:2310:HOH:O	2.17	0.43
1:D:90:LEU:HB3	1:D:92:LEU:HG	1.98	0.43
1:D:180:THR:CG2	1:D:192:SER:HB3	2.48	0.43
1:A:106:TRP:CD1	1:A:139:THR:CG2	3.02	0.43
1:A:182:ASN:ND2	1:A:192:SER:OG	2.51	0.43
1:B:60:ARG:O	1:B:64:ARG:HD2	2.19	0.43
1:B:329:THR:HA	1:B:332:LEU:HD12	2.00	0.43
1:C:6:VAL:HG22	1:C:47:THR:CG2	2.47	0.43
1:C:119:VAL:HG12	1:C:132:TRP:HE3	1.83	0.43
1:C:168:ARG:HA	1:C:173:SER:O	2.18	0.43
1:D:119:VAL:O	1:D:131:GLN:HA	2.19	0.43
1:D:137:ASN:HD22	1:D:137:ASN:N	2.07	0.43
1:B:106:TRP:N	1:B:107:PRO:CD	2.80	0.43
1:B:182:ASN:HD22	1:B:192:SER:CB	2.32	0.43
1:C:56:THR:OG1	1:C:59:THR:HG23	2.18	0.43
1:C:81:LEU:HD12	1:C:97:TRP:HZ3	1.83	0.43
1:C:324:ASP:OD1	1:C:326:SER:HB2	2.19	0.43
1:A:3:GLN:HG2	1:A:26:ALA:HB3	2.00	0.43
1:A:144:ALA:CA	1:A:147:TYR:HD2	2.32	0.43
1:A:336:ILE:CB	1:A:337:PRO:HD3	2.48	0.43
1:D:32:LEU:HA	1:D:58:LEU:HD23	2.00	0.43
1:A:119:VAL:O	1:A:119:VAL:HG23	2.18	0.43
1:C:336:ILE:HG22	1:C:337:PRO:N	2.32	0.43
1:D:74:PHE:N	1:D:75:PRO:HD2	2.34	0.43
1:A:103:ARG:C	1:A:105:GLU:H	2.24	0.43
1:A:217:LEU:HD12	1:A:217:LEU:HA	1.81	0.43
1:B:2:LYS:HE2	1:B:267:THR:HB	2.00	0.43
1:B:271:LEU:HD12	1:B:271:LEU:HA	1.68	0.43
1:C:2:LYS:HE3	1:C:269:LEU:HD11	2.00	0.43
1:C:106:TRP:CD1	1:C:139:THR:HG21	2.54	0.43
1:C:195:PHE:CZ	1:C:354:PHE:CE1	3.07	0.43
1:D:168:ARG:HG3	1:D:174:THR:CG2	2.49	0.43
1:A:108:ALA:CB	1:A:112:ARG:NH1	2.80	0.43
1:A:301:HIS:HB2	1:A:319:ASN:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:LEU:O	1:C:147:TYR:HA	2.19	0.43
1:D:77:ILE:HD13	1:D:77:ILE:N	2.34	0.43
1:A:81:LEU:CD2	1:A:122:ARG:NH2	2.82	0.43
1:A:83:GLN:O	1:A:86:LEU:HB3	2.19	0.43
1:A:110:PHE:HE1	1:A:135:ARG:HA	1.83	0.43
1:B:196:PRO:HG3	1:B:278:ASN:HA	2.01	0.43
1:C:17:ARG:HA	1:C:27:VAL:HB	2.01	0.43
1:D:39:VAL:HA	1:D:40:PRO:HD3	1.84	0.43
1:C:21:GLU:HB3	1:C:22:PRO:HD3	2.01	0.42
1:C:76:ILE:O	1:C:82:THR:OG1	2.32	0.42
1:D:90:LEU:HD12	1:D:90:LEU:HA	1.83	0.42
1:A:90:LEU:CD1	1:A:90:LEU:N	2.82	0.42
1:A:157:ASN:HB3	1:C:232:GLN:CB	2.49	0.42
1:A:288:SER:OG	1:A:343:TYR:OH	2.35	0.42
1:A:336:ILE:HG22	1:A:337:PRO:N	2.33	0.42
1:B:319:ASN:C	1:B:320:LEU:HD12	2.44	0.42
1:C:287:GLY:HA2	1:C:310:ARG:O	2.19	0.42
1:C:336:ILE:HD11	1:C:347:VAL:CG1	2.49	0.42
1:D:158:PHE:CD2	1:D:228:PHE:CD1	3.07	0.42
1:B:7:LEU:HB3	1:B:48:ALA:CB	2.49	0.42
1:B:63:ALA:HA	1:B:68:PHE:HD2	1.84	0.42
1:C:21:GLU:CB	1:C:22:PRO:HD3	2.49	0.42
1:C:144:ALA:C	1:C:147:TYR:HD1	2.27	0.42
1:D:329:THR:O	1:D:332:LEU:HB2	2.18	0.42
1:A:120:LYS:HA	1:A:130:GLY:O	2.20	0.42
1:B:295:LEU:HD12	1:B:295:LEU:HA	1.68	0.42
1:D:21:GLU:N	1:D:22:PRO:HD2	2.35	0.42
1:A:116:LEU:CD2	1:A:118:ILE:HD12	2.49	0.42
1:A:282:MET:HG2	1:A:283:ILE:N	2.33	0.42
1:B:23:LEU:HA	1:B:23:LEU:HD12	1.65	0.42
1:B:106:TRP:O	1:B:109:VAL:HB	2.20	0.42
1:C:62:LEU:HA	1:C:62:LEU:HD12	1.73	0.42
1:C:282:MET:HG2	1:C:283:ILE:N	2.32	0.42
1:D:164:LEU:HB2	1:D:179:LEU:HD23	2.00	0.42
1:B:86:LEU:HD11	1:B:90:LEU:CD2	2.45	0.42
1:C:119:VAL:CG1	1:C:132:TRP:CE3	3.03	0.42
1:D:223:MET:HE3	1:D:223:MET:HB2	1.59	0.42
1:A:41:PHE:N	1:A:42:GLN:HE21	2.18	0.42
1:A:185:GLN:HB2	1:A:190:ARG:HG3	2.01	0.42
1:B:105:GLU:C	1:B:107:PRO:HD2	2.45	0.42
1:D:182:ASN:ND2	1:D:192:SER:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ILE:HG22	1:A:337:PRO:HD3	2.01	0.42
1:A:74:PHE:N	1:A:75:PRO:HD2	2.35	0.42
1:C:32:LEU:HD21	1:C:50:ILE:CD1	2.50	0.42
1:C:119:VAL:CG1	1:C:132:TRP:HE3	2.31	0.42
1:A:144:ALA:HA	1:A:147:TYR:HD2	1.76	0.41
1:A:164:LEU:HD12	1:A:165:VAL:N	2.33	0.41
1:B:291:ASN:HB3	1:B:294:TRP:CE2	2.55	0.41
1:A:205:ARG:HD2	1:A:205:ARG:O	2.20	0.41
1:C:96:PRO:O	1:C:154:GLN:N	2.44	0.41
1:B:28:TRP:CE2	1:B:40:PRO:HG2	2.55	0.41
1:C:118:ILE:HD13	1:C:155:GLY:HA2	2.02	0.41
1:C:320:LEU:HD12	1:C:320:LEU:N	2.35	0.41
1:D:52:ARG:NH2	1:D:123:THR:CG2	2.79	0.41
1:D:106:TRP:HB2	1:D:107:PRO:HD3	2.03	0.41
1:D:335:LEU:HD23	1:D:335:LEU:HA	1.76	0.41
1:A:227:CYS:CB	1:A:234:LEU:HD23	2.46	0.41
1:B:344:ALA:O	1:B:348:ILE:HD12	2.21	0.41
1:C:60:ARG:O	1:C:63:ALA:HB3	2.19	0.41
1:D:4:VAL:HB	1:D:27:VAL:HG22	2.03	0.41
1:D:106:TRP:CD1	1:D:139:THR:HG21	2.55	0.41
1:A:340:PRO:HA	1:A:341:PRO:HD3	1.87	0.41
1:C:46:ILE:HD12	1:C:65:HIS:CE1	2.55	0.41
1:B:241:PRO:O	1:B:242:ARG:HB3	2.19	0.41
1:B:273:GLN:NE2	4:B:2147:HOH:O	2.52	0.41
1:B:278:ASN:HB3	1:B:279:PRO:CD	2.43	0.41
1:A:144:ALA:CA	1:A:147:TYR:CD2	3.00	0.41
1:B:7:LEU:HB3	1:B:48:ALA:HB2	2.03	0.41
1:C:39:VAL:C	1:C:41:PHE:H	2.28	0.41
1:C:158:PHE:CD2	1:C:228:PHE:CD1	3.08	0.41
1:C:336:ILE:N	1:C:337:PRO:HD2	2.34	0.41
1:A:6:VAL:O	1:A:30:VAL:HG12	2.20	0.41
1:A:144:ALA:C	1:A:147:TYR:HD2	2.28	0.41
1:A:209:MET:HG2	1:A:236:ILE:HD11	2.02	0.41
1:A:243:VAL:HG12	1:A:258:GLN:HG3	2.03	0.41
1:B:63:ALA:HB1	1:B:71:ARG:NH2	2.36	0.41
1:B:79:ASP:OD1	1:B:81:LEU:HB3	2.20	0.41
1:B:151:ILE:HG13	1:B:152:VAL:N	2.34	0.41
1:B:283:ILE:O	1:B:317:HIS:HA	2.21	0.41
1:C:295:LEU:HD12	1:C:295:LEU:HA	1.73	0.41
1:D:14:ARG:O	1:D:18:GLN:HG3	2.21	0.41
1:D:138:GLU:O	1:D:140:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:THR:HG22	1:D:192:SER:HB3	2.02	0.41
1:A:194:ALA:O	1:A:279:PRO:HA	2.21	0.41
1:C:103:ARG:HA	1:C:147:TYR:HE2	1.86	0.41
1:D:133:ARG:O	1:D:134:LEU:HD12	2.21	0.41
1:A:53:TRP:HB2	1:A:54:PRO:HD2	2.03	0.40
1:B:28:TRP:CD2	1:B:40:PRO:HG2	2.56	0.40
1:B:90:LEU:HB3	1:B:92:LEU:CG	2.49	0.40
1:B:217:LEU:HA	1:B:217:LEU:HD23	1.84	0.40
1:C:42:GLN:CD	1:C:42:GLN:H	2.27	0.40
1:A:40:PRO:C	1:A:42:GLN:NE2	2.80	0.40
1:A:84:LYS:HB3	1:A:97:TRP:CE2	2.57	0.40
1:C:11:GLN:O	1:C:15:MET:HE2	2.20	0.40
1:D:10:GLY:N	1:D:49:GLU:OE2	2.51	0.40
1:B:11:GLN:HG3	1:B:305:TYR:CE2	2.56	0.40
1:B:97:TRP:HA	1:B:152:VAL:O	2.21	0.40
1:C:139:THR:C	1:C:141:GLN:N	2.80	0.40
1:D:158:PHE:CB	1:D:228:PHE:HB3	2.52	0.40
1:A:318:LEU:HD23	1:A:318:LEU:HA	1.84	0.40
1:C:71:ARG:HH11	1:C:71:ARG:HD3	1.69	0.40
1:C:103:ARG:C	1:C:105:GLU:N	2.79	0.40
1:C:132:TRP:CD2	1:C:142:LEU:HD12	2.56	0.40
1:C:144:ALA:O	1:C:147:TYR:HD1	2.03	0.40
1:C:288:SER:OG	1:C:343:TYR:OH	2.31	0.40
1:C:293:ASP:O	1:C:296:LYS:HG3	2.21	0.40
1:D:297:LEU:HA	1:D:298:PRO:HD3	1.89	0.40
1:A:96:PRO:O	1:A:153:GLU:HA	2.22	0.40
1:B:332:LEU:O	1:B:335:LEU:HB2	2.22	0.40
1:C:79:ASP:HB3	1:C:82:THR:OG1	2.22	0.40
1:C:133:ARG:C	1:C:134:LEU:HD13	2.47	0.40
1:C:245:ASN:HA	1:C:248:HIS:CE1	2.56	0.40
1:C:297:LEU:HA	1:C:298:PRO:HD2	1.88	0.40
1:D:68:PHE:C	1:D:68:PHE:CD1	3.00	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2439:HOH:O	4:D:2477:HOH:O[1_454]	0.20	2.00

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	347/355 (98%)	329 (95%)	14 (4%)	4 (1%)	10	20
1	B	353/355 (99%)	326 (92%)	21 (6%)	6 (2%)	7	13
1	C	346/355 (98%)	321 (93%)	19 (6%)	6 (2%)	7	13
1	D	346/355 (98%)	331 (96%)	10 (3%)	5 (1%)	9	17
All	All	1392/1420 (98%)	1307 (94%)	64 (5%)	21 (2%)	8	16

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	129	ARG
1	C	146	CYS
1	A	139	THR
1	A	146	CYS
1	C	136	ALA
1	C	140	GLU
1	D	34	ALA
1	D	139	THR
1	A	292	TYR
1	B	139	THR
1	B	104	SER
1	C	104	SER
1	C	113	LEU
1	D	136	ALA
1	A	136	ALA
1	C	139	THR
1	D	40	PRO
1	B	124	GLY
1	B	298	PRO
1	B	125	GLY
1	D	287	GLY

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	293/296 (99%)	254 (87%)	39 (13%)	4	8
1	B	296/296 (100%)	244 (82%)	52 (18%)	2	3
1	C	293/296 (99%)	245 (84%)	48 (16%)	2	4
1	D	293/296 (99%)	256 (87%)	37 (13%)	4	9
All	All	1175/1184 (99%)	999 (85%)	176 (15%)	3	6

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	9	ASN
1	A	21	GLU
1	A	23	LEU
1	A	33	ASP
1	A	35	GLU
1	A	39	VAL
1	A	42	GLN
1	A	43	GLN
1	A	44	SER
1	A	90	LEU
1	A	98	GLN
1	A	104	SER
1	A	105	GLU
1	A	112	ARG
1	A	118	ILE
1	A	121	ARG
1	A	134	LEU
1	A	149	GLU
1	A	151	ILE
1	A	197	GLN
1	A	201	GLN
1	A	209	MET
1	A	215	GLN

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Mol	Chain	Res	Type
1	A	216	GLU
1	A	217	LEU
1	A	230	THR
1	A	234	LEU
1	A	239	LEU
1	A	243	VAL
1	A	290	VAL
1	A	295	LEU
1	A	306	ASP
1	A	310	ARG
1	A	325	THR
1	A	327	ARG
1	A	336	ILE
1	A	342	GLU
1	A	345	SER
1	B	1	MET
1	B	2	LYS
1	B	9	ASN
1	B	23	LEU
1	B	30	VAL
1	B	32	LEU
1	B	39	VAL
1	B	42	GLN
1	B	43	GLN
1	B	44	SER
1	B	49	GLU
1	B	52	ARG
1	B	61	GLU
1	B	86	LEU
1	B	90	LEU
1	B	104	SER
1	B	111	ASP
1	B	115	GLU
1	B	118	ILE
1	B	121	ARG
1	B	131	GLN
1	B	134	LEU
1	B	137	ASN
1	B	140	GLU
1	B	141	GLN
1	B	142	LEU
1	B	145	GLU

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Mol	Chain	Res	Type
1	B	146	CYS
1	B	151	ILE
1	B	152	VAL
1	B	154	GLN
1	B	159	SER
1	B	192	SER
1	B	197	GLN
1	B	201	GLN
1	B	211	SER
1	B	230	THR
1	B	232	GLN
1	B	235	LEU
1	B	239	LEU
1	B	260	GLU
1	B	271	LEU
1	B	280	SER
1	B	288	SER
1	B	295	LEU
1	B	306	ASP
1	B	326	SER
1	B	328	LEU
1	B	333	GLU
1	B	342	GLU
1	B	345	SER
1	B	352	SER
1	C	1	MET
1	C	30	VAL
1	C	32	LEU
1	C	33	ASP
1	C	35	GLU
1	C	39	VAL
1	C	42	GLN
1	C	44	SER
1	C	50	ILE
1	C	51	GLU
1	C	60	ARG
1	C	62	LEU
1	C	71	ARG
1	C	99	LEU
1	C	102	GLU
1	C	103	ARG
1	C	104	SER

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Mol	Chain	Res	Type
1	C	111	ASP
1	C	112	ARG
1	C	115	GLU
1	C	116	LEU
1	C	134	LEU
1	C	139	THR
1	C	142	LEU
1	C	146	CYS
1	C	149	GLU
1	C	151	ILE
1	C	152	VAL
1	C	168	ARG
1	C	188	ILE
1	C	192	SER
1	C	197	GLN
1	C	201	GLN
1	C	202	GLN
1	C	211	SER
1	C	235	LEU
1	C	269	LEU
1	C	286	ILE
1	C	288	SER
1	C	293	ASP
1	C	295	LEU
1	C	296	LYS
1	C	306	ASP
1	C	308	GLU
1	C	327	ARG
1	C	333	GLU
1	C	336	ILE
1	C	342	GLU
1	D	9	ASN
1	D	23	LEU
1	D	33	ASP
1	D	44	SER
1	D	47	THR
1	D	52	ARG
1	D	61	GLU
1	D	82	THR
1	D	90	LEU
1	D	104	SER
1	D	111	ASP

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Mol	Chain	Res	Type
1	D	116	LEU
1	D	118	ILE
1	D	123	THR
1	D	137	ASN
1	D	141	GLN
1	D	145	GLU
1	D	146	CYS
1	D	149	GLU
1	D	151	ILE
1	D	175	VAL
1	D	188	ILE
1	D	190	ARG
1	D	192	SER
1	D	211	SER
1	D	215	GLN
1	D	232	GLN
1	D	239	LEU
1	D	257	SER
1	D	271	LEU
1	D	288	SER
1	D	295	LEU
1	D	306	ASP
1	D	308	GLU
1	D	342	GLU
1	D	345	SER
1	D	348	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	9	ASN
1	A	42	GLN
1	A	43	GLN
1	A	83	GLN
1	A	91	HIS
1	A	98	GLN
1	A	182	ASN
1	A	185	GLN
1	A	215	GLN
1	A	251	GLN
1	B	3	GLN

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Mol	Chain	Res	Type
1	B	9	ASN
1	B	141	GLN
1	B	182	ASN
1	B	184	HIS
1	B	291	ASN
1	C	9	ASN
1	C	42	GLN
1	C	83	GLN
1	C	85	GLN
1	C	98	GLN
1	C	182	ASN
1	C	251	GLN
1	C	252	ASN
1	C	319	ASN
1	D	9	ASN
1	D	18	GLN
1	D	137	ASN
1	D	141	GLN
1	D	182	ASN
1	D	185	GLN
1	D	215	GLN
1	D	301	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	A	1100	2	28,29,29	1.20	4 (14%)	43,45,45	1.42	5 (11%)
3	ADP	C	1300	2	28,29,29	1.10	2 (7%)	43,45,45	1.13	3 (6%)
3	ADP	B	1200	2	28,29,29	1.13	2 (7%)	43,45,45	0.99	2 (4%)
3	ADP	D	1400	2	28,29,29	1.10	4 (14%)	43,45,45	0.96	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	1100	2	-	4/16/32/32	0/3/3/3
3	ADP	C	1300	2	-	5/16/32/32	0/3/3/3
3	ADP	B	1200	2	-	5/16/32/32	0/3/3/3
3	ADP	D	1400	2	-	4/16/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1100	ADP	O3'-C3'	2.89	1.50	1.43
3	C	1300	ADP	O2'-C2'	2.80	1.49	1.43
3	A	1100	ADP	O2'-C2'	2.76	1.49	1.43
3	B	1200	ADP	O3'-C3'	2.74	1.49	1.43
3	B	1200	ADP	O2'-C2'	2.72	1.49	1.43
3	C	1300	ADP	C2-N1	2.71	1.38	1.33
3	D	1400	ADP	O2'-C2'	2.67	1.49	1.43
3	D	1400	ADP	O3'-C3'	2.45	1.49	1.43
3	A	1100	ADP	C2-N1	2.32	1.38	1.33
3	D	1400	ADP	C2-N1	2.05	1.37	1.33
3	A	1100	ADP	PA-O3A	-2.01	1.57	1.59
3	D	1400	ADP	C2-N3	-2.00	1.30	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1100	ADP	O3'-C3'-C2'	4.72	126.94	111.82
3	C	1300	ADP	O3'-C3'-C2'	4.16	125.17	111.82
3	D	1400	ADP	O3'-C3'-C2'	3.66	123.56	111.82
3	A	1100	ADP	C2'-C3'-C4'	-3.41	96.02	102.61
3	A	1100	ADP	O4'-C4'-C3'	-3.32	98.56	105.15
3	B	1200	ADP	C2'-C3'-C4'	-3.28	96.26	102.61
3	A	1100	ADP	O2A-PA-O3A	3.01	115.41	107.27
3	C	1300	ADP	O2'-C2'-C3'	2.87	121.02	111.82
3	B	1200	ADP	O3'-C3'-C2'	2.76	120.66	111.82
3	C	1300	ADP	C2'-C3'-C4'	-2.25	98.27	102.61
3	A	1100	ADP	O2'-C2'-C3'	2.16	118.73	111.82
3	D	1400	ADP	O2'-C2'-C3'	2.15	118.69	111.82
3	D	1400	ADP	O2A-PA-O1A	-2.02	103.04	112.44

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1100	ADP	C5'-O5'-PA-O1A
3	A	1100	ADP	C5'-O5'-PA-O2A
3	C	1300	ADP	C5'-O5'-PA-O2A
3	D	1400	ADP	PA-O3A-PB-O3B
3	D	1400	ADP	C5'-O5'-PA-O2A
3	D	1400	ADP	C5'-O5'-PA-O3A
3	A	1100	ADP	O4'-C4'-C5'-O5'
3	B	1200	ADP	O4'-C4'-C5'-O5'
3	C	1300	ADP	O4'-C4'-C5'-O5'
3	B	1200	ADP	C3'-C4'-C5'-O5'
3	D	1400	ADP	O4'-C4'-C5'-O5'
3	B	1200	ADP	PA-O3A-PB-O3B
3	A	1100	ADP	C5'-O5'-PA-O3A
3	B	1200	ADP	C5'-O5'-PA-O2A
3	B	1200	ADP	C5'-O5'-PA-O3A
3	C	1300	ADP	C5'-O5'-PA-O1A
3	C	1300	ADP	C5'-O5'-PA-O3A
3	C	1300	ADP	PB-O3A-PA-O2A

There are no ring outliers.

2 monomers are involved in 2 short contacts:

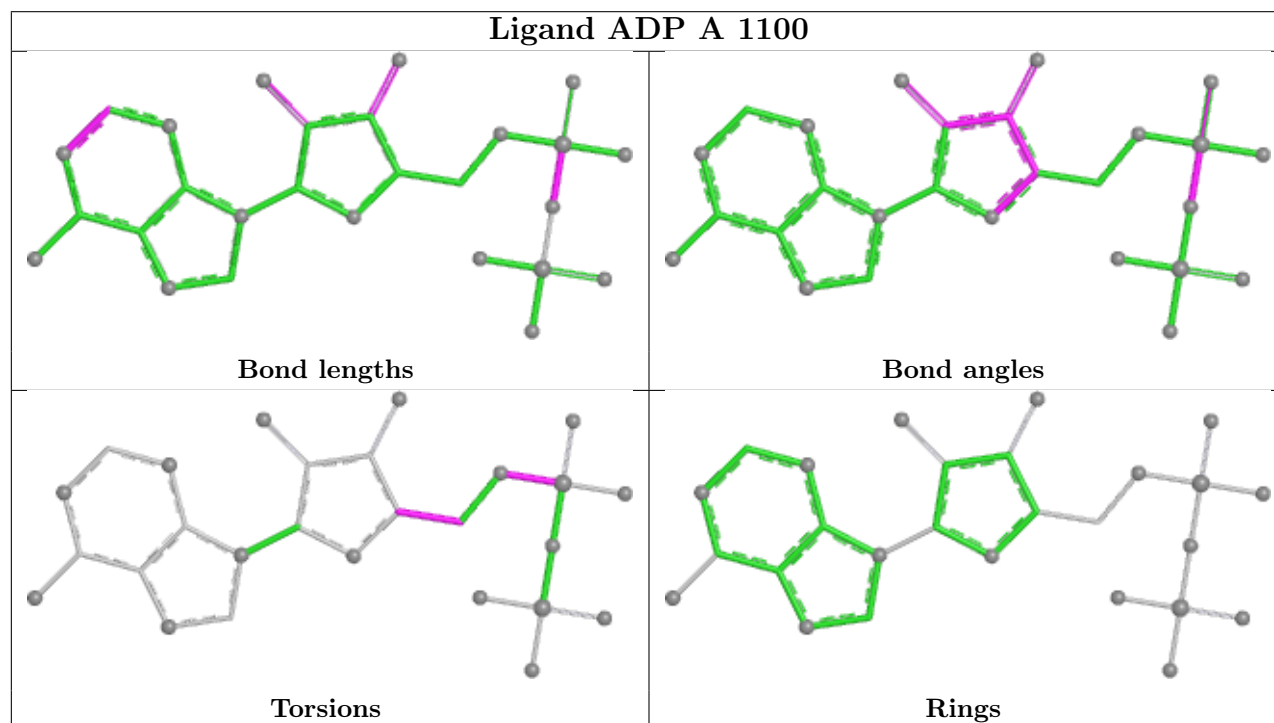
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1300	ADP	1	0

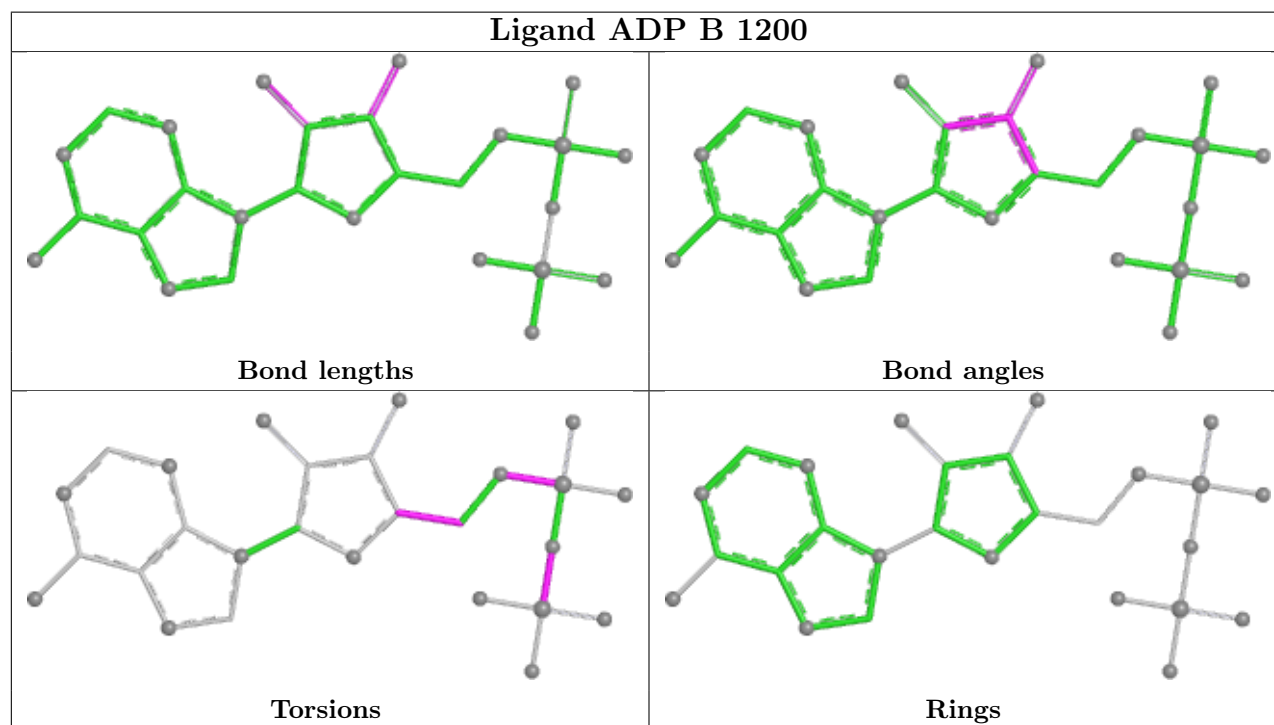
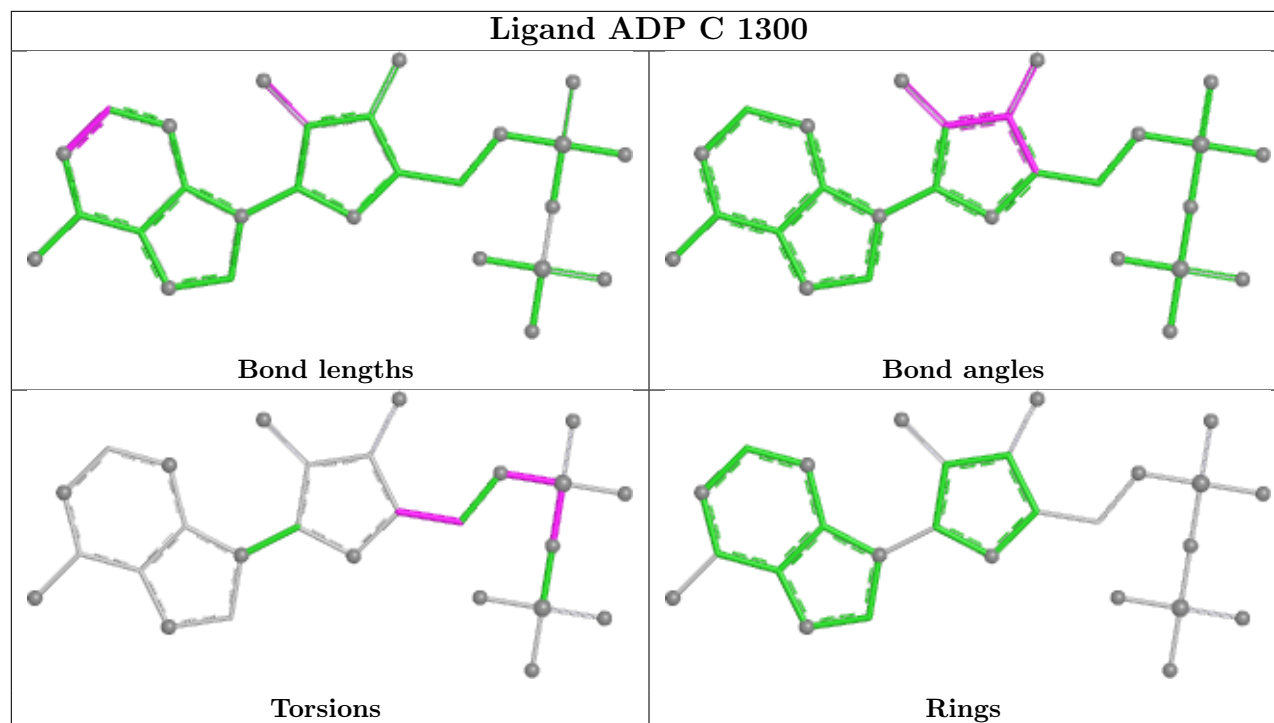
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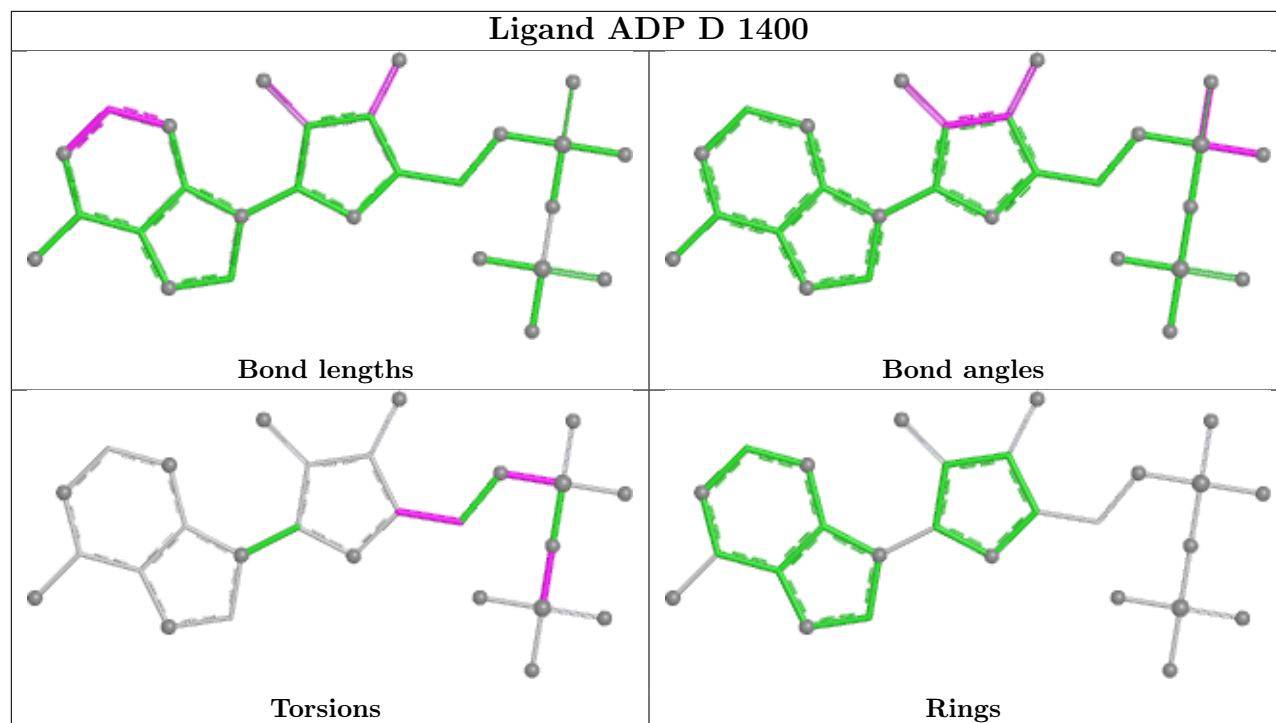
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1200	ADP	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.