



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:45 AM UTC

PDB ID : 1LRT / pdb_00001lrt
Title : CRYSTAL STRUCTURE OF TERNARY COMPLEX OF TRITRICHOMONAS FOETUS INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE: STRUCTURAL CHARACTERIZATION OF NAD⁺ SITE IN MICROBIAL ENZYME
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Deposited on : 2002-05-15
Resolution : 2.20 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

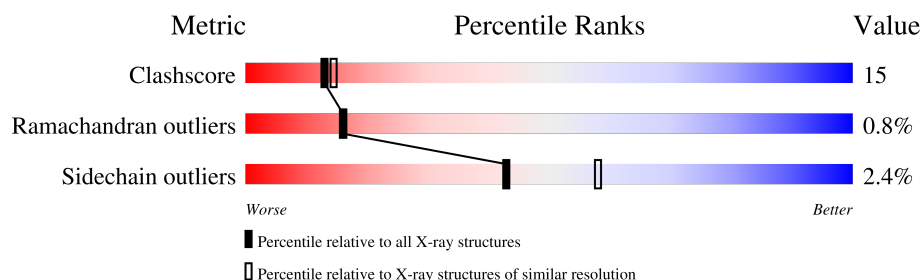
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	376	
1	B	376	
1	C	376	
1	D	376	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11238 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.

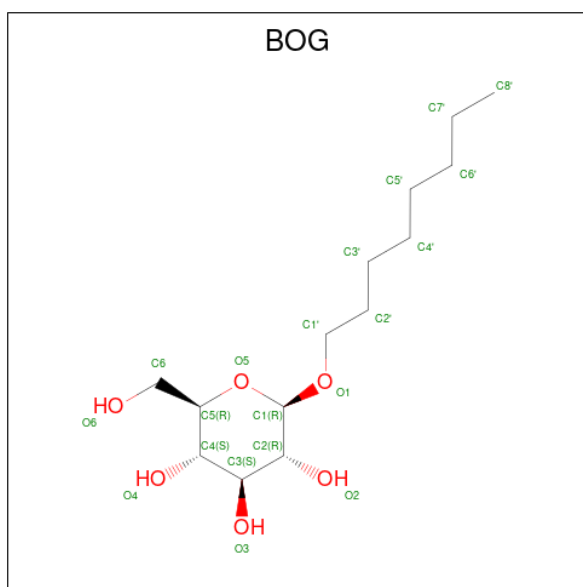
- Molecule 1 is a protein called INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2583	1638	437	493	15			
1	B	334	Total	C	N	O	S	0	0	0
			2554	1621	433	485	15			
1	C	334	Total	C	N	O	S	0	0	0
			2554	1621	433	485	15			
1	D	340	Total	C	N	O	S	0	0	0
			2600	1649	442	494	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	ASP	GLU	SEE REMARK 999	UNP P50097
B	279	ASP	GLU	SEE REMARK 999	UNP P50097
C	279	ASP	GLU	SEE REMARK 999	UNP P50097
D	279	ASP	GLU	SEE REMARK 999	UNP P50097

- Molecule 2 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).

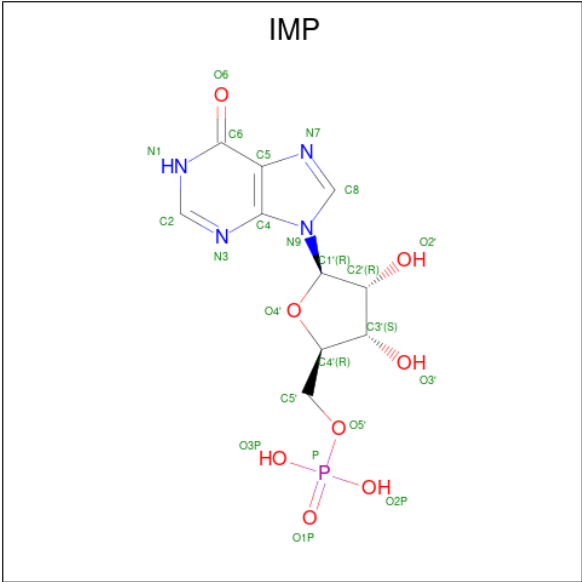


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C O	0	0
			20	14 6		
2	A	1	Total	C O	0	0
			20	14 6		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

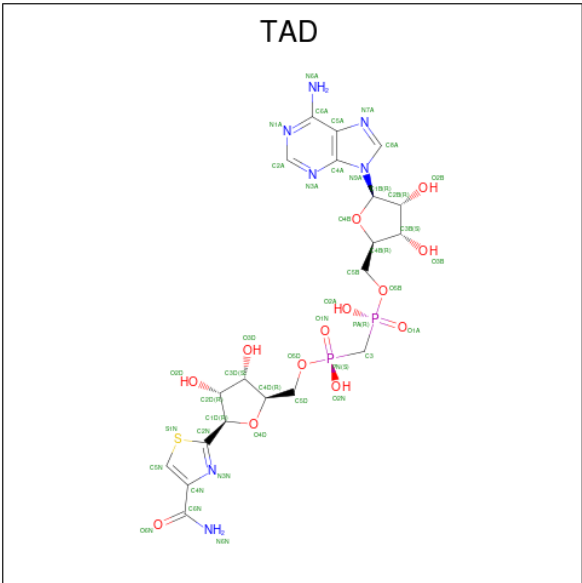
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		
3	B	1	Total	K	0	0
			1	1		
3	C	1	Total	K	0	0
			1	1		
3	D	1	Total	K	0	0
			1	1		

- Molecule 4 is INOSINIC ACID (CCD ID: IMP) (formula: C₁₀H₁₃N₄O₈P).



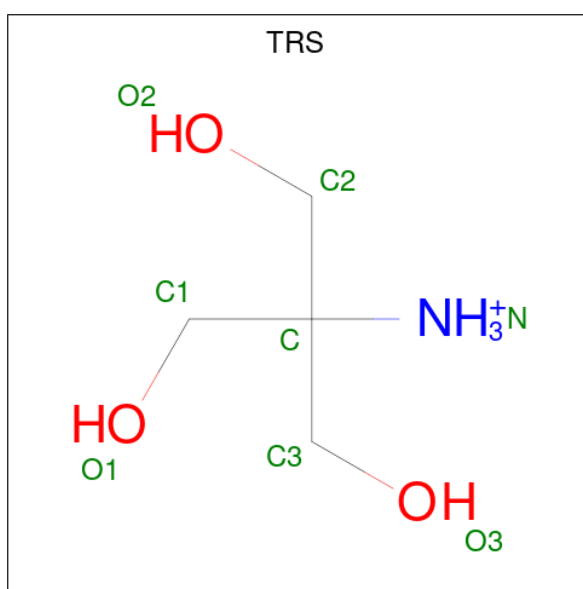
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
4	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
4	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 5 is BETA-METHYLENE-THIAZOLE-4-CARBOXYAMIDE-ADENINE DINUCLEOTIDE (CCD ID: TAD) (formula: C₂₀H₂₇N₇O₁₃P₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	
			43	20	7	13	2	1	
5	B	1	Total	C	N	O	P	S	
			43	20	7	13	2	1	
5	C	1	Total	C	N	O	P	S	
			43	20	7	13	2	1	
5	D	1	Total	C	N	O	P	S	
			43	20	7	13	2	1	

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O		
			8	4	1	3	0	0
6	A	1	Total	C	N	O		
			8	4	1	3	0	0
6	A	1	Total	C	N	O		
			8	4	1	3	0	0
6	A	1	Total	C	N	O		
			8	4	1	3	0	0
6	B	1	Total	C	N	O		
			8	4	1	3	0	0
6	B	1	Total	C	N	O		
			8	4	1	3	0	0
6	B	1	Total	C	N	O		
			8	4	1	3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			8	4	1	3		
6	C	1	Total	C	N	O	0	0
			8	4	1	3		
6	D	1	Total	C	N	O	0	0
			8	4	1	3		
6	D	1	Total	C	N	O	0	0
			8	4	1	3		
6	D	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 7 is water.

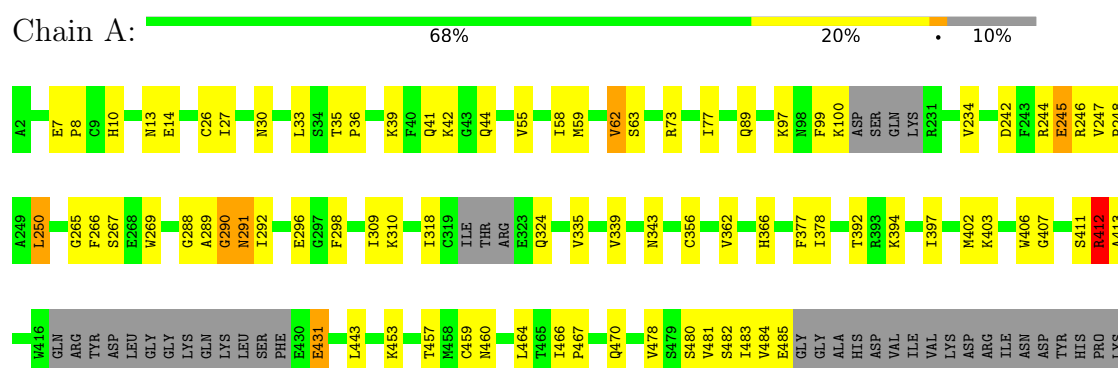
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	160	Total	O	0	0
			160	160		
7	B	128	Total	O	0	0
			128	128		
7	C	122	Total	O	0	0
			122	122		
7	D	133	Total	O	0	0
			133	133		

3 Residue-property plots

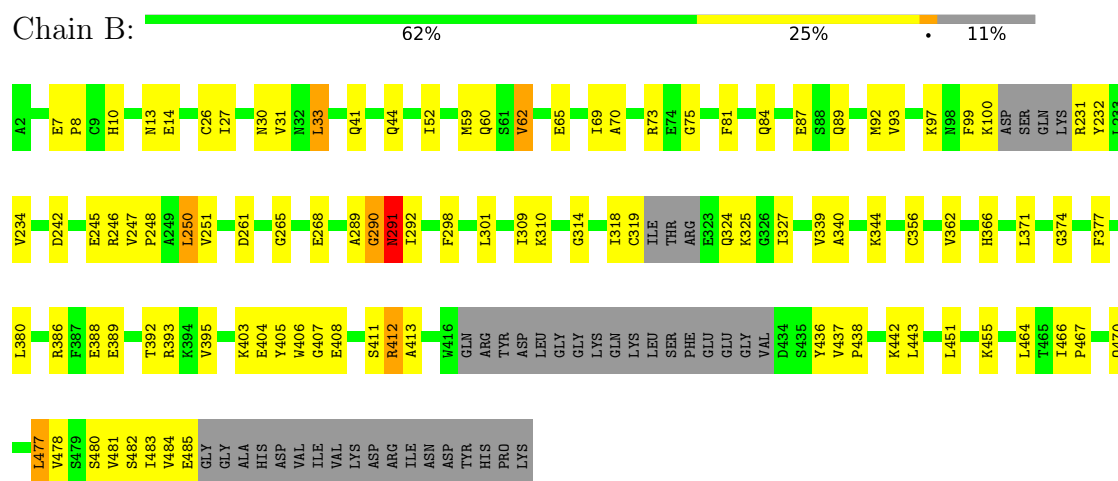
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

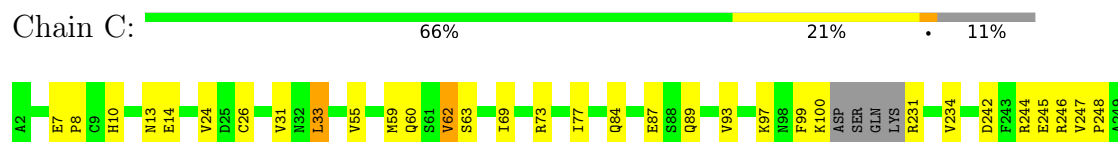
• Molecule 1: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE

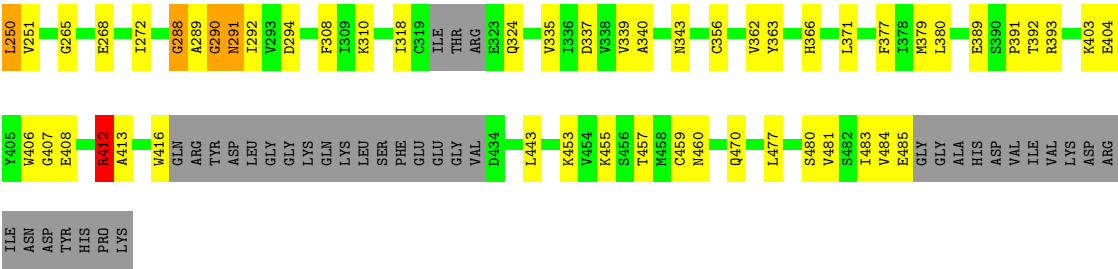


• Molecule 1: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE

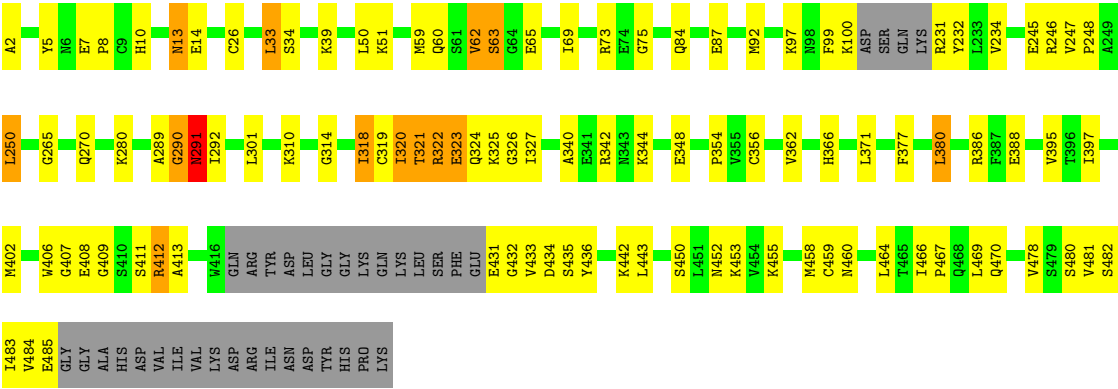


• Molecule 1: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE





● Molecule 1: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.14Å 112.37Å 162.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.86 – 2.20	Depositor
% Data completeness (in resolution range)	91.4 (29.86-2.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.212 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11238	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: TRS, IMP, K, BOG, TAD

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	0.40	0/2627	0.92	5/3541 (0.1%)
1	B	0.37	0/2598	0.89	3/3502 (0.1%)
1	C	0.38	0/2598	0.92	4/3502 (0.1%)
1	D	0.38	0/2645	0.92	9/3567 (0.3%)
All	All	0.38	0/10468	0.91	21/14112 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	290	GLY	N-CA-C	15.69	130.18	111.35
1	D	323	GLU	N-CA-C	-11.85	98.47	113.16
1	D	289	ALA	N-CA-C	7.40	119.99	108.96
1	B	289	ALA	N-CA-C	7.19	119.68	108.96
1	A	290	GLY	N-CA-C	7.19	130.22	113.18
1	D	290	GLY	N-CA-C	7.09	129.99	113.18
1	B	290	GLY	N-CA-C	6.46	128.50	113.18
1	A	289	ALA	N-CA-C	6.45	118.88	109.07
1	B	477	LEU	N-CA-C	-6.14	102.26	110.55
1	C	288	GLY	N-CA-C	-6.13	104.36	112.82
1	A	63	SER	N-CA-C	5.99	118.15	109.71
1	C	289	ALA	N-CA-C	5.78	117.04	108.60
1	D	460	ASN	N-CA-C	-5.70	105.15	111.71
1	D	63	SER	N-CA-C	5.65	118.47	108.24
1	D	280	LYS	N-CA-C	5.63	117.49	111.36
1	C	63	SER	N-CA-C	5.46	118.06	108.56
1	D	452	ASN	N-CA-C	-5.32	105.56	111.36
1	D	435	SER	N-CA-C	5.19	114.68	107.73
1	D	322	ARG	N-CA-C	5.17	118.96	111.56
1	A	378	ILE	N-CA-C	5.17	115.35	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	GLY	N-CA-C	-5.01	105.91	112.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2583	0	2572	69	0
1	B	2554	0	2548	83	0
1	C	2554	0	2548	73	0
1	D	2600	0	2598	106	0
2	A	40	0	56	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	23	0	11	0	0
4	B	23	0	11	0	0
4	C	23	0	11	0	0
4	D	23	0	11	2	0
5	A	43	0	24	0	0
5	B	43	0	24	1	0
5	C	43	0	24	0	0
5	D	43	0	24	3	0
6	A	32	0	48	5	0
6	B	24	0	36	2	0
6	C	16	0	24	3	0
6	D	24	0	36	6	0
7	A	160	0	0	3	0
7	B	128	0	0	0	0
7	C	122	0	0	2	0
7	D	133	0	0	1	0
All	All	11238	0	10606	320	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 15.

All (320) 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:322:ARG:HH22	5:D:904:TAD:H5N	1.25	1.02
1:D:322:ARG:HB3	1:D:326:GLY:H	1.35	0.89
1:D:322:ARG:HG2	1:D:327:ILE:H	1.36	0.89
1:C:7:GLU:HG3	1:C:8:PRO:HD2	1.60	0.83
1:C:343:ASN:ND2	6:C:605:TRS:H11	1.93	0.83
1:D:320:ILE:HD13	1:D:320:ILE:H	1.44	0.82
1:B:41:GLN:HB3	1:B:44:GLN:HE21	1.44	0.82
1:C:362:VAL:H	1:C:366:HIS:HD2	1.27	0.82
1:D:433:VAL:HG12	1:D:434:ASP:H	1.42	0.82
1:D:322:ARG:HB3	1:D:326:GLY:N	1.95	0.80
1:B:89:GLN:HG2	1:B:250:LEU:HD11	1.64	0.80
1:D:322:ARG:NH2	5:D:904:TAD:H5N	1.97	0.79
1:B:59:MET:HB2	1:B:62:VAL:HG13	1.66	0.78
1:A:411:SER:O	1:A:412:ARG:HB3	1.82	0.77
1:C:343:ASN:HD22	6:C:605:TRS:H11	1.50	0.77
1:D:59:MET:HE1	1:D:318:ILE:HD11	1.66	0.76
1:A:59:MET:HB2	1:A:62:VAL:HG13	1.68	0.76
1:D:290:GLY:O	1:D:291:ASN:HB2	1.88	0.72
1:A:412:ARG:HG3	1:A:413:ALA:N	2.02	0.71
1:B:242:ASP:OD1	1:B:246:ARG:HD2	1.91	0.71
1:A:291:ASN:HA	1:A:310:LYS:O	1.91	0.71
1:D:483:ILE:C	1:D:485:GLU:H	1.97	0.70
1:B:291:ASN:HA	1:B:310:LYS:O	1.92	0.70
1:A:265:GLY:HA3	1:A:290:GLY:HA2	1.73	0.70
1:B:59:MET:HE1	1:B:318:ILE:HD11	1.71	0.70
1:C:412:ARG:HG3	1:C:413:ALA:N	2.06	0.69
1:B:10:HIS:HD2	1:B:14:GLU:OE1	1.76	0.69
1:C:59:MET:HB2	1:C:62:VAL:HG13	1.74	0.68
1:C:10:HIS:HD2	1:C:14:GLU:OE1	1.77	0.68
1:D:291:ASN:HA	1:D:310:LYS:O	1.94	0.68
1:B:362:VAL:H	1:B:366:HIS:HD2	1.41	0.68
1:B:7:GLU:HG3	1:B:8:PRO:HD2	1.76	0.67
1:D:409:GLY:HA3	1:D:431:GLU:HB2	1.77	0.67
1:A:267:SER:HB3	6:A:600:TRS:H32	1.77	0.67
1:C:290:GLY:O	1:C:291:ASN:HB2	1.93	0.67
1:C:291:ASN:HA	1:C:310:LYS:O	1.94	0.67
1:C:483:ILE:C	1:C:485:GLU:H	2.01	0.67
1:B:483:ILE:C	1:B:485:GLU:H	2.01	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:PRO:HB3	6:A:610:TRS:H21	1.76	0.66
1:B:483:ILE:HD12	1:C:481:VAL:HG21	1.76	0.66
1:D:318:ILE:HD12	1:D:407:GLY:CA	2.25	0.66
1:D:318:ILE:HD12	1:D:407:GLY:HA2	1.77	0.66
1:D:5:TYR:HB3	6:D:609:TRS:H11	1.76	0.66
1:A:59:MET:HE1	1:A:318:ILE:HD11	1.77	0.66
1:B:265:GLY:HA3	1:B:290:GLY:HA2	1.77	0.66
1:C:324:GLN:O	1:D:453:LYS:HD3	1.96	0.66
1:A:290:GLY:O	1:A:291:ASN:HB2	1.96	0.65
1:C:483:ILE:HD12	1:D:481:VAL:HG21	1.76	0.65
1:A:481:VAL:HG21	1:D:483:ILE:HD12	1.79	0.65
1:D:362:VAL:H	1:D:366:HIS:HD2	1.44	0.65
1:B:290:GLY:O	1:B:291:ASN:HB2	1.96	0.64
1:B:388:GLU:HG2	1:B:442:LYS:HZ1	1.62	0.64
1:A:483:ILE:C	1:A:485:GLU:H	2.04	0.64
1:D:265:GLY:HA3	1:D:290:GLY:HA2	1.80	0.64
1:C:59:MET:HE1	1:C:318:ILE:HD11	1.78	0.64
1:D:411:SER:O	1:D:412:ARG:HB3	1.97	0.64
1:D:412:ARG:HG3	1:D:413:ALA:N	2.12	0.64
1:A:362:VAL:H	1:A:366:HIS:HD2	1.44	0.64
1:B:231:ARG:HG2	1:B:231:ARG:HH11	1.63	0.64
1:B:388:GLU:HG2	1:B:442:LYS:NZ	2.13	0.64
1:D:406:TRP:CD1	1:D:412:ARG:HD2	2.32	0.63
1:C:99:PHE:O	1:C:100:LYS:HB2	1.98	0.63
1:A:397:ILE:HD12	1:A:402:MET:HG3	1.81	0.62
1:B:412:ARG:HG3	1:B:413:ALA:N	2.12	0.62
1:A:55:VAL:HG12	1:A:77:ILE:HG22	1.82	0.62
1:A:457:THR:HG23	1:D:327:ILE:HD11	1.80	0.61
1:B:324:GLN:O	1:C:453:LYS:HD3	2.00	0.61
1:A:10:HIS:HD2	1:A:14:GLU:OE1	1.83	0.61
1:D:322:ARG:HG2	1:D:327:ILE:N	2.11	0.61
1:B:393:ARG:HG2	1:B:404:GLU:OE1	2.01	0.60
1:D:433:VAL:HG12	1:D:434:ASP:N	2.13	0.60
1:D:7:GLU:HG3	1:D:8:PRO:HD2	1.83	0.60
1:C:231:ARG:HG2	1:C:231:ARG:HH11	1.66	0.60
1:D:322:ARG:HH22	5:D:904:TAD:C5N	2.06	0.60
1:A:242:ASP:OD1	1:A:246:ARG:HD2	2.01	0.60
1:C:89:GLN:HG2	1:C:250:LEU:HD11	1.84	0.60
1:C:265:GLY:HA3	1:C:290:GLY:HA2	1.83	0.60
6:A:607:TRS:HO1	1:D:2:ALA:N	1.99	0.60
1:D:322:ARG:CG	1:D:327:ILE:H	2.09	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:ARG:HH21	1:D:99:PHE:HE2	1.49	0.59
1:A:99:PHE:O	1:A:100:LYS:HB2	2.00	0.59
1:A:266:PHE:CE2	1:A:296:GLU:HG2	2.37	0.59
1:B:393:ARG:HG2	1:B:404:GLU:CD	2.27	0.59
1:A:478:VAL:HG12	1:A:482:SER:HB2	1.85	0.59
1:C:483:ILE:C	1:C:485:GLU:N	2.59	0.58
1:C:13:ASN:ND2	1:C:366:HIS:CE1	2.71	0.58
1:C:480:SER:O	1:C:484:VAL:HG23	2.03	0.58
1:D:478:VAL:HG12	1:D:482:SER:HB2	1.84	0.58
1:A:394:LYS:HG2	1:A:403:LYS:HG2	1.86	0.57
1:B:97:LYS:HD3	1:B:234:VAL:HG12	1.85	0.57
1:A:324:GLN:HE22	1:A:431:GLU:C	2.11	0.57
1:B:65:GLU:HG3	1:B:92:MET:HG2	1.86	0.57
1:B:247:VAL:O	1:B:251:VAL:HG23	2.04	0.57
1:D:484:VAL:C	1:D:485:GLU:HG2	2.29	0.57
1:B:59:MET:HB2	1:B:62:VAL:CG1	2.32	0.57
1:A:483:ILE:HD12	1:B:481:VAL:HG21	1.86	0.57
1:B:483:ILE:C	1:B:485:GLU:N	2.63	0.56
1:D:7:GLU:CG	1:D:8:PRO:HD2	2.34	0.56
1:D:322:ARG:HB3	1:D:326:GLY:CA	2.36	0.56
1:D:265:GLY:HA3	1:D:290:GLY:CA	2.36	0.56
1:C:99:PHE:O	1:C:100:LYS:CB	2.53	0.56
1:A:483:ILE:C	1:A:485:GLU:N	2.63	0.56
1:D:483:ILE:C	1:D:485:GLU:N	2.60	0.56
1:A:480:SER:O	1:A:484:VAL:HG23	2.06	0.55
1:D:320:ILE:HD13	1:D:320:ILE:N	2.18	0.55
1:D:466:ILE:O	1:D:470:GLN:HG3	2.05	0.55
1:D:59:MET:HE1	1:D:318:ILE:CD1	2.35	0.55
1:B:340:ALA:O	1:B:344:LYS:HG3	2.06	0.55
1:C:380:LEU:N	1:C:380:LEU:HD12	2.20	0.55
1:D:322:ARG:HD2	1:D:322:ARG:N	2.22	0.55
1:B:318:ILE:HD12	1:B:407:GLY:CA	2.35	0.55
1:D:406:TRP:NE1	1:D:412:ARG:HD2	2.22	0.55
1:C:318:ILE:HD12	1:C:407:GLY:CA	2.36	0.55
1:C:484:VAL:C	1:C:485:GLU:HG2	2.32	0.55
1:A:406:TRP:NE1	1:A:412:ARG:HD2	2.23	0.54
1:D:99:PHE:O	1:D:100:LYS:HG3	2.08	0.54
1:D:340:ALA:O	1:D:344:LYS:HG3	2.07	0.54
1:A:59:MET:HB2	1:A:62:VAL:CG1	2.37	0.54
1:D:26:CYS:SG	1:D:464:LEU:HD22	2.47	0.54
1:C:242:ASP:OD1	1:C:246:ARG:HD2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:LYS:HB2	1:D:75:GLY:HA3	1.90	0.54
1:D:380:LEU:HD12	1:D:380:LEU:N	2.23	0.54
1:A:324:GLN:HE22	1:A:431:GLU:HA	1.72	0.54
1:B:99:PHE:O	1:B:100:LYS:HB2	2.07	0.54
1:B:99:PHE:O	1:B:100:LYS:CB	2.56	0.53
1:A:97:LYS:HD3	1:A:234:VAL:HG12	1.89	0.53
1:B:84:GLN:OE1	1:B:92:MET:HE3	2.09	0.53
1:A:99:PHE:O	1:A:100:LYS:CB	2.56	0.53
1:C:73:ARG:HH21	1:C:99:PHE:HE2	1.56	0.53
1:D:356:CYS:HB2	1:D:377:PHE:CE2	2.44	0.53
1:B:484:VAL:HG12	1:B:484:VAL:O	2.08	0.53
1:C:392:THR:OG1	1:C:403:LYS:HE2	2.08	0.53
1:A:59:MET:HE1	1:A:318:ILE:CD1	2.38	0.53
1:A:318:ILE:HD12	1:A:407:GLY:CA	2.39	0.53
1:C:356:CYS:HB2	1:C:377:PHE:CE2	2.44	0.53
1:D:231:ARG:HG2	1:D:231:ARG:HH11	1.73	0.53
1:B:411:SER:O	1:B:412:ARG:HB3	2.08	0.53
1:D:10:HIS:HD2	1:D:14:GLU:OE1	1.91	0.52
1:A:73:ARG:NH2	1:A:99:PHE:HE2	2.07	0.52
1:D:484:VAL:HG12	1:D:484:VAL:O	2.09	0.52
1:D:97:LYS:HD3	1:D:234:VAL:HG12	1.90	0.52
1:A:7:GLU:HG3	1:A:8:PRO:HD2	1.92	0.52
1:B:395:VAL:HG21	1:B:436:TYR:CE2	2.44	0.52
1:D:247:VAL:HB	1:D:248:PRO:HD3	1.92	0.52
1:D:322:ARG:C	1:D:324:GLN:H	2.13	0.52
1:C:484:VAL:HG12	1:C:484:VAL:O	2.09	0.52
1:A:484:VAL:HG12	1:A:484:VAL:O	2.11	0.51
1:A:356:CYS:HB2	1:A:377:PHE:CE2	2.46	0.51
1:B:231:ARG:HG2	1:B:231:ARG:NH1	2.26	0.51
1:A:26:CYS:SG	1:A:464:LEU:HD22	2.50	0.51
1:B:13:ASN:ND2	1:B:366:HIS:CE1	2.79	0.51
1:C:7:GLU:HG3	1:C:8:PRO:CD	2.37	0.50
1:A:484:VAL:C	1:A:485:GLU:HG2	2.37	0.50
1:B:380:LEU:N	1:B:380:LEU:HD12	2.26	0.50
1:D:320:ILE:O	1:D:322:ARG:N	2.44	0.50
1:C:60:GLN:HG3	1:C:408:GLU:OE2	2.11	0.50
1:A:89:GLN:HG2	1:A:250:LEU:HD11	1.93	0.50
1:D:99:PHE:O	1:D:100:LYS:CB	2.59	0.50
1:C:406:TRP:NE1	1:C:412:ARG:HD2	2.27	0.50
1:A:44:GLN:NE2	7:A:984:HOH:O	2.43	0.50
1:A:58:ILE:HD12	7:A:973:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ARG:HG2	1:C:231:ARG:NH1	2.28	0.49
1:B:395:VAL:HG21	1:B:436:TYR:HE2	1.76	0.49
1:C:97:LYS:HD3	1:C:234:VAL:HG12	1.93	0.49
1:A:324:GLN:HE22	1:A:431:GLU:CA	2.26	0.49
1:A:453:LYS:HD3	1:D:324:GLN:O	2.11	0.49
1:B:389:GLU:N	1:B:389:GLU:OE1	2.45	0.49
1:C:443:LEU:C	1:C:443:LEU:HD23	2.37	0.49
1:A:324:GLN:NE2	1:A:431:GLU:HA	2.28	0.49
1:C:292:ILE:C	1:C:292:ILE:HD12	2.37	0.49
1:B:478:VAL:HG12	1:B:482:SER:HB2	1.94	0.49
1:A:73:ARG:HH21	1:A:99:PHE:HE2	1.58	0.49
1:D:62:VAL:CG2	1:D:63:SER:N	2.76	0.49
1:A:26:CYS:C	1:A:459:CYS:SG	2.95	0.48
1:B:26:CYS:SG	1:B:464:LEU:HD22	2.53	0.48
1:C:55:VAL:HG12	1:C:77:ILE:HG22	1.95	0.48
1:D:290:GLY:HA3	1:D:301:LEU:HD11	1.95	0.48
1:C:413:ALA:O	1:C:416:TRP:HD1	1.95	0.48
1:A:247:VAL:HB	1:A:248:PRO:HD3	1.95	0.48
1:D:484:VAL:O	1:D:485:GLU:HG2	2.14	0.48
1:B:480:SER:O	1:B:484:VAL:HG23	2.14	0.48
1:C:340:ALA:HA	6:C:605:TRS:O1	2.13	0.48
1:D:478:VAL:CG1	1:D:482:SER:HB2	2.43	0.48
1:D:84:GLN:O	1:D:246:ARG:NH2	2.41	0.48
1:D:292:ILE:HD12	1:D:292:ILE:C	2.39	0.48
1:D:13:ASN:ND2	1:D:366:HIS:CE1	2.82	0.48
1:D:270:GLN:OE1	1:D:290:GLY:N	2.47	0.48
1:D:443:LEU:C	1:D:443:LEU:HD23	2.39	0.48
1:B:392:THR:OG1	1:B:403:LYS:HE2	2.14	0.48
1:B:443:LEU:HD23	1:B:443:LEU:C	2.38	0.48
1:D:322:ARG:C	1:D:324:GLN:N	2.68	0.47
1:A:266:PHE:CZ	1:A:296:GLU:HG2	2.49	0.47
1:D:60:GLN:HG3	1:D:408:GLU:OE2	2.14	0.47
1:B:406:TRP:CD1	1:B:412:ARG:HD2	2.49	0.47
1:A:41:GLN:HG2	1:A:42:LYS:N	2.29	0.47
1:D:33:LEU:HD22	1:D:455:LYS:HE3	1.97	0.47
1:B:31:VAL:HG12	1:B:33:LEU:HD13	1.97	0.46
1:D:362:VAL:H	1:D:366:HIS:CD2	2.29	0.46
1:B:87:GLU:H	1:B:87:GLU:CD	2.21	0.46
1:B:261:ASP:OD2	5:B:902:TAD:O3D	2.33	0.46
1:B:339:VAL:HG21	1:B:374:GLY:HA3	1.97	0.46
1:C:393:ARG:HG2	1:C:404:GLU:CD	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:THR:OG1	1:A:36:PRO:HD2	2.16	0.46
1:A:457:THR:HG23	1:D:327:ILE:CD1	2.45	0.46
1:D:65:GLU:HG3	1:D:92:MET:HG2	1.96	0.46
1:A:245:GLU:OE2	2:A:752:BOG:O4	2.31	0.46
1:C:69:ILE:O	1:C:73:ARG:HG3	2.16	0.46
1:D:458:MET:HG2	1:D:469:LEU:HD22	1.97	0.46
1:B:318:ILE:HD13	1:B:405:TYR:CE2	2.51	0.46
1:C:335:VAL:O	1:C:339:VAL:HG23	2.16	0.46
1:A:318:ILE:HD12	1:A:407:GLY:HA2	1.98	0.45
1:D:99:PHE:O	1:D:100:LYS:HB2	2.16	0.45
1:B:60:GLN:HG3	1:B:408:GLU:OE2	2.17	0.45
1:B:247:VAL:HB	1:B:248:PRO:HD3	1.99	0.45
1:D:26:CYS:C	1:D:459:CYS:SG	3.00	0.45
1:D:324:GLN:HE22	1:D:431:GLU:N	2.15	0.45
1:A:13:ASN:ND2	1:A:366:HIS:CE1	2.85	0.45
1:A:466:ILE:O	1:A:470:GLN:HG3	2.16	0.45
1:C:10:HIS:CD2	1:C:14:GLU:OE1	2.65	0.45
1:D:39:LYS:HA	1:D:354:PRO:HD3	1.98	0.45
1:B:14:GLU:HA	1:B:483:ILE:HD11	1.99	0.45
1:B:298:PHE:CE1	1:B:309:ILE:HD12	2.51	0.45
1:C:31:VAL:HG12	1:C:33:LEU:HD13	1.98	0.45
1:D:466:ILE:HB	1:D:467:PRO:HD3	1.99	0.45
1:D:319:CYS:SG	1:D:322:ARG:NH1	2.90	0.45
1:B:70:ALA:HB2	1:B:389:GLU:HG2	1.98	0.45
1:B:466:ILE:HB	1:B:467:PRO:HD3	1.99	0.45
1:A:292:ILE:HD12	1:A:292:ILE:C	2.42	0.45
1:A:443:LEU:C	1:A:443:LEU:HD23	2.42	0.45
1:D:33:LEU:HD22	1:D:455:LYS:CE	2.46	0.45
1:D:321:THR:O	1:D:321:THR:HG22	2.17	0.45
1:B:268:GLU:OE2	1:C:24:VAL:HG13	2.18	0.44
1:B:314:GLY:HA2	1:B:319:CYS:SG	2.57	0.44
1:B:327:ILE:HD11	1:C:457:THR:HG23	1.98	0.44
1:C:245:GLU:C	1:C:248:PRO:HD2	2.41	0.44
1:B:60:GLN:HA	1:B:81:PHE:CD2	2.53	0.44
1:B:93:VAL:O	1:B:97:LYS:HG2	2.16	0.44
1:B:290:GLY:HA3	1:B:301:LEU:CD1	2.48	0.44
1:B:339:VAL:HG12	6:B:608:TRS:O2	2.17	0.44
1:C:247:VAL:HB	1:C:248:PRO:HD3	1.98	0.44
1:C:389:GLU:OE1	1:C:389:GLU:N	2.50	0.44
1:D:5:TYR:HB3	6:D:609:TRS:H21	2.00	0.44
1:D:395:VAL:HG21	1:D:436:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:432:GLY:HA3	4:D:804:IMP:O6	2.16	0.44
1:C:268:GLU:O	1:C:272:ILE:HG13	2.18	0.44
1:A:343:ASN:ND2	6:A:607:TRS:H21	2.31	0.44
1:C:26:CYS:C	1:C:459:CYS:SG	3.01	0.44
1:C:371:LEU:O	1:C:470:GLN:HG2	2.18	0.44
1:C:484:VAL:O	1:C:485:GLU:HG2	2.18	0.44
1:D:397:ILE:HD12	1:D:402:MET:HG3	2.00	0.44
1:B:69:ILE:O	1:B:73:ARG:HG3	2.18	0.44
1:D:84:GLN:OE1	1:D:92:MET:HE3	2.18	0.43
1:B:386:ARG:HB3	1:B:438:PRO:O	2.17	0.43
1:C:244:ARG:HB2	7:C:916:HOH:O	2.17	0.43
1:B:84:GLN:O	1:B:246:ARG:NH2	2.41	0.43
1:C:33:LEU:HD22	1:C:455:LYS:HE3	2.00	0.43
1:D:69:ILE:HG23	1:D:232:TYR:CE1	2.54	0.43
1:C:87:GLU:H	1:C:87:GLU:CD	2.26	0.43
1:C:318:ILE:HD12	1:C:407:GLY:HA2	2.00	0.43
1:D:59:MET:CE	1:D:318:ILE:HD11	2.44	0.43
1:B:27:ILE:HG12	1:B:30:ASN:ND2	2.34	0.43
1:C:288:GLY:HA3	1:C:308:PHE:CZ	2.53	0.43
1:D:34:SER:HA	1:D:50:LEU:O	2.19	0.43
1:C:247:VAL:O	1:C:251:VAL:HG23	2.19	0.42
1:D:371:LEU:O	1:D:470:GLN:HG2	2.19	0.42
1:C:363:TYR:O	1:C:366:HIS:HB2	2.19	0.42
1:C:483:ILE:O	1:C:485:GLU:N	2.52	0.42
1:C:33:LEU:HD22	1:C:455:LYS:CE	2.49	0.42
1:D:319:CYS:HB2	4:D:804:IMP:H2	2.00	0.42
1:D:480:SER:O	1:D:484:VAL:HG23	2.19	0.42
1:A:7:GLU:CG	1:A:8:PRO:HD2	2.50	0.42
1:A:39:LYS:NZ	6:A:601:TRS:H12	2.34	0.42
1:B:356:CYS:HB2	1:B:377:PHE:CE2	2.55	0.42
1:D:322:ARG:CB	1:D:326:GLY:H	2.20	0.42
1:D:5:TYR:HB3	6:D:609:TRS:C1	2.45	0.42
1:A:244:ARG:HB2	7:A:953:HOH:O	2.19	0.42
1:C:84:GLN:O	1:C:246:ARG:NH2	2.39	0.42
1:A:460:ASN:OD1	1:D:325:LYS:NZ	2.43	0.42
1:B:318:ILE:HD12	1:B:407:GLY:HA2	2.00	0.42
1:B:386:ARG:HG2	1:B:437:VAL:HB	2.01	0.42
1:C:379:MET:C	1:C:380:LEU:HD12	2.45	0.42
1:B:242:ASP:O	1:B:246:ARG:HB2	2.20	0.42
1:D:250:LEU:HD12	1:D:250:LEU:HA	1.90	0.42
1:B:451:LEU:O	1:B:455:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:PRO:HD3	7:C:972:HOH:O	2.19	0.41
1:A:392:THR:OG1	1:A:403:LYS:HE2	2.20	0.41
1:A:466:ILE:HB	1:A:467:PRO:HD3	2.03	0.41
2:A:751:BOG:H3'2	2:A:752:BOG:H1	2.02	0.41
1:B:292:ILE:C	1:B:292:ILE:HD12	2.45	0.41
1:B:478:VAL:CG1	1:B:482:SER:HB2	2.50	0.41
1:D:450:SER:OG	6:D:604:TRS:H32	2.20	0.41
1:D:342:ARG:HD2	1:D:342:ARG:C	2.46	0.41
1:A:335:VAL:O	1:A:339:VAL:HG23	2.20	0.41
1:B:265:GLY:HA3	1:B:290:GLY:CA	2.48	0.41
1:B:406:TRP:NE1	1:B:412:ARG:HD2	2.35	0.41
1:C:93:VAL:O	1:C:97:LYS:HG2	2.19	0.41
1:D:386:ARG:NH2	6:D:604:TRS:O2	2.49	0.41
1:B:325:LYS:NZ	1:C:460:ASN:OD1	2.45	0.41
1:B:386:ARG:HH22	6:B:603:TRS:C1	2.34	0.41
1:C:87:GLU:CD	1:C:87:GLU:N	2.78	0.41
1:C:13:ASN:HD22	1:C:366:HIS:HE1	1.68	0.41
1:D:314:GLY:HA2	1:D:322:ARG:HH11	1.86	0.41
1:A:27:ILE:HG12	1:A:30:ASN:ND2	2.35	0.41
1:A:269:TRP:CE3	1:A:269:TRP:HA	2.56	0.41
1:B:371:LEU:O	1:B:470:GLN:HG2	2.21	0.41
1:D:320:ILE:O	1:D:321:THR:C	2.63	0.41
1:D:322:ARG:HG2	1:D:327:ILE:O	2.20	0.41
6:D:606:TRS:H21	7:D:930:HOH:O	2.20	0.41
1:A:318:ILE:H	1:A:318:ILE:HG12	1.69	0.41
1:C:294:ASP:HA	1:C:337:ASP:OD2	2.21	0.40
1:D:291:ASN:OD1	1:D:310:LYS:HB3	2.20	0.40
1:D:344:LYS:O	1:D:348:GLU:HG3	2.21	0.40
1:A:298:PHE:CE1	1:A:309:ILE:HD12	2.56	0.40
1:B:52:ILE:HG12	1:B:75:GLY:C	2.46	0.40
1:D:87:GLU:H	1:D:87:GLU:CD	2.27	0.40
1:B:69:ILE:HG23	1:B:232:TYR:CE1	2.57	0.40
1:B:99:PHE:O	1:B:100:LYS:HG3	2.21	0.40
1:C:292:ILE:HD12	1:C:292:ILE:O	2.22	0.40
1:D:388:GLU:HG2	1:D:442:LYS:NZ	2.36	0.40
1:B:65:GLU:CG	1:B:92:MET:HG2	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	330/376 (88%)	316 (96%)	12 (4%)	2 (1%)	21	23
1	B	326/376 (87%)	308 (94%)	16 (5%)	2 (1%)	21	23
1	C	326/376 (87%)	306 (94%)	18 (6%)	2 (1%)	21	23
1	D	334/376 (89%)	313 (94%)	17 (5%)	4 (1%)	10	8
All	All	1316/1504 (88%)	1243 (94%)	63 (5%)	10 (1%)	16	16

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	ASN
1	B	291	ASN
1	B	412	ARG
1	C	291	ASN
1	D	291	ASN
1	D	321	THR
1	A	412	ARG
1	C	412	ARG
1	D	412	ARG
1	D	318	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/308 (89%)	269 (98%)	6 (2%)	45	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	272/308 (88%)	266 (98%)	6 (2%)	45 61
1	C	272/308 (88%)	267 (98%)	5 (2%)	51 68
1	D	277/308 (90%)	268 (97%)	9 (3%)	34 47
All	All	1096/1232 (89%)	1070 (98%)	26 (2%)	43 58

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	62	VAL
1	A	245	GLU
1	A	250	LEU
1	A	412	ARG
1	A	431	GLU
1	B	33	LEU
1	B	62	VAL
1	B	245	GLU
1	B	250	LEU
1	B	291	ASN
1	B	477	LEU
1	C	33	LEU
1	C	62	VAL
1	C	250	LEU
1	C	412	ARG
1	C	477	LEU
1	D	13	ASN
1	D	33	LEU
1	D	62	VAL
1	D	245	GLU
1	D	250	LEU
1	D	291	ASN
1	D	320	ILE
1	D	323	GLU
1	D	380	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	13	ASN

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Mol	Chain	Res	Type
1	A	30	ASN
1	A	44	GLN
1	A	49	ASN
1	A	98	ASN
1	A	324	GLN
1	A	331	GLN
1	A	366	HIS
1	B	10	HIS
1	B	13	ASN
1	B	30	ASN
1	B	44	GLN
1	B	331	GLN
1	B	343	ASN
1	B	366	HIS
1	B	446	ASN
1	C	10	HIS
1	C	13	ASN
1	C	44	GLN
1	C	49	ASN
1	C	98	ASN
1	C	331	GLN
1	C	366	HIS
1	D	10	HIS
1	D	13	ASN
1	D	324	GLN
1	D	331	GLN
1	D	366	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 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
6	TRS	A	601	-	7,7,7	0.98	0	9,9,9	1.94	1 (11%)
6	TRS	A	607	-	7,7,7	1.04	1 (14%)	9,9,9	1.68	2 (22%)
4	IMP	C	803	-	25,25,25	1.93	7 (28%)	37,38,38	1.78	7 (18%)
6	TRS	C	605	-	7,7,7	0.98	0	9,9,9	1.74	2 (22%)
2	BOG	A	752	-	20,20,20	1.39	2 (10%)	25,25,25	0.63	0
5	TAD	B	902	-	42,47,47	1.44	7 (16%)	62,72,72	2.36	23 (37%)
5	TAD	C	903	-	42,47,47	1.44	6 (14%)	62,72,72	2.34	21 (33%)
6	TRS	C	602	-	7,7,7	0.97	0	9,9,9	1.81	2 (22%)
6	TRS	A	610	-	7,7,7	0.86	0	9,9,9	1.93	2 (22%)
4	IMP	D	804	-	25,25,25	1.83	5 (20%)	37,38,38	1.80	7 (18%)
6	TRS	B	603	-	7,7,7	0.98	0	9,9,9	1.86	2 (22%)
5	TAD	D	904	-	42,47,47	1.44	7 (16%)	62,72,72	2.88	24 (38%)
6	TRS	D	604	-	7,7,7	0.94	0	9,9,9	1.88	2 (22%)
6	TRS	B	608	-	7,7,7	0.90	0	9,9,9	1.93	1 (11%)
4	IMP	B	802	-	25,25,25	1.94	7 (28%)	37,38,38	1.80	7 (18%)
6	TRS	A	600	3	7,7,7	1.00	0	9,9,9	1.91	2 (22%)
6	TRS	D	606	-	7,7,7	0.87	0	9,9,9	1.94	2 (22%)
6	TRS	D	609	-	7,7,7	0.92	0	9,9,9	1.99	2 (22%)
4	IMP	A	801	-	25,25,25	1.88	6 (24%)	37,38,38	1.84	7 (18%)
2	BOG	A	751	-	20,20,20	1.34	1 (5%)	25,25,25	0.61	0
5	TAD	A	901	-	42,47,47	1.46	6 (14%)	62,72,72	2.32	21 (33%)
6	TRS	B	611	-	7,7,7	0.92	0	9,9,9	1.84	2 (22%)

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
6	TRS	A	601	-	-	3/9/9/9	-
6	TRS	A	607	-	-	4/9/9/9	-
4	IMP	C	803	-	-	4/10/26/26	0/3/3/3
6	TRS	C	605	-	-	3/9/9/9	-
2	BOG	A	752	-	-	2/11/31/31	0/1/1/1
5	TAD	B	902	-	-	4/30/62/62	0/5/5/5
5	TAD	C	903	-	-	1/30/62/62	0/5/5/5
6	TRS	C	602	-	-	1/9/9/9	-
6	TRS	A	610	-	-	4/9/9/9	-
4	IMP	D	804	-	-	5/10/26/26	0/3/3/3
6	TRS	B	603	-	-	4/9/9/9	-
5	TAD	D	904	-	-	3/30/62/62	0/5/5/5
6	TRS	D	604	-	-	2/9/9/9	-
6	TRS	B	608	-	-	4/9/9/9	-
4	IMP	B	802	-	-	4/10/26/26	0/3/3/3
6	TRS	A	600	3	-	6/9/9/9	-
6	TRS	D	606	-	-	3/9/9/9	-
6	TRS	D	609	-	-	5/9/9/9	-
4	IMP	A	801	-	-	1/10/26/26	0/3/3/3
2	BOG	A	751	-	-	1/11/31/31	0/1/1/1
5	TAD	A	901	-	-	1/30/62/62	0/5/5/5
6	TRS	B	611	-	-	3/9/9/9	-

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	803	IMP	C2-N1	5.18	1.44	1.35
4	B	802	IMP	C2-N1	5.07	1.44	1.35
2	A	752	BOG	C3-C2	-4.87	1.39	1.52
2	A	751	BOG	C3-C2	-4.73	1.40	1.52
4	A	801	IMP	C2-N1	4.69	1.43	1.35
4	D	804	IMP	C2-N1	4.68	1.43	1.35
4	A	801	IMP	C8-N7	4.01	1.43	1.32
5	D	904	TAD	C5A-N7A	-3.99	1.31	1.39
5	A	901	TAD	C5A-N7A	-3.95	1.31	1.39
4	B	802	IMP	C8-N7	3.92	1.43	1.32
5	B	902	TAD	C5A-N7A	-3.87	1.32	1.39
4	C	803	IMP	C8-N7	3.87	1.43	1.32
4	D	804	IMP	C8-N7	3.83	1.43	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	802	IMP	P-O5'	-3.80	1.48	1.60
5	C	903	TAD	C5A-N7A	-3.76	1.32	1.39
5	C	903	TAD	C4A-N9A	-3.69	1.30	1.37
4	D	804	IMP	P-O5'	-3.60	1.48	1.60
5	A	901	TAD	C4A-N9A	-3.56	1.30	1.37
4	A	801	IMP	P-O5'	-3.53	1.49	1.60
4	C	803	IMP	P-O5'	-3.49	1.49	1.60
5	A	901	TAD	C2D-C1D	-3.36	1.49	1.53
5	D	904	TAD	C2D-C1D	-3.26	1.49	1.53
5	B	902	TAD	C2D-C1D	-3.26	1.49	1.53
5	C	903	TAD	C2D-C1D	-3.22	1.49	1.53
5	D	904	TAD	C4A-N9A	-3.09	1.31	1.37
5	B	902	TAD	C4A-N9A	-3.07	1.31	1.37
4	C	803	IMP	C5'-C4'	-3.00	1.42	1.51
4	A	801	IMP	C5'-C4'	-2.83	1.43	1.51
5	A	901	TAD	PN-O2N	-2.80	1.49	1.56
5	B	902	TAD	C2A-N1A	2.64	1.38	1.33
4	D	804	IMP	C5'-C4'	-2.61	1.43	1.51
4	B	802	IMP	C5'-C4'	-2.59	1.43	1.51
5	D	904	TAD	PN-O2N	-2.54	1.50	1.56
5	D	904	TAD	C2A-N1A	2.52	1.38	1.33
5	B	902	TAD	PN-O2N	-2.46	1.50	1.56
5	B	902	TAD	C4A-N3A	2.35	1.38	1.34
5	C	903	TAD	PN-O2N	-2.32	1.50	1.56
5	C	903	TAD	C2A-N1A	2.30	1.38	1.33
4	C	803	IMP	C2-N3	2.30	1.34	1.30
5	A	901	TAD	C2A-N1A	2.26	1.38	1.33
2	A	752	BOG	O1-C1	2.18	1.43	1.40
5	B	902	TAD	C4N-N3N	-2.17	1.34	1.38
4	B	802	IMP	O2'-C2'	-2.16	1.37	1.43
4	B	802	IMP	C2-N3	2.11	1.34	1.30
4	A	801	IMP	C2-N3	2.10	1.34	1.30
4	C	803	IMP	C8-N9	2.09	1.42	1.37
5	D	904	TAD	C4N-N3N	-2.07	1.34	1.38
4	A	801	IMP	O2'-C2'	-2.05	1.37	1.43
5	A	901	TAD	PA-O2A	-2.05	1.51	1.56
5	D	904	TAD	C4A-N3A	2.05	1.38	1.34
5	C	903	TAD	C4N-N3N	-2.04	1.34	1.38
4	B	802	IMP	C6-N1	2.04	1.43	1.39
6	A	607	TRS	C3-C	2.03	1.58	1.53
4	C	803	IMP	C6-N1	2.01	1.43	1.39
4	D	804	IMP	C2-N3	2.01	1.34	1.30

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	904	TAD	O6N-C6N-C4N	9.71	129.57	120.25
5	D	904	TAD	C4N-C6N-N6N	-8.64	107.49	116.28
5	D	904	TAD	N3A-C4A-N9A	6.11	137.56	127.17
5	B	902	TAD	N3A-C4A-N9A	6.04	137.45	127.17
5	B	902	TAD	N3A-C2A-N1A	-5.94	119.59	128.58
5	D	904	TAD	N3A-C2A-N1A	-5.92	119.63	128.58
5	A	901	TAD	N3A-C2A-N1A	-5.79	119.82	128.58
5	C	903	TAD	N3A-C2A-N1A	-5.77	119.84	128.58
5	A	901	TAD	N3A-C4A-N9A	5.77	136.99	127.17
5	D	904	TAD	C5A-C4A-N3A	-5.77	118.77	126.72
5	C	903	TAD	N3A-C4A-N9A	5.76	136.96	127.17
5	B	902	TAD	C5A-C4A-N3A	-5.62	118.97	126.72
5	C	903	TAD	C5A-C4A-N3A	-5.60	119.01	126.72
4	A	801	IMP	N1-C2-N3	-5.59	119.06	125.50
5	A	901	TAD	C5A-C4A-N3A	-5.55	119.07	126.72
4	B	802	IMP	N1-C2-N3	-5.41	119.27	125.50
4	C	803	IMP	N1-C2-N3	-5.34	119.36	125.50
4	D	804	IMP	N1-C2-N3	-5.29	119.41	125.50
4	A	801	IMP	O4'-C1'-N9	5.21	120.16	108.36
5	B	902	TAD	O4B-C4B-C5B	5.01	125.39	109.33
5	D	904	TAD	O4B-C4B-C5B	4.92	125.10	109.33
4	D	804	IMP	O4'-C1'-N9	4.91	119.49	108.36
4	B	802	IMP	O4'-C1'-N9	4.85	119.34	108.36
4	C	803	IMP	O4'-C1'-N9	4.82	119.29	108.36
5	A	901	TAD	O4D-C1D-C2D	4.78	111.76	105.15
5	A	901	TAD	O4B-C4B-C5B	4.66	124.27	109.33
5	C	903	TAD	O4D-C1D-C2D	4.59	111.50	105.15
6	D	609	TRS	C2-C-N	4.58	119.86	108.17
5	D	904	TAD	O4D-C1D-C2D	4.52	111.40	105.15
5	C	903	TAD	O4B-C4B-C5B	4.51	123.79	109.33
6	A	610	TRS	C2-C-N	4.47	119.57	108.17
6	D	606	TRS	C2-C-N	4.47	119.56	108.17
6	A	601	TRS	C2-C-N	4.46	119.54	108.17
5	C	903	TAD	O6N-C6N-C4N	4.41	124.48	120.25
6	A	600	TRS	C2-C-N	4.38	119.35	108.17
6	B	608	TRS	C2-C-N	4.35	119.28	108.17
6	B	611	TRS	C2-C-N	4.32	119.18	108.17
6	B	603	TRS	C2-C-N	4.24	118.97	108.17
5	B	902	TAD	O6N-C6N-C4N	4.23	124.31	120.25
6	D	604	TRS	C2-C-N	4.17	118.82	108.17
6	C	602	TRS	C2-C-N	4.14	118.74	108.17
5	B	902	TAD	O4D-C1D-C2D	4.08	110.79	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	605	TRS	C2-C-N	4.05	118.51	108.17
5	D	904	TAD	C5N-C4N-C6N	-4.04	117.31	123.90
6	A	607	TRS	C2-C-N	3.99	118.34	108.17
5	A	901	TAD	O6N-C6N-C4N	3.95	124.04	120.25
5	A	901	TAD	C2A-N3A-C4A	3.81	121.13	111.83
5	C	903	TAD	C2A-N3A-C4A	3.80	121.12	111.83
5	D	904	TAD	C2A-N3A-C4A	3.80	121.11	111.83
5	B	902	TAD	C2A-N3A-C4A	3.75	120.99	111.83
5	D	904	TAD	C6A-C5A-N7A	-3.72	124.91	132.09
5	B	902	TAD	C4N-C6N-N6N	-3.69	112.53	116.28
5	B	902	TAD	C6A-C5A-N7A	-3.68	124.99	132.09
4	D	804	IMP	O3'-C3'-C4'	3.55	121.27	111.08
5	D	904	TAD	O1N-PN-C3	-3.48	99.89	109.05
5	B	902	TAD	O1N-PN-C3	-3.45	99.95	109.05
5	C	903	TAD	O1N-PN-C3	-3.44	99.98	109.05
5	A	901	TAD	C6A-C5A-N7A	-3.44	125.46	132.09
4	A	801	IMP	O3'-C3'-C4'	3.42	120.89	111.08
5	C	903	TAD	C4N-C6N-N6N	-3.41	112.81	116.28
4	B	802	IMP	O3'-C3'-C4'	3.39	120.83	111.08
5	C	903	TAD	C6A-C5A-N7A	-3.38	125.57	132.09
4	C	803	IMP	O3'-C3'-C4'	3.37	120.76	111.08
5	A	901	TAD	O1N-PN-C3	-3.32	100.30	109.05
5	A	901	TAD	C4N-C6N-N6N	-3.26	112.97	116.28
5	B	902	TAD	C2B-C3B-C4B	3.22	108.83	102.61
4	A	801	IMP	C2-N3-C4	3.17	117.10	111.53
5	D	904	TAD	C2B-C3B-C4B	3.15	108.70	102.61
4	B	802	IMP	C2-N3-C4	3.09	116.96	111.53
5	A	901	TAD	C2B-C3B-C4B	3.04	108.49	102.61
5	A	901	TAD	C2D-C3D-C4D	2.98	108.36	102.61
4	B	802	IMP	C5'-C4'-C3'	2.97	125.92	115.21
5	D	904	TAD	C6A-C5A-C4A	2.97	121.23	117.18
4	C	803	IMP	C2-N3-C4	2.92	116.67	111.53
4	D	804	IMP	C2-N3-C4	2.90	116.63	111.53
5	B	902	TAD	C4A-C5A-N7A	2.89	113.89	110.58
5	B	902	TAD	C6A-C5A-C4A	2.89	121.12	117.18
5	C	903	TAD	C2B-C3B-C4B	2.88	108.18	102.61
5	C	903	TAD	C2D-C3D-C4D	2.87	108.16	102.61
4	A	801	IMP	C5'-C4'-C3'	2.87	125.55	115.21
5	D	904	TAD	C4A-C5A-N7A	2.86	113.85	110.58
4	D	804	IMP	C5'-C4'-C3'	2.86	125.50	115.21
4	A	801	IMP	N9-C8-N7	-2.85	108.12	113.40
5	C	903	TAD	C2A-N1A-C6A	2.84	123.40	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	803	IMP	N9-C8-N7	-2.83	108.16	113.40
5	A	901	TAD	C2A-N1A-C6A	2.83	123.38	118.73
5	B	902	TAD	C2D-C3D-C4D	2.80	108.01	102.61
5	C	903	TAD	O2B-C2B-C1B	2.77	119.65	110.10
5	D	904	TAD	C2D-C3D-C4D	2.76	107.94	102.61
4	C	803	IMP	C5'-C4'-C3'	2.74	125.08	115.21
5	B	902	TAD	C2A-N1A-C6A	2.74	123.23	118.73
5	A	901	TAD	C4A-C5A-N7A	2.74	113.71	110.58
5	C	903	TAD	C6A-C5A-C4A	2.73	120.91	117.18
4	B	802	IMP	N9-C8-N7	-2.71	108.37	113.40
5	D	904	TAD	C2A-N1A-C6A	2.70	123.16	118.73
5	A	901	TAD	O2B-C2B-C1B	2.69	119.36	110.10
5	D	904	TAD	O4D-C4D-C5D	2.68	117.92	109.33
4	D	804	IMP	N9-C8-N7	-2.68	108.43	113.40
5	A	901	TAD	C6A-C5A-C4A	2.68	120.83	117.18
5	D	904	TAD	C5N-S1N-C2N	-2.65	86.38	89.52
5	C	903	TAD	C5D-C4D-C3D	-2.63	105.73	115.21
5	D	904	TAD	O2N-PN-O1N	2.60	118.43	109.95
5	C	903	TAD	C4A-C5A-N7A	2.57	113.52	110.58
5	D	904	TAD	C6N-C4N-N3N	2.57	127.13	121.42
5	B	902	TAD	O2N-PN-O1N	2.49	118.05	109.95
6	B	603	TRS	C1-C-N	-2.46	101.90	108.17
6	C	605	TRS	C1-C-N	-2.42	102.00	108.17
6	B	611	TRS	C1-C-N	-2.42	102.01	108.17
6	C	602	TRS	C1-C-N	-2.41	102.01	108.17
5	B	902	TAD	O2B-C2B-C1B	2.40	118.36	110.10
5	A	901	TAD	C5D-C4D-C3D	-2.36	106.71	115.21
5	C	903	TAD	O2N-PN-O1N	2.36	117.62	109.95
5	A	901	TAD	O4D-C4D-C5D	2.33	116.81	109.33
5	C	903	TAD	O4D-C4D-C5D	2.32	116.78	109.33
5	D	904	TAD	O2B-C2B-C1B	2.32	118.08	110.10
5	A	901	TAD	O2N-PN-O1N	2.32	117.49	109.95
6	D	609	TRS	C1-C-N	-2.31	102.28	108.17
4	D	804	IMP	O3P-P-O5'	2.29	112.64	106.67
5	C	903	TAD	C5N-S1N-C2N	-2.28	86.82	89.52
5	D	904	TAD	C5D-C4D-C3D	-2.26	107.06	115.21
6	D	604	TRS	C1-C-N	-2.24	102.45	108.17
5	B	902	TAD	C5N-S1N-C2N	-2.24	86.88	89.52
5	D	904	TAD	C3D-C2D-C1D	2.24	104.33	101.69
5	C	903	TAD	C2D-C1D-C2N	2.24	119.17	114.94
5	B	902	TAD	C5D-C4D-C3D	-2.24	107.16	115.21
5	B	902	TAD	C3D-C2D-C1D	2.23	104.32	101.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	902	TAD	C1D-C2N-N3N	-2.22	121.48	124.48
4	B	802	IMP	O3P-P-O5'	2.22	112.45	106.67
5	B	902	TAD	O4D-C4D-C5D	2.20	116.38	109.33
4	A	801	IMP	O3P-P-O5'	2.19	112.37	106.67
6	A	600	TRS	C1-C-N	-2.14	102.70	108.17
5	A	901	TAD	C5N-S1N-C2N	-2.12	87.02	89.52
6	A	610	TRS	C2-C-C1	-2.11	105.05	110.66
5	A	901	TAD	C2D-C1D-C2N	2.10	118.91	114.94
6	A	607	TRS	C1-C-N	-2.08	102.86	108.17
6	D	606	TRS	C1-C-N	-2.08	102.87	108.17
4	C	803	IMP	O3P-P-O5'	2.06	112.04	106.67
5	B	902	TAD	C5A-C4A-N9A	-2.05	103.58	105.81
5	D	904	TAD	C4B-O4B-C1B	2.01	113.91	109.47

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	802	IMP	C5'-O5'-P-O2P
4	C	803	IMP	C5'-O5'-P-O2P
4	D	804	IMP	C5'-O5'-P-O2P
4	D	804	IMP	C5'-O5'-P-O3P
5	B	902	TAD	PA-C3-PN-O5D
5	D	904	TAD	PA-C3-PN-O5D
6	A	600	TRS	C1-C-C3-O3
6	A	600	TRS	C2-C-C3-O3
6	A	600	TRS	N-C-C3-O3
6	A	607	TRS	C1-C-C2-O2
6	A	607	TRS	C3-C-C2-O2
6	A	607	TRS	N-C-C2-O2
6	B	608	TRS	C1-C-C2-O2
6	B	608	TRS	C3-C-C2-O2
6	D	609	TRS	C1-C-C2-O2
6	D	609	TRS	C3-C-C2-O2
6	D	609	TRS	N-C-C2-O2
4	D	804	IMP	C3'-C4'-C5'-O5'
2	A	752	BOG	C2'-C1'-O1-C1
6	B	603	TRS	C2-C-C3-O3
6	C	605	TRS	C2-C-C1-O1
4	B	802	IMP	C3'-C4'-C5'-O5'
4	C	803	IMP	C3'-C4'-C5'-O5'
5	D	904	TAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
4	D	804	IMP	O4'-C4'-C5'-O5'
5	B	902	TAD	O4B-C4B-C5B-O5B
4	D	804	IMP	C5'-O5'-P-O1P
5	A	901	TAD	O4B-C4B-C5B-O5B
6	A	600	TRS	C3-C-C2-O2
6	A	601	TRS	N-C-C2-O2
6	A	610	TRS	C1-C-C2-O2
6	A	610	TRS	N-C-C2-O2
6	B	603	TRS	N-C-C1-O1
6	B	603	TRS	C1-C-C3-O3
6	B	608	TRS	N-C-C2-O2
6	B	611	TRS	N-C-C2-O2
6	C	605	TRS	N-C-C1-O1
6	D	606	TRS	C1-C-C2-O2
6	D	606	TRS	C3-C-C2-O2
2	A	752	BOG	C3'-C4'-C5'-C6'
4	B	802	IMP	C5'-O5'-P-O3P
4	C	803	IMP	C5'-O5'-P-O3P
4	A	801	IMP	C3'-C4'-C5'-O5'
2	A	751	BOG	C2'-C1'-O1-C1
6	A	600	TRS	C1-C-C2-O2
6	A	601	TRS	C1-C-C2-O2
6	A	601	TRS	C3-C-C2-O2
6	A	610	TRS	C3-C-C2-O2
6	B	611	TRS	C1-C-C2-O2
6	B	611	TRS	C3-C-C2-O2
6	C	602	TRS	C2-C-C1-O1
6	C	605	TRS	C3-C-C1-O1
5	B	902	TAD	PA-C3-PN-O2N
5	D	904	TAD	PA-C3-PN-O2N
4	B	802	IMP	C5'-O5'-P-O1P
4	C	803	IMP	C5'-O5'-P-O1P
5	C	903	TAD	O4B-C4B-C5B-O5B
6	A	600	TRS	N-C-C2-O2
6	B	603	TRS	N-C-C3-O3
6	D	604	TRS	C1-C-C3-O3
6	D	606	TRS	N-C-C2-O2
6	D	609	TRS	C2-C-C3-O3
6	D	604	TRS	C2-C-C3-O3
6	D	609	TRS	C1-C-C3-O3
6	A	607	TRS	N-C-C3-O3
6	A	610	TRS	N-C-C3-O3

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Mol	Chain	Res	Type	Atoms
6	B	608	TRS	N-C-C3-O3
5	B	902	TAD	C5D-O5D-PN-O1N

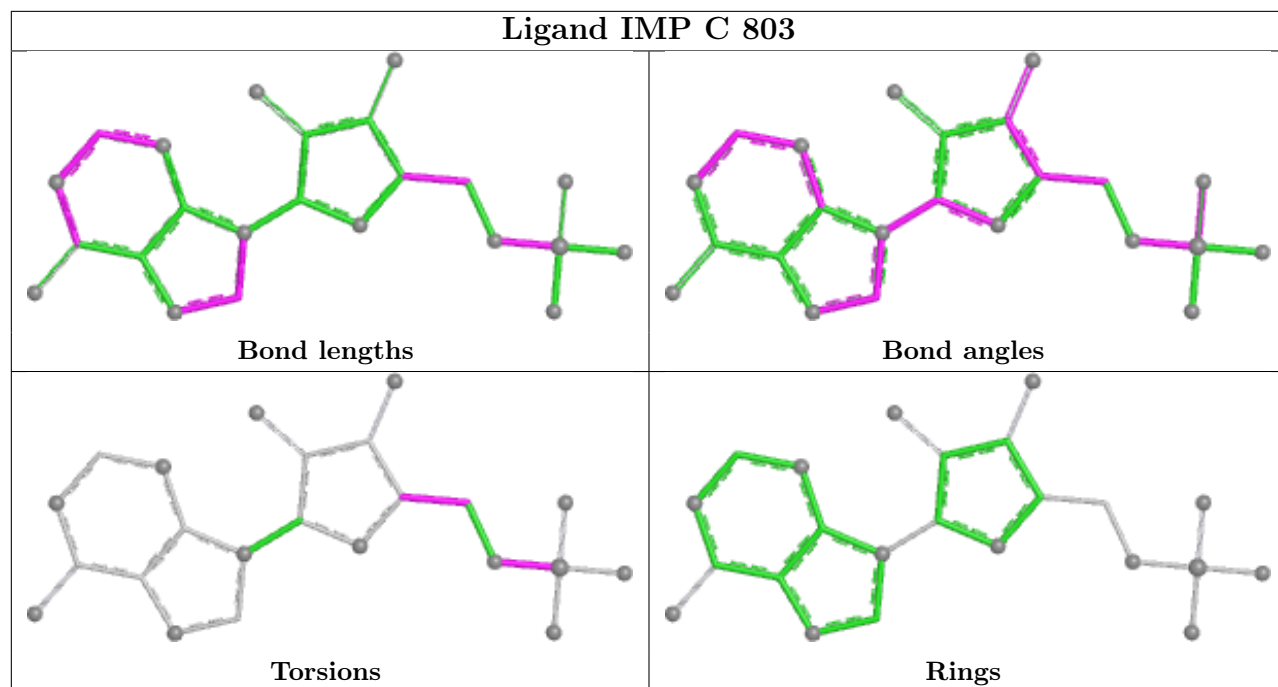
There are no ring outliers.

15 monomers are involved in 24 short contacts:

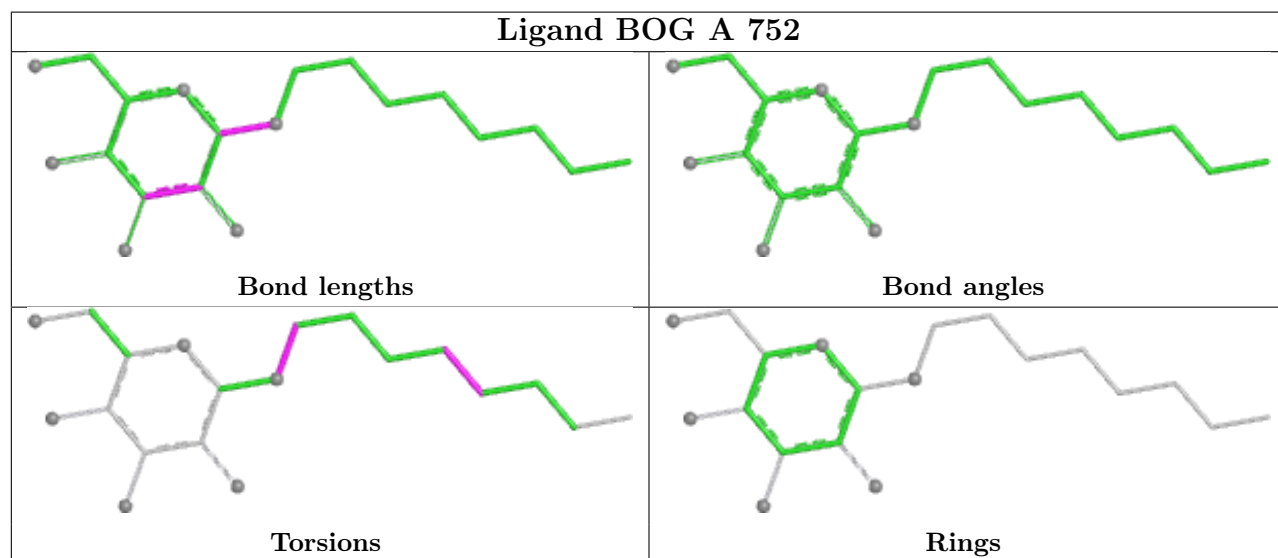
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	601	TRS	1	0
6	A	607	TRS	2	0
6	C	605	TRS	3	0
2	A	752	BOG	2	0
5	B	902	TAD	1	0
6	A	610	TRS	1	0
4	D	804	IMP	2	0
6	B	603	TRS	1	0
5	D	904	TAD	3	0
6	D	604	TRS	2	0
6	B	608	TRS	1	0
6	A	600	TRS	1	0
6	D	606	TRS	1	0
6	D	609	TRS	3	0
2	A	751	BOG	1	0

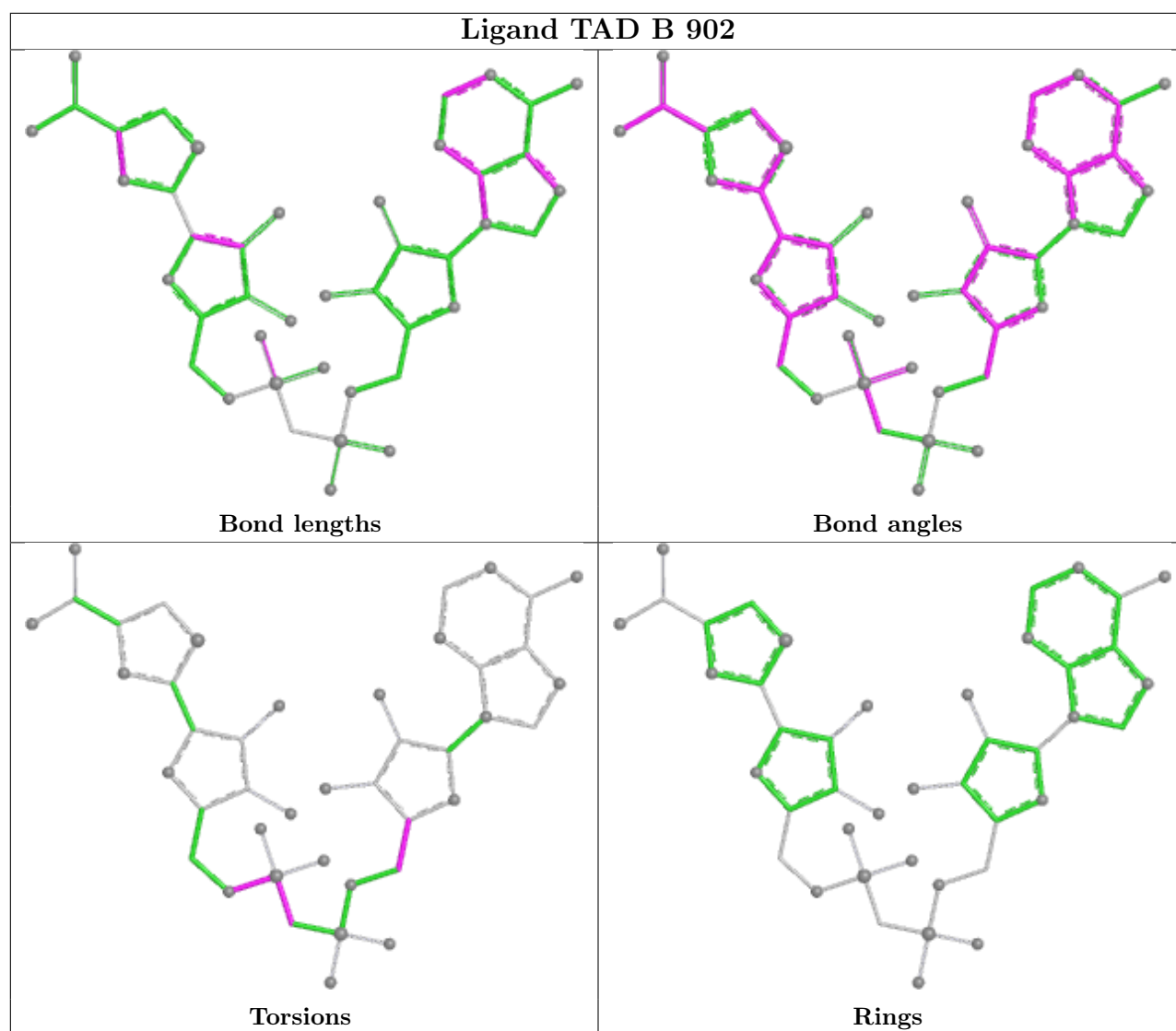
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand IMP C 803

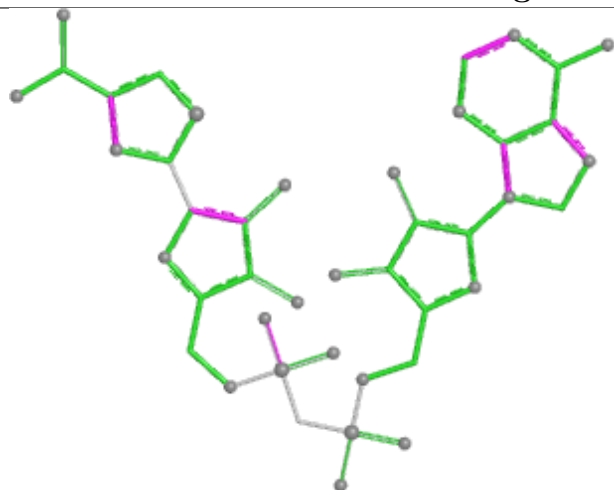


Ligand BOG A 752

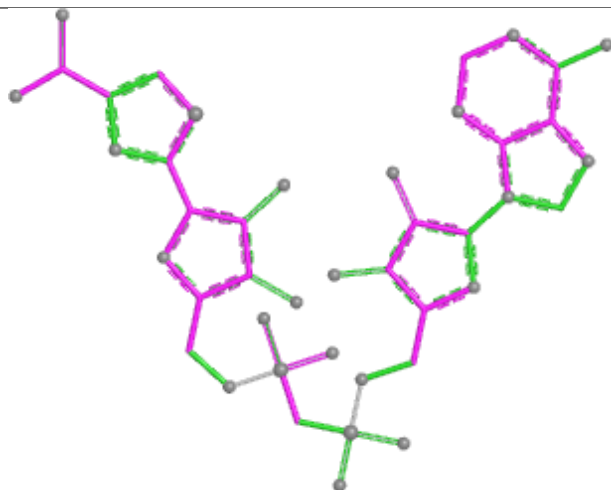




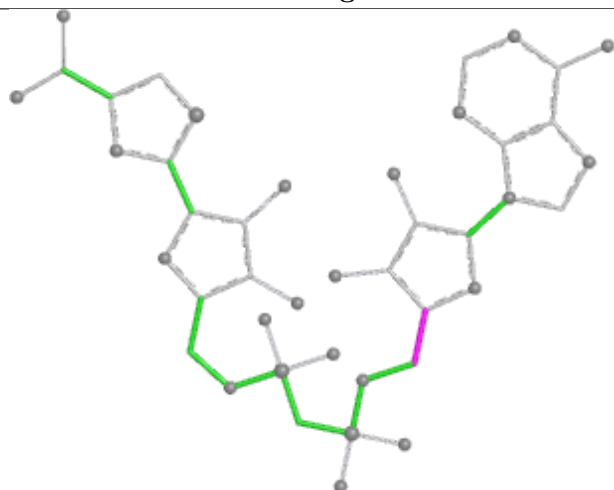
Ligand TAD C 903



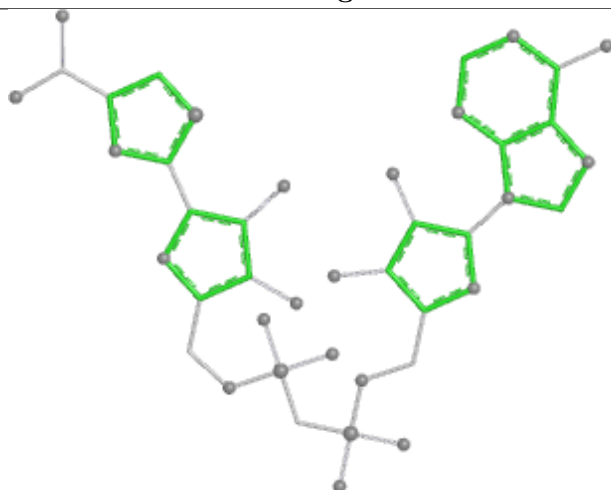
Bond lengths



Bond angles

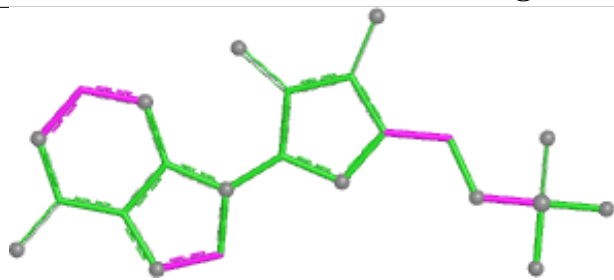


Torsions

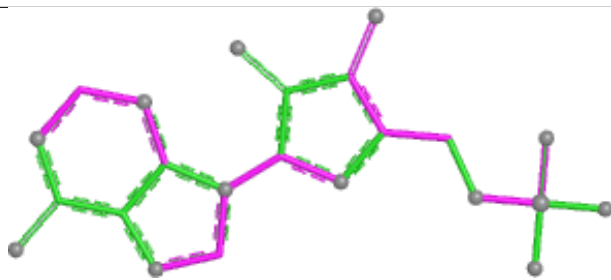


Rings

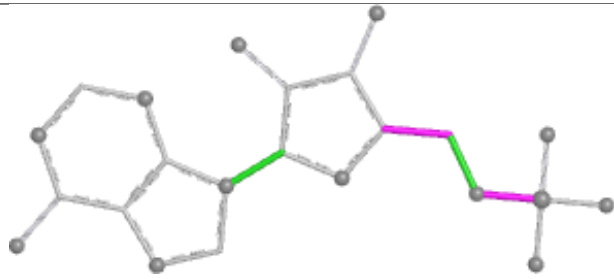
Ligand IMP D 804



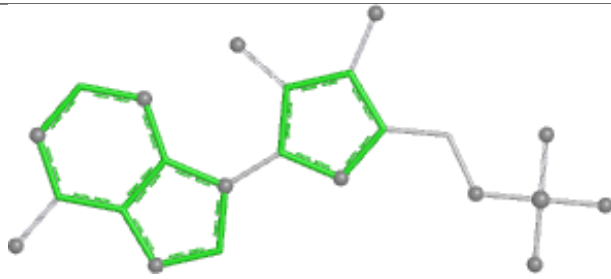
Bond lengths



Bond angles

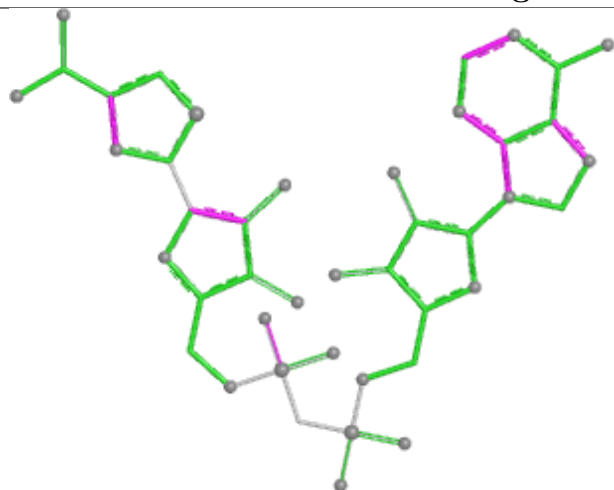


Torsions

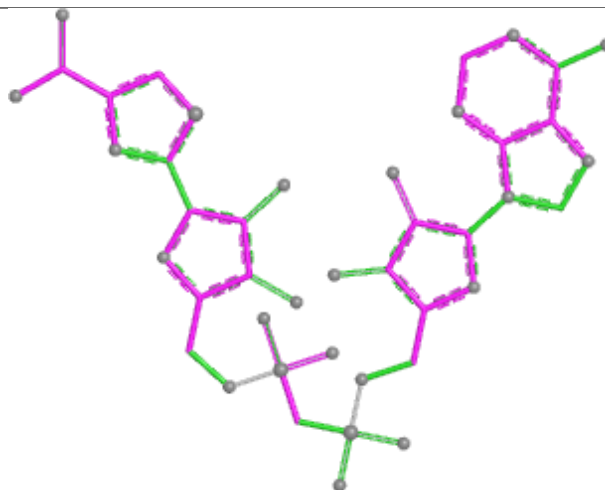


Rings

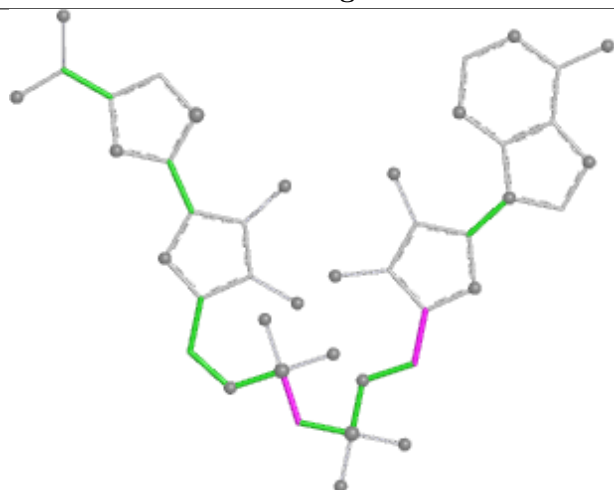
Ligand TAD D 904



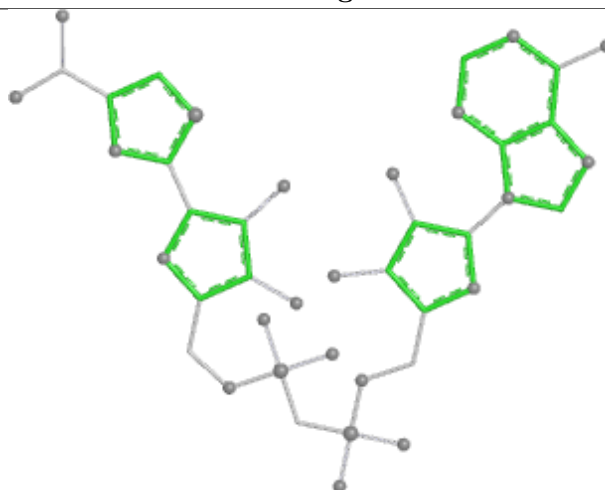
Bond lengths



Bond angles

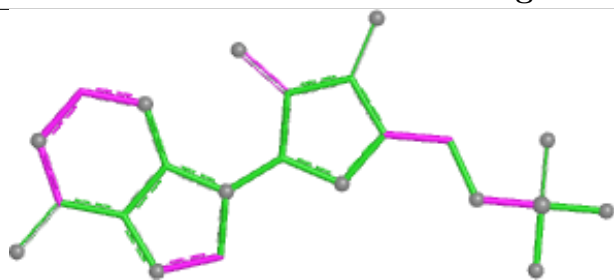


Torsions

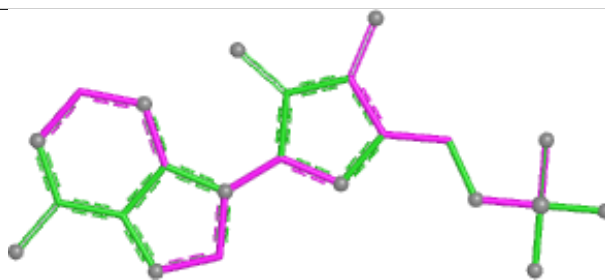


Rings

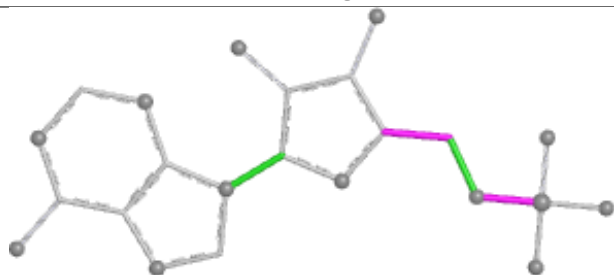
Ligand IMP B 802



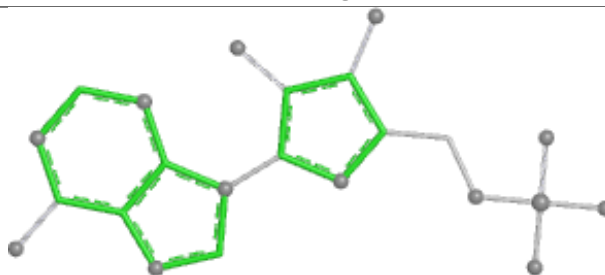
Bond lengths



Bond angles

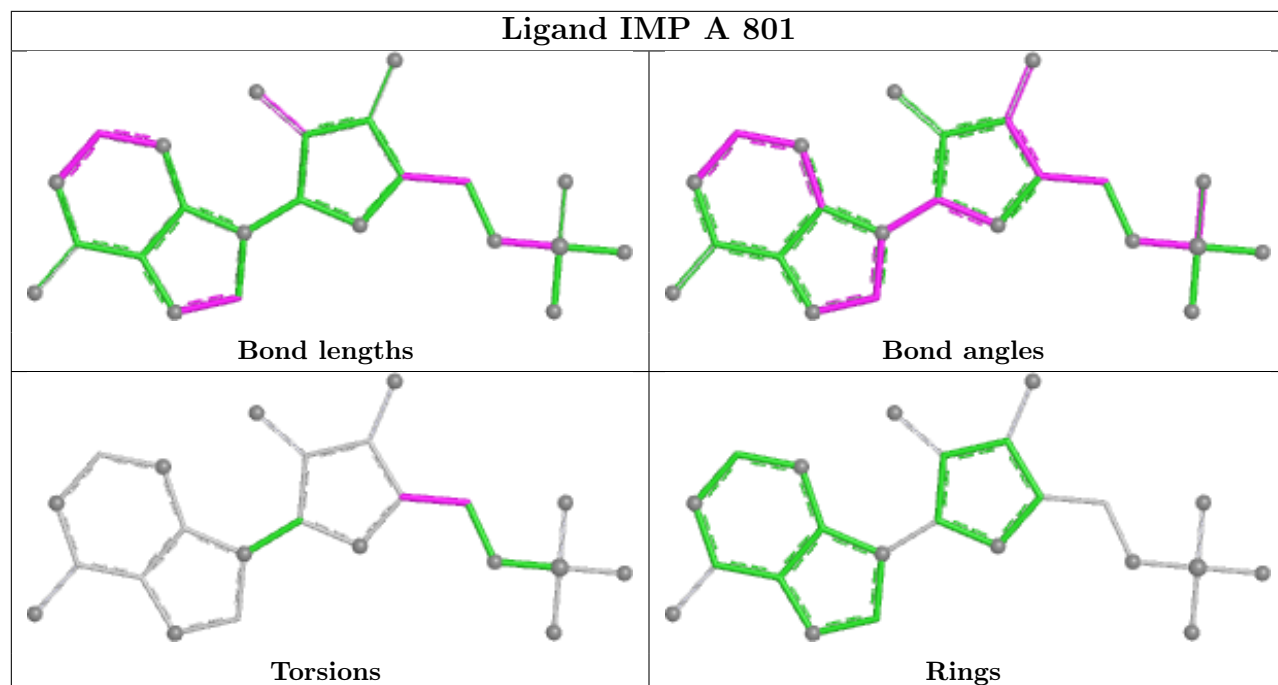


Torsions

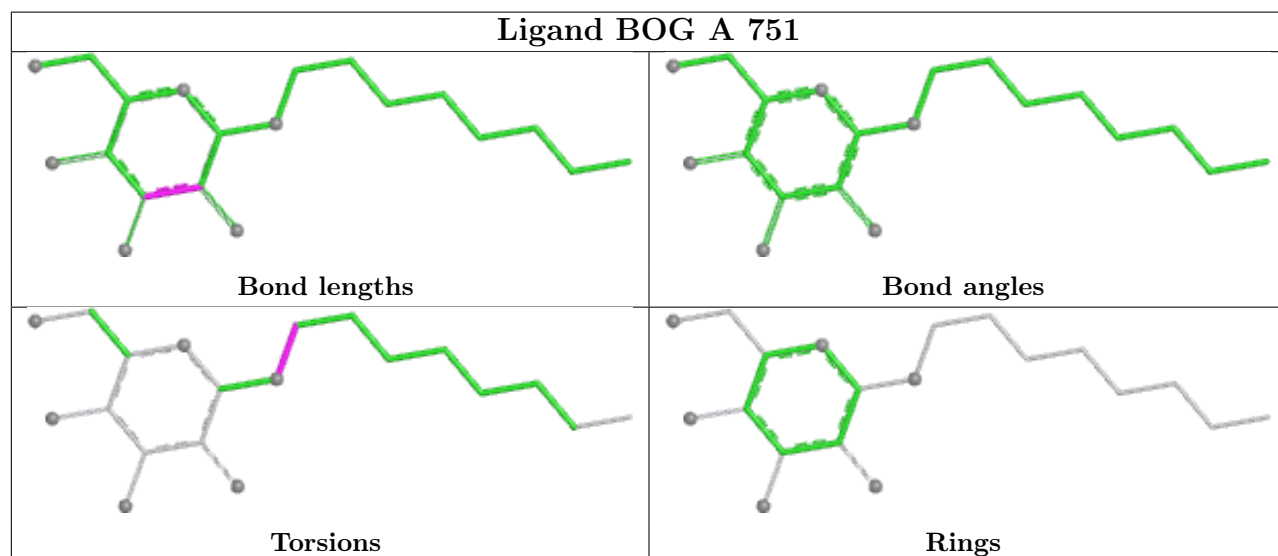


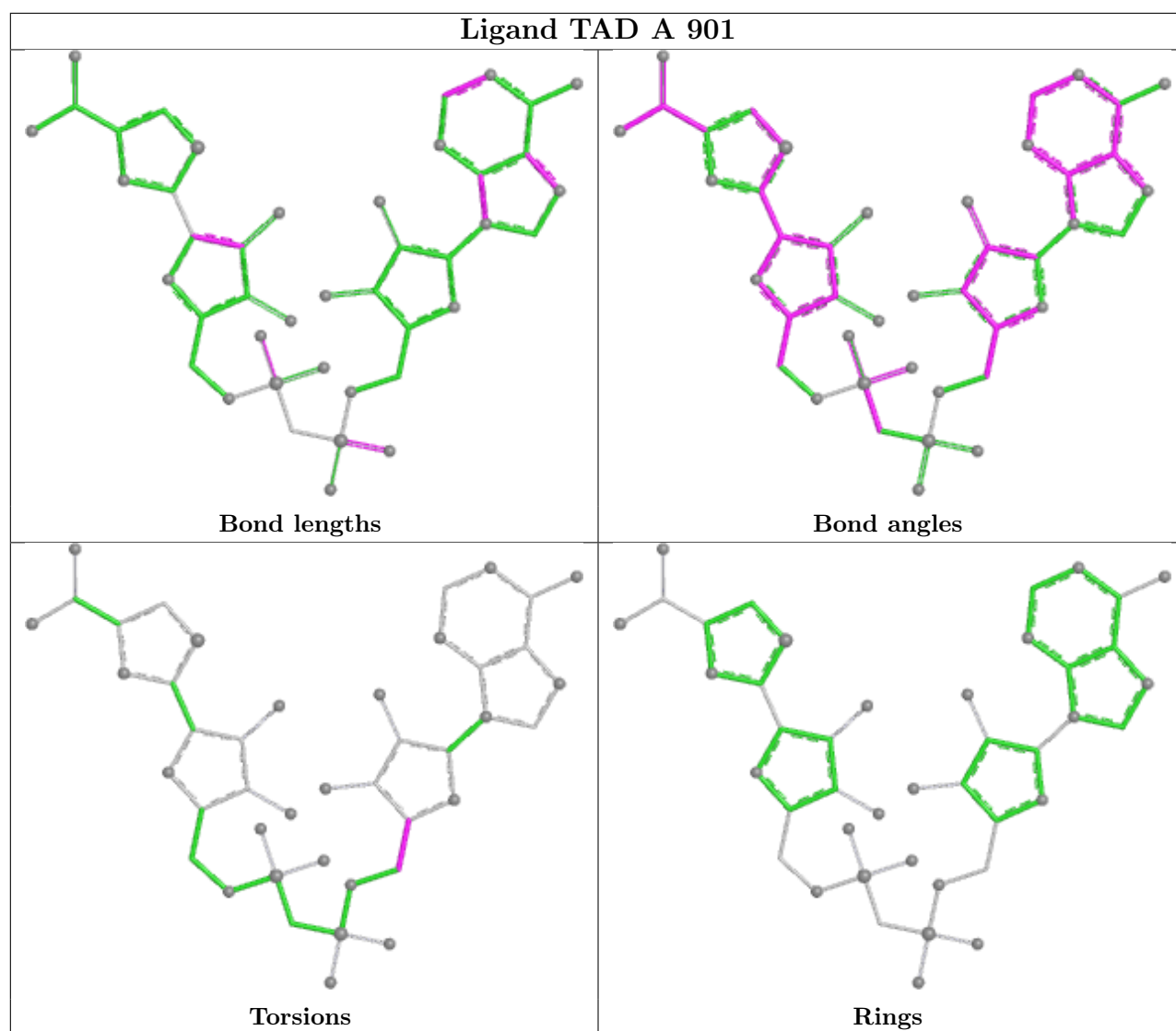
Rings

Ligand IMP A 801



Ligand BOG A 751





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.