



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:57 am BST

PDB ID : 1P19
Title : Hypoxanthine Phosphoribosyltransferase from *Trypanosoma cruzi*, in complex with the product IMP
Authors : Medrano, F.J.; Eakin, A.E.; Craig III, S.P.
Deposited on : 2003-04-11
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

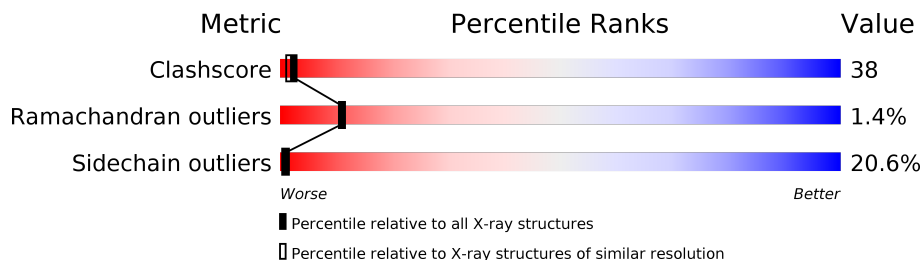
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	221	31% 43% 11% 15%
1	B	221	29% 41% 12% 17%
1	C	221	29% 44% 10% 16%
1	D	221	33% 40% 12% 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6928 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.

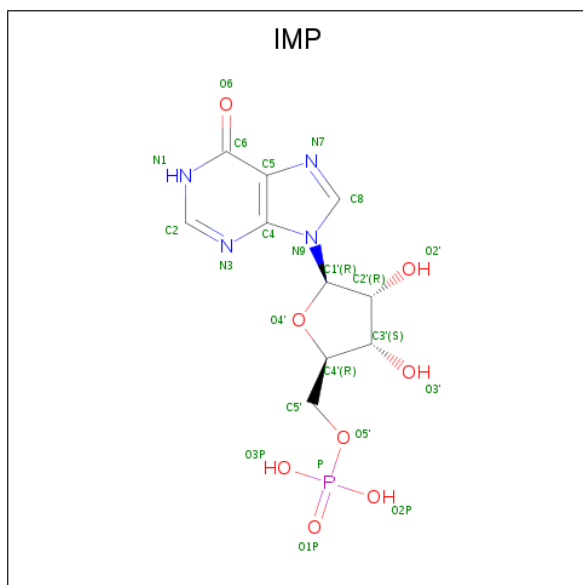
- Molecule 1 is a protein called hypoxanthine phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	187	1519	978	259	276	6	0	0	0
1	B	184	1507	967	262	272	6	0	0	0
1	C	185	1507	970	257	274	6	0	0	0
1	D	186	1523	977	265	275	6	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	LYS	MET	SEE REMARK 999	UNP Q27796
A	66	CYS	SER	SEE REMARK 999	UNP Q27796
A	86	LEU	VAL	SEE REMARK 999	UNP Q27796
B	23	LYS	MET	SEE REMARK 999	UNP Q27796
B	66	CYS	SER	SEE REMARK 999	UNP Q27796
B	86	LEU	VAL	SEE REMARK 999	UNP Q27796
C	23	LYS	MET	SEE REMARK 999	UNP Q27796
C	66	CYS	SER	SEE REMARK 999	UNP Q27796
C	86	LEU	VAL	SEE REMARK 999	UNP Q27796
D	23	LYS	MET	SEE REMARK 999	UNP Q27796
D	66	CYS	SER	SEE REMARK 999	UNP Q27796
D	86	LEU	VAL	SEE REMARK 999	UNP Q27796

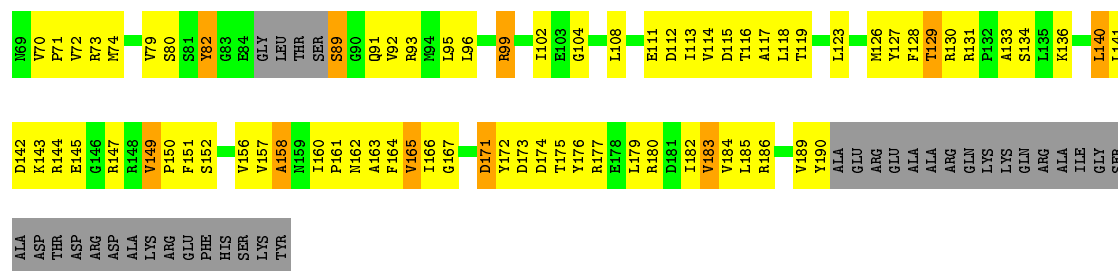
- Molecule 2 is INOSINIC ACID (three-letter code: IMP) (formula: C₁₀H₁₃N₄O₈P).



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

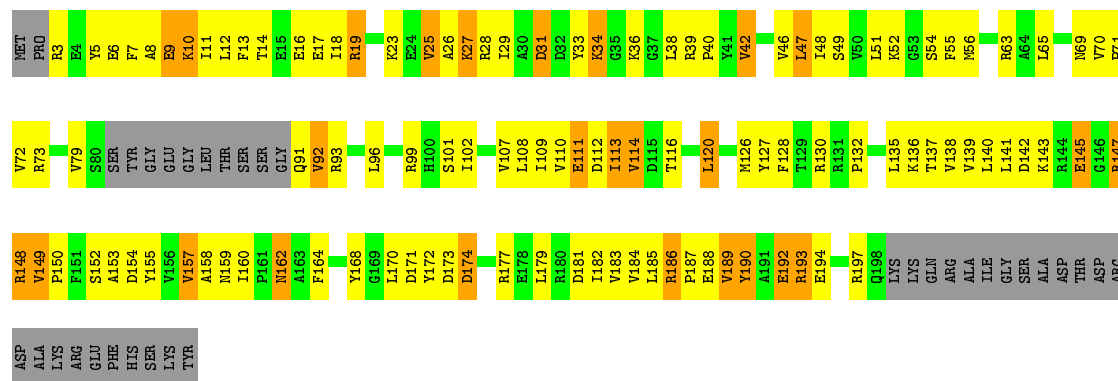
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	202	202	202	0	0
3	B	193	193	193	0	0
3	C	183	183	183	0	0
3	D	202	202	202	0	0



- Molecule 1: hypoxanthine phosphoribosyltransferase

Chain D: 33% 40% 12% 16%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	156.94Å 121.02Å 52.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.30)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.193 , 0.261	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6928	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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

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	0.34	0/1550	0.99	8/2099 (0.4%)
1	B	0.45	3/1536 (0.2%)	0.93	1/2078 (0.0%)
1	C	0.33	0/1538	0.91	4/2082 (0.2%)
1	D	0.30	0/1552	0.86	2/2100 (0.1%)
All	All	0.36	3/6176 (0.0%)	0.92	15/8359 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4	GLU	CB-CG	8.18	1.67	1.52
1	B	4	GLU	CD-OE1	5.56	1.31	1.25
1	B	4	GLU	CD-OE2	5.47	1.31	1.25

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	28	ARG	CD-NE-CZ	7.54	134.15	123.60
1	A	131	ARG	NE-CZ-NH2	6.45	123.52	120.30
1	A	28	ARG	CD-NE-CZ	6.22	132.31	123.60
1	A	28	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	A	131	ARG	CD-NE-CZ	5.98	131.98	123.60
1	A	99	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	D	190	TYR	CA-CB-CG	5.78	124.38	113.40
1	B	98	THR	C-N-CA	5.61	135.73	121.70
1	A	145	GLU	C-N-CA	5.54	133.93	122.30
1	A	63	ARG	CD-NE-CZ	5.39	131.14	123.60
1	C	171	ASP	C-N-CA	5.32	134.99	121.70
1	C	82	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	C	2	PRO	O-C-N	-5.26	114.28	122.70
1	A	124	TYR	CB-CG-CD1	-5.24	117.86	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	177	ARG	NE-CZ-NH2	-5.15	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1519	0	1526	116	0
1	B	1507	0	1514	117	0
1	C	1507	0	1509	123	0
1	D	1523	0	1531	124	0
2	A	23	0	11	6	0
2	B	23	0	11	1	0
2	C	23	0	11	4	0
2	D	23	0	11	1	0
3	A	202	0	0	14	0
3	B	193	0	0	16	0
3	C	183	0	0	13	0
3	D	202	0	0	12	0
All	All	6928	0	6124	463	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 38.

All (463) 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:B:102:ILE:HD12	1:B:107:VAL:HG21	1.43	0.97
1:A:15:GLU:HA	1:A:18:ILE:HD12	1.49	0.94
1:D:193:ARG:HH21	1:D:197:ARG:HD3	1.32	0.92
1:A:185:LEU:HD11	1:A:189:VAL:HG11	1.54	0.89
1:C:102:ILE:HD11	1:C:130:ARG:HB2	1.58	0.86
1:D:120:LEU:HD11	1:D:137:THR:HG21	1.59	0.84
1:D:39:ARG:HB3	1:D:42:VAL:HG23	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:ILE:HD11	1:D:143:LYS:HG3	1.59	0.83
1:A:9:GLU:HB3	1:A:186:ARG:HB3	1.60	0.83
1:D:127:TYR:HA	1:D:130:ARG:HG3	1.60	0.81
1:D:149:VAL:HG22	1:D:150:PRO:HD2	1.64	0.80
1:B:185:LEU:HD21	1:B:190:TYR:HB3	1.64	0.80
1:B:160:ILE:HD12	1:B:161:PRO:O	1.83	0.79
1:D:112:ASP:O	1:D:140:LEU:HB3	1.84	0.78
1:C:147:ARG:HB3	1:C:149:VAL:O	1.83	0.78
1:B:186:ARG:HD2	1:B:188:GLU:OE2	1.84	0.78
1:C:65:LEU:HD11	3:C:3456:HOH:O	1.83	0.77
1:C:149:VAL:HG22	1:C:150:PRO:HD2	1.65	0.77
1:D:39:ARG:HG2	1:D:40:PRO:HD2	1.64	0.77
1:C:11:ILE:HG23	1:C:183:VAL:HG12	1.67	0.77
1:B:10:LYS:O	1:B:184:VAL:HG12	1.86	0.76
1:A:5:TYR:HD1	1:A:11:ILE:HD11	1.51	0.76
1:D:79:VAL:HG11	1:D:92:VAL:HG13	1.69	0.75
1:C:9:GLU:HB3	1:C:186:ARG:HG2	1.69	0.74
1:C:11:ILE:HG22	1:C:182:ILE:O	1.86	0.74
1:C:21:ARG:O	1:C:25:VAL:HG23	1.87	0.74
2:B:2300:IMP:H1'	3:B:2317:HOH:O	1.86	0.74
1:B:143:LYS:HE2	1:B:160:ILE:HD11	1.70	0.73
1:A:16:GLU:HG3	1:A:19:ARG:HH21	1.53	0.73
1:C:141:LEU:HD11	1:C:182:ILE:HD13	1.70	0.73
1:C:179:LEU:HD22	3:D:4404:HOH:O	1.89	0.73
1:C:17:GLU:HG3	3:C:3395:HOH:O	1.88	0.73
1:D:3:ARG:HD2	1:D:181:ASP:OD2	1.89	0.73
1:D:38:LEU:HB3	1:D:71:PRO:HG2	1.70	0.73
1:D:141:LEU:HA	1:D:158:ALA:O	1.89	0.72
1:D:136:LYS:HD2	1:D:154:ASP:OD1	1.88	0.72
1:C:45:LEU:HB3	1:C:72:VAL:HG12	1.72	0.72
1:A:156:VAL:HB	3:A:1463:HOH:O	1.90	0.71
1:C:117:ALA:HB1	1:C:151:PHE:HB3	1.72	0.71
1:C:15:GLU:OE2	3:C:3452:HOH:O	2.09	0.71
1:D:142:ASP:HB3	1:D:159:ASN:ND2	2.05	0.71
1:A:153:ALA:HB3	3:A:1463:HOH:O	1.91	0.71
1:A:14:THR:HA	1:A:181:ASP:HB3	1.72	0.71
1:C:41:TYR:HB3	1:D:193:ARG:NH1	2.06	0.71
1:C:140:LEU:O	1:C:141:LEU:HD23	1.90	0.70
1:C:127:TYR:HA	1:C:130:ARG:HG3	1.73	0.70
1:B:170:LEU:HA	3:B:2434:HOH:O	1.90	0.70
1:B:113:ILE:HA	1:B:141:LEU:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:TYR:O	1:C:36:LYS:HB2	1.91	0.70
1:D:79:VAL:HG22	1:D:93:ARG:O	1.92	0.70
1:D:10:LYS:NZ	1:D:184:VAL:HG21	2.07	0.69
1:C:27:LYS:O	1:C:30:ALA:HB3	1.92	0.69
1:A:116:THR:HG23	2:A:1300:IMP:O1P	1.93	0.69
1:C:41:TYR:HB3	1:D:193:ARG:HH11	1.58	0.69
1:A:14:THR:OG1	1:A:17:GLU:HG3	1.92	0.69
1:B:190:TYR:O	1:B:194:GLU:HB2	1.93	0.69
1:C:80:SER:HB2	1:C:95:LEU:HD11	1.75	0.68
1:B:51:LEU:HD11	1:B:76:PHE:HB3	1.76	0.68
1:A:12:LEU:O	1:C:2:PRO:N	2.26	0.68
1:C:142:ASP:OD1	1:C:144:ARG:HG3	1.93	0.68
1:A:115:ASP:HB3	2:A:1300:IMP:P	2.34	0.68
1:A:143:LYS:HD3	1:A:162:ASN:HA	1.76	0.67
1:A:180:ARG:HG3	1:B:63:ARG:HG2	1.74	0.67
1:A:115:ASP:HB3	2:A:1300:IMP:O1P	1.94	0.67
1:C:14:THR:O	1:C:18:ILE:HG13	1.95	0.67
1:A:14:THR:O	1:A:18:ILE:HG13	1.95	0.66
1:A:87:THR:OG1	1:A:91:GLN:HB3	1.94	0.66
1:B:145:GLU:HB2	1:B:162:ASN:HD21	1.60	0.66
1:C:104:GLY:O	1:C:133:ALA:HB2	1.95	0.66
1:C:113:ILE:HD11	1:C:143:LYS:HE3	1.78	0.66
1:C:14:THR:HG23	1:C:16:GLU:H	1.59	0.66
1:B:145:GLU:HB2	1:B:162:ASN:ND2	2.10	0.66
1:C:140:LEU:HG	1:C:141:LEU:HG	1.79	0.65
1:A:47:LEU:HD12	1:A:74:MET:SD	2.38	0.64
1:B:144:ARG:HD3	1:B:159:ASN:HD22	1.62	0.64
1:D:33:TYR:HB3	1:D:36:LYS:HB2	1.79	0.64
1:B:93:ARG:NH2	1:B:95:LEU:HD21	2.11	0.64
1:D:102:ILE:HG22	3:D:4454:HOH:O	1.97	0.64
1:B:34:LYS:HA	3:B:2308:HOH:O	1.96	0.64
1:D:187:PRO:HA	1:D:190:TYR:CE1	2.33	0.64
1:D:70:VAL:O	1:D:72:VAL:HG13	1.97	0.64
1:C:89:SER:OG	1:C:91:GLN:HG3	1.98	0.64
1:D:14:THR:OG1	1:D:17:GLU:HG3	1.97	0.64
1:D:172:TYR:OH	1:D:194:GLU:HG2	1.97	0.64
1:C:96:LEU:HA	3:C:3384:HOH:O	1.97	0.63
1:A:52:LYS:HE3	1:B:74:MET:O	1.99	0.62
1:C:172:TYR:O	1:C:175:THR:HB	1.99	0.62
1:C:180:ARG:HG2	1:D:63:ARG:HD2	1.81	0.62
1:D:25:VAL:O	1:D:29:ILE:HG13	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:THR:HG23	2:D:4300:IMP:O1P	2.00	0.61
1:D:10:LYS:HZ3	1:D:184:VAL:HG21	1.65	0.61
1:C:176:TYR:O	1:C:179:LEU:HG	2.00	0.61
1:B:3:ARG:HD3	1:B:3:ARG:N	2.16	0.61
1:D:10:LYS:HE2	1:D:12:LEU:HD21	1.83	0.61
1:B:101:SER:HB3	3:B:2425:HOH:O	1.99	0.61
1:A:113:ILE:HD12	1:A:141:LEU:HB3	1.83	0.61
1:C:12:LEU:HD13	1:C:160:ILE:HG21	1.83	0.61
1:C:15:GLU:OE2	1:C:180:ARG:HD3	2.00	0.61
1:B:45:LEU:HB3	1:B:72:VAL:HG12	1.83	0.60
1:D:46:VAL:HG11	3:D:4454:HOH:O	2.00	0.60
1:D:114:VAL:HB	1:D:139:VAL:HG11	1.84	0.60
1:D:3:ARG:O	1:D:11:ILE:HD11	2.02	0.60
1:B:34:LYS:HE2	3:B:2322:HOH:O	2.02	0.60
1:A:171:ASP:HB3	1:A:177:ARG:HG2	1.83	0.59
1:A:64:ALA:O	1:A:67:ASP:HB2	2.01	0.59
1:C:99:ARG:HH21	1:C:99:ARG:HB2	1.67	0.59
1:D:194:GLU:O	1:D:197:ARG:HB2	2.02	0.59
1:B:18:ILE:HD11	1:B:182:ILE:HD12	1.83	0.59
1:D:150:PRO:HD3	3:D:4460:HOH:O	2.02	0.59
1:A:159:ASN:O	1:A:160:ILE:HG23	2.03	0.58
1:A:28:ARG:HG2	1:A:28:ARG:HH11	1.68	0.58
1:A:3:ARG:HD2	1:A:5:TYR:OH	2.02	0.58
1:A:93:ARG:HD2	1:A:95:LEU:CD2	2.34	0.58
1:B:14:THR:HG23	1:B:17:GLU:OE1	2.04	0.58
1:D:137:THR:O	1:D:154:ASP:HB2	2.02	0.58
1:B:26:ALA:HB1	1:B:65:LEU:HD23	1.86	0.58
1:C:79:VAL:HA	1:C:93:ARG:O	2.04	0.58
1:B:120:LEU:HD11	1:B:137:THR:HG21	1.85	0.58
1:B:79:VAL:HA	1:B:93:ARG:O	2.04	0.58
1:B:148:ARG:HD3	3:B:2481:HOH:O	2.03	0.57
1:D:79:VAL:CG1	1:D:92:VAL:HG13	2.34	0.57
1:B:125:HIS:O	1:B:129:THR:HG23	2.04	0.57
1:D:31:ASP:O	1:D:34:LYS:HB2	2.04	0.57
1:A:10:LYS:HD3	1:A:12:LEU:CD2	2.34	0.57
1:D:47:LEU:CD2	1:D:108:LEU:HD23	2.35	0.57
1:A:113:ILE:HD11	1:A:143:LYS:HE3	1.86	0.57
1:A:36:LYS:HB2	1:A:38:LEU:CD2	2.35	0.57
1:C:38:LEU:HD12	1:C:70:VAL:HG13	1.87	0.57
1:D:111:GLU:OE2	1:D:111:GLU:HA	2.05	0.57
1:A:17:GLU:OE1	1:C:2:PRO:HD3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:THR:HA	1:A:146:GLY:O	2.05	0.56
1:B:99:ARG:HB3	1:B:100:HIS:CE1	2.40	0.56
1:A:164:PHE:HZ	3:A:1454:HOH:O	1.88	0.56
1:D:114:VAL:HG11	1:D:147:ARG:HH22	1.70	0.56
1:D:102:ILE:HB	1:D:107:VAL:HG21	1.87	0.56
1:A:102:ILE:O	1:A:105:HIS:HB2	2.06	0.56
1:A:137:THR:HG23	3:A:1306:HOH:O	2.06	0.56
1:A:56:MET:SD	1:A:168:TYR:HA	2.45	0.56
1:A:15:GLU:OE2	1:A:180:ARG:HG2	2.06	0.56
1:B:18:ILE:CD1	1:B:182:ILE:HD12	2.35	0.56
1:C:41:TYR:CD2	1:D:193:ARG:HG2	2.41	0.56
1:C:96:LEU:HD13	1:D:96:LEU:HB2	1.88	0.56
1:D:16:GLU:HA	1:D:19:ARG:HE	1.70	0.56
1:D:65:LEU:HB3	1:D:70:VAL:HB	1.87	0.56
1:D:113:ILE:HD11	1:D:143:LYS:CG	2.34	0.56
1:B:193:ARG:HG3	3:B:2327:HOH:O	2.06	0.55
1:C:143:LYS:HG2	1:C:160:ILE:HD12	1.86	0.55
1:D:16:GLU:HA	1:D:19:ARG:NE	2.22	0.55
1:A:48:ILE:HD12	3:A:1420:HOH:O	2.05	0.55
1:C:143:LYS:HD3	1:C:161:PRO:O	2.07	0.55
1:D:102:ILE:HD11	1:D:130:ARG:HB2	1.88	0.55
1:D:39:ARG:HB3	1:D:42:VAL:CG2	2.35	0.55
1:A:21:ARG:O	1:A:25:VAL:HG23	2.06	0.55
1:B:144:ARG:HD3	1:B:159:ASN:ND2	2.21	0.55
1:A:109:ILE:HB	1:A:137:THR:HG22	1.89	0.54
1:B:79:VAL:HG13	1:B:93:ARG:O	2.07	0.54
1:D:18:ILE:HD11	1:D:182:ILE:HG13	1.89	0.54
1:D:56:MET:SD	1:D:168:TYR:HA	2.48	0.54
1:A:102:ILE:HB	1:A:107:VAL:HG21	1.89	0.54
1:B:22:ILE:O	1:B:25:VAL:HG12	2.07	0.54
1:B:33:TYR:O	1:B:36:LYS:HB2	2.07	0.54
1:C:186:ARG:HB2	1:C:189:VAL:HG23	1.89	0.54
1:B:125:HIS:HA	1:B:128:PHE:HB3	1.89	0.54
1:B:15:GLU:HA	1:B:18:ILE:HD12	1.88	0.54
1:A:10:LYS:HD3	1:A:12:LEU:HD23	1.89	0.54
1:A:79:VAL:HG23	3:A:1358:HOH:O	2.07	0.53
1:B:167:GLY:HA2	1:B:176:TYR:O	2.08	0.53
1:C:38:LEU:HB3	1:C:71:PRO:HG2	1.90	0.53
1:D:112:ASP:HB2	1:D:170:LEU:HD21	1.90	0.53
1:C:11:ILE:HA	1:C:183:VAL:HA	1.90	0.53
1:B:162:ASN:N	1:B:162:ASN:HD22	2.05	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:ALA:HB2	1:C:183:VAL:HG21	1.91	0.53
1:B:167:GLY:CA	1:B:179:LEU:HB2	2.38	0.53
1:D:92:VAL:O	1:D:92:VAL:HG12	2.09	0.53
1:A:172:TYR:HE2	1:B:41:TYR:HH	1.53	0.52
1:A:87:THR:HG1	1:A:91:GLN:HB3	1.73	0.52
1:B:193:ARG:HD2	3:B:2327:HOH:O	2.09	0.52
1:B:24:GLU:O	1:B:27:LYS:HB3	2.09	0.52
1:C:41:TYR:CE2	1:D:193:ARG:HG2	2.43	0.52
1:B:99:ARG:HD3	1:B:100:HIS:CE1	2.44	0.52
1:B:9:GLU:O	1:B:10:LYS:HB3	2.09	0.52
1:C:52:LYS:O	1:C:55:PHE:HD2	1.92	0.52
1:C:5:TYR:HB2	1:C:8:ALA:HB3	1.90	0.52
1:A:136:LYS:HA	3:A:1306:HOH:O	2.08	0.52
1:A:18:ILE:O	1:A:22:ILE:HG13	2.09	0.52
1:D:113:ILE:HG13	1:D:141:LEU:HB2	1.92	0.52
1:C:115:ASP:O	1:C:147:ARG:HD3	2.09	0.52
1:B:143:LYS:CE	1:B:160:ILE:HD11	2.38	0.52
1:A:16:GLU:CG	1:A:19:ARG:HH21	2.21	0.51
1:B:10:LYS:HG2	1:B:184:VAL:CG1	2.41	0.51
1:C:117:ALA:CB	1:C:151:PHE:HB3	2.40	0.51
1:A:78:CYS:HA	3:A:1391:HOH:O	2.09	0.51
1:B:171:ASP:HB3	1:B:177:ARG:CG	2.40	0.51
1:A:140:LEU:O	1:A:157:VAL:HB	2.11	0.51
1:A:21:ARG:HB3	1:A:157:VAL:HG13	1.93	0.51
1:A:5:TYR:CE2	1:A:179:LEU:HD22	2.46	0.51
1:B:48:ILE:HG13	1:B:107:VAL:HG13	1.93	0.51
1:C:27:LYS:HG3	1:C:68:PHE:CE2	2.45	0.51
1:D:47:LEU:HD22	1:D:108:LEU:HD23	1.93	0.51
1:B:12:LEU:HD12	1:B:165:VAL:HG11	1.93	0.51
1:C:21:ARG:HA	1:C:24:GLU:HG3	1.92	0.51
1:D:9:GLU:OE1	1:D:184:VAL:HG11	2.11	0.51
1:C:175:THR:HG22	1:C:176:TYR:CG	2.46	0.51
1:C:99:ARG:HB2	1:C:99:ARG:NH2	2.26	0.51
1:C:185:LEU:HD23	1:C:190:TYR:CD2	2.46	0.51
1:C:113:ILE:HD13	2:C:3300:IMP:N7	2.25	0.51
1:C:116:THR:O	1:C:149:VAL:HG12	2.11	0.51
1:C:4:GLU:HG2	3:C:3424:HOH:O	2.09	0.50
1:D:13:PHE:HA	1:D:17:GLU:OE2	2.11	0.50
1:C:102:ILE:HG12	3:C:3349:HOH:O	2.11	0.50
1:B:113:ILE:HD11	1:B:143:LYS:HD2	1.93	0.50
1:D:188:GLU:OE2	1:D:192:GLU:OE1	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ASP:HB3	1:A:177:ARG:NH1	2.26	0.50
1:C:11:ILE:CG2	1:C:183:VAL:HG12	2.40	0.50
1:C:9:GLU:HB2	3:C:3353:HOH:O	2.12	0.50
1:D:48:ILE:O	1:D:48:ILE:HG22	2.10	0.50
1:A:55:PHE:HE2	1:A:169:GLY:HA2	1.76	0.50
1:A:13:PHE:O	1:A:181:ASP:HB3	2.12	0.50
1:A:184:VAL:HG12	1:A:184:VAL:O	2.10	0.50
1:B:47:LEU:CD2	1:B:108:LEU:HD23	2.42	0.50
1:C:136:LYS:HG3	3:C:3426:HOH:O	2.12	0.50
1:D:137:THR:HG22	1:D:138:VAL:N	2.27	0.50
1:D:173:ASP:O	1:D:173:ASP:OD1	2.30	0.50
1:D:5:TYR:CD1	1:D:183:VAL:HG11	2.47	0.50
1:B:167:GLY:HA2	1:B:179:LEU:HB2	1.93	0.49
1:B:188:GLU:OE1	1:B:188:GLU:O	2.30	0.49
1:D:23:LYS:O	1:D:26:ALA:HB3	2.12	0.49
1:B:99:ARG:HB3	1:B:100:HIS:ND1	2.27	0.49
1:A:158:ALA:HA	3:A:1324:HOH:O	2.12	0.49
1:C:163:ALA:HB1	3:C:3322:HOH:O	2.13	0.49
1:B:113:ILE:HD11	1:B:143:LYS:CD	2.42	0.49
1:B:113:ILE:HD11	1:B:143:LYS:HE3	1.94	0.49
1:D:120:LEU:CD1	1:D:137:THR:HG21	2.39	0.49
1:C:15:GLU:OE2	1:C:180:ARG:HB3	2.12	0.49
1:D:148:ARG:HA	3:D:4458:HOH:O	2.11	0.49
1:A:143:LYS:HE2	1:A:160:ILE:HD12	1.95	0.49
1:B:14:THR:OG1	1:B:17:GLU:HG3	2.12	0.49
1:B:45:LEU:O	1:B:72:VAL:HA	2.12	0.49
1:A:112:ASP:HB2	1:A:170:LEU:CD2	2.42	0.48
1:A:93:ARG:HD2	1:A:95:LEU:HD21	1.95	0.48
1:C:93:ARG:HD3	1:C:95:LEU:HD21	1.95	0.48
1:B:140:LEU:HD23	1:B:141:LEU:HG	1.95	0.48
1:B:114:VAL:HG13	1:B:142:ASP:OD1	2.14	0.48
1:A:124:TYR:CE1	1:A:135:LEU:HG	2.48	0.48
1:A:169:GLY:O	1:A:177:ARG:HB3	2.13	0.48
1:D:116:THR:HB	1:D:148:ARG:HD3	1.96	0.48
1:C:143:LYS:HD3	1:C:162:ASN:HA	1.96	0.48
1:A:172:TYR:HD2	1:A:176:TYR:HE1	1.61	0.48
1:A:5:TYR:HB2	1:A:8:ALA:HB3	1.95	0.48
1:A:76:PHE:HE2	3:A:1410:HOH:O	1.95	0.48
1:C:18:ILE:HG22	1:C:22:ILE:HD12	1.94	0.48
1:D:107:VAL:O	1:D:135:LEU:HA	2.12	0.48
1:D:145:GLU:HB3	1:D:162:ASN:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LEU:HB3	1:B:71:PRO:HG2	1.94	0.48
1:C:33:TYR:OH	1:C:136:LYS:HD3	2.14	0.48
1:D:171:ASP:OD2	1:D:174:ASP:HA	2.14	0.48
1:A:106:HIS:HD1	1:A:134:SER:HG	1.60	0.48
1:B:24:GLU:HG2	1:B:25:VAL:N	2.27	0.48
1:C:161:PRO:HD2	3:C:3441:HOH:O	2.14	0.48
1:A:111:GLU:HG3	1:A:112:ASP:N	2.29	0.47
1:B:10:LYS:HG2	1:B:184:VAL:HG12	1.95	0.47
1:C:116:THR:HA	1:C:147:ARG:HA	1.95	0.47
1:C:175:THR:HG22	1:C:176:TYR:CD2	2.50	0.47
1:A:169:GLY:C	1:A:177:ARG:HB3	2.34	0.47
1:C:58:THR:HG22	1:C:74:MET:HE1	1.97	0.47
1:D:172:TYR:CZ	1:D:190:TYR:HB2	2.49	0.47
1:A:9:GLU:HG3	1:A:10:LYS:N	2.30	0.47
1:A:175:THR:HG22	1:A:176:TYR:CG	2.50	0.47
1:C:46:VAL:HG22	1:C:73:ARG:HD2	1.96	0.47
1:C:157:VAL:O	1:C:158:ALA:HB2	2.15	0.47
1:C:37:GLY:O	1:C:39:ARG:HG2	2.13	0.47
1:D:141:LEU:HD23	1:D:158:ALA:HB3	1.96	0.47
1:D:46:VAL:HB	1:D:107:VAL:HG22	1.96	0.47
1:D:138:VAL:HG23	1:D:155:TYR:HB2	1.96	0.47
1:B:47:LEU:HD22	1:B:108:LEU:HD23	1.97	0.47
1:B:116:THR:HG21	3:B:2484:HOH:O	2.14	0.47
1:B:47:LEU:HD12	1:B:74:MET:HE1	1.97	0.47
1:B:173:ASP:OD1	1:B:197:ARG:HD2	2.15	0.46
1:D:186:ARG:NH2	3:D:4344:HOH:O	2.47	0.46
1:B:116:THR:HB	1:B:148:ARG:HB2	1.97	0.46
1:D:111:GLU:HG3	1:D:120:LEU:HG	1.97	0.46
1:B:105:HIS:O	1:B:132:PRO:HB2	2.15	0.46
1:C:156:VAL:HG12	1:C:158:ALA:H	1.80	0.46
1:C:164:PHE:O	1:C:184:VAL:HA	2.15	0.46
1:B:5:TYR:HE2	1:B:179:LEU:HD22	1.80	0.46
1:B:6:GLU:O	1:B:186:ARG:NH2	2.49	0.46
1:D:102:ILE:HD11	1:D:127:TYR:O	2.16	0.46
1:D:185:LEU:HD21	1:D:190:TYR:HB3	1.97	0.46
1:A:27:LYS:NZ	3:A:1475:HOH:O	2.49	0.46
1:A:28:ARG:HG2	1:A:28:ARG:NH1	2.29	0.46
1:D:8:ALA:C	1:D:186:ARG:HG3	2.35	0.46
1:C:167:GLY:HA2	1:C:179:LEU:HG	1.98	0.46
1:C:28:ARG:HB2	1:C:28:ARG:NH1	2.31	0.46
1:D:47:LEU:HD21	1:D:108:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:TYR:HA	3:A:1315:HOH:O	2.14	0.46
1:B:51:LEU:HA	1:B:52:LYS:HA	1.42	0.46
1:C:114:VAL:O	1:C:114:VAL:HG13	2.16	0.46
1:D:112:ASP:HB2	1:D:170:LEU:CD2	2.45	0.46
1:D:188:GLU:HG3	1:D:188:GLU:O	2.15	0.46
1:D:33:TYR:HA	1:D:36:LYS:HG2	1.97	0.46
1:D:73:ARG:NH1	3:D:4402:HOH:O	2.49	0.46
1:A:28:ARG:NH1	1:A:155:TYR:HE2	2.14	0.45
1:A:2:PRO:N	1:C:17:GLU:OE1	2.49	0.45
1:A:86:LEU:HD13	3:A:1478:HOH:O	2.16	0.45
1:B:116:THR:O	1:B:117:ALA:HB3	2.16	0.45
1:C:20:THR:O	1:C:24:GLU:HG2	2.15	0.45
1:C:165:VAL:O	2:C:3300:IMP:N1	2.49	0.45
1:A:27:LYS:HG2	3:A:1357:HOH:O	2.16	0.45
1:C:143:LYS:HG2	1:C:160:ILE:CD1	2.47	0.45
1:A:45:LEU:O	1:A:72:VAL:HA	2.16	0.45
1:B:171:ASP:HB3	1:B:177:ARG:HG3	1.97	0.45
1:B:194:GLU:OE1	1:B:194:GLU:O	2.34	0.45
1:C:165:VAL:HG23	2:C:3300:IMP:C6	2.47	0.45
1:C:61:LEU:O	1:C:65:LEU:HG	2.16	0.45
1:D:109:ILE:HD11	1:D:135:LEU:HD11	1.99	0.45
1:C:113:ILE:HG23	2:C:3300:IMP:H3'	1.98	0.45
1:C:161:PRO:HD3	3:C:3358:HOH:O	2.15	0.45
1:D:112:ASP:OD1	1:D:113:ILE:N	2.50	0.45
1:A:55:PHE:CE2	1:A:169:GLY:HA2	2.51	0.45
1:B:36:LYS:HD3	1:B:36:LYS:HA	1.36	0.45
1:C:12:LEU:HB2	1:C:182:ILE:HG22	1.97	0.45
1:A:13:PHE:HA	1:C:2:PRO:CD	2.47	0.45
1:A:3:ARG:NH2	1:A:181:ASP:OD1	2.50	0.45
1:B:36:LYS:NZ	3:B:2433:HOH:O	2.49	0.45
1:C:12:LEU:HD13	1:C:160:ILE:CG2	2.46	0.45
1:C:15:GLU:OE1	1:C:180:ARG:NH1	2.50	0.45
1:C:51:LEU:HB3	1:C:52:LYS:HG2	1.97	0.45
1:D:128:PHE:HA	1:D:135:LEU:HD22	1.98	0.45
1:A:105:HIS:N	1:A:133:ALA:H	2.14	0.45
1:B:97:ASP:CG	1:B:130:ARG:HH22	2.19	0.45
1:D:194:GLU:OE2	1:D:197:ARG:NH2	2.50	0.45
1:D:173:ASP:OD2	1:D:197:ARG:NH1	2.50	0.45
1:B:143:LYS:NZ	1:B:163:ALA:O	2.50	0.45
1:C:175:THR:O	1:C:176:TYR:HB2	2.17	0.45
1:A:165:VAL:HG12	1:A:166:ILE:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLU:N	1:A:16:GLU:OE1	2.50	0.45
1:B:79:VAL:HG12	1:B:80:SER:N	2.32	0.45
1:C:179:LEU:HD23	1:C:179:LEU:N	2.31	0.45
1:B:136:LYS:NZ	1:B:155:TYR:OH	2.50	0.44
1:D:8:ALA:HA	1:D:184:VAL:O	2.16	0.44
1:C:119:THR:O	1:C:123:LEU:HG	2.18	0.44
1:C:18:ILE:HD11	1:C:182:ILE:HG13	1.99	0.44
1:A:39:ARG:HB3	1:A:39:ARG:HE	1.63	0.44
1:B:130:ARG:NE	3:B:2399:HOH:O	2.50	0.44
1:C:112:ASP:N	1:C:112:ASP:OD1	2.50	0.44
1:D:92:VAL:HB	3:D:4405:HOH:O	2.16	0.44
1:D:116:THR:HB	1:D:148:ARG:HB2	1.98	0.44
1:D:91:GLN:HG3	1:D:92:VAL:N	2.33	0.44
1:A:5:TYR:CB	1:A:8:ALA:HB3	2.48	0.44
1:C:140:LEU:O	1:C:157:VAL:HB	2.17	0.44
1:D:139:VAL:HG13	1:D:153:ALA:CB	2.47	0.44
1:A:105:HIS:H	1:A:133:ALA:H	1.66	0.44
1:B:109:ILE:O	1:B:137:THR:HG23	2.18	0.44
1:D:102:ILE:HD12	1:D:132:PRO:HB3	1.99	0.44
1:A:52:LYS:NZ	1:A:174:ASP:OD2	2.50	0.44
1:B:42:VAL:HG23	1:B:43:ASN:H	1.83	0.44
1:C:39:ARG:NH2	3:C:3467:HOH:O	2.50	0.44
1:D:136:LYS:HD2	1:D:154:ASP:CG	2.38	0.44
1:B:136:LYS:HG3	1:B:154:ASP:CG	2.38	0.44
1:B:57:PHE:CD2	1:B:140:LEU:HB2	2.53	0.44
1:A:115:ASP:HB3	2:A:1300:IMP:O2P	2.17	0.43
1:A:82:TYR:CE1	1:A:93:ARG:HB2	2.53	0.43
1:C:113:ILE:HD11	1:C:143:LYS:CE	2.47	0.43
1:B:12:LEU:CD1	1:B:165:VAL:HG11	2.48	0.43
1:B:3:ARG:HD2	3:B:2470:HOH:O	2.17	0.43
1:C:22:ILE:HG22	1:C:23:LYS:N	2.32	0.43
1:A:106:HIS:ND1	1:A:134:SER:OG	2.50	0.43
1:A:27:LYS:HB2	1:A:68:PHE:CZ	2.54	0.43
1:B:14:THR:HG23	1:B:17:GLU:CD	2.38	0.43
1:B:170:LEU:N	1:B:170:LEU:HD23	2.32	0.43
1:C:36:LYS:HD3	1:C:36:LYS:HA	1.67	0.43
1:D:5:TYR:HB3	1:D:7:PHE:CZ	2.54	0.43
1:D:186:ARG:NH1	3:D:4363:HOH:O	2.50	0.43
1:C:45:LEU:O	1:C:72:VAL:HB	2.19	0.43
1:D:27:LYS:HZ3	1:D:31:ASP:CG	2.22	0.43
1:D:29:ILE:O	1:D:33:TYR:HD1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:PHE:CE1	1:D:179:LEU:HD11	2.53	0.43
1:A:175:THR:HG22	1:A:176:TYR:CD1	2.54	0.43
1:C:186:ARG:NH1	3:C:3353:HOH:O	2.50	0.43
1:D:9:GLU:HG2	1:D:184:VAL:CG1	2.49	0.43
1:A:113:ILE:HA	1:A:141:LEU:O	2.19	0.43
1:D:47:LEU:HD13	1:D:110:VAL:HG21	2.01	0.43
1:D:140:LEU:HG	1:D:141:LEU:HG	2.00	0.43
1:D:28:ARG:NH1	3:D:4333:HOH:O	2.48	0.43
1:A:31:ASP:OD2	1:A:31:ASP:N	2.51	0.43
1:A:75:GLU:CD	1:A:98:THR:HB	2.39	0.43
1:A:54:SER:HB2	1:A:110:VAL:HG12	2.01	0.42
1:D:185:LEU:HD11	1:D:189:VAL:HG12	2.01	0.42
1:A:116:THR:H	2:A:1300:IMP:P	2.42	0.42
1:A:112:ASP:HB2	1:A:170:LEU:HD21	2.00	0.42
1:A:187:PRO:HA	1:A:190:TYR:CE1	2.55	0.42
1:B:166:ILE:HG12	1:B:183:VAL:HG22	2.01	0.42
1:D:162:ASN:ND2	3:D:4372:HOH:O	2.52	0.42
1:A:165:VAL:O	1:A:166:ILE:HG23	2.20	0.42
1:B:189:VAL:HA	1:B:192:GLU:HB3	2.01	0.42
1:C:15:GLU:CD	1:C:180:ARG:HB3	2.40	0.42
1:C:186:ARG:HB2	1:C:189:VAL:CG2	2.48	0.42
1:B:13:PHE:HB2	1:B:182:ILE:HB	2.00	0.42
1:B:47:LEU:HD23	1:B:108:LEU:HB3	2.01	0.42
1:A:115:ASP:N	2:A:1300:IMP:O2P	2.50	0.42
1:A:176:TYR:O	1:A:179:LEU:HD12	2.19	0.42
1:D:157:VAL:HG12	1:D:158:ALA:N	2.33	0.42
1:C:5:TYR:HB3	1:C:7:PHE:CE1	2.55	0.42
1:C:99:ARG:HG2	3:D:4306:HOH:O	2.20	0.42
1:A:29:ILE:O	1:A:33:TYR:HD1	2.02	0.42
1:B:77:ILE:HG21	1:B:127:TYR:OH	2.20	0.42
1:C:65:LEU:HD23	1:C:65:LEU:HA	1.87	0.42
1:D:138:VAL:O	1:D:138:VAL:HG13	2.19	0.42
1:C:113:ILE:HA	1:C:141:LEU:O	2.20	0.42
1:C:39:ARG:HA	1:C:40:PRO:HD3	1.95	0.42
1:A:12:LEU:C	1:C:2:PRO:HD2	2.40	0.41
1:D:12:LEU:N	1:D:182:ILE:O	2.50	0.41
1:D:51:LEU:HA	1:D:52:LYS:HA	1.53	0.41
1:D:9:GLU:HG2	1:D:184:VAL:HB	2.02	0.41
1:B:45:LEU:HB3	1:B:72:VAL:CG1	2.50	0.41
1:B:57:PHE:HA	1:B:168:TYR:HE2	1.84	0.41
1:B:93:ARG:HD3	3:B:2444:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:PHE:CZ	1:C:158:ALA:HB1	2.55	0.41
1:D:147:ARG:HA	1:D:147:ARG:HD3	1.54	0.41
1:D:10:LYS:CE	1:D:184:VAL:HG21	2.50	0.41
1:B:144:ARG:H	1:B:144:ARG:HG3	1.53	0.41
1:B:185:LEU:CD2	1:B:190:TYR:HD2	2.33	0.41
1:B:133:ALA:O	1:B:134:SER:HB3	2.20	0.41
1:B:22:ILE:HA	1:B:25:VAL:HG12	2.01	0.41
1:B:51:LEU:CD1	1:B:76:PHE:HB3	2.49	0.41
1:A:9:GLU:HA	1:A:186:ARG:NH2	2.36	0.41
1:B:167:GLY:HA3	1:B:179:LEU:HB2	2.02	0.41
1:D:5:TYR:CE1	1:D:183:VAL:HG11	2.56	0.41
1:A:123:LEU:O	1:A:126:MET:HB3	2.21	0.41
1:A:169:GLY:O	1:A:177:ARG:NH1	2.49	0.41
1:C:108:LEU:CD1	1:C:136:LYS:HB2	2.50	0.41
1:D:159:ASN:O	1:D:160:ILE:HG23	2.20	0.41
1:D:193:ARG:HH21	1:D:197:ARG:CD	2.17	0.41
1:D:193:ARG:NH2	1:D:197:ARG:HD3	2.15	0.41
1:D:29:ILE:HD12	1:D:65:LEU:HD21	2.02	0.41
1:C:74:MET:HE2	1:D:55:PHE:CE1	2.55	0.41
1:D:52:LYS:O	1:D:55:PHE:HD2	2.03	0.41
1:B:126:MET:HB2	3:B:2363:HOH:O	2.21	0.41
1:B:113:ILE:CD1	1:B:143:LYS:HE3	2.51	0.41
1:D:36:LYS:HA	1:D:36:LYS:HD3	1.79	0.41
1:B:112:ASP:N	1:B:112:ASP:OD1	2.49	0.41
1:B:40:PRO:HG3	3:B:2323:HOH:O	2.19	0.41
1:D:193:ARG:HE	1:D:197:ARG:CG	2.34	0.41
1:A:3:ARG:HE	1:A:181:ASP:CG	2.24	0.41
1:A:70:VAL:HA	1:A:71:PRO:HD2	1.98	0.41
1:B:41:TYR:HB3	3:B:2318:HOH:O	2.21	0.41
1:A:167:GLY:O	1:A:170:LEU:HD12	2.20	0.41
1:B:124:TYR:O	1:B:128:PHE:HB2	2.21	0.41
1:A:21:ARG:NH1	1:A:158:ALA:HB2	2.36	0.40
1:B:120:LEU:CD1	1:B:137:THR:HG21	2.51	0.40
1:B:140:LEU:HD21	1:B:182:ILE:HD11	2.03	0.40
1:B:31:ASP:O	1:B:34:LYS:HB2	2.21	0.40
1:C:108:LEU:HD12	1:C:108:LEU:HA	1.83	0.40
1:A:99:ARG:NH2	1:B:52:LYS:HD2	2.36	0.40
1:A:13:PHE:CA	1:C:2:PRO:HD2	2.51	0.40
1:A:13:PHE:HA	1:C:2:PRO:HD2	2.02	0.40
1:B:15:GLU:HB2	1:B:180:ARG:O	2.22	0.40
1:B:64:ALA:O	1:B:67:ASP:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:LYS:HE2	1:C:177:ARG:NH2	2.37	0.40
1:D:149:VAL:CG2	1:D:150:PRO:HD2	2.43	0.40
1:C:126:MET:O	1:C:129:THR:HG22	2.21	0.40
1:A:140:LEU:HD12	1:A:157:VAL:HG11	2.04	0.40
1:A:69:ASN:O	1:A:71:PRO:HD3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	183/221 (83%)	167 (91%)	15 (8%)	1 (0%)	29	35
1	B	180/221 (81%)	163 (91%)	13 (7%)	4 (2%)	6	5
1	C	181/221 (82%)	162 (90%)	16 (9%)	3 (2%)	9	8
1	D	182/221 (82%)	163 (90%)	17 (9%)	2 (1%)	14	15
All	All	726/884 (82%)	655 (90%)	61 (8%)	10 (1%)	11	11

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	173	ASP
1	D	162	ASN
1	A	146	GLY
1	B	197	ARG
1	B	10	LYS
1	C	10	LYS
1	C	32	ASP
1	C	158	ALA
1	B	131	ARG
1	D	92	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	166/194 (86%)	134 (81%)	32 (19%)	1	1
1	B	162/194 (84%)	128 (79%)	34 (21%)	1	1
1	C	164/194 (84%)	127 (77%)	37 (23%)	1	0
1	D	164/194 (84%)	132 (80%)	32 (20%)	1	1
All	All	656/776 (84%)	521 (79%)	135 (21%)	1	1

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	9	GLU
1	A	10	LYS
1	A	11	ILE
1	A	27	LYS
1	A	28	ARG
1	A	31	ASP
1	A	39	ARG
1	A	48	ILE
1	A	80	SER
1	A	82	TYR
1	A	88	SER
1	A	89	SER
1	A	92	VAL
1	A	101	SER
1	A	114	VAL
1	A	125	HIS
1	A	126	MET
1	A	129	THR
1	A	144	ARG
1	A	145	GLU
1	A	148	ARG
1	A	160	ILE
1	A	166	ILE

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Mol	Chain	Res	Type
1	A	170	LEU
1	A	171	ASP
1	A	172	TYR
1	A	174	ASP
1	A	177	ARG
1	A	181	ASP
1	A	186	ARG
1	A	189	VAL
1	B	3	ARG
1	B	4	GLU
1	B	10	LYS
1	B	11	ILE
1	B	12	LEU
1	B	14	THR
1	B	15	GLU
1	B	34	LYS
1	B	36	LYS
1	B	39	ARG
1	B	49	SER
1	B	52	LYS
1	B	63	ARG
1	B	72	VAL
1	B	80	SER
1	B	94	MET
1	B	98	THR
1	B	99	ARG
1	B	100	HIS
1	B	113	ILE
1	B	120	LEU
1	B	125	HIS
1	B	129	THR
1	B	130	ARG
1	B	136	LYS
1	B	149	VAL
1	B	152	SER
1	B	162	ASN
1	B	166	ILE
1	B	174	ASP
1	B	188	GLU
1	B	193	ARG
1	B	194	GLU
1	B	198	GLN

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Mol	Chain	Res	Type
1	C	3	ARG
1	C	4	GLU
1	C	6	GLU
1	C	7	PHE
1	C	9	GLU
1	C	10	LYS
1	C	11	ILE
1	C	16	GLU
1	C	22	ILE
1	C	24	GLU
1	C	28	ARG
1	C	31	ASP
1	C	36	LYS
1	C	39	ARG
1	C	49	SER
1	C	58	THR
1	C	63	ARG
1	C	82	TYR
1	C	89	SER
1	C	92	VAL
1	C	99	ARG
1	C	111	GLU
1	C	118	LEU
1	C	128	PHE
1	C	129	THR
1	C	131	ARG
1	C	134	SER
1	C	140	LEU
1	C	145	GLU
1	C	149	VAL
1	C	152	SER
1	C	165	VAL
1	C	166	ILE
1	C	171	ASP
1	C	173	ASP
1	C	174	ASP
1	C	183	VAL
1	D	6	GLU
1	D	9	GLU
1	D	10	LYS
1	D	19	ARG
1	D	25	VAL

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Mol	Chain	Res	Type
1	D	27	LYS
1	D	31	ASP
1	D	34	LYS
1	D	42	VAL
1	D	47	LEU
1	D	49	SER
1	D	54	SER
1	D	69	ASN
1	D	99	ARG
1	D	101	SER
1	D	111	GLU
1	D	113	ILE
1	D	114	VAL
1	D	120	LEU
1	D	126	MET
1	D	145	GLU
1	D	147	ARG
1	D	148	ARG
1	D	149	VAL
1	D	152	SER
1	D	157	VAL
1	D	164	PHE
1	D	174	ASP
1	D	186	ARG
1	D	189	VAL
1	D	192	GLU
1	D	193	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	B	159	ASN
1	B	162	ASN
1	B	198	GLN
1	D	43	ASN
1	D	105	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	IMP	B	2300	-	21,25,25	1.71	3 (14%)	23,38,38	1.55	4 (17%)
2	IMP	A	1300	-	21,25,25	1.66	3 (14%)	23,38,38	1.77	7 (30%)
2	IMP	D	4300	-	21,25,25	1.69	3 (14%)	23,38,38	1.78	5 (21%)
2	IMP	C	3300	-	21,25,25	1.65	3 (14%)	23,38,38	1.67	6 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMP	B	2300	-	-	3/6/26/26	0/3/3/3
2	IMP	A	1300	-	-	2/6/26/26	0/3/3/3
2	IMP	D	4300	-	-	3/6/26/26	0/3/3/3
2	IMP	C	3300	-	-	1/6/26/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2300	IMP	C6-N1	5.41	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4300	IMP	C6-N1	5.27	1.42	1.33
2	C	3300	IMP	C6-N1	5.25	1.42	1.33
2	A	1300	IMP	C6-N1	5.05	1.41	1.33
2	D	4300	IMP	C2-N1	2.93	1.39	1.33
2	A	1300	IMP	C2-N1	2.92	1.39	1.33
2	B	2300	IMP	C8-N7	-2.86	1.29	1.34
2	A	1300	IMP	C8-N7	-2.75	1.29	1.34
2	C	3300	IMP	C8-N7	-2.73	1.29	1.34
2	D	4300	IMP	C8-N7	-2.71	1.29	1.34
2	B	2300	IMP	C2-N1	2.68	1.38	1.33
2	C	3300	IMP	C2-N1	2.61	1.38	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3300	IMP	C2-N1-C6	3.95	122.50	115.88
2	A	1300	IMP	C2-N1-C6	3.76	122.18	115.88
2	D	4300	IMP	C2-N1-C6	3.69	122.06	115.88
2	B	2300	IMP	C2-N1-C6	3.65	122.00	115.88
2	D	4300	IMP	N3-C2-N1	-3.45	123.28	128.68
2	C	3300	IMP	N3-C2-N1	-3.38	123.40	128.68
2	D	4300	IMP	C6-C5-C4	-3.29	117.65	120.80
2	A	1300	IMP	N3-C2-N1	-3.20	123.68	128.68
2	B	2300	IMP	N3-C2-N1	-3.15	123.75	128.68
2	D	4300	IMP	C1'-N9-C4	-3.11	121.17	126.64
2	B	2300	IMP	O4'-C4'-C5'	-2.99	99.52	109.37
2	A	1300	IMP	C1'-N9-C4	-2.84	121.65	126.64
2	A	1300	IMP	O5'-C5'-C4'	2.81	118.67	108.99
2	A	1300	IMP	C6-C5-C4	-2.74	118.18	120.80
2	C	3300	IMP	C6-C5-C4	-2.71	118.21	120.80
2	D	4300	IMP	O4'-C4'-C5'	-2.71	100.47	109.37
2	A	1300	IMP	O4'-C4'-C5'	-2.50	101.15	109.37
2	C	3300	IMP	O4'-C4'-C5'	-2.44	101.34	109.37
2	B	2300	IMP	C6-C5-C4	-2.40	118.51	120.80
2	A	1300	IMP	C5'-C4'-C3'	2.38	124.10	115.18
2	C	3300	IMP	C1'-N9-C4	-2.31	122.59	126.64
2	C	3300	IMP	O5'-C5'-C4'	2.06	116.08	108.99

There are no chirality outliers.

All (9) torsion outliers are listed below:

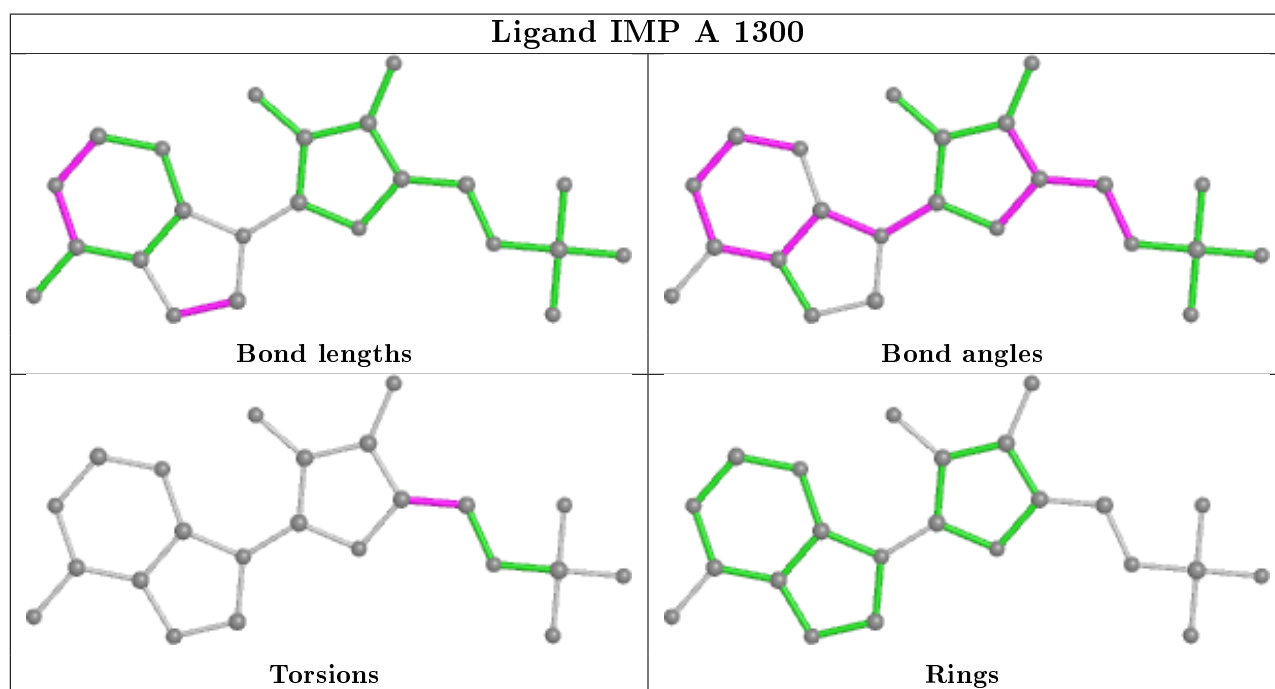
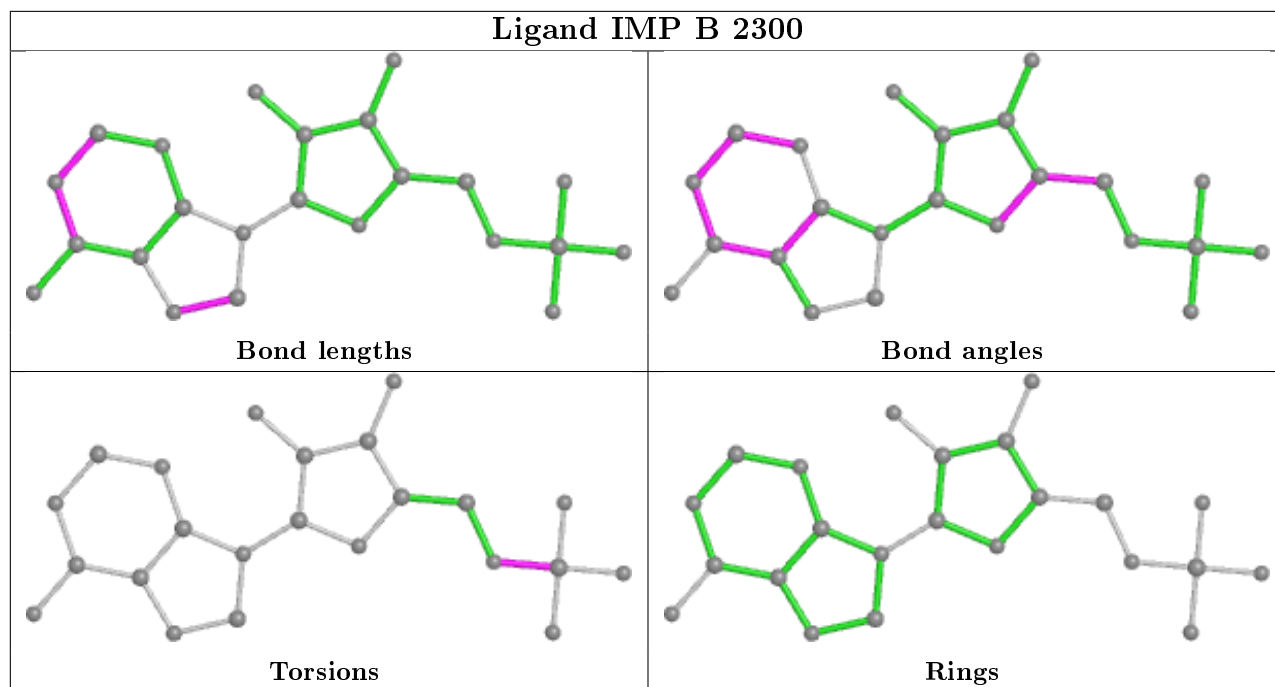
Mol	Chain	Res	Type	Atoms
2	B	2300	IMP	C5'-O5'-P-O1P
2	B	2300	IMP	C5'-O5'-P-O2P
2	B	2300	IMP	C5'-O5'-P-O3P
2	C	3300	IMP	O4'-C4'-C5'-O5'
2	A	1300	IMP	C3'-C4'-C5'-O5'
2	A	1300	IMP	O4'-C4'-C5'-O5'
2	D	4300	IMP	C3'-C4'-C5'-O5'
2	D	4300	IMP	O4'-C4'-C5'-O5'
2	D	4300	IMP	C5'-O5'-P-O1P

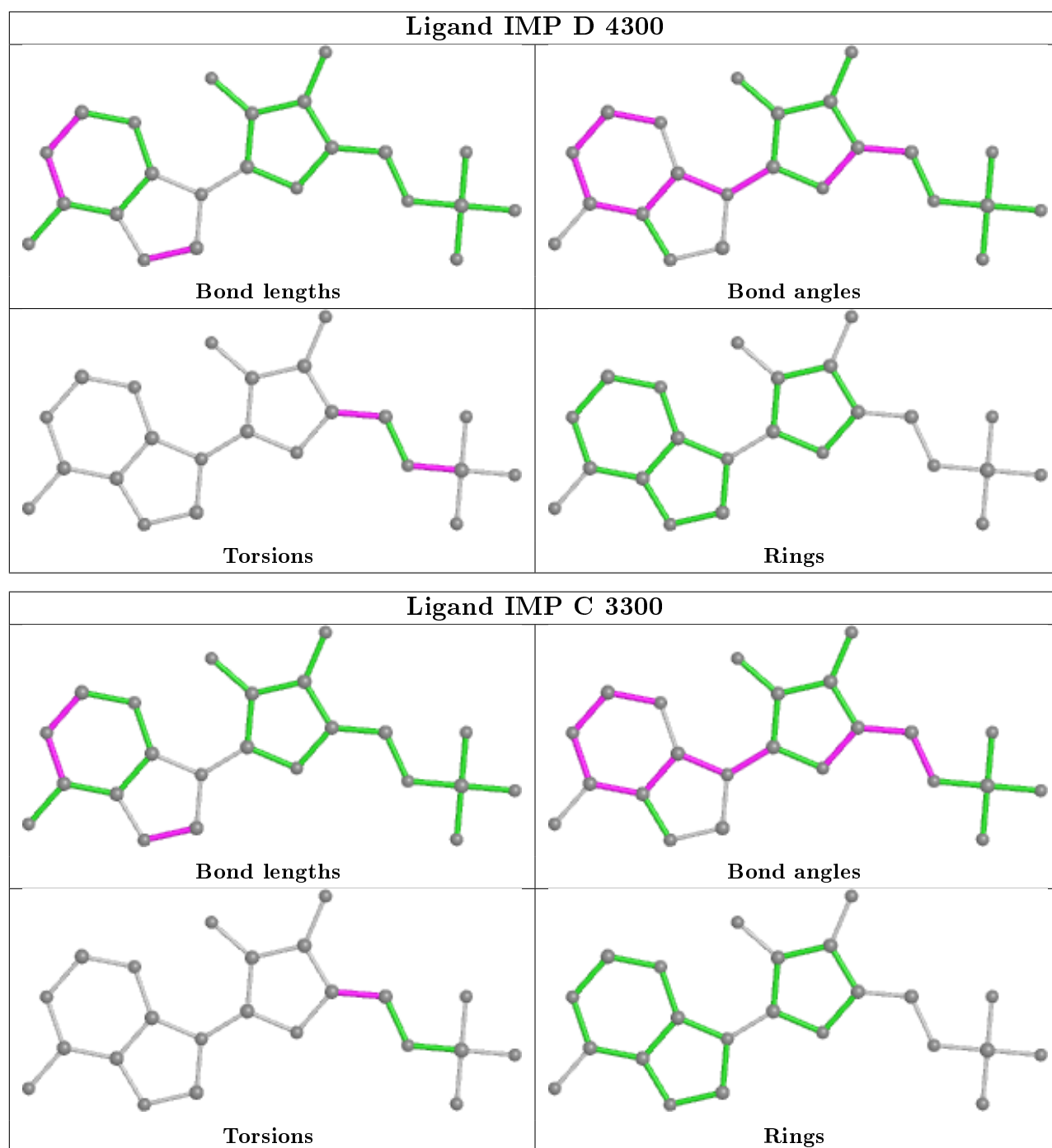
There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2300	IMP	1	0
2	A	1300	IMP	6	0
2	D	4300	IMP	1	0
2	C	3300	IMP	4	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.