



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:07 am BST

PDB ID : 3IRM
Title : Trypanosoma cruzi Dihydrofolate Reductase-Thymidylate Synthase COM-
PLEXED WITH Cycloguanil
Authors : Chitnumsub, P.; Yuvaniyama, J.; Yuthavong, Y.
Deposited on : 2009-08-24
Resolution : 2.10 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)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

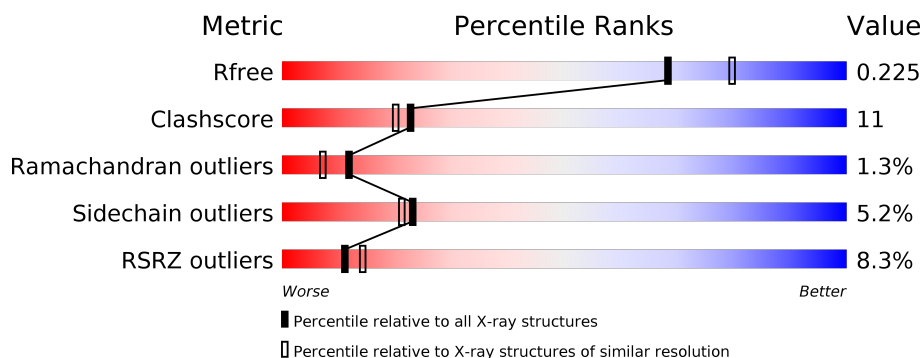
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	521	<div> <div>7%</div> <div>79%18%</div> <div>.</div> </div>
1	B	521	<div> <div>10%</div> <div>72%23%</div> <div>.</div> </div>
1	C	521	<div> <div>7%</div> <div>77%19%</div> <div>..</div> </div>
1	D	521	<div> <div>7%</div> <div>69%27%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACT	D	808	-	-	X	-

2 Entry composition [i](#)

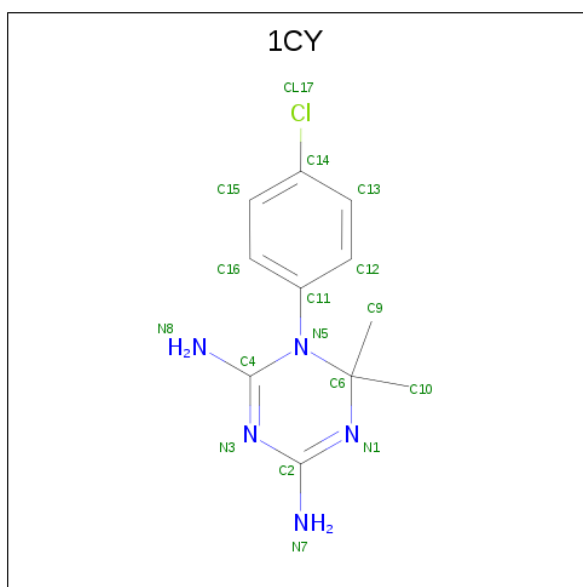
There are 5 unique types of molecules in this entry. The entry contains 17255 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	0	0
			4137	2624	731	761	21			
1	B	519	Total	C	N	O	S	0	0	0
			4131	2621	730	760	20			
1	C	516	Total	C	N	O	S	0	0	0
			4107	2605	726	757	19			
1	D	513	Total	C	N	O	S	0	0	0
			4087	2594	723	752	18			

- Molecule 2 is 1-(4-chlorophenyl)-6,6-dimethyl-1,6-dihydro-1,3,5-triazine-2,4-diamine (three-letter code: 1CY) (formula: C₁₁H₁₄ClN₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	0	0
			17	11	1	5		
2	B	1	Total	C	Cl	N	0	0
			17	11	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	Cl	N	0	0
			17	11	1	5		
2	D	1	Total	C	Cl	N	0	0
			17	11	1	5		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

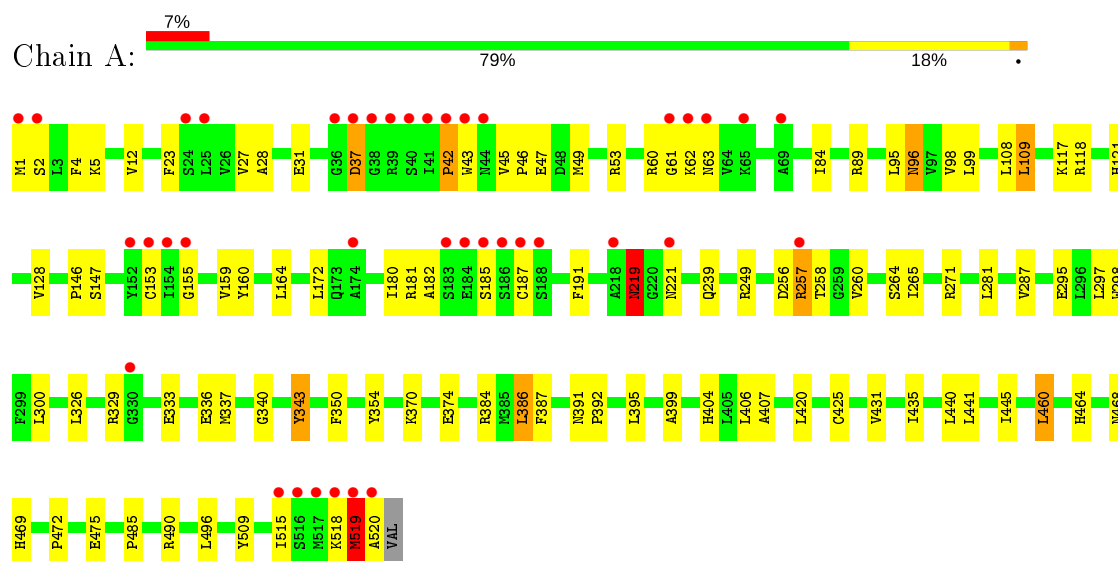
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	193	Total O 193 193	0	0
5	B	123	Total O 123 123	0	0
5	C	189	Total O 189 189	0	0
5	D	148	Total O 148 148	0	0

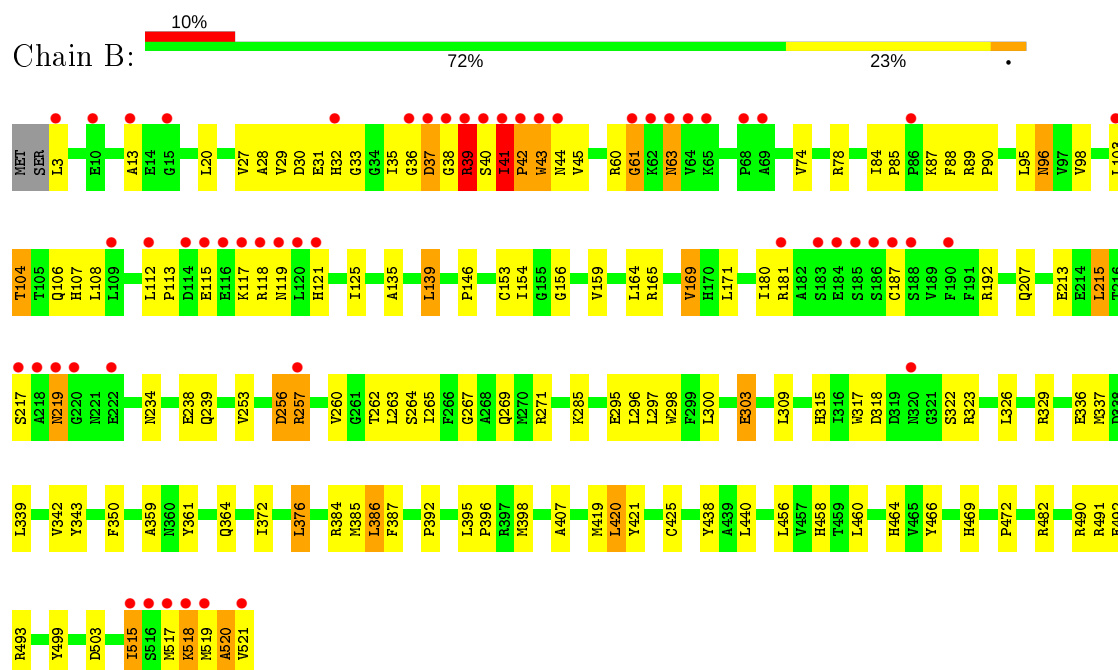
3 Residue-property plots [i](#)

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

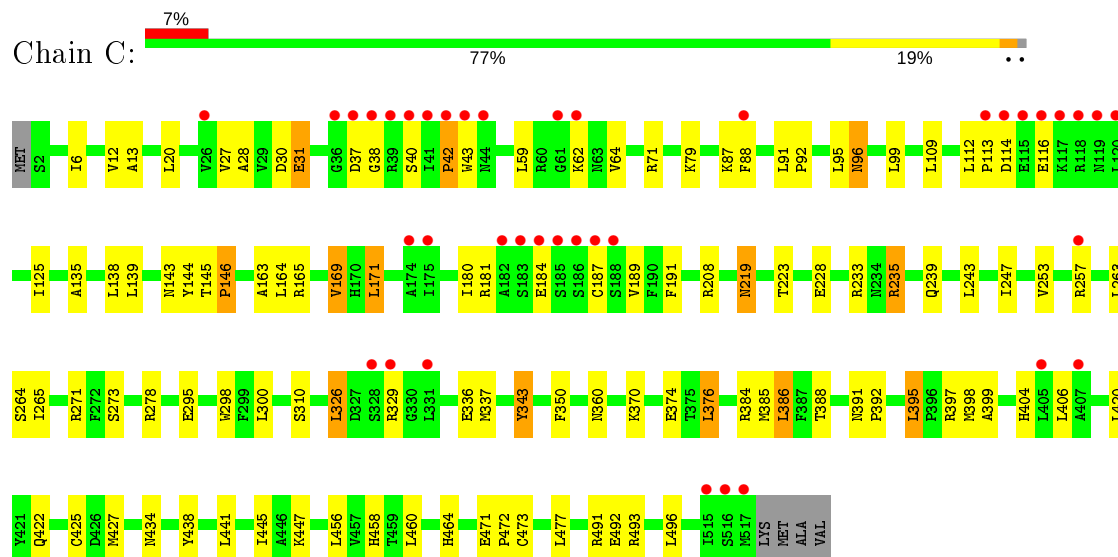
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



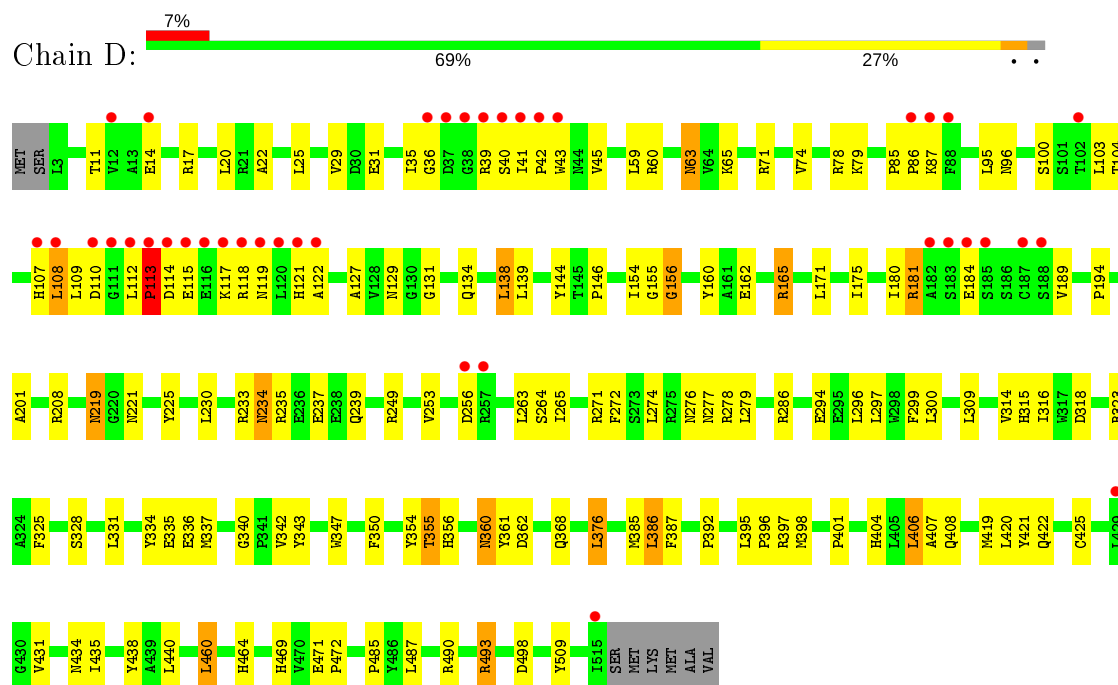
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.44Å 165.79Å 84.77Å 90.00° 113.39° 90.00°	Depositor
Resolution (Å)	29.97 – 2.10 29.97 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.5 (29.97-2.10) 91.5 (29.97-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.10Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.202 , 0.245 0.194 , 0.225	Depositor DCC
R_{free} test set	5532 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17255	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: 1CY, PO4, ACT

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	0/4237	0.63	0/5746
1	B	0.34	0/4231	0.62	1/5738 (0.0%)
1	C	0.34	0/4207	0.64	0/5708
1	D	0.34	0/4187	0.64	1/5682 (0.0%)
All	All	0.34	0/16862	0.63	2/22874 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	156	GLY	N-CA-C	-5.35	99.72	113.10
1	B	156	GLY	N-CA-C	-5.33	99.78	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4137	0	4099	75	0
1	B	4131	0	4091	120	0
1	C	4107	0	4060	75	0
1	D	4087	0	4041	121	0
2	A	17	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	17	0	14	0	0
2	C	17	0	14	0	0
2	D	17	0	14	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
4	A	12	0	9	1	0
4	B	12	0	9	1	0
4	C	4	0	3	1	0
4	D	4	0	3	4	0
5	A	193	0	0	5	0
5	B	123	0	0	4	0
5	C	189	0	0	1	0
5	D	148	0	0	5	0
All	All	17255	0	16371	379	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 11.

All (379) 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:257:ARG:H	1:B:257:ARG:HD3	1.23	1.00
1:B:41:ILE:H	1:B:42:PRO:HD3	1.26	1.00
1:D:79:LYS:HB2	4:D:808:ACT:H1	1.42	1.00
1:B:41:ILE:H	1:B:42:PRO:CD	1.79	0.96
1:C:300:LEU:HD13	1:C:496:LEU:HD11	1.50	0.93
1:B:239:GLN:HE22	1:B:271:ARG:H	1.18	0.91
1:D:112:LEU:HD12	1:D:113:PRO:HD2	1.54	0.89
1:A:1:MET:HB2	1:A:5:LYS:HG3	1.54	0.87
1:B:115:GLU:HG3	1:B:118:ARG:HD3	1.58	0.85
1:C:239:GLN:HE22	1:C:271:ARG:H	1.29	0.79
1:D:131:GLY:H	1:D:134:GLN:NE2	1.79	0.79
1:C:376:LEU:HD13	1:C:385:MET:SD	2.23	0.79
1:B:491:ARG:HD3	1:B:493:ARG:HH12	1.49	0.77
1:D:114:ASP:HB3	1:D:117:LYS:CB	2.16	0.76
1:B:112:LEU:HB3	1:B:117:LYS:HE3	1.66	0.76
1:B:376:LEU:HD13	1:B:385:MET:SD	2.26	0.75
1:D:114:ASP:HB3	1:D:117:LYS:HB2	1.66	0.75
1:C:425:CYS:SG	1:C:460:LEU:HD22	2.28	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:GLU:OE2	1:C:181:ARG:HG3	1.87	0.74
1:B:41:ILE:N	1:B:42:PRO:CD	2.51	0.73
1:D:355:THR:HG22	1:D:356:HIS:N	2.03	0.73
1:D:397:ARG:HG2	1:D:397:ARG:HH11	1.54	0.72
1:B:104:THR:HG22	1:B:107:HIS:H	1.55	0.72
1:C:253:VAL:HG22	1:C:263:LEU:CD2	2.19	0.72
1:D:117:LYS:HE2	1:D:121:HIS:NE2	2.03	0.72
1:D:45:VAL:HG21	1:D:180:ILE:HD12	1.71	0.72
1:A:42:PRO:HD2	5:A:1608:HOH:O	1.89	0.72
1:C:40:SER:O	1:C:42:PRO:HD3	1.89	0.71
1:D:115:GLU:HA	1:D:118:ARG:NH1	2.06	0.71
1:A:425:CYS:SG	1:A:460:LEU:HD12	2.31	0.69
1:B:115:GLU:HA	1:B:118:ARG:HB2	1.75	0.69
1:A:518:LYS:HG2	1:A:519:MET:H	1.55	0.69
1:A:239:GLN:HE22	1:A:271:ARG:H	1.41	0.69
1:B:491:ARG:HD3	1:B:493:ARG:NH1	2.07	0.69
1:C:164:LEU:HA	1:C:169:VAL:HG13	1.75	0.69
1:D:360:ASN:HD22	1:D:360:ASN:C	1.96	0.68
1:B:104:THR:H	1:B:107:HIS:HB2	1.58	0.67
1:D:360:ASN:ND2	1:D:362:ASP:H	1.93	0.67
1:D:117:LYS:C	1:D:119:ASN:H	1.96	0.67
1:A:257:ARG:CD	1:A:257:ARG:H	2.08	0.66
1:D:376:LEU:HD13	1:D:385:MET:SD	2.34	0.66
1:C:392:PRO:HA	1:C:395:LEU:HD22	1.78	0.65
1:A:1:MET:HG2	5:A:1587:HOH:O	1.96	0.65
1:A:518:LYS:O	1:A:519:MET:HB3	1.95	0.65
1:A:62:LYS:O	1:A:63:ASN:HB2	1.97	0.65
1:B:234:ASN:O	1:B:238:GLU:HG3	1.97	0.65
1:D:115:GLU:HA	1:D:118:ARG:HH11	1.62	0.64
1:D:425:CYS:SG	1:D:460:LEU:HD12	2.38	0.64
1:D:155:GLY:HA2	1:D:160:TYR:CZ	2.33	0.64
1:A:256:ASP:HB2	1:A:257:ARG:HH11	1.62	0.64
1:B:45:VAL:HG21	1:B:180:ILE:HD12	1.80	0.63
1:C:404:HIS:HB2	1:C:420:LEU:HD11	1.81	0.63
1:A:37:ASP:HA	1:A:187:CYS:HA	1.82	0.62
1:D:239:GLN:HE22	1:D:271:ARG:H	1.48	0.62
1:B:239:GLN:NE2	1:B:271:ARG:H	1.92	0.62
1:B:285:LYS:HE2	1:B:515:ILE:HD11	1.82	0.62
1:B:135:ALA:O	1:B:139:LEU:HD22	2.00	0.61
1:C:164:LEU:HA	1:C:169:VAL:CG1	2.30	0.61
1:C:40:SER:C	1:C:42:PRO:HD3	2.20	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HB3	1:A:4:PHE:HB2	1.82	0.61
1:B:87:LYS:HE3	1:B:88:PHE:CE2	2.36	0.61
1:D:234:ASN:C	1:D:234:ASN:HD22	2.04	0.61
1:B:78:ARG:HG3	1:B:103:LEU:HD12	1.83	0.61
1:B:74:VAL:HG11	1:B:154:ILE:HD13	1.81	0.60
1:C:278:ARG:HD3	5:C:1530:HOH:O	2.00	0.60
1:A:109:LEU:O	1:A:118:ARG:HD3	2.02	0.60
1:B:257:ARG:N	1:B:257:ARG:HD3	2.05	0.59
1:B:303:GLU:HG3	5:B:1463:HOH:O	2.02	0.59
1:C:388:THR:HB	1:C:406:LEU:HD12	1.84	0.59
1:D:360:ASN:HD22	1:D:361:TYR:N	2.01	0.59
1:D:490:ARG:NH1	1:D:490:ARG:HB3	2.18	0.58
1:B:213:GLU:O	1:B:215:LEU:HD13	2.03	0.58
1:A:46:PRO:HG2	1:A:47:GLU:OE1	2.04	0.58
1:B:29:VAL:HG21	1:B:33:GLY:HA2	1.85	0.58
1:D:253:VAL:HG22	1:D:263:LEU:CD2	2.34	0.58
1:A:404:HIS:HB2	1:A:420:LEU:HD11	1.84	0.58
1:B:104:THR:HG23	1:B:106:GLN:H	1.69	0.57
1:C:6:ILE:HD11	1:C:370:LYS:HB2	1.86	0.57
1:C:59:LEU:HD21	1:C:71:ARG:HA	1.86	0.57
1:B:336:GLU:O	1:B:337:MET:HB2	2.04	0.57
1:B:39:ARG:O	1:B:39:ARG:HD3	2.04	0.57
1:D:110:ASP:HA	1:D:118:ARG:HE	1.70	0.57
1:A:98:VAL:HB	1:A:108:LEU:HD21	1.86	0.57
1:B:364:GLN:HG3	5:B:1198:HOH:O	2.03	0.57
1:D:404:HIS:HB2	1:D:420:LEU:HD11	1.86	0.56
1:B:387:PHE:CE2	1:B:407:ALA:HB3	2.41	0.56
1:B:491:ARG:CD	1:B:493:ARG:NH1	2.69	0.56
1:B:96:ASN:N	1:B:96:ASN:HD22	2.04	0.56
1:A:468:ASN:O	1:A:520:ALA:HB1	2.06	0.56
1:D:74:VAL:CG1	1:D:154:ILE:HD13	2.36	0.56
1:D:60:ARG:NH2	5:D:1044:HOH:O	2.37	0.56
1:D:340:GLY:HA2	1:D:354:TYR:CE2	2.41	0.56
1:C:273:SER:HB3	1:C:278:ARG:HH21	1.71	0.56
1:D:490:ARG:HB3	1:D:490:ARG:HH11	1.71	0.56
1:B:29:VAL:HG22	1:B:30:ASP:N	2.21	0.55
1:B:3:LEU:O	1:B:3:LEU:HD23	2.05	0.55
1:B:207:GLN:NE2	1:D:249:ARG:HH21	2.03	0.55
1:A:60:ARG:NH2	5:A:1086:HOH:O	2.38	0.55
1:B:84:ILE:CG2	1:B:89:ARG:HG2	2.36	0.55
1:C:59:LEU:HB2	1:C:64:VAL:HG13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:PRO:HD2	1:D:350:PHE:CE1	2.41	0.55
1:B:517:MET:O	1:B:518:LYS:C	2.45	0.55
1:D:335:GLU:HB2	5:D:1359:HOH:O	2.06	0.55
1:D:100:SER:O	1:D:129:ASN:HA	2.06	0.54
1:D:78:ARG:HE	1:D:103:LEU:HD11	1.71	0.54
1:D:264:SER:HB3	1:D:464:HIS:HB3	1.90	0.54
1:D:59:LEU:HD21	1:D:71:ARG:HA	1.90	0.54
4:D:808:ACT:H2	5:D:1497:HOH:O	2.07	0.54
1:C:165:ARG:C	1:C:169:VAL:HG22	2.28	0.54
1:D:219:ASN:ND2	1:D:221:ASN:H	2.06	0.54
1:B:60:ARG:NH2	5:B:1053:HOH:O	2.40	0.54
1:A:256:ASP:OD2	1:A:260:VAL:HB	2.08	0.53
1:B:519:MET:O	1:B:520:ALA:HB2	2.07	0.53
1:A:370:LYS:O	1:A:374:GLU:HG2	2.08	0.53
1:B:315:HIS:HB3	1:B:318:ASP:OD1	2.09	0.53
1:A:31:GLU:HG3	1:A:181:ARG:HA	1.90	0.53
1:B:31:GLU:HG3	1:B:181:ARG:HA	1.91	0.53
1:D:138:LEU:HD22	1:D:144:TYR:CE2	2.44	0.53
1:D:315:HIS:HB3	1:D:318:ASP:OD1	2.09	0.53
1:A:386:LEU:HD12	1:A:406:LEU:HD11	1.91	0.53
1:C:253:VAL:HG22	1:C:263:LEU:HD22	1.91	0.53
1:B:420:LEU:HD22	1:B:438:TYR:CD2	2.44	0.53
1:D:336:GLU:O	1:D:337:MET:HB2	2.09	0.53
1:D:342:VAL:HG12	1:D:398:MET:HB3	1.90	0.53
1:D:355:THR:CG2	1:D:356:HIS:N	2.72	0.53
1:B:519:MET:HG2	1:B:519:MET:O	2.08	0.53
1:B:395:LEU:HB2	1:B:396:PRO:HD3	1.91	0.52
1:A:257:ARG:HD3	1:A:257:ARG:H	1.73	0.52
1:B:493:ARG:HB2	1:B:499:TYR:CE1	2.44	0.52
1:D:397:ARG:HG2	1:D:397:ARG:NH1	2.24	0.52
1:B:85:PRO:HB2	1:B:88:PHE:HD2	1.74	0.52
1:C:20:LEU:HB2	1:C:171:LEU:HD13	1.91	0.52
1:C:392:PRO:HD2	1:D:350:PHE:CZ	2.44	0.52
1:B:207:GLN:HE21	1:D:249:ARG:HH21	1.58	0.52
1:C:336:GLU:O	1:C:337:MET:HB2	2.08	0.52
1:C:13:ALA:HB2	1:C:492:GLU:HG3	1.91	0.52
1:D:114:ASP:HB3	1:D:117:LYS:HB3	1.89	0.52
1:D:493:ARG:HG2	1:D:498:ASP:HB2	1.91	0.52
1:B:253:VAL:HG22	1:B:263:LEU:HG	1.91	0.52
1:A:45:VAL:HG21	1:A:180:ILE:HD13	1.91	0.52
1:B:296:LEU:HG	1:B:300:LEU:CD2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ILE:O	1:B:89:ARG:HD3	2.11	0.51
1:B:164:LEU:C	1:B:169:VAL:HG13	2.30	0.51
1:B:165:ARG:C	1:B:169:VAL:HG22	2.30	0.51
1:D:460:LEU:N	1:D:460:LEU:HD22	2.26	0.51
1:A:490:ARG:HB2	1:A:490:ARG:HH11	1.75	0.51
1:B:74:VAL:CG1	1:B:154:ILE:HD13	2.40	0.51
1:B:39:ARG:NH2	1:B:41:ILE:HB	2.26	0.51
1:D:180:ILE:HD13	1:D:225:TYR:HB2	1.91	0.51
1:A:300:LEU:HD21	1:A:441:LEU:CD1	2.41	0.51
1:A:384:ARG:C	1:A:386:LEU:HD23	2.31	0.50
1:D:355:THR:HG23	1:D:356:HIS:CD2	2.46	0.50
1:A:336:GLU:O	1:A:337:MET:HB2	2.11	0.50
1:B:20:LEU:HB2	1:B:171:LEU:CD1	2.42	0.50
1:B:296:LEU:CD2	1:B:440:LEU:HG	2.41	0.50
1:B:425:CYS:SG	1:B:460:LEU:HD22	2.51	0.50
1:A:350:PHE:CE1	1:B:392:PRO:HD2	2.47	0.50
1:A:84:ILE:CG2	1:A:89:ARG:HG3	2.41	0.50
1:A:271:ARG:NH2	1:B:267:GLY:O	2.44	0.50
1:A:329:ARG:HH11	1:A:329:ARG:HG3	1.77	0.50
1:C:143:ASN:ND2	1:C:144:TYR:CE2	2.80	0.50
1:D:325:PHE:O	1:D:328:SER:HB3	2.12	0.50
1:D:420:LEU:HD13	1:D:438:TYR:CZ	2.46	0.49
1:D:96:ASN:HD22	1:D:96:ASN:N	2.10	0.49
1:A:431:VAL:O	1:A:435:ILE:HG13	2.11	0.49
1:B:420:LEU:HD12	1:B:421:TYR:N	2.27	0.49
1:C:329:ARG:NH1	1:C:399:ALA:O	2.46	0.49
1:D:265:ILE:HD12	1:D:265:ILE:C	2.32	0.49
1:A:387:PHE:CE1	1:A:407:ALA:HB3	2.47	0.49
1:C:109:LEU:HD12	1:C:125:ILE:HD12	1.93	0.49
1:C:79:LYS:HD2	4:C:807:ACT:H2	1.94	0.49
1:D:233:ARG:CZ	1:D:235:ARG:NH1	2.76	0.49
1:A:153:CYS:SG	1:A:159:VAL:HG12	2.53	0.49
1:D:31:GLU:HG3	1:D:181:ARG:HA	1.94	0.49
1:D:74:VAL:HG11	1:D:154:ILE:HD13	1.93	0.49
1:B:164:LEU:C	1:B:169:VAL:CG1	2.81	0.49
1:C:163:ALA:O	1:C:169:VAL:HG13	2.12	0.49
1:D:175:ILE:HB	1:D:230:LEU:HB2	1.95	0.48
1:A:265:ILE:C	1:A:265:ILE:HD12	2.33	0.48
1:B:372:ILE:HG22	1:B:376:LEU:HD22	1.94	0.48
1:D:156:GLY:HA3	4:D:808:ACT:O	2.13	0.48
1:B:41:ILE:HD13	1:B:44:ASN:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:ARG:NH1	1:B:503:ASP:OD2	2.47	0.48
1:A:117:LYS:HG3	1:A:121:HIS:HD2	1.78	0.48
1:A:257:ARG:CD	1:A:257:ARG:N	2.76	0.48
1:D:331:LEU:HD13	1:D:334:TYR:CE2	2.49	0.48
1:D:36:GLY:O	1:D:40:SER:HB2	2.14	0.48
1:B:84:ILE:HG22	1:B:89:ARG:HG2	1.95	0.48
1:A:147:SER:HB2	5:A:1320:HOH:O	2.13	0.48
1:D:162:GLU:HG3	1:D:165:ARG:NH1	2.29	0.48
1:B:87:LYS:HE3	1:B:88:PHE:HE2	1.79	0.48
1:C:164:LEU:CA	1:C:169:VAL:HG13	2.44	0.48
1:C:384:ARG:HD3	1:D:401:PRO:HG2	1.95	0.48
1:C:59:LEU:HB2	1:C:64:VAL:CG1	2.44	0.47
1:B:37:ASP:C	1:B:39:ARG:H	2.18	0.47
1:A:27:VAL:HG22	1:A:28:ALA:N	2.29	0.47
1:D:407:ALA:HA	1:D:419:MET:O	2.14	0.47
1:A:257:ARG:HD3	1:A:257:ARG:N	2.29	0.47
1:B:38:GLY:O	1:B:39:ARG:CB	2.63	0.47
1:B:219:ASN:C	1:B:219:ASN:HD22	2.16	0.47
1:B:265:ILE:HD12	1:B:265:ILE:C	2.34	0.47
1:A:392:PRO:HD2	1:B:350:PHE:CZ	2.49	0.47
1:C:350:PHE:CE1	1:D:392:PRO:HD2	2.50	0.47
1:D:63:ASN:HD22	1:D:63:ASN:C	2.18	0.47
1:C:458:HIS:CE1	1:C:460:LEU:HD21	2.50	0.47
1:C:350:PHE:CZ	1:D:392:PRO:HD2	2.50	0.47
1:A:518:LYS:CG	1:A:519:MET:H	2.20	0.47
1:D:41:ILE:N	1:D:42:PRO:HD3	2.30	0.47
1:D:420:LEU:HD22	1:D:438:TYR:CD2	2.49	0.47
1:B:295:GLU:O	1:B:298:TRP:HB3	2.15	0.46
1:A:45:VAL:CG2	1:A:180:ILE:HD13	2.45	0.46
1:B:29:VAL:CG2	1:B:33:GLY:C	2.84	0.46
1:B:329:ARG:HE	1:B:329:ARG:HB3	1.56	0.46
1:C:114:ASP:N	1:C:114:ASP:OD1	2.48	0.46
1:D:286:ARG:NH2	5:D:1268:HOH:O	2.49	0.46
1:A:485:PRO:HB3	1:A:509:TYR:HA	1.97	0.46
1:B:61:GLY:O	1:B:63:ASN:N	2.45	0.46
1:A:1:MET:HB2	1:A:5:LYS:CG	2.37	0.46
1:A:460:LEU:HD22	1:A:460:LEU:N	2.31	0.46
1:B:98:VAL:HB	1:B:108:LEU:HD21	1.97	0.46
1:C:386:LEU:HD23	1:C:386:LEU:N	2.30	0.46
1:D:386:LEU:HD23	1:D:386:LEU:N	2.31	0.46
1:D:272:PHE:CZ	1:D:435:ILE:HD13	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:PRO:HD2	1:B:350:PHE:CE1	2.50	0.46
1:D:296:LEU:CD2	1:D:440:LEU:HG	2.46	0.46
1:A:329:ARG:NH1	1:A:399:ALA:O	2.49	0.46
1:D:156:GLY:HA3	4:D:808:ACT:C	2.46	0.46
1:A:219:ASN:N	1:A:219:ASN:HD22	2.11	0.46
1:C:96:ASN:N	1:C:96:ASN:HD22	2.13	0.46
1:C:422:GLN:HE22	1:C:434:ASN:ND2	2.13	0.46
1:B:45:VAL:HG13	1:B:217:SER:OG	2.15	0.46
1:B:264:SER:HB3	1:B:464:HIS:HB3	1.97	0.46
1:B:466:TYR:O	1:B:469:HIS:HB2	2.16	0.46
1:B:31:GLU:OE1	1:B:181:ARG:CZ	2.64	0.45
1:B:29:VAL:HG22	1:B:30:ASP:H	1.81	0.45
1:B:20:LEU:HB2	1:B:171:LEU:HD11	1.96	0.45
1:D:108:LEU:HD22	1:D:127:ALA:HB2	1.98	0.45
1:D:323:ARG:NE	1:D:323:ARG:HA	2.31	0.45
1:B:256:ASP:HB2	1:B:260:VAL:H	1.81	0.45
1:B:407:ALA:HA	1:B:419:MET:O	2.16	0.45
1:C:138:LEU:HD11	1:C:144:TYR:CE2	2.52	0.45
1:C:264:SER:HB3	1:C:464:HIS:HB3	1.97	0.45
1:D:131:GLY:H	1:D:134:GLN:CD	2.19	0.45
1:B:384:ARG:C	1:B:386:LEU:HD23	2.37	0.45
1:A:239:GLN:NE2	1:A:271:ARG:H	2.12	0.45
1:B:103:LEU:HB3	1:B:108:LEU:CD1	2.47	0.45
1:B:322:SER:O	1:B:326:LEU:HD13	2.16	0.45
1:A:256:ASP:OD1	1:A:258:THR:N	2.48	0.45
1:D:234:ASN:ND2	1:D:237:GLU:H	2.15	0.45
1:A:281:LEU:HD22	1:A:287:VAL:HB	1.99	0.44
1:A:96:ASN:HD22	1:A:96:ASN:N	2.14	0.44
1:C:233:ARG:CZ	1:C:235:ARG:NH1	2.80	0.44
1:D:314:VAL:HG12	1:D:316:ILE:HG12	1.99	0.44
1:D:360:ASN:ND2	1:D:360:ASN:C	2.69	0.44
1:A:386:LEU:N	1:A:386:LEU:HD23	2.32	0.44
1:C:265:ILE:C	1:C:265:ILE:HD12	2.38	0.44
1:B:35:ILE:HG13	1:B:36:GLY:N	2.33	0.44
1:A:350:PHE:CZ	1:B:392:PRO:HD2	2.52	0.44
1:B:253:VAL:HA	1:B:262:THR:O	2.17	0.44
1:C:441:LEU:HD23	1:C:441:LEU:C	2.38	0.44
1:A:182:ALA:HB1	1:A:185:SER:HB2	1.98	0.44
1:D:294:GLU:HA	1:D:294:GLU:OE1	2.17	0.44
1:D:78:ARG:HG3	1:D:103:LEU:HD12	1.99	0.44
1:D:331:LEU:HB3	1:D:334:TYR:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:THR:HG22	1:D:356:HIS:H	1.78	0.44
1:C:406:LEU:HD22	1:D:406:LEU:HD23	2.00	0.44
1:B:13:ALA:HB2	1:B:492:GLU:HG3	1.99	0.44
1:D:490:ARG:CB	1:D:490:ARG:NH1	2.80	0.44
1:A:249:ARG:HD3	5:A:1235:HOH:O	2.18	0.44
1:B:256:ASP:OD2	1:B:260:VAL:HB	2.18	0.44
1:C:471:GLU:N	1:C:472:PRO:HD2	2.33	0.44
1:C:496:LEU:C	1:C:496:LEU:HD13	2.38	0.44
1:D:25:LEU:HD23	1:D:25:LEU:C	2.37	0.44
1:B:115:GLU:CG	1:B:118:ARG:HD3	2.40	0.43
1:B:520:ALA:O	1:B:521:VAL:HB	2.17	0.43
1:D:485:PRO:HB3	1:D:509:TYR:HA	2.00	0.43
1:B:296:LEU:HD23	1:B:440:LEU:HG	2.00	0.43
1:D:41:ILE:HG13	1:D:41:ILE:O	2.18	0.43
1:D:490:ARG:CB	1:D:490:ARG:CZ	2.96	0.43
1:D:117:LYS:C	1:D:119:ASN:N	2.66	0.43
1:D:299:PHE:HB3	1:D:347:TRP:CZ3	2.54	0.43
1:A:155:GLY:HA2	1:A:160:TYR:CZ	2.53	0.43
1:A:23:PHE:CE1	1:A:172:LEU:HD13	2.54	0.43
1:B:342:VAL:HG12	1:B:398:MET:HB3	2.01	0.43
1:D:296:LEU:HG	1:D:300:LEU:HD23	2.00	0.43
1:D:490:ARG:HB2	1:D:490:ARG:CZ	2.48	0.43
1:C:247:ILE:HD12	1:C:427:MET:HG3	1.99	0.43
1:B:43:TRP:HH2	1:B:187:CYS:HG	1.66	0.43
1:C:295:GLU:O	1:C:298:TRP:HB3	2.18	0.43
1:D:360:ASN:HD22	1:D:362:ASP:H	1.65	0.43
1:D:78:ARG:NE	1:D:103:LEU:HD11	2.32	0.43
1:D:431:VAL:O	1:D:435:ILE:HG13	2.18	0.43
1:A:295:GLU:O	1:A:298:TRP:HB3	2.19	0.43
1:A:475:GLU:HB2	1:A:515:ILE:HG21	2.00	0.43
1:B:387:PHE:CZ	1:B:407:ALA:HB3	2.54	0.43
1:C:208:ARG:NE	1:C:228:GLU:OE2	2.43	0.43
1:B:117:LYS:C	1:B:119:ASN:H	2.22	0.42
1:B:359:ALA:HB3	1:B:361:TYR:CZ	2.54	0.42
1:B:90:PRO:HD3	1:B:125:ILE:HD11	2.01	0.42
1:D:104:THR:O	1:D:107:HIS:HB2	2.20	0.42
1:D:386:LEU:HB3	1:D:408:GLN:HA	2.00	0.42
1:C:441:LEU:O	1:C:445:ILE:HG12	2.19	0.42
1:D:11:THR:HG22	1:D:14:GLU:OE2	2.19	0.42
4:B:806:ACT:H1	1:D:208:ARG:HB3	2.02	0.42
1:D:422:GLN:HE22	1:D:434:ASN:ND2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:ASN:HD21	1:C:223:THR:H	1.67	0.42
1:A:350:PHE:CE2	1:A:391:ASN:HB2	2.54	0.42
1:B:153:CYS:SG	1:B:159:VAL:HG12	2.59	0.42
1:B:285:LYS:CE	1:B:515:ILE:HD11	2.49	0.42
1:C:219:ASN:HD22	1:C:219:ASN:C	2.22	0.42
1:C:329:ARG:NH1	1:C:398:MET:O	2.51	0.42
1:C:447:LYS:NZ	1:C:492:GLU:OE1	2.51	0.42
1:B:317:TRP:CE3	1:B:339:LEU:HD13	2.54	0.42
1:B:490:ARG:N	1:B:503:ASP:O	2.51	0.42
1:C:91:LEU:HA	1:C:92:PRO:HD3	1.87	0.42
1:C:187:CYS:SG	1:C:187:CYS:O	2.77	0.42
1:C:420:LEU:HD13	1:C:438:TYR:CZ	2.55	0.42
1:D:20:LEU:HB2	1:D:171:LEU:HD13	2.02	0.42
1:A:441:LEU:O	1:A:445:ILE:HG12	2.20	0.42
1:B:74:VAL:HG13	1:B:154:ILE:HG12	2.02	0.42
1:B:90:PRO:HB2	1:B:96:ASN:CG	2.39	0.42
1:D:194:PRO:HB3	1:D:201:ALA:HA	2.02	0.42
1:D:368:GLN:OE1	1:D:387:PHE:HA	2.19	0.42
1:D:39:ARG:HG2	1:D:79:LYS:O	2.19	0.42
1:D:469:HIS:O	1:D:472:PRO:HG2	2.19	0.42
1:A:340:GLY:HA2	1:A:354:TYR:CE2	2.55	0.42
1:B:482:ARG:NH1	5:B:1580:HOH:O	2.52	0.42
1:C:391:ASN:O	1:C:395:LEU:HD13	2.19	0.42
1:D:278:ARG:NE	5:D:1590:HOH:O	2.53	0.42
1:D:17:ARG:HH11	1:D:17:ARG:HG2	1.84	0.41
1:A:99:LEU:HD23	1:A:128:VAL:HG22	2.01	0.41
1:C:30:ASP:HA	1:C:180:ILE:O	2.20	0.41
1:D:420:LEU:HD13	1:D:438:TYR:CE1	2.54	0.41
1:C:99:LEU:HD21	1:C:135:ALA:HB2	2.03	0.41
1:B:269:GLN:HA	1:B:458:HIS:O	2.20	0.41
1:B:492:GLU:O	1:B:493:ARG:HD2	2.20	0.41
1:C:27:VAL:HG22	1:C:28:ALA:N	2.35	0.41
1:C:473:CYS:O	1:C:477:LEU:HG	2.20	0.41
1:B:115:GLU:HA	1:B:118:ARG:CB	2.48	0.41
1:D:431:VAL:HA	1:D:434:ASN:HD22	1.85	0.41
1:C:164:LEU:HD11	1:C:191:PHE:CE1	2.55	0.41
1:C:343:TYR:CE1	1:C:404:HIS:CE1	3.08	0.41
1:D:180:ILE:HD13	1:D:225:TYR:CB	2.51	0.41
1:B:117:LYS:HB2	1:B:121:HIS:CD2	2.56	0.41
1:B:493:ARG:NH1	1:B:503:ASP:CG	2.73	0.41
1:A:469:HIS:O	1:A:472:PRO:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ARG:HB3	1:B:181:ARG:NH1	2.36	0.41
1:B:323:ARG:NE	1:B:323:ARG:HA	2.36	0.41
1:C:145:THR:HA	1:C:146:PRO:HA	1.91	0.41
1:D:471:GLU:N	1:D:472:PRO:HD2	2.35	0.41
1:D:85:PRO:O	1:D:87:LYS:N	2.54	0.41
1:A:84:ILE:HG21	1:A:89:ARG:HG3	2.03	0.41
1:B:38:GLY:O	1:B:39:ARG:HB3	2.21	0.41
1:C:326:LEU:HD12	1:C:326:LEU:HA	1.91	0.41
1:D:29:VAL:HG12	1:D:35:ILE:HG22	2.03	0.41
1:D:406:LEU:HG	1:D:421:TYR:HB3	2.03	0.41
1:A:164:LEU:HD11	1:A:191:PHE:CE1	2.56	0.41
1:A:343:TYR:CE2	1:A:404:HIS:CE1	3.08	0.41
1:C:310:SER:OG	1:C:337:MET:HE1	2.20	0.41
1:C:397:ARG:HG3	1:C:397:ARG:HH11	1.86	0.41
1:C:496:LEU:O	1:C:496:LEU:HD13	2.21	0.41
1:D:279:LEU:HD22	1:D:487:LEU:HB2	2.03	0.41
1:D:63:ASN:ND2	1:D:65:LYS:H	2.19	0.41
1:C:30:ASP:C	1:C:30:ASP:OD1	2.60	0.41
1:D:112:LEU:HD23	1:D:118:ARG:HA	2.03	0.41
1:B:27:VAL:HG22	1:B:28:ALA:N	2.36	0.40
1:C:87:LYS:HG3	1:C:88:PHE:CD2	2.56	0.40
1:A:62:LYS:O	1:A:63:ASN:CB	2.67	0.40
1:C:12:VAL:HG13	1:C:13:ALA:N	2.37	0.40
1:D:395:LEU:HB2	1:D:396:PRO:HD3	2.02	0.40
1:A:159:VAL:HG23	4:A:801:ACT:H3	2.03	0.40
1:A:264:SER:HB3	1:A:464:HIS:HB3	2.04	0.40
1:B:469:HIS:O	1:B:472:PRO:HG2	2.21	0.40
1:C:112:LEU:HA	1:C:113:PRO:HD3	1.90	0.40
1:A:518:LYS:HG2	1:A:519:MET:N	2.29	0.40
1:A:53:ARG:HH11	1:A:53:ARG:HG2	1.87	0.40
1:B:219:ASN:ND2	1:B:219:ASN:C	2.75	0.40
1:D:22:ALA:HA	1:D:171:LEU:HB3	2.02	0.40
1:D:276:ASN:O	1:D:277:ASN:HB2	2.21	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	518/521 (99%)	484 (93%)	27 (5%)	7 (1%)	11	6
1	B	517/521 (99%)	484 (94%)	23 (4%)	10 (2%)	8	3
1	C	514/521 (99%)	486 (95%)	23 (4%)	5 (1%)	15	11
1	D	511/521 (98%)	480 (94%)	26 (5%)	5 (1%)	15	11
All	All	2060/2084 (99%)	1934 (94%)	99 (5%)	27 (1%)	12	7

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	219	ASN
1	A	343	TYR
1	B	39	ARG
1	B	41	ILE
1	B	63	ASN
1	B	113	PRO
1	B	518	LYS
1	B	520	ALA
1	C	62	LYS
1	C	343	TYR
1	D	113	PRO
1	D	343	TYR
1	A	519	MET
1	D	122	ALA
1	B	37	ASP
1	B	61	GLY
1	B	343	TYR
1	A	61	GLY
1	D	184	GLU
1	C	42	PRO
1	C	189	VAL

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Mol	Chain	Res	Type
1	D	86	PRO
1	B	42	PRO
1	C	38	GLY
1	A	12	VAL
1	A	42	PRO

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	445/446 (100%)	426 (96%)	19 (4%)	29	29
1	B	444/446 (100%)	420 (95%)	24 (5%)	22	20
1	C	442/446 (99%)	418 (95%)	24 (5%)	22	20
1	D	439/446 (98%)	414 (94%)	25 (6%)	20	18
All	All	1770/1784 (99%)	1678 (95%)	92 (5%)	23	21

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASP
1	A	43	TRP
1	A	49	MET
1	A	95	LEU
1	A	96	ASN
1	A	109	LEU
1	A	146	PRO
1	A	219	ASN
1	A	221	ASN
1	A	257	ARG
1	A	297	LEU
1	A	326	LEU
1	A	333	GLU
1	A	386	LEU
1	A	395	LEU
1	A	440	LEU

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Mol	Chain	Res	Type
1	A	460	LEU
1	A	496	LEU
1	A	519	MET
1	B	32	HIS
1	B	39	ARG
1	B	40	SER
1	B	41	ILE
1	B	43	TRP
1	B	95	LEU
1	B	96	ASN
1	B	104	THR
1	B	139	LEU
1	B	146	PRO
1	B	169	VAL
1	B	192	ARG
1	B	215	LEU
1	B	219	ASN
1	B	256	ASP
1	B	257	ARG
1	B	297	LEU
1	B	303	GLU
1	B	309	LEU
1	B	376	LEU
1	B	386	LEU
1	B	420	LEU
1	B	456	LEU
1	B	515	ILE
1	C	31	GLU
1	C	37	ASP
1	C	43	TRP
1	C	95	LEU
1	C	96	ASN
1	C	116	GLU
1	C	139	LEU
1	C	146	PRO
1	C	169	VAL
1	C	171	LEU
1	C	184	GLU
1	C	219	ASN
1	C	235	ARG
1	C	243	LEU
1	C	257	ARG

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Mol	Chain	Res	Type
1	C	326	LEU
1	C	360	ASN
1	C	374	GLU
1	C	376	LEU
1	C	386	LEU
1	C	395	LEU
1	C	456	LEU
1	C	491	ARG
1	C	493	ARG
1	D	43	TRP
1	D	63	ASN
1	D	95	LEU
1	D	108	LEU
1	D	109	LEU
1	D	113	PRO
1	D	138	LEU
1	D	139	LEU
1	D	146	PRO
1	D	165	ARG
1	D	181	ARG
1	D	189	VAL
1	D	219	ASN
1	D	234	ASN
1	D	256	ASP
1	D	274	LEU
1	D	297	LEU
1	D	309	LEU
1	D	355	THR
1	D	360	ASN
1	D	376	LEU
1	D	386	LEU
1	D	406	LEU
1	D	460	LEU
1	D	493	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	HIS
1	A	173	GLN
1	A	219	ASN
1	A	239	GLN

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Mol	Chain	Res	Type
1	A	255	HIS
1	A	320	ASN
1	A	434	ASN
1	A	476	GLN
1	B	121	HIS
1	B	207	GLN
1	B	219	ASN
1	B	239	GLN
1	B	277	ASN
1	B	434	ASN
1	B	476	GLN
1	C	106	GLN
1	C	173	GLN
1	C	207	GLN
1	C	219	ASN
1	C	239	GLN
1	C	320	ASN
1	C	360	ASN
1	C	434	ASN
1	C	476	GLN
1	D	63	ASN
1	D	106	GLN
1	D	143	ASN
1	D	219	ASN
1	D	234	ASN
1	D	239	GLN
1	D	276	ASN
1	D	277	ASN
1	D	320	ASN
1	D	360	ASN
1	D	434	ASN
1	D	464	HIS
1	D	476	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

20 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
3	PO4	C	703	-	4,4,4	2.54	1 (25%)	6,6,6	0.82	0
4	ACT	C	807	-	1,3,3	3.49	1 (100%)	0,3,3	0.00	-
2	1CY	D	604	-	15,18,18	1.57	3 (20%)	15,27,27	0.92	1 (6%)
3	PO4	B	706	-	4,4,4	2.53	1 (25%)	6,6,6	0.82	0
4	ACT	B	804	-	1,3,3	2.59	1 (100%)	0,3,3	0.00	-
3	PO4	D	704	-	4,4,4	2.60	1 (25%)	6,6,6	0.79	0
3	PO4	D	708	-	4,4,4	2.57	1 (25%)	6,6,6	0.83	0
2	1CY	C	603	-	15,18,18	1.60	3 (20%)	15,27,27	0.84	0
3	PO4	C	707	-	4,4,4	2.62	1 (25%)	6,6,6	0.83	0
3	PO4	A	701	-	4,4,4	2.49	1 (25%)	6,6,6	0.86	0
4	ACT	B	806	-	1,3,3	2.36	1 (100%)	0,3,3	0.00	-
4	ACT	A	803	-	1,3,3	2.78	1 (100%)	0,3,3	0.00	-
2	1CY	B	602	-	15,18,18	1.55	3 (20%)	15,27,27	0.95	1 (6%)
4	ACT	D	808	-	1,3,3	1.75	0	0,3,3	0.00	-
3	PO4	B	702	-	4,4,4	2.52	1 (25%)	6,6,6	0.83	0
4	ACT	A	802	-	1,3,3	2.76	1 (100%)	0,3,3	0.00	-
4	ACT	A	801	-	1,3,3	2.17	1 (100%)	0,3,3	0.00	-
2	1CY	A	601	-	15,18,18	1.58	3 (20%)	15,27,27	0.84	0
3	PO4	A	705	-	4,4,4	2.44	1 (25%)	6,6,6	0.87	0
4	ACT	B	805	-	1,3,3	2.72	1 (100%)	0,3,3	0.00	-

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	1CY	B	602	-	-	0/4/23/23	0/2/2/2
2	1CY	A	601	-	-	0/4/23/23	0/2/2/2
2	1CY	D	604	-	-	0/4/23/23	0/2/2/2
2	1CY	C	603	-	-	0/4/23/23	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	704	PO4	P-O1	4.96	1.62	1.50
3	C	707	PO4	P-O1	4.88	1.62	1.50
3	D	708	PO4	P-O1	4.80	1.62	1.50
3	C	703	PO4	P-O1	4.79	1.62	1.50
3	B	702	PO4	P-O1	4.75	1.62	1.50
3	B	706	PO4	P-O1	4.75	1.62	1.50
3	A	701	PO4	P-O1	4.67	1.61	1.50
3	A	705	PO4	P-O1	4.57	1.61	1.50
2	A	601	1CY	C2-N3	-3.89	1.27	1.36
2	D	604	1CY	C2-N3	-3.88	1.27	1.36
2	C	603	1CY	C2-N3	-3.78	1.27	1.36
2	B	602	1CY	C2-N3	-3.73	1.28	1.36
4	C	807	ACT	CH3-C	3.49	1.53	1.48
2	C	603	1CY	C4-N3	-3.20	1.28	1.34
2	A	601	1CY	C4-N3	-3.07	1.28	1.34
2	B	602	1CY	C4-N3	-3.00	1.28	1.34
2	D	604	1CY	C4-N3	-2.91	1.28	1.34
4	A	803	ACT	CH3-C	2.78	1.52	1.48
4	A	802	ACT	CH3-C	2.76	1.52	1.48
4	B	805	ACT	CH3-C	2.72	1.52	1.48
4	B	804	ACT	CH3-C	2.59	1.52	1.48
2	D	604	1CY	C2-N1	-2.52	1.27	1.34
2	B	602	1CY	C2-N1	-2.45	1.27	1.34
2	C	603	1CY	C2-N1	-2.44	1.27	1.34
4	B	806	ACT	CH3-C	2.36	1.51	1.48
2	A	601	1CY	C2-N1	-2.29	1.28	1.34
4	A	801	ACT	CH3-C	2.17	1.51	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	1CY	C16-C11-N5	2.06	122.45	120.08
2	D	604	1CY	C16-C11-N5	2.04	122.43	120.08

There are no chirality outliers.

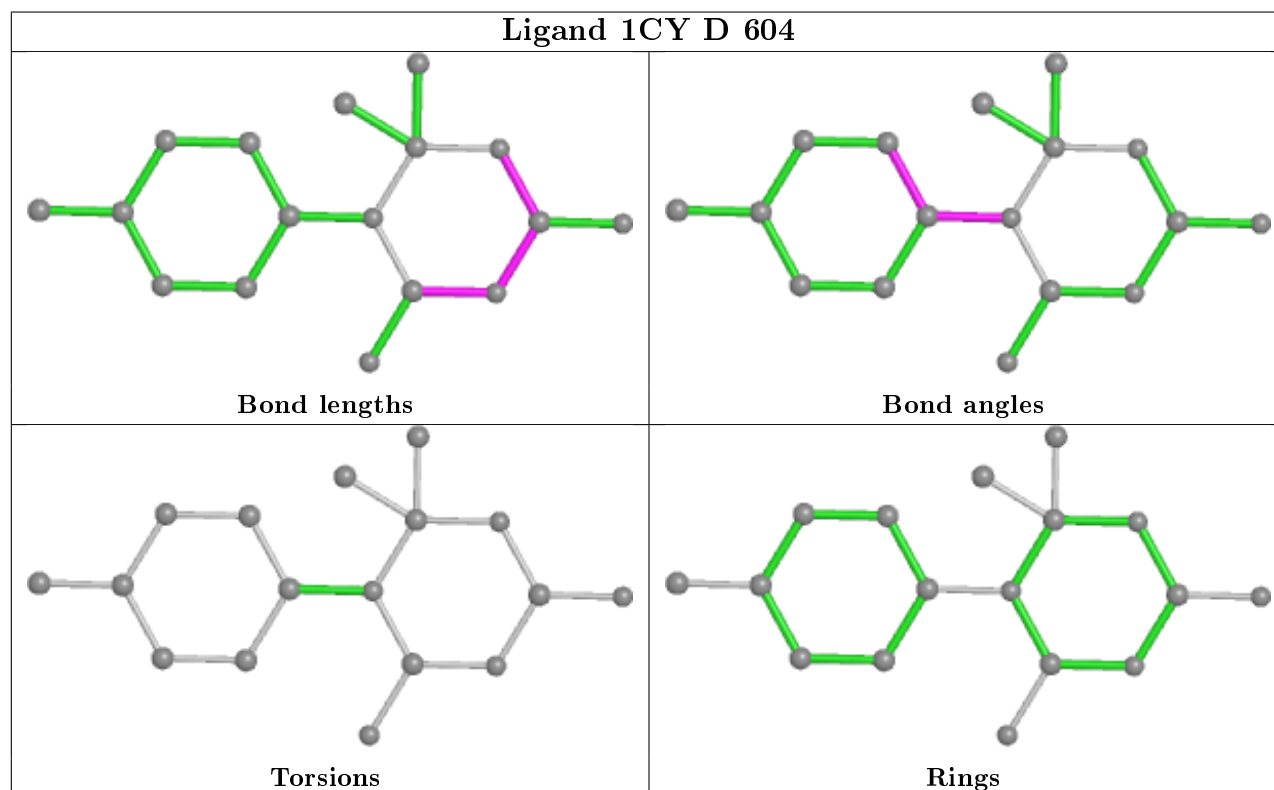
There are no torsion outliers.

There are no ring outliers.

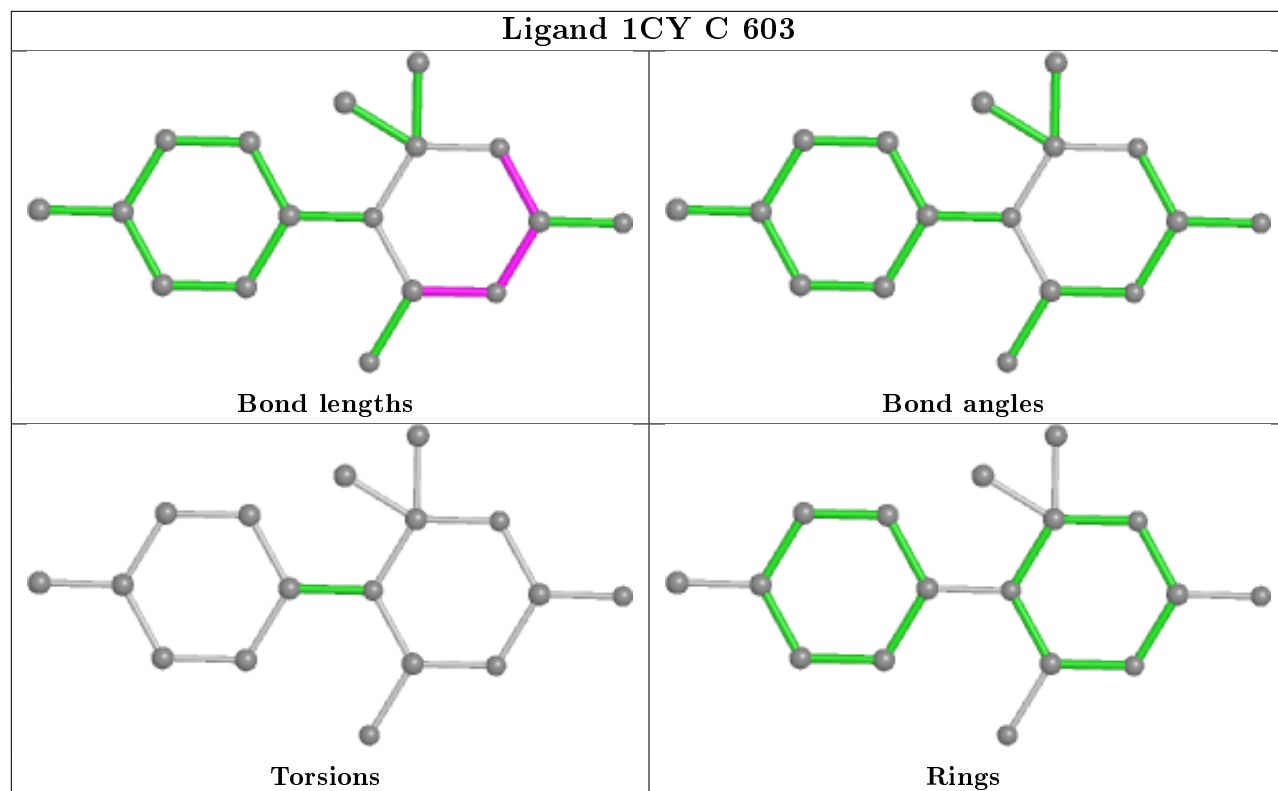
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	807	ACT	1	0
4	B	806	ACT	1	0
4	D	808	ACT	4	0
4	A	801	ACT	1	0

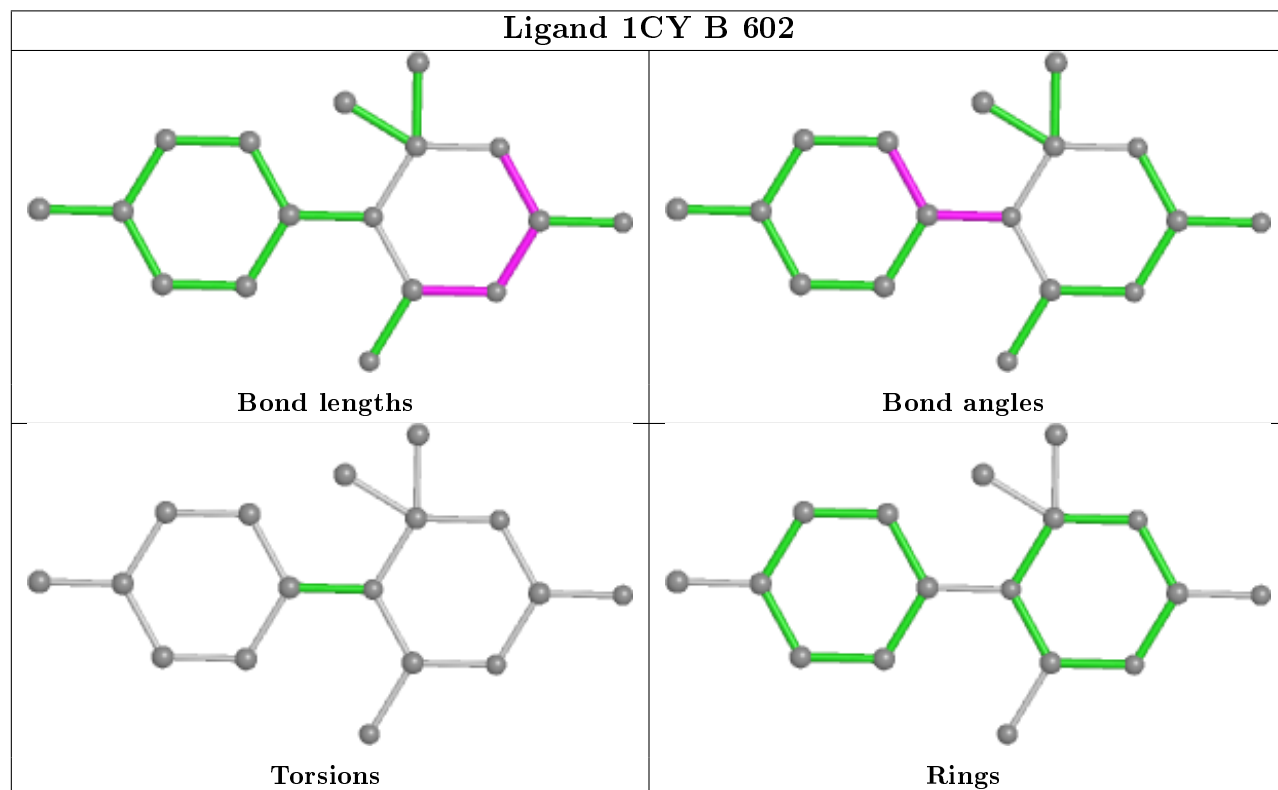
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

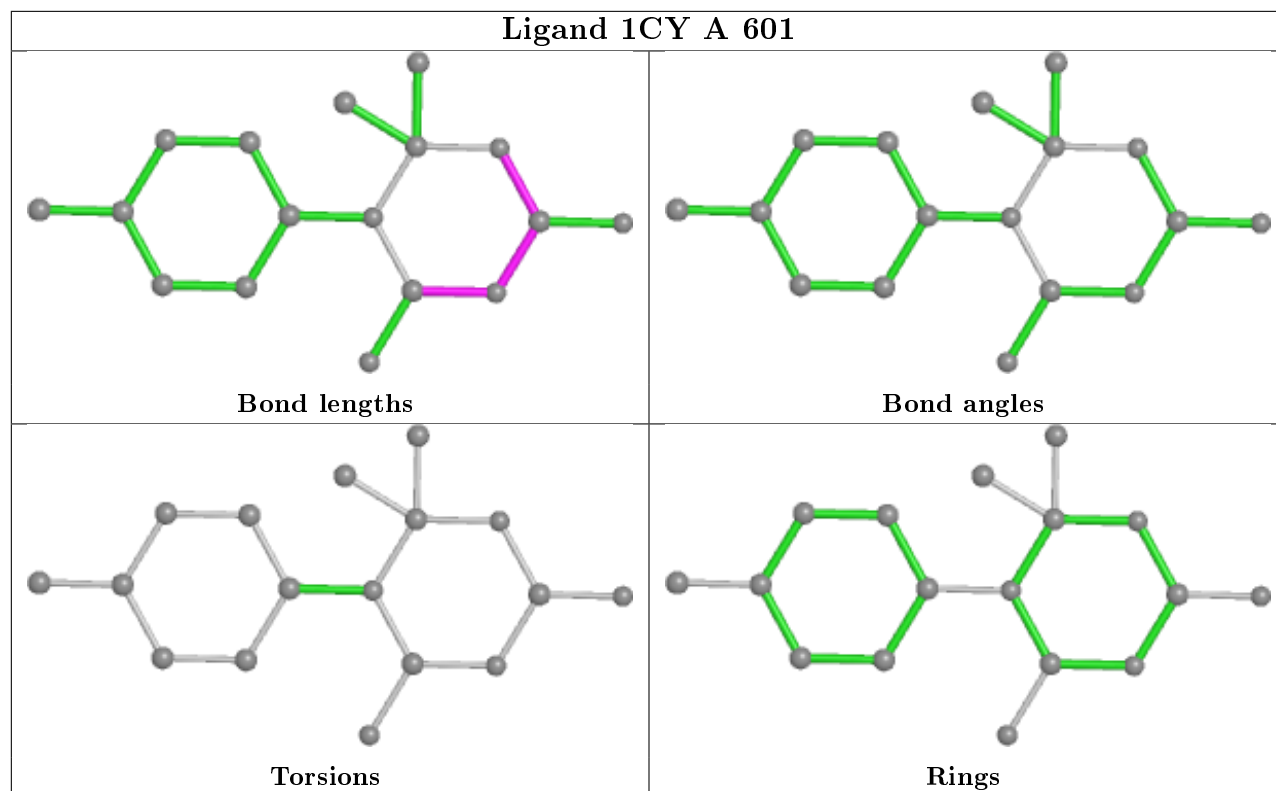


Ligand 1CY C 603



Ligand 1CY B 602





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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	520/521 (99%)	0.41	39 (7%) 14 18	18, 28, 57, 90	0
1	B	519/521 (99%)	0.56	54 (10%) 6 8	20, 33, 73, 90	0
1	C	516/521 (99%)	0.37	39 (7%) 13 18	17, 27, 62, 88	0
1	D	513/521 (98%)	0.37	39 (7%) 13 18	19, 30, 68, 90	0
All	All	2068/2084 (99%)	0.43	171 (8%) 11 14	17, 30, 66, 90	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	38	GLY	11.7
1	A	517	MET	10.9
1	B	521	VAL	9.9
1	A	38	GLY	9.9
1	B	186	SER	9.7
1	C	42	PRO	9.2
1	A	520	ALA	8.6
1	B	187	CYS	8.1
1	C	185	SER	8.0
1	A	519	MET	7.9
1	C	39	ARG	7.9
1	C	187	CYS	7.6
1	B	41	ILE	7.2
1	C	186	SER	7.1
1	D	120	LEU	7.0
1	D	119	ASN	7.0
1	A	186	SER	6.8
1	D	41	ILE	6.8
1	A	184	GLU	6.5
1	B	43	TRP	6.4
1	A	187	CYS	6.4

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Mol	Chain	Res	Type	RSRZ
1	C	44	ASN	6.3
1	A	42	PRO	6.3
1	C	41	ILE	6.2
1	B	188	SER	6.1
1	B	36	GLY	6.0
1	A	516	SER	5.9
1	C	37	ASP	5.9
1	D	39	ARG	5.9
1	C	183	SER	5.8
1	D	38	GLY	5.8
1	D	114	ASP	5.7
1	D	43	TRP	5.6
1	A	183	SER	5.5
1	A	44	ASN	5.4
1	D	257	ARG	5.3
1	B	183	SER	5.3
1	C	43	TRP	5.3
1	D	42	PRO	5.2
1	B	515	ILE	5.2
1	A	62	LYS	5.2
1	C	182	ALA	5.2
1	A	39	ARG	5.1
1	D	112	LEU	5.1
1	B	37	ASP	5.1
1	B	185	SER	5.0
1	B	61	GLY	5.0
1	C	115	GLU	5.0
1	C	517	MET	4.9
1	A	185	SER	4.9
1	D	185	SER	4.8
1	B	119	ASN	4.7
1	D	113	PRO	4.7
1	B	44	ASN	4.7
1	A	41	ILE	4.6
1	D	36	GLY	4.6
1	D	188	SER	4.6
1	A	515	ILE	4.6
1	B	38	GLY	4.5
1	C	116	GLU	4.5
1	B	64	VAL	4.4
1	B	519	MET	4.4
1	A	1	MET	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	516	SER	4.4
1	A	37	ASP	4.1
1	B	257	ARG	4.1
1	B	40	SER	4.0
1	C	119	ASN	4.0
1	A	518	LYS	4.0
1	D	187	CYS	4.0
1	D	115	GLU	4.0
1	B	220	GLY	3.9
1	B	184	GLU	3.9
1	C	62	LYS	3.9
1	A	188	SER	3.9
1	C	40	SER	3.8
1	A	2	SER	3.8
1	A	43	TRP	3.8
1	C	36	GLY	3.8
1	C	184	GLU	3.7
1	B	39	ARG	3.7
1	C	516	SER	3.7
1	A	61	GLY	3.6
1	C	61	GLY	3.6
1	D	40	SER	3.6
1	D	37	ASP	3.6
1	B	517	MET	3.6
1	C	515	ILE	3.6
1	D	118	ARG	3.6
1	D	515	ILE	3.6
1	A	257	ARG	3.5
1	C	257	ARG	3.5
1	B	42	PRO	3.4
1	B	13	ALA	3.3
1	D	122	ALA	3.3
1	D	184	GLU	3.3
1	B	15	GLY	3.3
1	A	25	LEU	3.3
1	B	109	LEU	3.3
1	B	114	ASP	3.3
1	B	32	HIS	3.2
1	A	63	ASN	3.2
1	B	112	LEU	3.2
1	A	36	GLY	3.2
1	B	116	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	114	ASP	3.2
1	C	188	SER	3.2
1	B	190	PHE	3.1
1	C	88	PHE	3.1
1	B	63	ASN	3.1
1	D	116	GLU	3.1
1	D	183	SER	3.1
1	C	113	PRO	3.1
1	D	86	PRO	3.1
1	D	110	ASP	3.0
1	D	429	LEU	3.0
1	A	65	LYS	3.0
1	C	117	LYS	2.9
1	A	221	ASN	2.9
1	D	107	HIS	2.9
1	B	217	SER	2.8
1	B	62	LYS	2.8
1	D	12	VAL	2.7
1	D	256	ASP	2.7
1	C	175	ILE	2.7
1	B	120	LEU	2.7
1	B	117	LYS	2.7
1	D	117	LYS	2.7
1	C	331	LEU	2.7
1	B	103	LEU	2.7
1	B	65	LYS	2.6
1	C	174	ALA	2.6
1	B	219	ASN	2.6
1	C	328	SER	2.6
1	B	69	ALA	2.5
1	B	181	ARG	2.5
1	B	68	PRO	2.5
1	B	86	PRO	2.5
1	C	405	LEU	2.5
1	A	154	ILE	2.5
1	D	182	ALA	2.4
1	B	121	HIS	2.4
1	C	120	LEU	2.4
1	A	330	GLY	2.4
1	A	174	ALA	2.4
1	A	153	CYS	2.4
1	B	118	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	118	ARG	2.4
1	D	102	THR	2.4
1	B	222	GLU	2.4
1	A	24	SER	2.3
1	B	218	ALA	2.3
1	B	115	GLU	2.3
1	B	518	LYS	2.2
1	C	26	VAL	2.2
1	A	155	GLY	2.2
1	D	108	LEU	2.2
1	D	14	GLU	2.2
1	B	3	LEU	2.1
1	A	152	TYR	2.1
1	B	320	ASN	2.1
1	D	87	LYS	2.1
1	A	69	ALA	2.1
1	D	88	PHE	2.1
1	D	111	GLY	2.1
1	A	40	SER	2.1
1	B	10	GLU	2.0
1	A	218	ALA	2.0
1	C	407	ALA	2.0
1	C	329	ARG	2.0
1	D	121	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

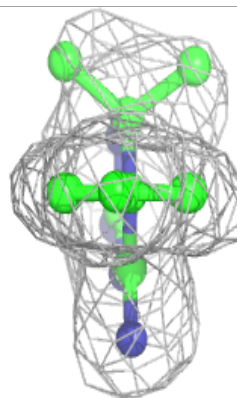
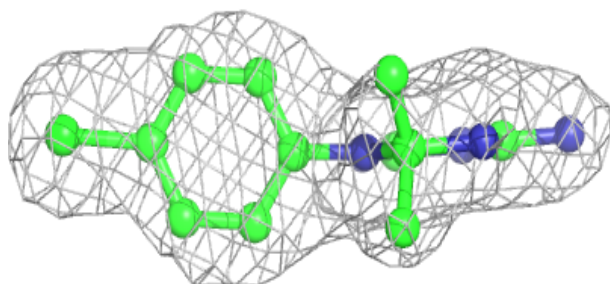
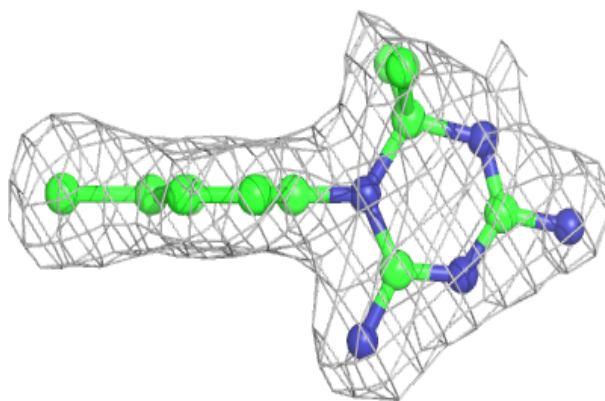
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ACT	B	805	4/4	0.82	0.28	44,44,45,45	0
4	ACT	A	801	4/4	0.85	0.17	24,29,30,31	0
3	PO4	C	703	5/5	0.86	0.13	73,73,73,74	0
4	ACT	B	804	4/4	0.86	0.18	40,43,45,45	0
4	ACT	C	807	4/4	0.87	0.19	31,36,36,36	0
4	ACT	A	802	4/4	0.89	0.16	44,44,44,45	0
2	1CY	B	602	17/17	0.91	0.14	33,39,43,46	0
3	PO4	C	707	5/5	0.92	0.16	49,51,52,53	0
3	PO4	B	702	5/5	0.92	0.17	73,74,75,75	0
3	PO4	B	706	5/5	0.93	0.20	78,78,79,80	0
3	PO4	D	704	5/5	0.93	0.16	63,63,65,65	0
2	1CY	A	601	17/17	0.94	0.15	26,31,34,36	0
3	PO4	A	705	5/5	0.94	0.23	53,54,55,56	0
4	ACT	A	803	4/4	0.94	0.40	44,47,47,48	0
3	PO4	D	708	5/5	0.95	0.21	67,69,69,70	0
2	1CY	C	603	17/17	0.95	0.13	22,26,32,35	0
2	1CY	D	604	17/17	0.95	0.13	25,29,34,40	0
4	ACT	B	806	4/4	0.95	0.16	42,42,43,43	0
3	PO4	A	701	5/5	0.96	0.10	51,52,52,53	0
4	ACT	D	808	4/4	0.96	0.15	34,34,37,37	0

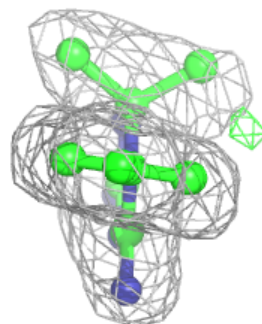
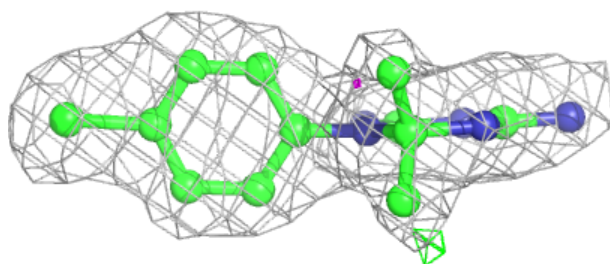
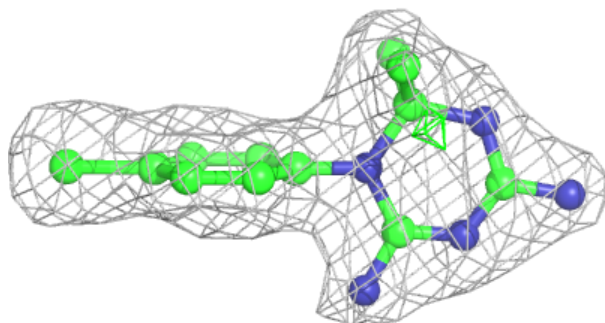
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 1CY B 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

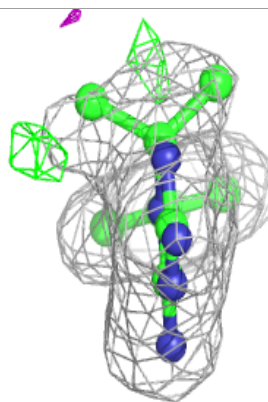
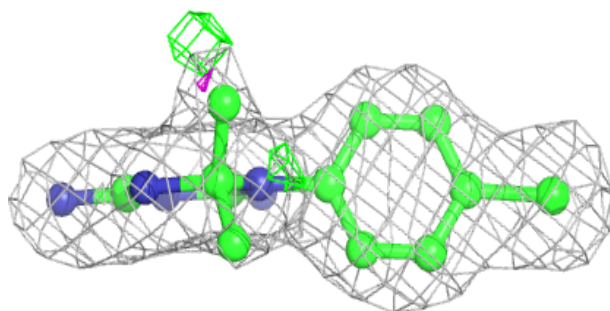
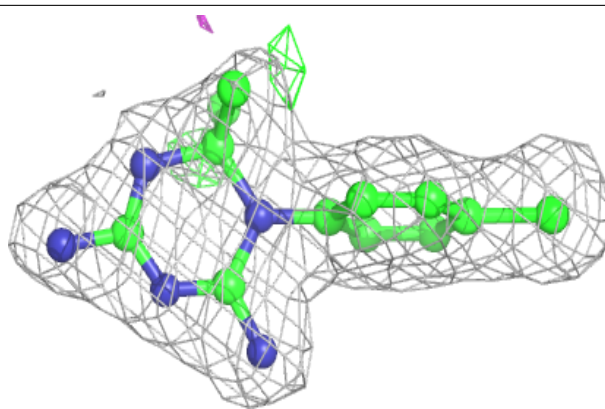
**Electron density around 1CY A 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

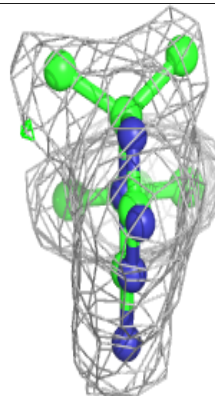
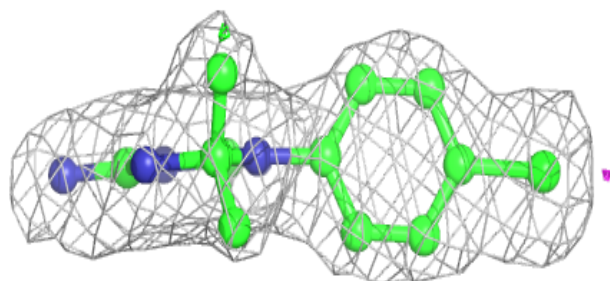
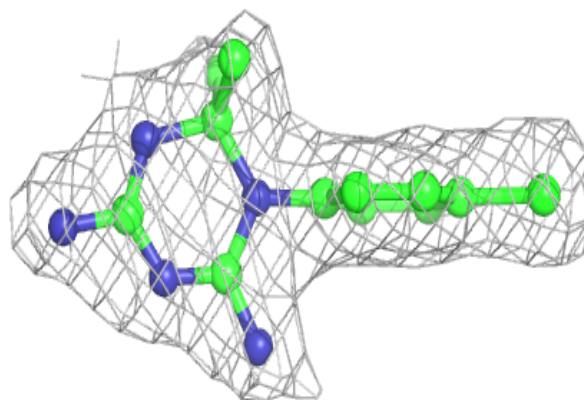


Electron density around 1CY C 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 1CY D 604:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.