



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:40 AM UTC

PDB ID : 3IRM / pdb_00003irm
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 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

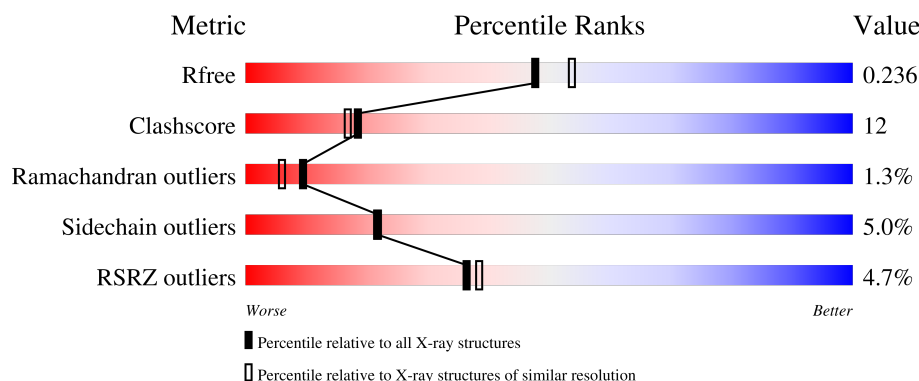
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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 $\leq 5\%$. 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	4% 77% 20% .
1	B	521	6% 70% 24% 5%
1	C	521	4% 74% 21% ..
1	D	521	5% 66% 28% ..

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 criteria:

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

2 Entry composition [i](#)

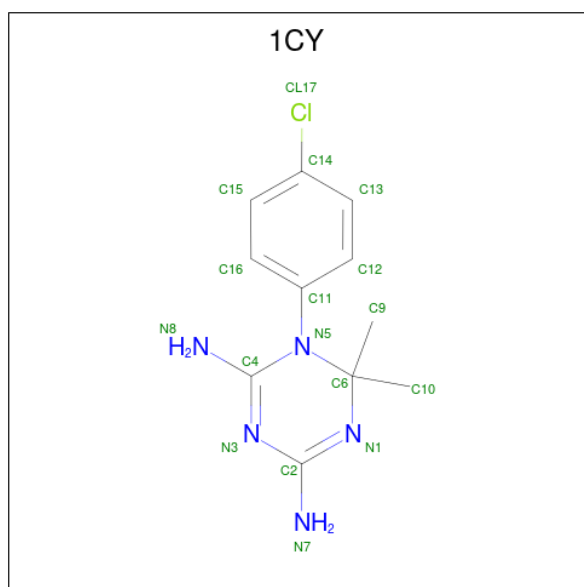
There are 5 unique types of molecules in this entry. The entry contains 17255 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 1CY) (formula: C₁₁H₁₄ClN₅).



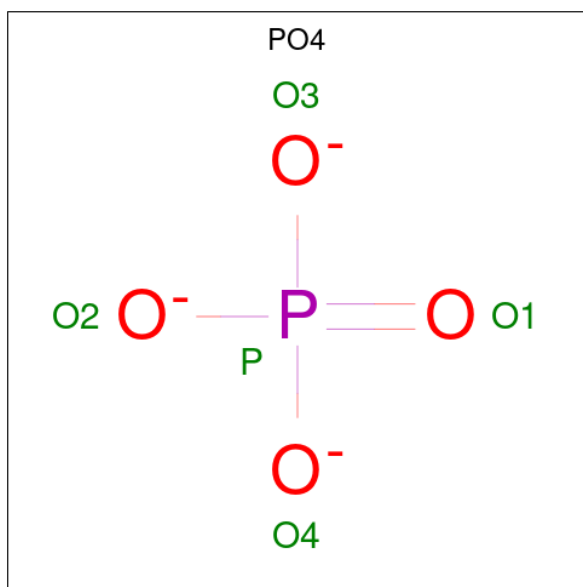
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	0	0
			17	11	1	5		
2	B	1	Total	C	Cl	N	0	0
			17	11	1	5		

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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 (CCD ID: PO4) (formula: O_4P).



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 (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

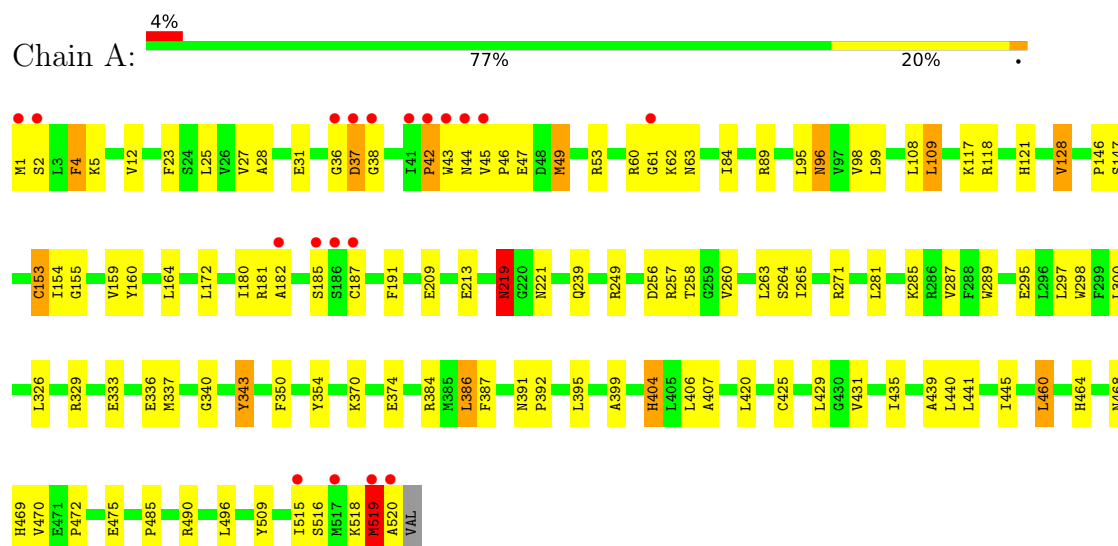
- Molecule 5 is water.

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

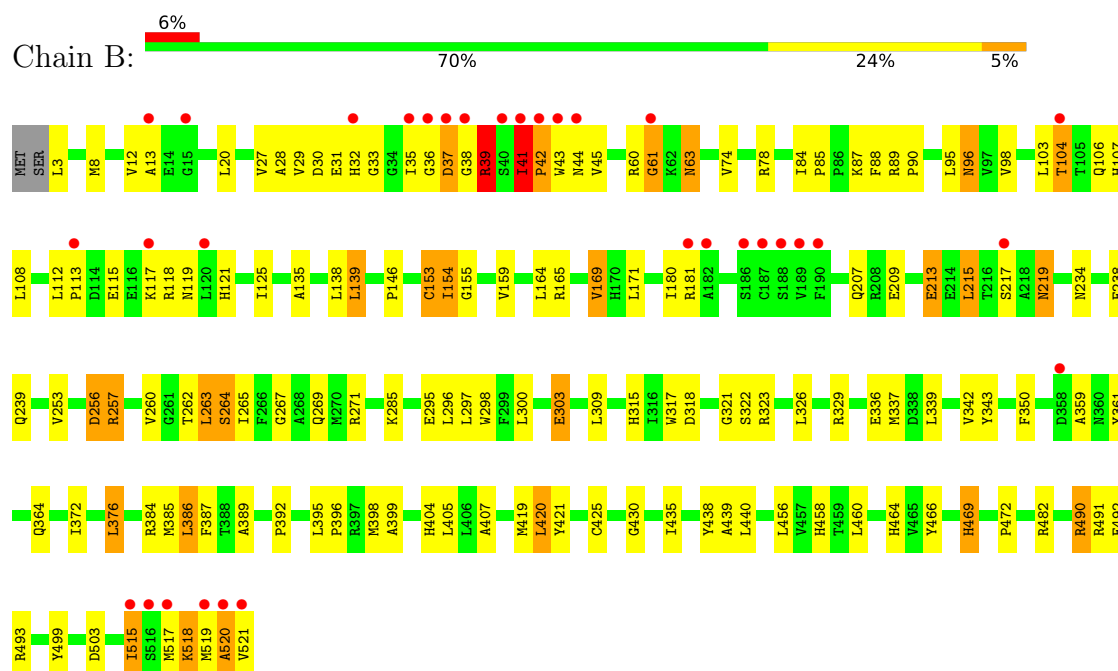
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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 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.

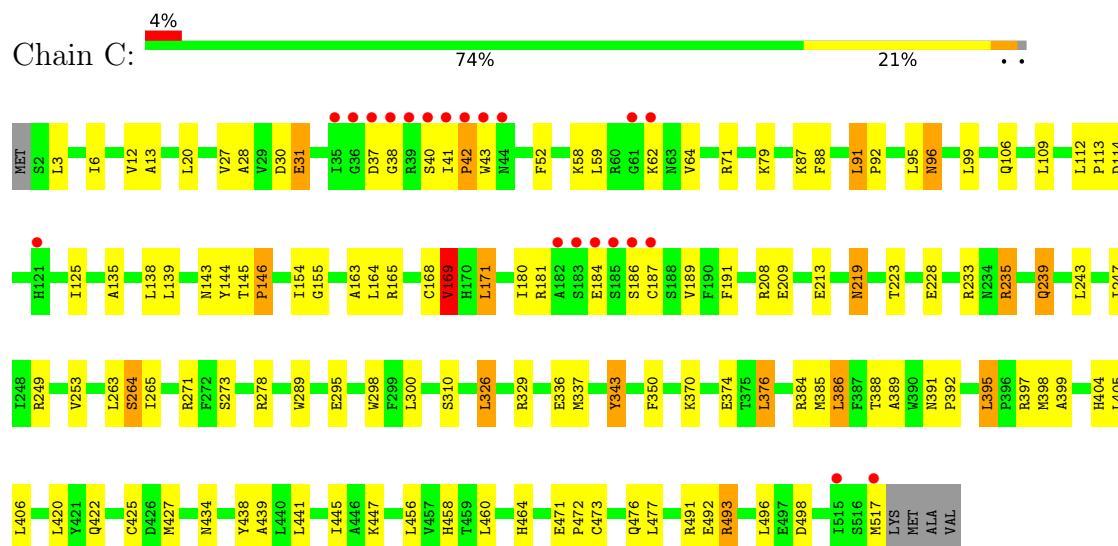
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



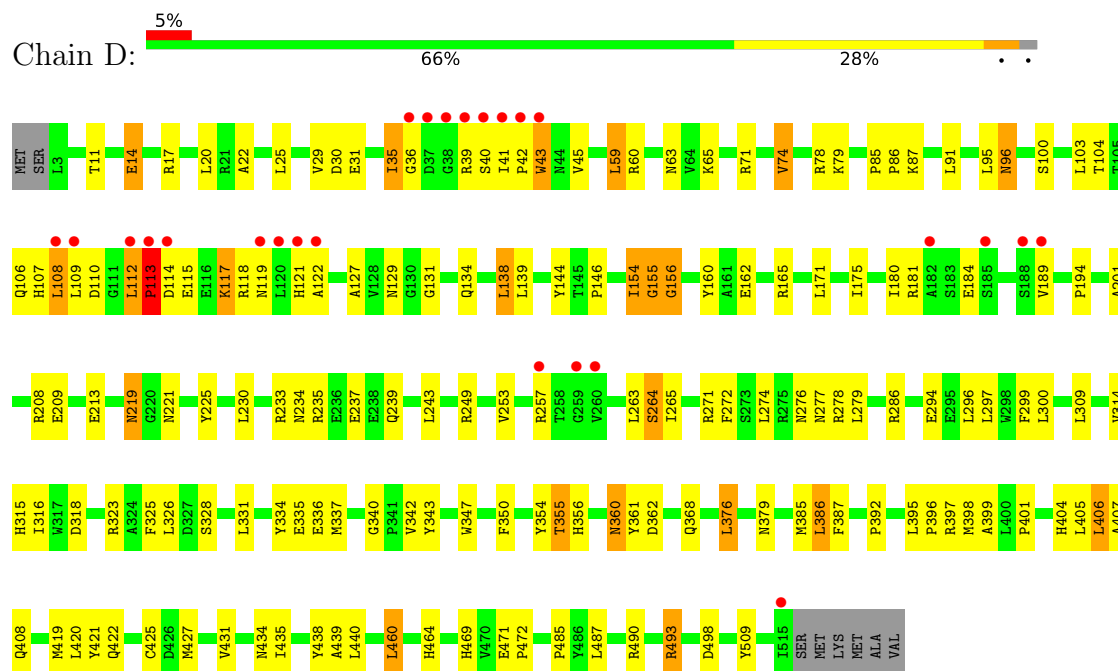
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



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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 0.202 , 0.236	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)	0.35 , 37.1	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1CY, ACT, PO4

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	0.41	0/4237	0.91	11/5746 (0.2%)
1	B	0.39	0/4231	0.91	18/5738 (0.3%)
1	C	0.40	0/4207	0.95	20/5708 (0.4%)
1	D	0.39	0/4187	0.93	20/5682 (0.4%)
All	All	0.40	0/16862	0.93	69/22874 (0.3%)

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	ILE	N-CA-C	8.18	119.94	112.17
1	A	154	ILE	N-CA-C	7.94	119.72	112.17
1	C	154	ILE	N-CA-C	7.93	119.73	112.43
1	C	3	LEU	N-CA-C	-7.90	103.63	113.18
1	A	209	GLU	N-CA-C	-7.68	102.25	111.69
1	C	209	GLU	N-CA-C	-7.36	101.44	112.04
1	B	430	GLY	N-CA-C	7.19	121.19	112.49
1	B	209	GLU	N-CA-C	-7.09	102.60	112.45
1	A	439	ALA	N-CA-C	-7.05	103.67	111.36
1	B	439	ALA	N-CA-C	-6.92	103.67	111.14
1	C	186	SER	N-CA-C	-6.89	103.16	112.26
1	D	439	ALA	N-CA-C	-6.74	103.87	111.14
1	B	155	GLY	N-CA-C	6.73	120.95	111.00
1	D	405	LEU	N-CA-C	6.70	121.62	113.38
1	C	91	LEU	CA-C-N	6.57	126.60	119.90
1	C	91	LEU	C-N-CA	6.57	126.60	119.90
1	D	209	GLU	N-CA-C	-6.45	103.48	112.45
1	B	257	ARG	N-CA-C	-6.43	105.29	113.01
1	A	213	GLU	N-CA-C	-6.38	101.93	110.55
1	C	155	GLY	N-CA-C	6.36	120.42	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	257	ARG	N-CA-C	-6.34	105.03	112.89
1	C	439	ALA	N-CA-C	-6.29	104.35	111.14
1	C	41	ILE	CA-C-N	6.20	127.58	119.84
1	C	41	ILE	C-N-CA	6.20	127.58	119.84
1	D	117	LYS	N-CA-C	-6.19	103.85	111.40
1	C	168	CYS	N-CA-C	6.15	117.99	111.28
1	D	91	LEU	CA-C-N	6.10	126.06	119.78
1	D	91	LEU	C-N-CA	6.10	126.06	119.78
1	D	213	GLU	N-CA-C	-6.02	102.77	110.53
1	B	263	LEU	N-CA-C	-5.88	100.12	109.59
1	B	405	LEU	N-CA-C	5.85	121.14	113.30
1	B	389	ALA	N-CA-C	-5.84	106.13	113.72
1	A	470	VAL	N-CA-C	5.83	116.30	110.23
1	C	239	GLN	N-CA-C	-5.80	104.86	111.07
1	B	469	HIS	N-CA-C	-5.74	106.07	114.39
1	D	35	ILE	N-CA-C	5.72	119.38	112.80
1	D	154	ILE	N-CA-C	5.71	117.59	112.17
1	B	264	SER	N-CA-C	5.71	117.75	109.07
1	C	264	SER	N-CA-C	5.69	117.83	109.24
1	D	156	GLY	N-CA-C	-5.68	99.72	113.18
1	A	404	HIS	N-CA-C	-5.56	98.69	108.20
1	A	153	CYS	N-CA-C	-5.53	100.78	109.25
1	A	263	LEU	N-CA-C	-5.53	100.39	109.40
1	D	399	ALA	N-CA-C	-5.47	105.41	111.71
1	C	169	VAL	CB-CA-C	-5.46	103.70	112.16
1	B	43	TRP	N-CA-C	-5.42	106.45	112.57
1	B	399	ALA	N-CA-C	-5.42	105.38	111.28
1	C	405	LEU	N-CA-C	5.42	120.76	113.72
1	A	289	TRP	N-CA-C	5.40	117.16	111.28
1	B	153	CYS	N-CA-C	-5.40	100.99	109.25
1	D	264	SER	N-CA-C	5.39	117.26	109.07
1	B	213	GLU	N-CA-C	-5.38	103.59	110.53
1	C	249	ARG	N-CA-C	5.36	117.20	111.36
1	A	4	PHE	N-CA-C	-5.33	106.28	112.89
1	B	435	ILE	N-CA-C	-5.33	105.34	110.72
1	D	59	LEU	N-CA-C	-5.31	102.89	110.59
1	D	14	GLU	N-CA-C	5.25	117.75	111.71
1	C	289	TRP	N-CA-C	5.23	117.39	111.11
1	C	213	GLU	N-CA-C	-5.18	103.84	110.53
1	C	389	ALA	N-CA-C	-5.18	106.35	113.30
1	B	404	HIS	N-CA-C	-5.17	100.09	108.41
1	C	58	LYS	N-CA-C	5.08	117.67	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	112	LEU	CA-C-N	5.08	126.19	119.84
1	D	112	LEU	C-N-CA	5.08	126.19	119.84
1	D	155	GLY	N-CA-C	5.06	125.18	113.18
1	D	379	ASN	CA-C-N	5.05	124.72	119.56
1	D	379	ASN	C-N-CA	5.05	124.72	119.56
1	B	154	ILE	CB-CA-C	-5.04	105.45	111.85
1	A	516	SER	N-CA-C	5.01	117.74	110.42

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	4137	0	4099	80	0
1	B	4131	0	4091	123	0
1	C	4107	0	4060	81	0
1	D	4087	0	4041	125	0
2	A	17	0	14	0	0
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	397	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 12.

All (397) 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
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:360:ASN:C	1:D:360:ASN:HD22	1.96	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:D:117:LYS:C	1:D:119:ASN:H	1.96	0.70
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:40:SER:C	1:C:42:PRO:HD3	2.20	0.66
1:D:234:ASN:C	1:D:234:ASN:HD22	2.04	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: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: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:HD3	1:B:257:ARG:N	2.05	0.59
1:B:303:GLU:HG3	5:B:1463:HOH:O	2.02	0.59
1:B:321:GLY:O	1:B:337:MET:HE2	2.02	0.59
1:B:517:MET:O	1:B:518:LYS:C	2.45	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:HB3	1:D:490:ARG:NH1	2.18	0.58
1:C:165:ARG:C	1:C:169:VAL:HG22	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD22	1:B:96:ASN:N	2.04	0.56
1:B:164:LEU:C	1:B:169:VAL:HG13	2.30	0.56
1:A:468:ASN:O	1:A:520:ALA:HB1	2.06	0.56
1:B:165:ARG:C	1:B:169:VAL:HG22	2.30	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:3:LEU:HD23	1:B:3:LEU:O	2.05	0.55
1:B:29:VAL:HG22	1:B:30:ASP:N	2.21	0.55
1:B:207:GLN:NE2	1:D:249:ARG:HH21	2.03	0.55
1:A:384:ARG:C	1:A:386:LEU:HD23	2.31	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
1:C:392:PRO:HD2	1:D:350:PHE:CE1	2.41	0.55
1:D:335:GLU:HB2	5:D:1359:HOH:O	2.06	0.55
1:D:265:ILE:HD12	1:D:265:ILE:C	2.32	0.55
1:D:100:SER:O	1:D:129:ASN:HA	2.06	0.54
1:D:117:LYS:C	1:D:119:ASN:N	2.66	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: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:C:476:GLN:NE2	1:C:517:MET:HE1	2.23	0.54
1:B:164:LEU:C	1:B:169:VAL:CG1	2.81	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ASP:OD2	1:A:260:VAL:HB	2.08	0.53
1:A:265:ILE:HD12	1:A:265:ILE:C	2.33	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:265:ILE:C	1:B:265:ILE:HD12	2.34	0.53
1:B:420:LEU:HD22	1:B:438:TYR:CD2	2.44	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:395:LEU:HB2	1:B:396:PRO:HD3	1.91	0.52
1:D:336:GLU:O	1:D:337:MET:HB2	2.09	0.52
1:A:257:ARG:H	1:A:257:ARG:HD3	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:A:44:ASN:OD1	1:A:49:MET:HE2	2.08	0.52
1:B:37:ASP:C	1:B:39:ARG:H	2.18	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:13:ALA:HB2	1:C:492:GLU:HG3	1.91	0.52
1:C:336:GLU:O	1:C:337:MET:HB2	2.08	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
1:B:84:ILE:O	1:B:89:ARG:HD3	2.11	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:219:ASN:C	1:B:219:ASN:HD22	2.16	0.51
1:B:74:VAL:CG1	1:B:154:ILE:HD13	2.40	0.51
1:B:519:MET:O	1:B:519:MET:HG2	2.08	0.51
1:B:29:VAL:CG2	1:B:33:GLY:C	2.84	0.51
1:B:39:ARG:NH2	1:B:41:ILE:HB	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:63:ASN:C	1:D:63:ASN:HD22	2.18	0.51
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:D:131:GLY:H	1:D:134:GLN:CD	2.19	0.50
1:A:329:ARG:HG3	1:A:329:ARG:HH11	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:B:384:ARG:C	1:B:386:LEU:HD23	2.37	0.49
1:D:420:LEU:HD13	1:D:438:TYR:CZ	2.46	0.49
1:D:96:ASN:N	1:D:96:ASN:HD22	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: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:25:LEU:HD23	1:D:25:LEU:C	2.37	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:C:265:ILE:C	1:C:265:ILE:HD12	2.38	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:C:441:LEU:C	1:C:441:LEU:HD23	2.38	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:C:496:LEU:HD13	1:C:496:LEU:C	2.38	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
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:36:GLY:O	1:D:40:SER:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:LEU:HD13	1:D:334:TYR:CE2	2.49	0.48
1:B:84:ILE:HG22	1:B:89:ARG:HG2	1.95	0.48
1:C:476:GLN:HE21	1:C:517:MET:HE1	1.77	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:B:117:LYS:C	1:B:119:ASN:H	2.22	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: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:90:PRO:HB2	1:B:96:ASN:CG	2.39	0.47
1:A:392:PRO:HD2	1:B:350:PHE:CZ	2.49	0.47
1:C:219:ASN:C	1:C:219:ASN:HD22	2.22	0.47
1:C:350:PHE:CE1	1:D:392:PRO:HD2	2.50	0.47
1:C:350:PHE:CZ	1:D:392:PRO:HD2	2.50	0.47
1:C:458:HIS:CE1	1:C:460:LEU:HD21	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:329:ARG:HE	1:B:329:ARG:HB3	1.56	0.46
1:C:114:ASP:OD1	1:C:114:ASP:N	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:N	1:A:460:LEU:HD22	2.31	0.46
1:B:98:VAL:HB	1:B:108:LEU:HD21	1.97	0.46
1:C:386:LEU:N	1:C:386:LEU:HD23	2.30	0.46
1:D:272:PHE:CZ	1:D:435:ILE:HD13	2.50	0.46
1:D:386:LEU:N	1:D:386:LEU:HD23	2.31	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:493:ARG:NH1	1:B:503:ASP:CG	2.73	0.46
1:B:29:VAL:HG22	1:B:30:ASP:H	1.81	0.45
1:B:31:GLU:OE1	1:B:181:ARG:CZ	2.64	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:HA	1:D:323:ARG:NE	2.31	0.45
1:C:30:ASP:OD1	1:C:30:ASP:C	2.60	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: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:B:219:ASN:C	1:B:219:ASN:ND2	2.75	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:96:ASN:N	1:A:96:ASN:HD22	2.14	0.44
1:A:281:LEU:HD22	1:A:287:VAL:HB	1.99	0.44
1:C:219:ASN:C	1:C:219:ASN:ND2	2.75	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:A:36:GLY:C	1:A:38:GLY:H	2.26	0.44
1:A:386:LEU:HD23	1:A:386:LEU:N	2.32	0.44
1:B:8:MET:HE3	1:B:12:VAL:HG23	2.00	0.44
1:A:350:PHE:CZ	1:B:392:PRO:HD2	2.52	0.44
1:B:35:ILE:HG13	1:B:36:GLY:N	2.33	0.44
1:B:253:VAL:HA	1:B:262:THR:O	2.17	0.44
1:A:182:ALA:HB1	1:A:185:SER:HB2	1.98	0.44
1:A:36:GLY:C	1:A:38:GLY:N	2.75	0.44
1:D:294:GLU:OE1	1:D:294:GLU:HA	2.17	0.44
1:C:406:LEU:HD22	1:D:406:LEU:HD23	2.00	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
1:D:355:THR:HG22	1:D:356:HIS:H	1.78	0.44
1:B:13:ALA:HB2	1:B:492:GLU:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:490:ARG:NH1	1:D:490:ARG:CB	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: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:336:GLU:CD	1:D:336:GLU:H	2.26	0.43
1:D:490:ARG:CB	1:D:490:ARG:CZ	2.96	0.43
1:B:3:LEU:HD23	1:B:3:LEU:C	2.44	0.43
1:C:52:PHE:CD1	1:C:52:PHE:C	2.96	0.43
1:D:299:PHE:HB3	1:D:347:TRP:CZ3	2.54	0.43
1:A:23:PHE:CE1	1:A:172:LEU:HD13	2.54	0.43
1:A:155:GLY:HA2	1:A:160:TYR:CZ	2.53	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:CZ	1:D:490:ARG:HB2	2.48	0.43
1:C:247:ILE:HD12	1:C:427:MET:HG3	1.99	0.43
1:C:295:GLU:O	1:C:298:TRP:HB3	2.18	0.43
1:D:78:ARG:NE	1:D:103:LEU:HD11	2.32	0.43
1:D:360:ASN:HD22	1:D:362:ASP:H	1.65	0.43
1:D:431:VAL:O	1:D:435:ILE:HG13	2.18	0.43
1:A:36:GLY:C	1:A:187:CYS:HB3	2.43	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:90:PRO:HD3	1:B:125:ILE:HD11	2.01	0.42
1:B:359:ALA:HB3	1:B:361:TYR:CZ	2.54	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
4:B:806:ACT:H1	1:D:208:ARG:HB3	2.02	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
1:D:30:ASP:C	1:D:30:ASP:OD2	2.62	0.42
1:D:422:GLN:HE22	1:D:434:ASN:ND2	2.17	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:LYS:CE	1:B:515:ILE:HD11	2.49	0.42
1:C:310:SER:OG	1:C:337:MET:HE2	2.19	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:D:243:LEU:HD23	1:D:427:MET:HE1	2.02	0.42
1:C:187:CYS:O	1:C:187:CYS:SG	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:D:194:PRO:HB3	1:D:201:ALA:HA	2.02	0.42
1:D:39:ARG:HG2	1:D:79:LYS:O	2.19	0.42
1:D:368:GLN:OE1	1:D:387:PHE:HA	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:HG2	1:D:17:ARG:HH11	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:C:350:PHE:CD1	1:C:350:PHE:C	2.99	0.41
1:D:43:TRP:CD1	1:D:43:TRP:H	2.35	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:D:234:ASN:C	1:D:234:ASN:ND2	2.73	0.41
1:B:115:GLU:HA	1:B:118:ARG:CB	2.48	0.41
1:C:493:ARG:HG2	1:C:498:ASP:C	2.44	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: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:NH1	1:B:181:ARG:HB3	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:85:PRO:O	1:D:87:LYS:N	2.54	0.41
1:D:471:GLU:N	1:D:472:PRO:HD2	2.35	0.41
1:A:84:ILE:HG21	1:A:89:ARG:HG3	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:B:38:GLY:O	1:B:39:ARG:HB3	2.21	0.41
1:B:117:LYS:C	1:B:119:ASN:N	2.78	0.41
1:C:326:LEU:HD12	1:C:326:LEU:HA	1.91	0.41
1:C:397:ARG:HH11	1:C:397:ARG:HG3	1.86	0.41
1:C:496:LEU:HD13	1:C:496:LEU:O	2.21	0.41
1:D:29:VAL:HG12	1:D:35:ILE:HG22	2.03	0.41
1:D:63:ASN:ND2	1:D:65:LYS:H	2.19	0.41
1:D:279:LEU:HD22	1:D:487:LEU:HB2	2.03	0.41
1:D:406:LEU:HG	1:D:421:TYR:HB3	2.03	0.41
1:A:25:LEU:HD23	1:A:25:LEU:C	2.46	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:53:ARG:HH11	1:A:53:ARG:HG2	1.87	0.40
1:A:518:LYS:HG2	1:A:519:MET:N	2.29	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%)	9	5
1	B	517/521 (99%)	484 (94%)	23 (4%)	10 (2%)	6	3
1	C	514/521 (99%)	486 (95%)	23 (4%)	5 (1%)	12	9
1	D	511/521 (98%)	480 (94%)	26 (5%)	5 (1%)	12	9
All	All	2060/2084 (99%)	1934 (94%)	99 (5%)	27 (1%)	9	6

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
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%)	424 (95%)	21 (5%)	23	24
1	B	444/446 (100%)	422 (95%)	22 (5%)	22	22
1	C	442/446 (99%)	420 (95%)	22 (5%)	22	22
1	D	439/446 (98%)	415 (94%)	24 (6%)	19	18
All	All	1770/1784 (99%)	1681 (95%)	89 (5%)	22	22

All (89) 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	128	VAL
1	A	146	PRO
1	A	219	ASN
1	A	221	ASN
1	A	285	LYS
1	A	297	LEU
1	A	326	LEU
1	A	333	GLU
1	A	386	LEU
1	A	395	LEU
1	A	429	LEU
1	A	440	LEU
1	A	460	LEU
1	A	496	LEU
1	A	519	MET
1	B	32	HIS
1	B	39	ARG
1	B	41	ILE

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Mol	Chain	Res	Type
1	B	95	LEU
1	B	96	ASN
1	B	104	THR
1	B	138	LEU
1	B	139	LEU
1	B	146	PRO
1	B	169	VAL
1	B	215	LEU
1	B	219	ASN
1	B	256	ASP
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	490	ARG
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	106	GLN
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	326	LEU
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

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Mol	Chain	Res	Type
1	D	74	VAL
1	D	95	LEU
1	D	96	ASN
1	D	106	GLN
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	189	VAL
1	D	219	ASN
1	D	274	LEU
1	D	297	LEU
1	D	309	LEU
1	D	326	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

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

Mol	Chain	Res	Type
1	A	121	HIS
1	A	173	GLN
1	A	219	ASN
1	A	239	GLN
1	A	255	HIS
1	A	320	ASN
1	A	364	GLN
1	A	434	ASN
1	B	106	GLN
1	B	121	HIS
1	B	207	GLN
1	B	219	ASN
1	B	239	GLN
1	B	315	HIS
1	B	357	HIS

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Mol	Chain	Res	Type
1	B	360	ASN
1	B	434	ASN
1	B	476	GLN
1	C	173	GLN
1	C	207	GLN
1	C	219	ASN
1	C	239	GLN
1	C	320	ASN
1	C	434	ASN
1	C	476	GLN
1	D	32	HIS
1	D	63	ASN
1	D	119	ASN
1	D	143	ASN
1	D	207	GLN
1	D	219	ASN
1	D	234	ASN
1	D	239	GLN
1	D	255	HIS
1	D	277	ASN
1	D	320	ASN
1	D	360	ASN
1	D	434	ASN
1	D	464	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 ⓘ

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	2.62	1 (25%)	6,6,6	0.87	0
4	ACT	A	802	-	3,3,3	0.63	0	3,3,3	1.38	0
3	PO4	C	707	-	4,4,4	2.71	1 (25%)	6,6,6	0.88	0
4	ACT	C	807	-	3,3,3	0.79	0	3,3,3	1.25	0
4	ACT	B	806	-	3,3,3	0.61	0	3,3,3	1.42	0
2	1CY	C	603	-	16,18,18	1.69	3 (18%)	18,27,27	2.08	2 (11%)
3	PO4	B	702	-	4,4,4	2.61	1 (25%)	6,6,6	0.88	0
4	ACT	A	801	-	3,3,3	0.70	0	3,3,3	1.50	0
2	1CY	B	602	-	16,18,18	1.64	3 (18%)	18,27,27	2.08	4 (22%)
4	ACT	B	804	-	3,3,3	0.62	0	3,3,3	1.39	0
3	PO4	D	704	-	4,4,4	2.69	1 (25%)	6,6,6	0.83	0
3	PO4	B	706	-	4,4,4	2.61	1 (25%)	6,6,6	0.87	0
3	PO4	D	708	-	4,4,4	2.65	1 (25%)	6,6,6	0.88	0
4	ACT	A	803	-	3,3,3	0.66	0	3,3,3	1.38	0
4	ACT	D	808	-	3,3,3	0.47	0	3,3,3	1.45	0
2	1CY	A	601	-	16,18,18	1.67	3 (18%)	18,27,27	2.06	2 (11%)
2	1CY	D	604	-	16,18,18	1.63	3 (18%)	18,27,27	2.12	3 (16%)
3	PO4	A	705	-	4,4,4	2.52	1 (25%)	6,6,6	0.91	0
4	ACT	B	805	-	3,3,3	0.68	0	3,3,3	1.42	0
3	PO4	A	701	-	4,4,4	2.58	1 (25%)	6,6,6	0.91	0

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

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	704	PO4	P-O1	5.13	1.62	1.50
3	C	707	PO4	P-O1	5.05	1.62	1.50
3	D	708	PO4	P-O1	4.97	1.62	1.50
3	C	703	PO4	P-O1	4.95	1.62	1.50
3	B	702	PO4	P-O1	4.92	1.62	1.50
3	B	706	PO4	P-O1	4.91	1.62	1.50
3	A	701	PO4	P-O1	4.83	1.61	1.50
3	A	705	PO4	P-O1	4.73	1.61	1.50
2	A	601	1CY	C2-N3	-4.01	1.27	1.36
2	D	604	1CY	C2-N3	-3.99	1.27	1.36
2	C	603	1CY	C2-N3	-3.89	1.27	1.36
2	B	602	1CY	C2-N3	-3.85	1.28	1.36
2	C	603	1CY	C4-N3	-3.72	1.28	1.33
2	A	601	1CY	C4-N3	-3.56	1.28	1.33
2	B	602	1CY	C4-N3	-3.48	1.28	1.33
2	D	604	1CY	C4-N3	-3.37	1.28	1.33
2	D	604	1CY	C2-N1	-2.53	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
2	A	601	1CY	C2-N1	-2.28	1.28	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	1CY	N8-C4-N5	6.58	124.08	118.79
2	C	603	1CY	N8-C4-N5	6.57	124.07	118.79
2	D	604	1CY	N8-C4-N5	6.53	124.04	118.79
2	A	601	1CY	N8-C4-N5	6.32	123.87	118.79
2	D	604	1CY	C9-C6-N5	4.91	113.91	110.24
2	A	601	1CY	C9-C6-N5	4.74	113.79	110.24
2	C	603	1CY	C9-C6-N5	4.69	113.75	110.24
2	B	602	1CY	C9-C6-N5	3.95	113.20	110.24
2	B	602	1CY	C16-C11-N5	2.13	122.45	120.08
2	D	604	1CY	C16-C11-N5	2.11	122.43	120.08
2	B	602	1CY	C10-C6-N5	2.03	111.75	110.24

There are no chirality outliers.

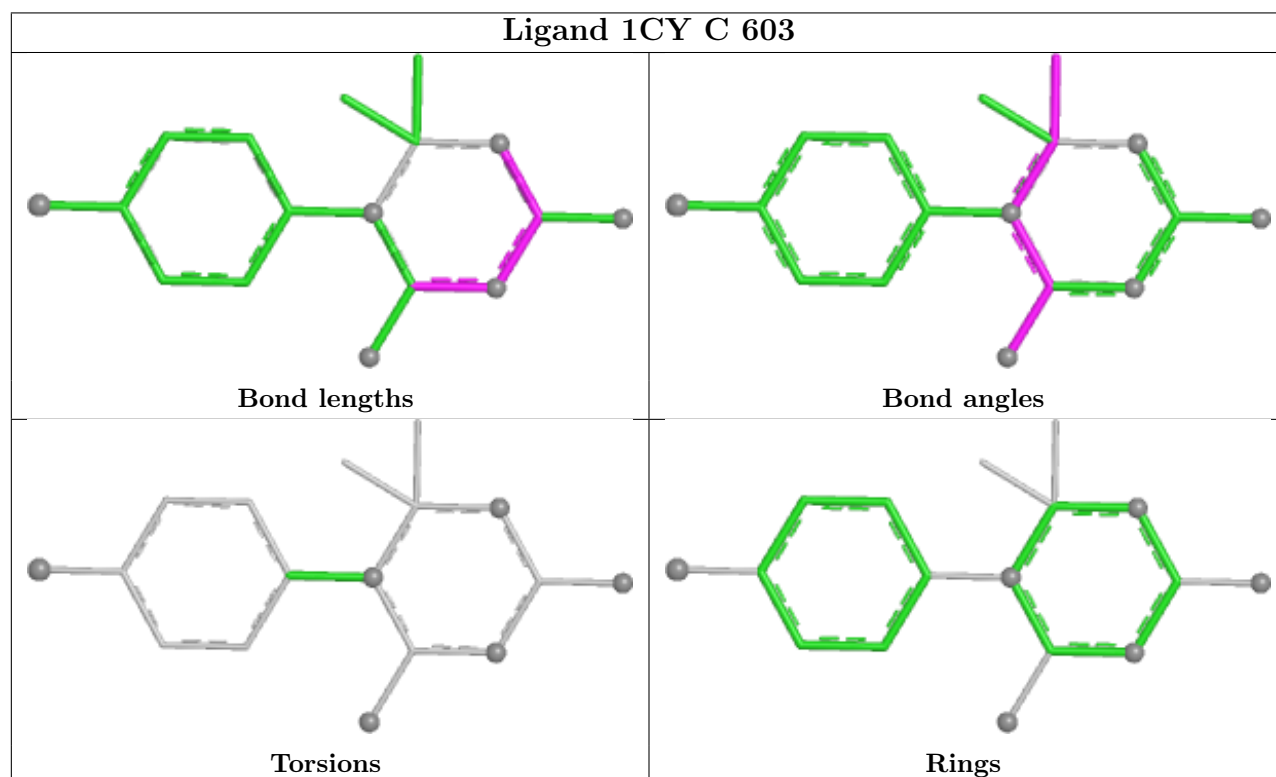
There are no torsion outliers.

There are no ring outliers.

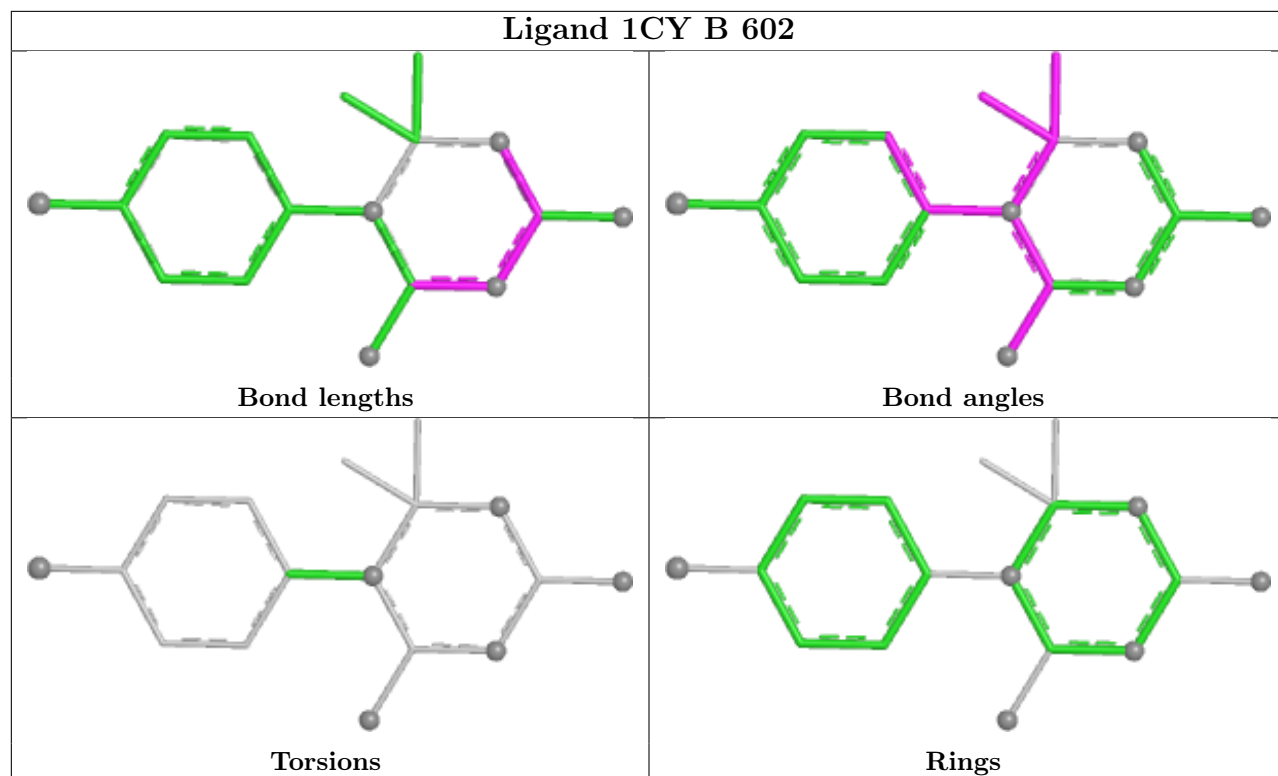
4 monomers are involved in 7 short contacts:

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

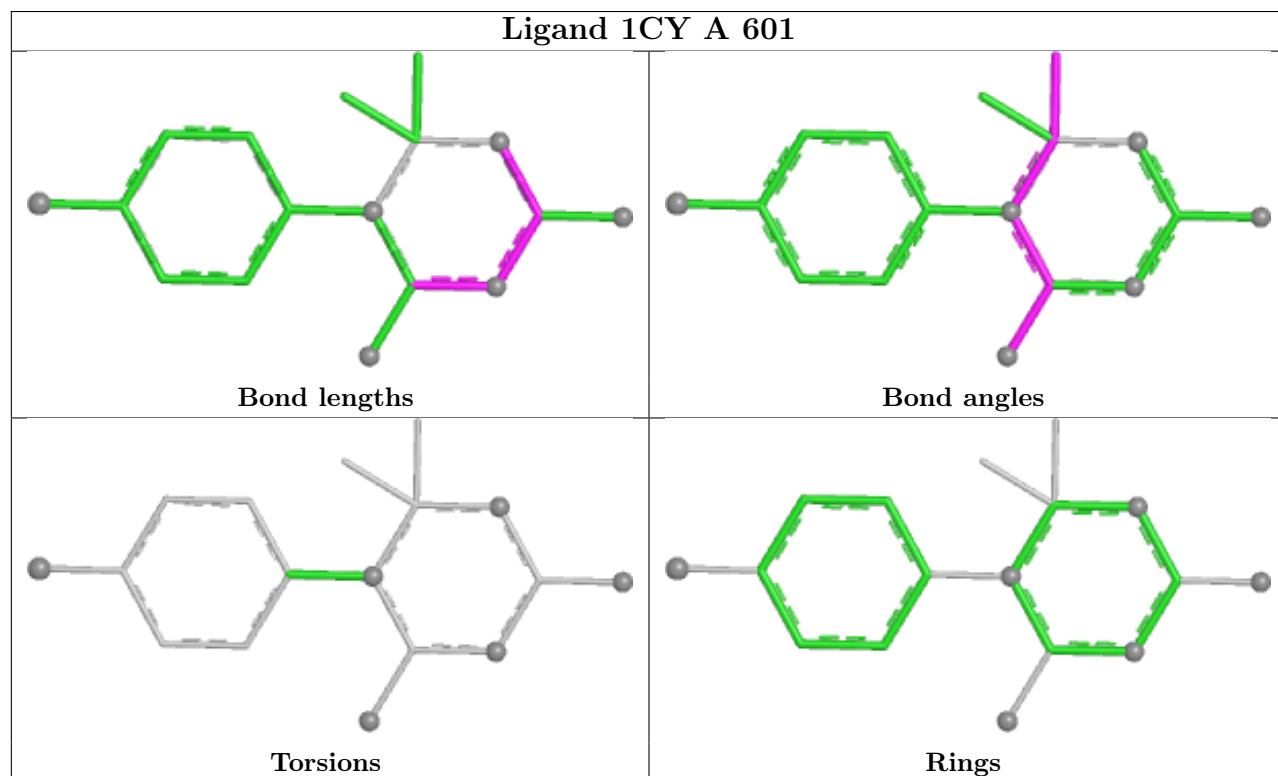
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

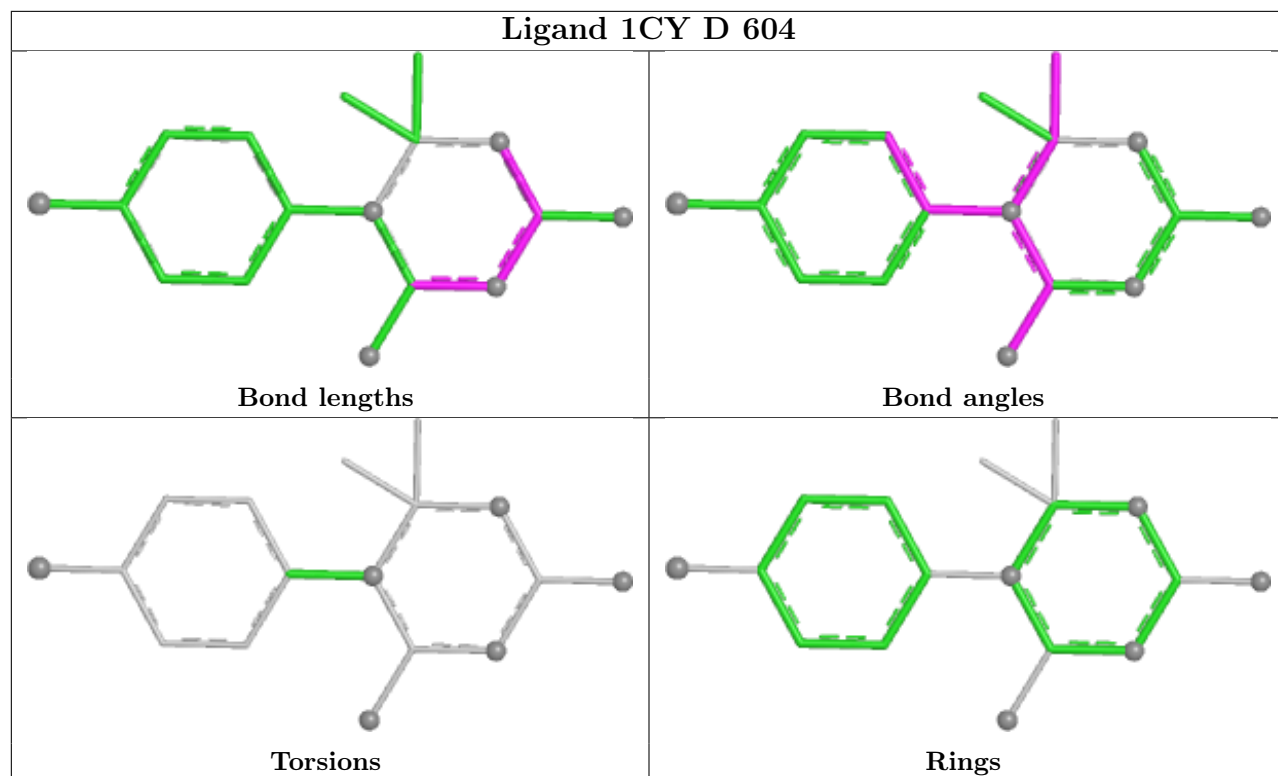


Ligand 1CY B 602



Ligand 1CY A 601





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%)	0.01	19 (3%) 45 47	18, 28, 57, 90	0
1	B	519/521 (99%)	0.25	32 (6%) 26 28	20, 33, 73, 90	0
1	C	516/521 (99%)	0.00	21 (4%) 41 43	16, 27, 62, 88	0
1	D	513/521 (98%)	0.17	25 (4%) 35 37	19, 30, 68, 90	0
All	All	2068/2084 (99%)	0.11	97 (4%) 36 38	16, 30, 66, 90	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	41	ILE	5.9
1	D	41	ILE	5.7
1	C	42	PRO	5.2
1	A	520	ALA	5.2
1	B	521	VAL	5.2
1	C	41	ILE	4.7
1	C	517	MET	4.6
1	B	186	SER	4.5
1	D	42	PRO	4.5
1	D	43	TRP	4.4
1	A	38	GLY	4.1
1	B	519	MET	4.0
1	A	41	ILE	4.0
1	B	36	GLY	3.9
1	D	36	GLY	3.9
1	A	1	MET	3.9
1	A	517	MET	3.8
1	A	2	SER	3.7
1	D	188	SER	3.7
1	D	515	ILE	3.7
1	C	187	CYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	43	TRP	3.5
1	C	43	TRP	3.4
1	C	38	GLY	3.4
1	A	519	MET	3.3
1	C	182	ALA	3.3
1	D	112	LEU	3.3
1	C	37	ASP	3.3
1	B	520	ALA	3.2
1	D	120	LEU	3.1
1	A	186	SER	3.1
1	B	188	SER	3.1
1	D	37	ASP	3.0
1	B	42	PRO	2.9
1	A	43	TRP	2.9
1	C	515	ILE	2.9
1	D	259	GLY	2.9
1	B	187	CYS	2.8
1	B	515	ILE	2.8
1	C	44	ASN	2.8
1	D	40	SER	2.8
1	D	122	ALA	2.8
1	C	121	HIS	2.7
1	B	38	GLY	2.7
1	B	61	GLY	2.7
1	D	108	LEU	2.7
1	D	38	GLY	2.7
1	A	42	PRO	2.7
1	B	40	SER	2.7
1	B	190	PHE	2.7
1	B	37	ASP	2.7
1	C	186	SER	2.6
1	A	44	ASN	2.5
1	A	182	ALA	2.5
1	D	185	SER	2.5
1	D	109	LEU	2.5
1	D	260	VAL	2.5
1	C	183	SER	2.5
1	B	13	ALA	2.5
1	D	39	ARG	2.5
1	C	61	GLY	2.5
1	A	187	CYS	2.4
1	D	257	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	185	SER	2.4
1	B	35	ILE	2.4
1	B	104	THR	2.3
1	B	120	LEU	2.3
1	C	39	ARG	2.3
1	C	35	ILE	2.3
1	A	37	ASP	2.3
1	A	185	SER	2.3
1	B	32	HIS	2.3
1	D	119	ASN	2.3
1	B	117	LYS	2.3
1	B	516	SER	2.2
1	C	40	SER	2.2
1	A	515	ILE	2.2
1	B	44	ASN	2.2
1	B	182	ALA	2.2
1	B	517	MET	2.2
1	D	121	HIS	2.2
1	B	189	VAL	2.2
1	C	62	LYS	2.2
1	D	113	PRO	2.2
1	B	15	GLY	2.2
1	B	217	SER	2.2
1	A	45	VAL	2.2
1	B	358	ASP	2.1
1	B	113	PRO	2.1
1	C	36	GLY	2.1
1	B	181	ARG	2.1
1	D	182	ALA	2.1
1	A	61	GLY	2.0
1	C	184	GLU	2.0
1	D	189	VAL	2.0
1	D	114	ASP	2.0
1	A	36	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

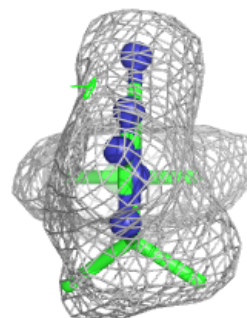
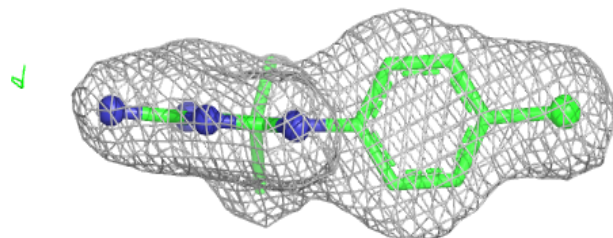
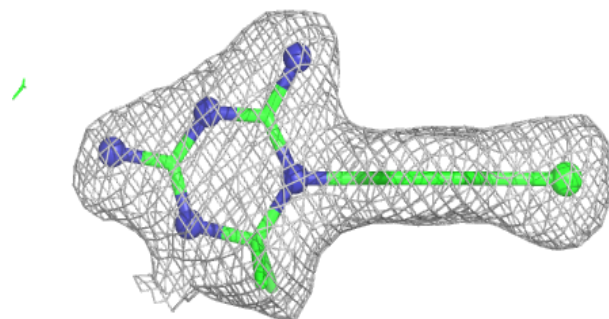
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	C	807	4/4	0.72	0.17	31,36,36,36	0
4	ACT	A	802	4/4	0.78	0.13	44,44,44,45	0
3	PO4	B	702	5/5	0.78	0.13	73,74,75,75	0
4	ACT	A	803	4/4	0.80	0.21	44,47,47,48	0
3	PO4	B	706	5/5	0.81	0.10	78,78,79,80	0
4	ACT	B	804	4/4	0.82	0.14	40,43,45,45	0
3	PO4	D	708	5/5	0.84	0.11	67,69,69,70	0
3	PO4	C	703	5/5	0.85	0.11	73,73,73,74	0
4	ACT	B	805	4/4	0.86	0.18	44,44,45,45	0
4	ACT	A	801	4/4	0.86	0.12	24,29,30,31	0
3	PO4	D	704	5/5	0.87	0.10	63,63,65,65	0
3	PO4	A	705	5/5	0.89	0.12	53,54,55,56	0
3	PO4	C	707	5/5	0.90	0.09	49,51,52,53	0
2	1CY	B	602	17/17	0.91	0.09	33,39,43,46	0
2	1CY	A	601	17/17	0.91	0.09	26,31,34,36	0
4	ACT	D	808	4/4	0.91	0.12	34,34,37,37	0
3	PO4	A	701	5/5	0.92	0.11	51,52,52,53	0
4	ACT	B	806	4/4	0.93	0.13	42,42,43,43	0
2	1CY	D	604	17/17	0.93	0.08	25,29,34,40	0
2	1CY	C	603	17/17	0.93	0.08	22,26,32,35	0

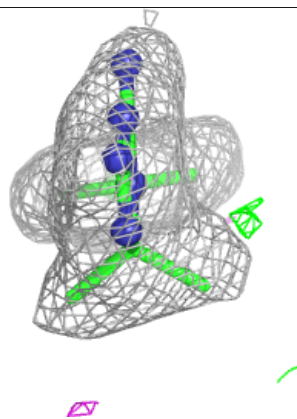
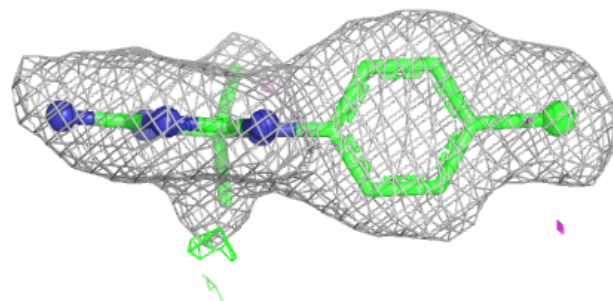
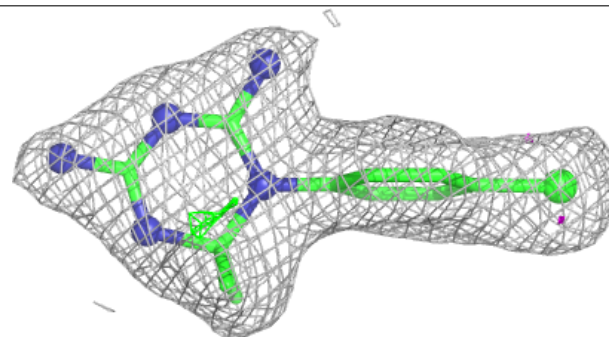
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

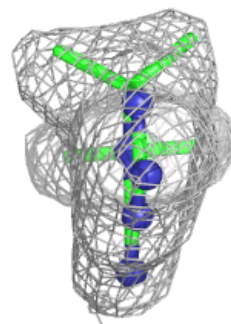
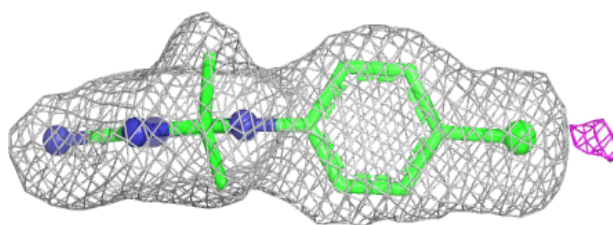
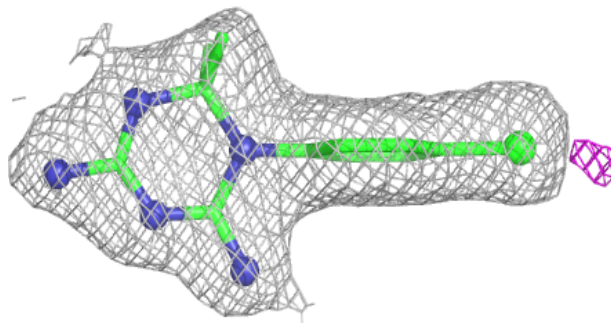
**Electron density around 1CY A 601:**

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

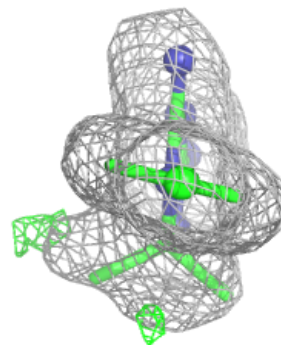
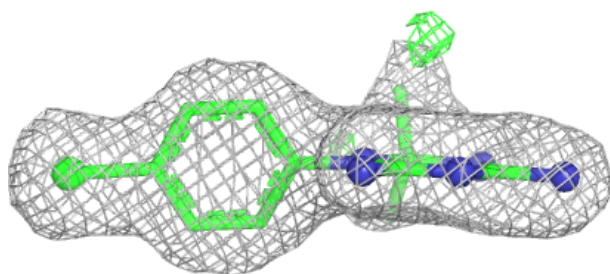
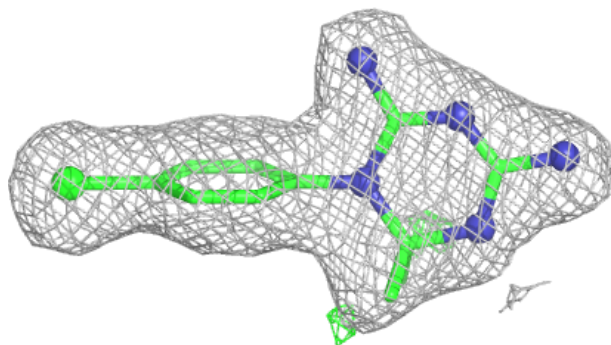


Electron density around 1CY D 604:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.