



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:56 AM UTC

PDB ID : 7XB6 / pdb_00007xb6
Title : Crystal structure of the O-carbamoyltransferase VtdB in complex with carbamoyl adenylate intermediate
Authors : Zhang, H.; Teng, Y.
Deposited on : 2022-03-20
Resolution : 2.90 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

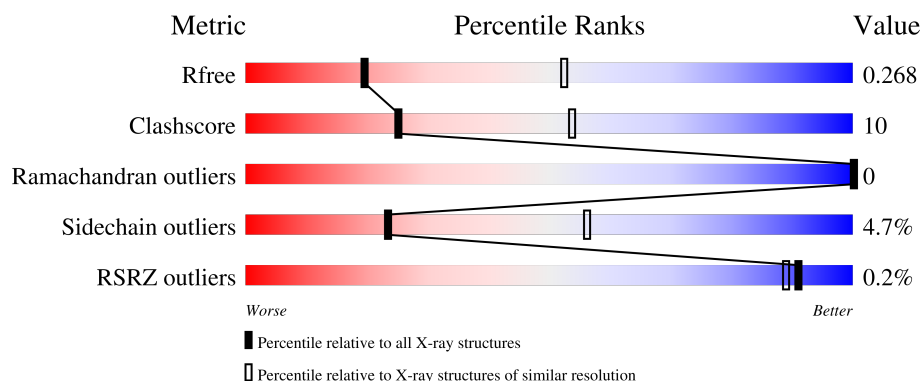
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	597	 77% 21% 2% 2%
1	B	597	 79% 20% 1% 1%
1	C	597	 78% 20% 2% 2%
1	D	597	 75% 23% 2% 2%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18838 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.

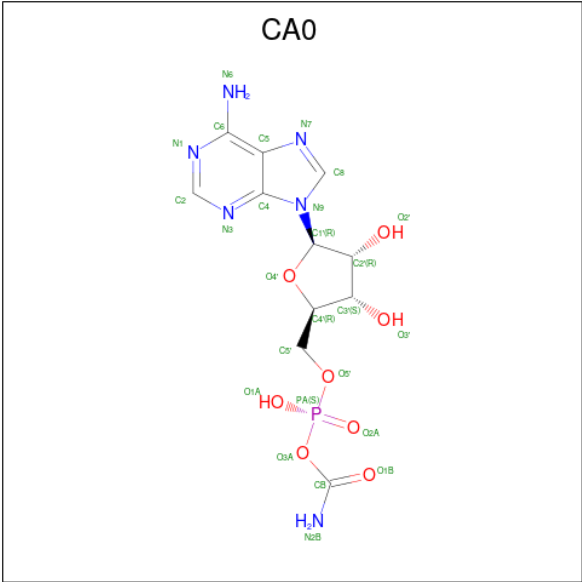
- Molecule 1 is a protein called Carbamoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	0	0
			4642	2936	796	895	15			
1	B	597	Total	C	N	O	S	0	0	0
			4642	2936	796	895	15			
1	C	597	Total	C	N	O	S	0	0	0
			4642	2936	796	895	15			
1	D	597	Total	C	N	O	S	0	0	0
			4642	2936	796	895	15			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

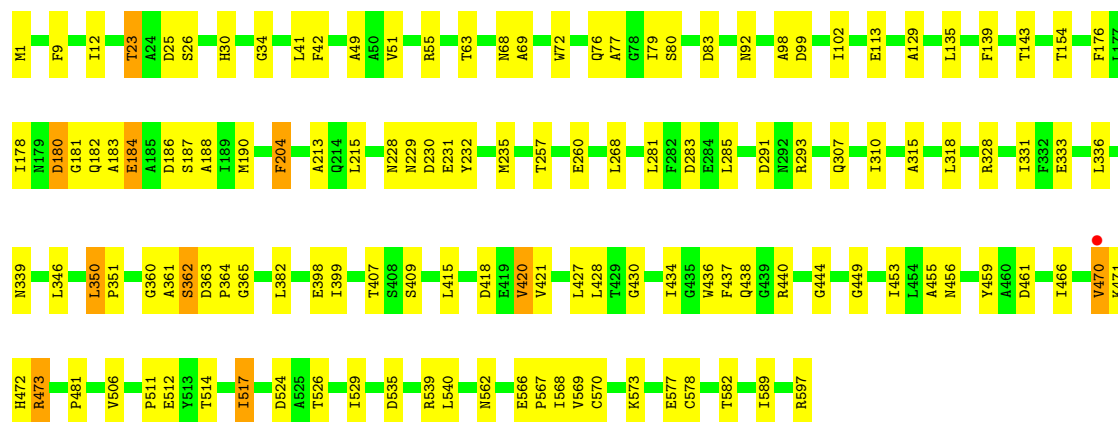
- Molecule 3 is 5'-O-[(S)-(carbamoyloxy)(hydroxy)phosphoryl]adenosine (CCD ID: CA0) (formula: C₁₁H₁₅N₆O₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			26	11	6	8	1		
3	B	1	Total	C	N	O	P	0	0
			26	11	6	8	1		
3	C	1	Total	C	N	O	P	0	0
			26	11	6	8	1		
3	D	1	Total	C	N	O	P	0	0
			26	11	6	8	1		

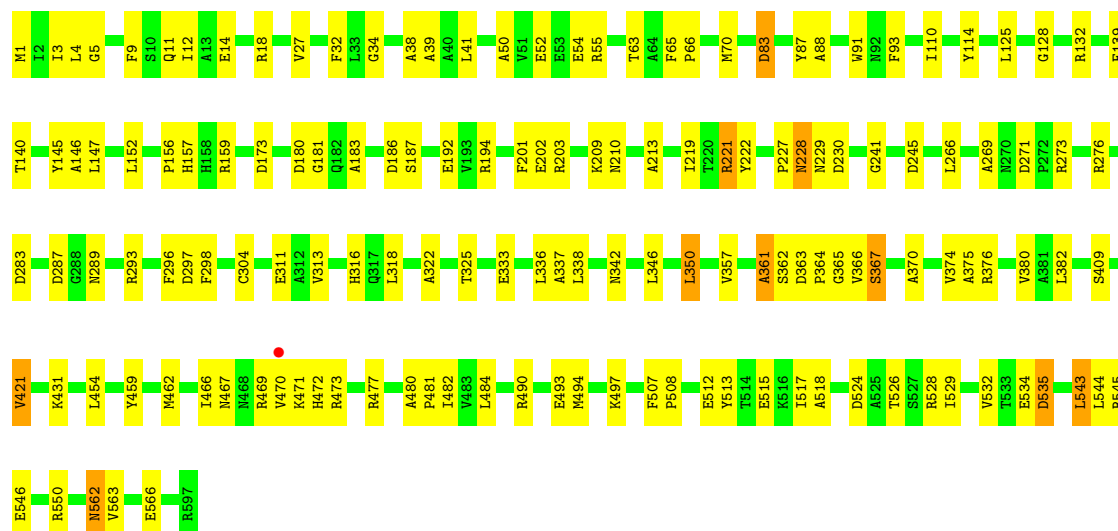
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O	0	0
			41	41		
4	B	41	Total	O	0	0
			41	41		
4	C	46	Total	O	0	0
			46	46		
4	D	34	Total	O	0	0
			34	34		



● Molecule 1: Carbamoyltransferase

Chain D: 75% 23% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.39Å 245.57Å 96.95Å 90.00° 92.04° 90.00°	Depositor
Resolution (Å)	48.19 – 2.90 48.19 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.19-2.90) 98.2 (48.19-2.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.187 , 0.269 0.187 , 0.268	Depositor DCC
R_{free} test set	2743 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	60.9	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.059 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18838	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: MG, CA0

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.01	0/4746	1.46	9/6448 (0.1%)
1	B	1.00	0/4746	1.47	8/6448 (0.1%)
1	C	1.02	1/4746 (0.0%)	1.47	4/6448 (0.1%)
1	D	1.01	0/4746	1.47	7/6448 (0.1%)
All	All	1.01	1/18984 (0.0%)	1.47	28/25792 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	473	ARG	N-CA	7.08	1.54	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	ASN	N-CA-C	-7.98	102.82	114.39
1	D	229	ASN	N-CA-C	-7.40	105.43	114.75
1	C	472	HIS	N-CA-C	-6.38	104.07	112.24
1	B	230	ASP	CB-CA-C	-6.19	101.52	111.86
1	B	180	ASP	CA-CB-CG	6.06	118.66	112.60
1	B	559	THR	CA-CB-OG1	-5.75	100.98	109.60
1	D	221	ARG	CA-C-N	5.73	128.27	120.54
1	D	221	ARG	C-N-CA	5.73	128.27	120.54
1	A	229	ASN	N-CA-C	-5.72	107.55	114.75
1	A	471	LYS	N-CA-C	-5.71	102.97	110.33
1	D	287	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	180	ASP	CA-CB-CG	5.51	118.11	112.60
1	C	187	SER	N-CA-C	-5.46	107.17	113.88
1	B	99	ASP	CA-CB-CG	5.44	118.04	112.60
1	D	535	ASP	CA-CB-CG	5.40	118.00	112.60
1	C	461	ASP	CA-CB-CG	5.21	117.81	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	ASP	CA-CB-CG	5.19	117.79	112.60
1	B	238	ALA	CA-C-N	5.11	125.76	120.03
1	B	238	ALA	C-N-CA	5.11	125.76	120.03
1	D	361	ALA	N-CA-C	-5.09	106.17	112.38
1	B	524	ASP	CA-CB-CG	5.08	117.68	112.60
1	C	204	PHE	N-CA-C	-5.07	107.14	113.38
1	A	98	ALA	CA-C-N	5.04	126.99	120.44
1	A	98	ALA	C-N-CA	5.04	126.99	120.44
1	A	501	PRO	N-CA-C	5.04	120.25	114.20
1	D	230	ASP	N-CA-C	5.03	118.95	112.41
1	A	368	ILE	CA-C-N	5.01	125.51	119.94
1	A	368	ILE	C-N-CA	5.01	125.51	119.94

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	4642	0	4497	98	0
1	B	4642	0	4497	80	0
1	C	4642	0	4497	87	0
1	D	4642	0	4497	95	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	26	0	13	6	0
3	B	26	0	14	1	0
3	C	26	0	14	7	0
3	D	26	0	13	1	0
4	A	41	0	0	0	0
4	B	41	0	0	2	0
4	C	46	0	0	1	0
4	D	34	0	0	0	0
All	All	18838	0	18042	357	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 10.

All (357) 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:A:335:GLY:HA3	3:A:602:CA0:H5'	1.22	1.12
1:C:471:LYS:HB3	1:C:473:ARG:HG3	1.42	1.00
1:A:102:ILE:HD12	1:A:119:ILE:HG23	1.63	0.78
1:B:140:THR:OG1	1:B:146:ALA:HA	1.86	0.76
1:A:421:VAL:HG12	1:A:546:GLU:HG3	1.67	0.75
1:C:350:LEU:HB3	1:C:351:PRO:HD2	1.70	0.74
1:C:92:ASN:HA	1:C:154:THR:HB	1.70	0.74
1:D:333:GLU:OE1	1:D:361:ALA:HA	1.88	0.72
1:D:11:GLN:HG3	1:D:128:GLY:O	1.90	0.72
1:B:183:ALA:HB3	1:B:186:ASP:O	1.89	0.71
1:D:283:ASP:OD1	1:D:293:ARG:NH2	2.24	0.71
1:A:231:GLU:HG3	3:A:602:CA0:C8	2.22	0.70
1:A:481:PRO:HG2	1:A:529:ILE:HG22	1.73	0.69
1:D:471:LYS:HB2	1:D:472:HIS:CE1	2.28	0.69
1:C:360:GLY:O	1:C:365:GLY:HA3	1.93	0.68
1:D:110:ILE:CG2	1:D:114:TYR:HB2	2.22	0.68
1:C:23:THR:O	1:C:26:SER:HB3	1.94	0.68
1:D:14:GLU:OE2	1:D:18:ARG:NH1	2.26	0.67
1:B:512:GLU:HB2	4:B:730:HOH:O	1.94	0.67
1:C:228:ASN:ND2	3:C:602:CA0:H3'	2.10	0.66
1:A:9:PHE:HB2	1:A:12:ILE:HB	1.75	0.66
1:C:183:ALA:HB3	1:C:186:ASP:O	1.96	0.66
1:C:362:SER:C	1:C:364:PRO:HD2	2.21	0.66
1:C:350:LEU:HB3	1:C:351:PRO:CD	2.25	0.66
1:D:466:ILE:O	1:D:470:VAL:HG22	1.96	0.65
1:C:9:PHE:O	1:C:12:ILE:HG22	1.96	0.65
1:A:30:HIS:HD2	1:A:229:ASN:HB2	1.62	0.64
1:C:430:GLY:HA2	1:C:459:TYR:OH	1.98	0.64
1:B:201:PHE:HB2	1:B:204:PHE:CD2	2.33	0.64
1:A:319:ARG:O	1:A:322:ALA:HB3	1.99	0.63
1:C:511:PRO:HA	1:C:514:THR:HG23	1.80	0.63
1:B:315:ALA:HA	1:B:350:LEU:HD11	1.81	0.63
1:A:102:ILE:CD1	1:A:119:ILE:HG23	2.28	0.63
1:D:534:GLU:OE2	1:D:545:ARG:NH1	2.33	0.62
1:D:110:ILE:HG22	1:D:114:TYR:HB2	1.82	0.62
1:A:230:ASP:HB3	1:A:233:LYS:HD2	1.82	0.61
1:A:350:LEU:HB3	1:A:351:PRO:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:ARG:HA	1:D:298:PHE:CE2	2.35	0.61
1:A:221:ARG:HB2	1:A:227:PRO:HG3	1.81	0.61
1:B:147:LEU:HD12	1:B:148:PRO:HD2	1.83	0.60
1:D:27:VAL:O	1:D:227:PRO:HD2	2.01	0.60
1:B:201:PHE:HB2	1:B:204:PHE:HD2	1.67	0.60
1:A:362:SER:HB2	1:A:364:PRO:HD2	1.84	0.59
1:B:28:ASP:OD2	1:B:221:ARG:NH2	2.36	0.59
1:D:183:ALA:HB3	1:D:186:ASP:O	2.02	0.59
1:C:449:GLY:HA3	1:C:540:LEU:HD22	1.85	0.58
1:A:181:GLY:HA2	1:A:213:ALA:HB3	1.84	0.58
1:A:455:ALA:HB1	1:A:462:MET:HE2	1.86	0.58
1:B:310:ILE:O	1:B:314:THR:OG1	2.20	0.58
1:B:226:THR:HB	1:B:229:ASN:HD21	1.69	0.58
1:D:480:ALA:HB1	1:D:528:ARG:O	2.04	0.58
1:A:235:MET:HE2	3:A:602:CA0:HN6	1.67	0.57
1:C:190:MET:HE3	1:C:204:PHE:HB3	1.85	0.57
1:B:473:ARG:HB3	1:B:477:ARG:NH1	2.20	0.57
1:A:363:ASP:N	1:A:364:PRO:HD2	2.20	0.57
1:D:88:ALA:HB1	1:D:370:ALA:HB1	1.87	0.57
1:A:5:GLY:HA2	1:A:88:ALA:O	2.05	0.56
1:A:408:SER:O	1:A:597:ARG:HD2	2.04	0.56
1:B:30:HIS:ND1	1:B:229:ASN:HB3	2.20	0.56
1:C:453:ILE:HD13	1:C:470:VAL:HG21	1.86	0.56
1:D:462:MET:HE3	1:D:466:ILE:HG13	1.87	0.56
1:C:455:ALA:HB3	1:C:466:ILE:HD11	1.87	0.56
1:A:481:PRO:HB3	1:A:520:ALA:HB1	1.88	0.56
1:C:230:ASP:HA	1:C:232:TYR:CE2	2.40	0.56
1:D:276:ARG:NE	1:D:276:ARG:HA	2.19	0.56
1:C:363:ASP:N	1:C:364:PRO:CD	2.69	0.56
1:D:375:ALA:CB	1:D:382:LEU:HD21	2.35	0.56
1:A:451:ARG:HD3	1:A:569:VAL:O	2.06	0.55
1:C:228:ASN:H	1:C:231:GLU:CD	2.14	0.55
1:D:311:GLU:HA	1:D:342:ASN:ND2	2.21	0.55
1:A:421:VAL:HG13	1:A:543:LEU:HA	1.89	0.55
1:D:38:ALA:HB2	1:D:52:GLU:HA	1.88	0.55
1:C:283:ASP:OD1	1:C:293:ARG:NH1	2.39	0.55
1:B:41:LEU:HD11	1:B:79:ILE:HD11	1.89	0.55
1:B:407:THR:HG22	1:B:412:TRP:HH2	1.71	0.55
1:C:180:ASP:OD2	1:C:181:GLY:N	2.40	0.55
1:C:228:ASN:HD22	3:C:602:CA0:H3'	1.73	0.54
1:B:1:MET:HE3	1:B:1:MET:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:SER:HA	1:A:516:LYS:O	2.07	0.54
1:D:1:MET:HG2	1:D:380:VAL:HG21	1.90	0.54
1:B:374:VAL:O	1:B:378:LYS:HB2	2.08	0.54
1:C:49:ALA:HB1	1:C:72:TRP:CZ3	2.43	0.54
1:D:363:ASP:N	1:D:364:PRO:HD2	2.23	0.54
1:A:187:SER:HB3	1:A:208:ALA:HA	1.90	0.54
1:A:326:GLU:O	1:A:328:ARG:NH1	2.41	0.54
1:B:256:VAL:HG22	1:B:266:LEU:CD2	2.38	0.54
1:C:180:ASP:CG	1:C:181:GLY:N	2.66	0.53
1:D:266:LEU:O	1:D:269:ALA:HB2	2.08	0.53
1:B:1:MET:HG2	1:B:380:VAL:HG21	1.90	0.53
1:B:431:LYS:HD3	1:B:465:VAL:HG21	1.89	0.53
1:D:210:ASN:HB2	1:D:266:LEU:HG	1.89	0.53
1:A:30:HIS:CD2	1:A:229:ASN:HB2	2.43	0.53
1:B:276:ARG:HA	1:B:276:ARG:NE	2.23	0.53
1:D:157:HIS:CE1	1:D:366:VAL:HG11	2.44	0.53
1:D:363:ASP:N	1:D:364:PRO:CD	2.71	0.53
1:C:182:GLN:CD	1:C:182:GLN:H	2.17	0.53
1:B:425:ALA:O	1:B:429:THR:HG23	2.09	0.53
1:D:11:GLN:HE21	1:D:11:GLN:HA	1.74	0.53
1:A:235:MET:HE2	3:A:602:CA0:N6	2.23	0.52
1:C:398:GLU:HG2	1:D:296:PHE:CE2	2.44	0.52
1:D:173:ASP:OD1	1:D:194:ARG:HA	2.09	0.52
1:D:421:VAL:HG13	1:D:543:LEU:HA	1.91	0.52
1:C:76:GLN:HE21	1:C:440:ARG:NH1	2.07	0.52
1:C:511:PRO:HA	1:C:514:THR:CG2	2.39	0.52
1:B:132:ARG:HE	1:B:149:ASP:CG	2.18	0.52
1:C:566:GLU:CG	1:C:567:PRO:HD2	2.39	0.52
1:D:376:ARG:NH1	1:D:382:LEU:HD12	2.25	0.52
1:A:237:LEU:HD13	1:A:299:ARG:HB3	1.91	0.52
1:B:470:VAL:HG13	1:B:471:LYS:H	1.74	0.52
1:C:407:THR:HG21	1:D:467:ASN:HB3	1.90	0.52
1:A:420:VAL:HG21	1:A:591:ASP:HA	1.92	0.52
1:A:470:VAL:O	1:A:470:VAL:HG22	2.09	0.52
1:C:307:GLN:HE22	1:C:339:ASN:HD21	1.56	0.52
1:D:9:PHE:HB2	1:D:12:ILE:HB	1.91	0.52
1:D:228:ASN:N	1:D:228:ASN:HD22	2.07	0.52
1:D:562:ASN:C	1:D:562:ASN:HD22	2.18	0.52
1:A:190:MET:HE1	1:A:317:GLN:O	2.10	0.52
1:D:517:ILE:O	1:D:517:ILE:HG13	2.09	0.52
1:D:293:ARG:HA	1:D:298:PHE:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:VAL:HG13	1:A:517:ILE:HD11	1.91	0.51
1:B:407:THR:HG22	1:B:412:TRP:CH2	2.45	0.51
1:A:249:ASN:HD21	1:A:305:ALA:HB1	1.75	0.51
1:C:235:MET:HE2	3:C:602:CA0:HN6	1.76	0.51
1:C:281:LEU:O	1:C:285:LEU:HG	2.10	0.51
1:C:407:THR:O	1:C:597:ARG:NH1	2.44	0.51
1:D:431:LYS:O	1:D:469:ARG:NH2	2.43	0.51
1:B:470:VAL:HG22	1:B:471:LYS:HG3	1.93	0.51
1:C:213:ALA:HB1	3:C:602:CA0:O3'	2.11	0.51
1:A:517:ILE:O	1:A:521:THR:HG23	2.11	0.51
1:B:362:SER:C	1:B:364:PRO:HD2	2.35	0.51
1:D:221:ARG:HB2	1:D:227:PRO:HB3	1.91	0.51
1:B:363:ASP:N	1:B:364:PRO:CD	2.74	0.51
1:A:287:ASP:O	1:A:292:ASN:ND2	2.44	0.51
1:C:182:GLN:N	3:C:602:CA0:O1B	2.44	0.51
1:B:563:VAL:HG23	1:B:566:GLU:HB2	1.92	0.51
1:A:339:ASN:HB2	3:A:602:CA0:N1	2.25	0.50
1:D:481:PRO:HG2	1:D:529:ILE:HG22	1.93	0.50
1:C:79:ILE:HG23	1:C:83:ASP:HB2	1.92	0.50
1:D:65:PHE:CZ	1:D:139:PHE:HA	2.46	0.50
1:B:34:GLY:O	1:B:63:THR:HA	2.12	0.50
1:A:511:PRO:HA	1:A:514:THR:HG23	1.94	0.50
1:B:342:ASN:O	1:B:346:LEU:HG	2.11	0.50
1:C:113:GLU:OE1	1:C:113:GLU:N	2.40	0.50
1:C:79:ILE:CG2	1:C:80:SER:N	2.75	0.50
1:D:473:ARG:NH2	1:D:477:ARG:O	2.44	0.50
1:A:346:LEU:O	1:A:350:LEU:HB2	2.12	0.50
1:A:33:LEU:HD21	1:A:130:LEU:HD21	1.94	0.50
1:D:192:GLU:HG2	1:D:201:PHE:CZ	2.47	0.49
1:A:228:ASN:H	1:A:231:GLU:CD	2.20	0.49
1:A:7:ASN:O	1:A:37:ALA:HA	2.12	0.49
1:B:369:GLY:O	1:B:370:ALA:C	2.55	0.49
1:C:427:LEU:HB3	1:C:434:ILE:HD11	1.93	0.49
1:A:4:LEU:HD13	1:A:4:LEU:C	2.38	0.49
1:C:566:GLU:HG2	1:C:567:PRO:HD2	1.93	0.49
1:B:267:ALA:O	1:B:268:LEU:HB2	2.12	0.49
1:C:428:LEU:HG	1:C:434:ILE:HD12	1.95	0.49
1:C:481:PRO:HG2	1:C:529:ILE:HG22	1.94	0.49
1:C:437:PHE:HB3	1:C:589:ILE:HA	1.94	0.49
1:C:578:CYS:O	1:C:582:THR:HG23	2.13	0.49
1:B:182:GLN:OE1	1:B:182:GLN:HA	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:GLY:HA2	1:D:213:ALA:HB3	1.96	0.48
1:B:350:LEU:HB3	1:B:351:PRO:CD	2.43	0.48
1:C:178:ILE:O	1:C:188:ALA:HA	2.12	0.48
1:A:363:ASP:N	1:A:364:PRO:CD	2.77	0.48
1:D:515:GLU:HA	1:D:518:ALA:HB2	1.94	0.48
1:A:310:ILE:HD12	1:A:336:LEU:HD11	1.95	0.48
1:A:363:ASP:O	1:A:366:VAL:HG22	2.13	0.48
1:B:61:LYS:HE2	1:B:228:ASN:O	2.14	0.48
1:C:339:ASN:HB2	3:C:602:CA0:N1	2.29	0.48
1:D:459:TYR:HB2	1:D:462:MET:HG2	1.95	0.48
1:B:129:ALA:O	1:B:130:LEU:HB2	2.13	0.47
1:D:507:PHE:CD2	1:D:529:ILE:HG12	2.49	0.47
1:A:180:ASP:HB2	3:A:602:CA0:O2A	2.15	0.47
1:A:33:LEU:HD12	1:A:33:LEU:H	1.79	0.47
1:A:342:ASN:O	1:A:346:LEU:HG	2.15	0.47
1:C:139:PHE:CE1	1:C:143:THR:HG21	2.49	0.47
1:C:453:ILE:CD1	1:C:470:VAL:HG21	2.44	0.47
1:D:4:LEU:C	1:D:4:LEU:HD23	2.39	0.47
1:A:347:LEU:HD21	1:A:497:LYS:HG2	1.96	0.47
1:A:523:VAL:C	1:A:525:ALA:H	2.22	0.47
1:B:57:ASN:HD21	1:B:62:THR:HG21	1.80	0.47
1:B:157:HIS:CE1	1:B:366:VAL:HG11	2.49	0.47
1:D:562:ASN:ND2	1:D:562:ASN:O	2.48	0.47
1:A:70:MET:HE1	1:A:143:THR:HG21	1.97	0.47
1:C:176:PHE:HA	1:C:331:ILE:O	2.15	0.47
1:D:346:LEU:O	1:D:350:LEU:HB2	2.15	0.47
1:A:470:VAL:O	1:A:470:VAL:HG13	2.15	0.47
1:D:524:ASP:OD1	1:D:526:THR:OG1	2.24	0.47
1:D:140:THR:OG1	1:D:146:ALA:HA	2.14	0.47
1:A:469:ARG:NH1	1:A:585:ASP:OD2	2.48	0.46
1:C:399:ILE:HD12	1:C:589:ILE:HG12	1.96	0.46
1:D:132:ARG:NH2	1:D:152:LEU:O	2.41	0.46
1:C:30:HIS:ND1	1:C:229:ASN:HB2	2.30	0.46
1:A:54:GLU:OE2	1:A:55:ARG:NH1	2.49	0.46
1:C:41:LEU:CD2	1:C:77:ALA:HB2	2.45	0.46
1:B:363:ASP:O	1:B:364:PRO:C	2.57	0.46
1:C:34:GLY:O	1:C:63:THR:HA	2.15	0.46
1:D:83:ASP:N	1:D:83:ASP:OD1	2.48	0.46
1:A:292:ASN:O	1:A:295:GLU:HB2	2.15	0.46
1:C:41:LEU:HD23	1:C:77:ALA:HB2	1.98	0.46
1:A:16:PHE:CD2	1:A:32:PHE:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:SER:C	1:A:364:PRO:HD2	2.41	0.46
1:B:1:MET:CE	1:B:85:ASP:CB	2.94	0.46
1:D:337:ALA:HB1	1:D:357:VAL:CG1	2.46	0.46
1:A:462:MET:O	1:A:466:ILE:HG13	2.15	0.46
1:C:23:THR:HG22	1:C:26:SER:HB2	1.98	0.46
1:C:428:LEU:O	1:C:456:ASN:HB2	2.16	0.46
1:D:546:GLU:OE2	1:D:550:ARG:NE	2.49	0.46
1:A:288:GLY:HA2	1:A:292:ASN:HD21	1.81	0.46
1:D:110:ILE:HG21	1:D:114:TYR:HB2	1.95	0.45
1:A:160:ALA:O	1:A:369:GLY:HA3	2.16	0.45
1:D:5:GLY:HA2	1:D:88:ALA:O	2.17	0.45
1:D:54:GLU:OE2	1:D:55:ARG:NH1	2.49	0.45
1:D:507:PHE:HD2	1:D:529:ILE:HG12	1.81	0.45
1:B:467:ASN:HA	1:B:471:LYS:O	2.17	0.45
1:B:56:MET:HE3	4:B:726:HOH:O	2.17	0.45
1:A:70:MET:HE1	1:A:139:PHE:CE2	2.52	0.45
1:A:451:ARG:HG2	1:A:569:VAL:HG23	1.97	0.45
1:A:461:ASP:O	1:A:465:VAL:HG23	2.17	0.45
1:C:42:PHE:CE1	1:C:382:LEU:HD12	2.51	0.45
1:D:271:ASP:OD2	1:D:273:ARG:NH1	2.50	0.45
1:A:520:ALA:O	1:A:527:SER:OG	2.32	0.45
1:B:1:MET:HE2	1:B:85:ASP:HB2	1.98	0.45
1:D:38:ALA:CB	1:D:52:GLU:HA	2.45	0.45
1:B:61:LYS:NZ	1:B:229:ASN:HA	2.32	0.45
1:C:573:LYS:HE3	1:C:577:GLU:HG3	1.99	0.45
1:C:362:SER:C	1:C:364:PRO:CD	2.88	0.44
1:A:362:SER:CB	1:A:364:PRO:HD2	2.47	0.44
1:A:470:VAL:C	1:A:471:LYS:O	2.59	0.44
1:B:220:THR:OG1	1:B:231:GLU:HG3	2.17	0.44
1:C:55:ARG:NH2	1:C:444:GLY:O	2.50	0.44
1:D:34:GLY:O	1:D:63:THR:HA	2.18	0.44
1:D:87:TYR:CD1	1:D:147:LEU:HD11	2.53	0.44
1:A:527:SER:O	1:A:529:ILE:HG23	2.18	0.44
1:B:279:ASP:HB2	1:B:280:PRO:HD3	2.00	0.44
1:C:98:ALA:O	1:C:102:ILE:HG13	2.18	0.44
1:A:360:GLY:O	1:A:365:GLY:HA3	2.18	0.44
1:B:461:ASP:OD1	1:B:461:ASP:N	2.50	0.44
1:A:258:LEU:HD12	1:A:316:HIS:ND1	2.33	0.44
1:A:322:ALA:O	1:A:325:THR:O	2.35	0.44
1:D:563:VAL:HG22	1:D:566:GLU:OE1	2.18	0.44
1:A:32:PHE:CE2	1:A:63:THR:HG21	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ALA:HB1	1:B:72:TRP:CZ3	2.53	0.44
1:B:201:PHE:HD2	1:B:204:PHE:HE2	1.65	0.44
1:B:466:ILE:HG23	1:B:470:VAL:CG1	2.47	0.44
1:D:27:VAL:HG22	1:D:227:PRO:HD3	1.99	0.44
1:D:490:ARG:NE	1:D:513:TYR:OH	2.51	0.44
1:A:33:LEU:H	1:A:33:LEU:CD1	2.31	0.44
1:A:251:LEU:HD12	1:A:305:ALA:HB1	2.00	0.44
1:C:455:ALA:CB	1:C:466:ILE:HD11	2.47	0.44
1:B:87:TYR:HB2	1:B:147:LEU:HD21	2.00	0.43
1:D:375:ALA:HB1	1:D:382:LEU:HD21	2.00	0.43
1:B:27:VAL:O	1:B:226:THR:HG23	2.18	0.43
1:B:60:LYS:HA	1:B:567:PRO:HG3	1.99	0.43
1:C:9:PHE:HB2	1:C:12:ILE:HB	2.00	0.43
1:D:484:LEU:HA	1:D:532:VAL:O	2.18	0.43
1:C:310:ILE:HD12	1:C:336:LEU:HD11	2.01	0.43
1:A:228:ASN:N	1:A:231:GLU:OE1	2.51	0.43
1:D:39:ALA:O	1:D:50:ALA:HA	2.18	0.43
1:D:140:THR:HA	1:D:145:TYR:O	2.19	0.43
1:D:484:LEU:HD11	1:D:544:LEU:HB3	2.00	0.43
1:B:43:VAL:O	1:B:46:GLU:CG	2.66	0.43
1:B:350:LEU:HB3	1:B:351:PRO:HD2	2.00	0.43
1:B:363:ASP:N	1:B:364:PRO:HD2	2.34	0.43
1:C:268:LEU:HD12	1:C:268:LEU:N	2.34	0.43
1:C:466:ILE:O	1:C:470:VAL:HG13	2.18	0.43
1:A:481:PRO:HB3	1:A:520:ALA:CB	2.47	0.43
1:B:471:LYS:HB3	1:B:473:ARG:HG3	2.00	0.43
1:D:4:LEU:HD12	1:D:41:LEU:HD13	2.00	0.43
1:D:363:ASP:C	1:D:365:GLY:N	2.77	0.43
1:A:12:ILE:CG2	1:A:63:THR:HB	2.49	0.43
1:A:35:HIS:N	1:A:63:THR:HG22	2.34	0.43
1:A:481:PRO:CG	1:A:529:ILE:HG22	2.47	0.43
1:B:376:ARG:CZ	1:B:382:LEU:HD12	2.49	0.43
1:B:404:GLU:HA	1:B:412:TRP:CH2	2.54	0.43
1:C:524:ASP:O	1:C:526:THR:HG23	2.19	0.43
1:D:493:GLU:HB2	1:D:508:PRO:HD2	2.01	0.43
1:D:5:GLY:HA3	1:D:367:SER:O	2.19	0.43
1:B:328:ARG:HD2	1:B:328:ARG:HA	1.72	0.42
1:C:315:ALA:HA	1:C:350:LEU:HD11	2.01	0.42
1:C:436:TRP:CE2	1:C:438:GLN:HG3	2.54	0.42
1:B:7:ASN:ND2	1:B:91:TRP:HE1	2.16	0.42
1:B:45:GLY:HA2	1:B:382:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:362:SER:CB	1:D:364:PRO:HD2	2.49	0.42
1:D:362:SER:C	1:D:364:PRO:HD2	2.44	0.42
1:D:462:MET:CE	1:D:466:ILE:HG13	2.48	0.42
1:A:434:ILE:O	1:A:453:ILE:HA	2.19	0.42
1:B:281:LEU:O	1:B:285:LEU:HD13	2.20	0.42
1:C:176:PHE:CD1	1:C:176:PHE:C	2.97	0.42
1:D:322:ALA:O	1:D:325:THR:O	2.38	0.42
1:A:138:ASP:O	1:A:142:HIS:HD2	2.03	0.42
1:A:221:ARG:CB	1:A:227:PRO:HG3	2.46	0.42
1:B:311:GLU:HA	1:B:342:ASN:OD1	2.20	0.42
1:D:156:PRO:HB2	1:D:159:ARG:HB2	2.02	0.42
1:D:219:ILE:O	1:D:222:TYR:HB3	2.19	0.42
1:D:338:LEU:HD12	3:D:602:CA0:H8	2.01	0.42
1:A:454:LEU:HA	1:A:557:VAL:O	2.19	0.42
1:B:235:MET:SD	1:B:341:VAL:HG23	2.60	0.42
1:B:235:MET:HE2	3:B:602:CA0:HN6	1.85	0.42
1:A:221:ARG:HB2	1:A:227:PRO:CG	2.46	0.42
1:A:258:LEU:N	1:A:258:LEU:HD22	2.35	0.42
1:A:466:ILE:O	1:A:470:VAL:HG12	2.19	0.42
1:D:313:VAL:O	1:D:316:HIS:HB3	2.20	0.42
1:D:562:ASN:C	1:D:562:ASN:ND2	2.78	0.42
1:A:523:VAL:C	1:A:525:ALA:N	2.78	0.42
1:B:158:HIS:NE2	1:B:183:ALA:HB2	2.35	0.42
1:D:3:ILE:HD13	1:D:374:VAL:HG12	2.02	0.42
1:C:55:ARG:HB3	1:C:570:CYS:HB2	2.01	0.41
1:C:182:GLN:H	1:C:182:GLN:NE2	2.18	0.41
1:C:470:VAL:HG22	1:C:471:LYS:HG2	2.01	0.41
1:A:82:GLU:HG3	1:A:145:TYR:CE1	2.55	0.41
1:B:84:VAL:CG1	1:B:87:TYR:CE1	3.03	0.41
1:B:481:PRO:HG2	1:B:529:ILE:HG22	2.02	0.41
1:D:202:GLU:O	1:D:203:ARG:C	2.62	0.41
1:B:473:ARG:HD2	1:B:477:ARG:CZ	2.50	0.41
1:C:346:LEU:O	1:C:350:LEU:HB2	2.20	0.41
1:C:415:LEU:HB2	1:C:420:VAL:HG12	2.02	0.41
1:A:410:VAL:CG1	1:A:580:LEU:HD21	2.49	0.41
1:B:28:ASP:CG	1:B:221:ARG:NH2	2.78	0.41
1:C:328:ARG:HD3	1:C:328:ARG:HA	1.77	0.41
1:C:517:ILE:HG12	1:C:517:ILE:O	2.20	0.41
1:D:494:MET:HB3	1:D:497:LYS:O	2.21	0.41
1:A:91:TRP:O	1:A:154:THR:HB	2.19	0.41
1:A:524:ASP:O	1:A:525:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:LYS:NZ	1:B:559:THR:OG1	2.45	0.41
1:C:9:PHE:HB3	1:C:129:ALA:HB1	2.02	0.41
1:D:91:TRP:HB3	1:D:93:PHE:CE2	2.55	0.41
1:B:347:LEU:CD2	1:B:497:LYS:HG2	2.51	0.41
1:C:562:ASN:ND2	1:C:566:GLU:O	2.44	0.41
1:A:293:ARG:HA	1:A:298:PHE:CD1	2.56	0.41
1:A:451:ARG:HG3	1:A:451:ARG:HH11	1.86	0.41
1:B:256:VAL:HG22	1:B:266:LEU:HD21	2.03	0.41
1:C:568:ILE:HG22	1:C:569:VAL:O	2.21	0.41
1:D:362:SER:HB2	1:D:364:PRO:HD2	2.03	0.41
1:A:509:VAL:CG1	1:A:517:ILE:HD11	2.51	0.41
1:B:23:THR:O	1:B:26:SER:HB3	2.20	0.41
1:B:171:LEU:HD13	1:B:329:ASP:HB3	2.02	0.41
1:B:226:THR:HB	1:B:229:ASN:ND2	2.35	0.41
1:A:140:THR:OG1	1:A:146:ALA:HA	2.21	0.40
1:C:333:GLU:OE1	1:C:361:ALA:HA	2.21	0.40
1:C:512:GLU:HB2	4:C:726:HOH:O	2.21	0.40
1:D:32:PHE:CE2	1:D:63:THR:HG21	2.56	0.40
1:D:66:PRO:O	1:D:70:MET:HB2	2.21	0.40
1:D:318:LEU:HD23	1:D:318:LEU:HA	1.98	0.40
1:A:132:ARG:NH2	1:A:149:ASP:O	2.54	0.40
1:B:84:VAL:HG11	1:B:87:TYR:CE1	2.56	0.40
1:B:338:LEU:HD23	1:B:338:LEU:HA	1.93	0.40
1:B:407:THR:O	1:B:597:ARG:NH1	2.50	0.40
1:C:51:VAL:HG13	1:C:69:ALA:CB	2.50	0.40
1:C:68:ASN:OD1	1:D:289:ASN:ND2	2.54	0.40
1:C:235:MET:HE2	3:C:602:CAO:N6	2.34	0.40
1:A:302:VAL:O	1:A:305:ALA:HB3	2.21	0.40
1:A:350:LEU:HB3	1:A:351:PRO:CD	2.48	0.40
1:D:363:ASP:O	1:D:366:VAL:HG22	2.22	0.40
1:A:65:PHE:CE2	1:A:139:PHE:HA	2.56	0.40
1:C:184:GLU:H	1:C:184:GLU:HG2	1.44	0.40
1:D:241:GLY:HA3	1:D:304:CYS:SG	2.61	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	595/597 (100%)	568 (96%)	27 (4%)	0	100	100
1	B	595/597 (100%)	567 (95%)	28 (5%)	0	100	100
1	C	595/597 (100%)	569 (96%)	26 (4%)	0	100	100
1	D	595/597 (100%)	559 (94%)	36 (6%)	0	100	100
All	All	2380/2388 (100%)	2263 (95%)	117 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	483/483 (100%)	461 (95%)	22 (5%)	24	57
1	B	483/483 (100%)	457 (95%)	26 (5%)	20	51
1	C	483/483 (100%)	460 (95%)	23 (5%)	23	55
1	D	483/483 (100%)	464 (96%)	19 (4%)	28	63
All	All	1932/1932 (100%)	1842 (95%)	90 (5%)	23	56

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	33	LEU

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Mol	Chain	Res	Type
1	A	56	MET
1	A	105	LEU
1	A	180	ASP
1	A	231	GLU
1	A	247	GLN
1	A	326	GLU
1	A	336	LEU
1	A	362	SER
1	A	377	GLU
1	A	413	GLU
1	A	421	VAL
1	A	429	THR
1	A	451	ARG
1	A	473	ARG
1	A	486	GLU
1	A	506	VAL
1	A	534	GLU
1	A	559	THR
1	A	573	LYS
1	A	597	ARG
1	B	1	MET
1	B	124	GLU
1	B	137	GLU
1	B	209	LYS
1	B	229	ASN
1	B	245	ASP
1	B	304	CYS
1	B	314	THR
1	B	327	LEU
1	B	336	LEU
1	B	358	SER
1	B	362	SER
1	B	402	THR
1	B	408	SER
1	B	409	SER
1	B	423	LYS
1	B	432	THR
1	B	442	GLU
1	B	470	VAL
1	B	477	ARG
1	B	499	ARG
1	B	506	VAL

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Mol	Chain	Res	Type
1	B	552	ASP
1	B	563	VAL
1	B	589	ILE
1	B	593	LEU
1	C	1	MET
1	C	23	THR
1	C	25	ASP
1	C	99	ASP
1	C	135	LEU
1	C	180	ASP
1	C	184	GLU
1	C	215	LEU
1	C	257	THR
1	C	260	GLU
1	C	291	ASP
1	C	318	LEU
1	C	350	LEU
1	C	362	SER
1	C	409	SER
1	C	418	ASP
1	C	420	VAL
1	C	421	VAL
1	C	470	VAL
1	C	506	VAL
1	C	517	ILE
1	C	535	ASP
1	C	539	ARG
1	D	83	ASP
1	D	125	LEU
1	D	180	ASP
1	D	187	SER
1	D	209	LYS
1	D	228	ASN
1	D	245	ASP
1	D	297	ASP
1	D	336	LEU
1	D	350	LEU
1	D	367	SER
1	D	409	SER
1	D	421	VAL
1	D	454	LEU
1	D	482	ILE

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Mol	Chain	Res	Type
1	D	512	GLU
1	D	535	ASP
1	D	543	LEU
1	D	562	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	35	HIS
1	A	142	HIS
1	A	179	ASN
1	A	214	GLN
1	A	249	ASN
1	A	294	GLN
1	A	317	GLN
1	A	373	HIS
1	A	467	ASN
1	A	472	HIS
1	B	7	ASN
1	B	59	GLN
1	B	127	ASN
1	B	179	ASN
1	B	214	GLN
1	B	229	ASN
1	B	270	ASN
1	B	294	GLN
1	B	317	GLN
1	B	537	ASN
1	C	92	ASN
1	C	210	ASN
1	C	214	GLN
1	C	218	ASN
1	C	228	ASN
1	C	247	GLN
1	C	307	GLN
1	D	11	GLN
1	D	30	HIS
1	D	59	GLN
1	D	76	GLN
1	D	210	ASN
1	D	228	ASN

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Mol	Chain	Res	Type
1	D	294	GLN
1	D	308	GLN
1	D	342	ASN
1	D	438	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	CA0	D	602	2	27,28,28	0.40	0	39,42,42	0.62	0
3	CA0	C	602	-	27,28,28	0.41	0	39,42,42	0.64	0
3	CA0	B	602	2	27,28,28	0.39	0	39,42,42	0.57	0
3	CA0	A	602	2	27,28,28	0.38	0	39,42,42	0.53	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
3	CA0	D	602	2	-	0/13/31/31	0/3/3/3
3	CA0	C	602	-	-	0/13/31/31	0/3/3/3
3	CA0	B	602	2	-	2/13/31/31	0/3/3/3
3	CA0	A	602	2	-	4/13/31/31	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

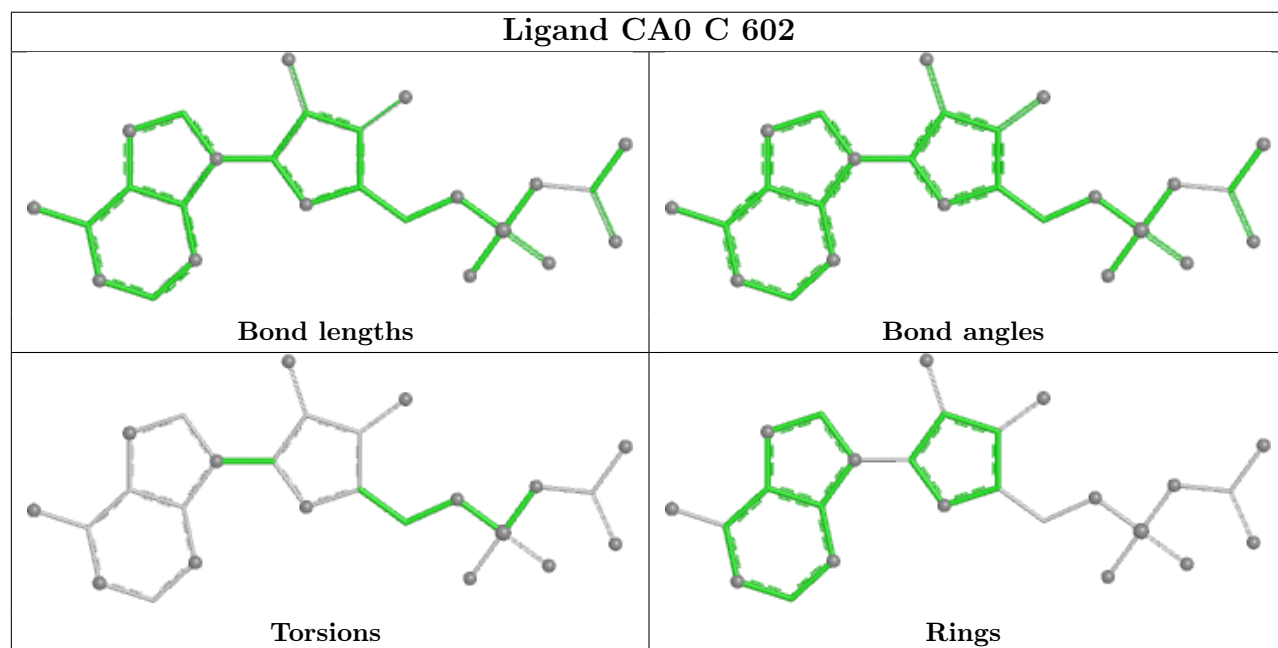
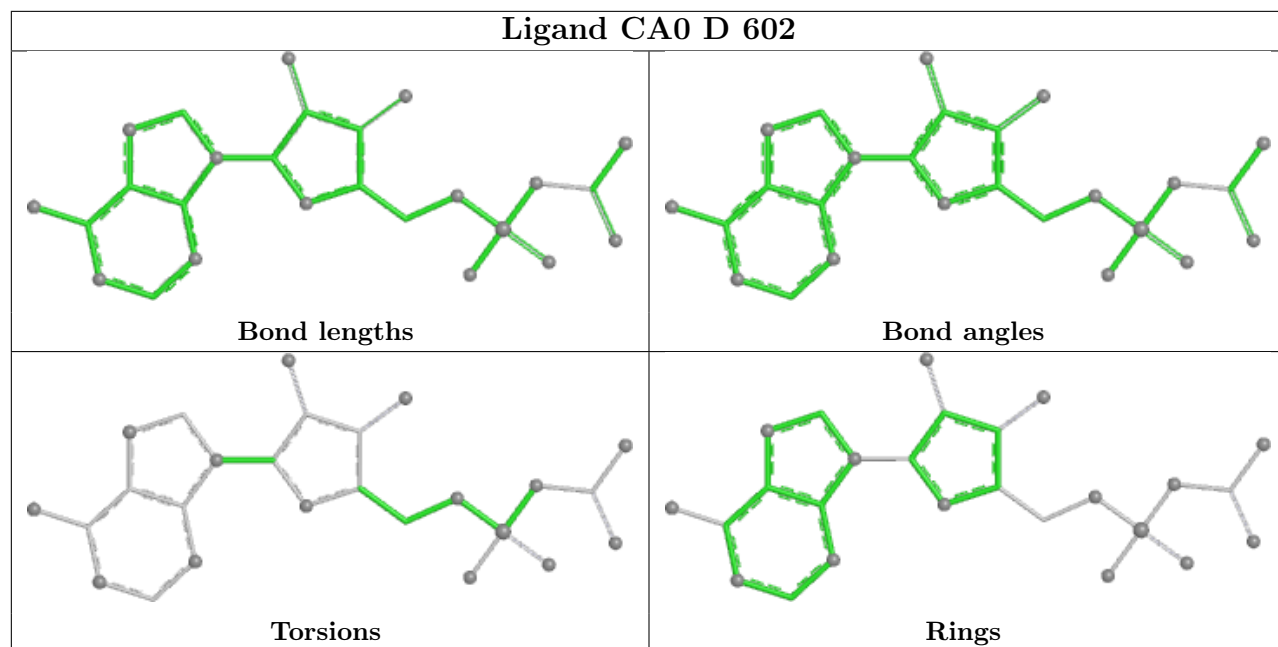
Mol	Chain	Res	Type	Atoms
3	A	602	CA0	C5'-O5'-PA-O2A
3	A	602	CA0	C5'-O5'-PA-O3A
3	B	602	CA0	C3'-C4'-C5'-O5'
3	B	602	CA0	C5'-O5'-PA-O2A
3	A	602	CA0	C2'-C1'-N9-C8
3	A	602	CA0	O4'-C4'-C5'-O5'

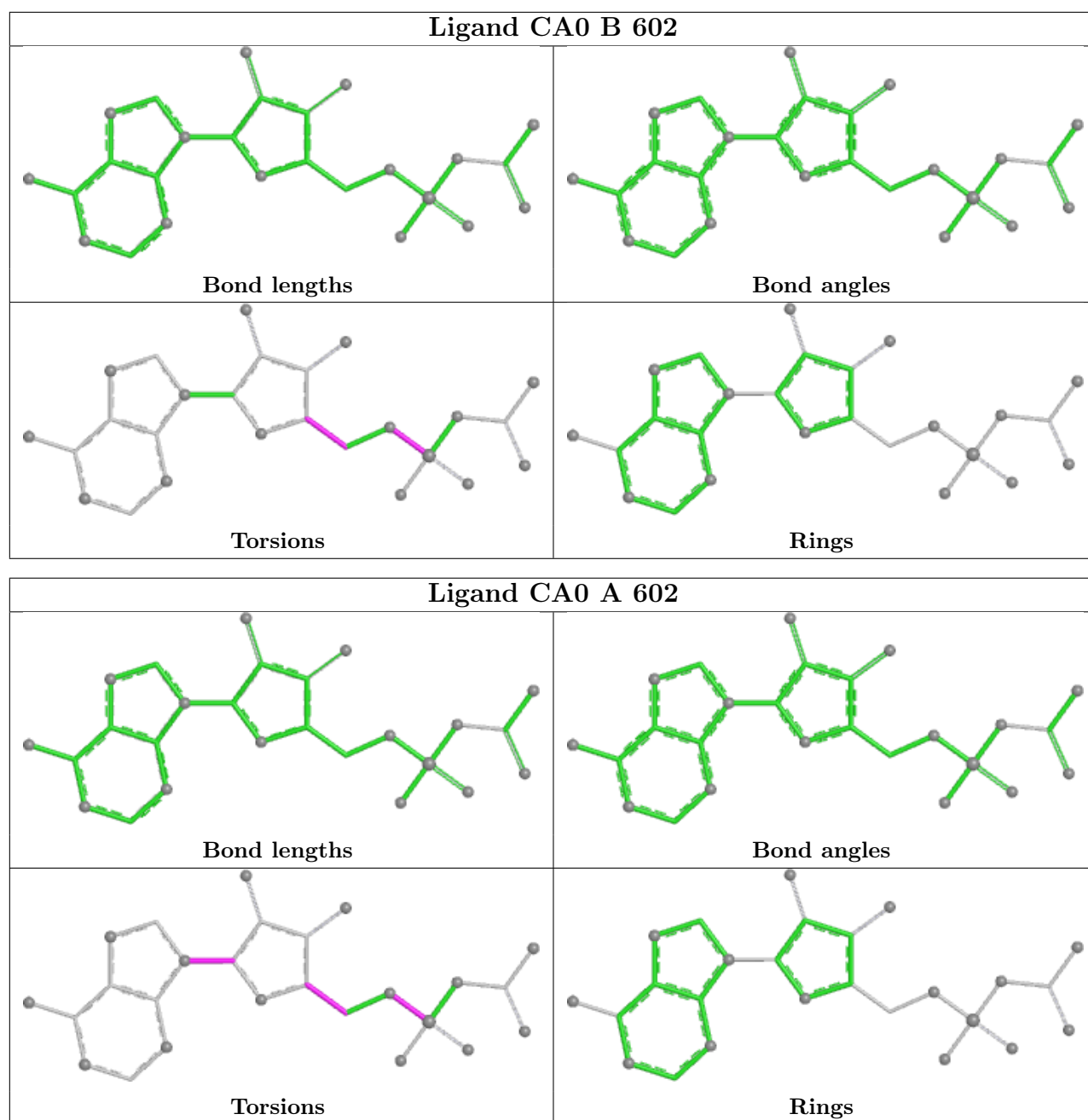
There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	602	CA0	1	0
3	C	602	CA0	7	0
3	B	602	CA0	1	0
3	A	602	CA0	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	597/597 (100%)	-0.38	0 100 100	36, 62, 87, 107	0
1	B	597/597 (100%)	-0.44	3 (0%) 87 83	42, 60, 81, 104	0
1	C	597/597 (100%)	-0.44	1 (0%) 91 89	37, 58, 81, 114	0
1	D	597/597 (100%)	-0.37	1 (0%) 91 89	41, 61, 85, 105	0
All	All	2388/2388 (100%)	-0.41	5 (0%) 91 89	36, 60, 85, 114	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	229	ASN	5.1
1	B	230	ASP	2.8
1	C	470	VAL	2.7
1	D	470	VAL	2.1
1	B	129	ALA	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 oligosaccharides 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,

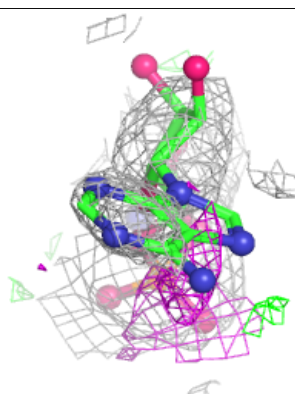
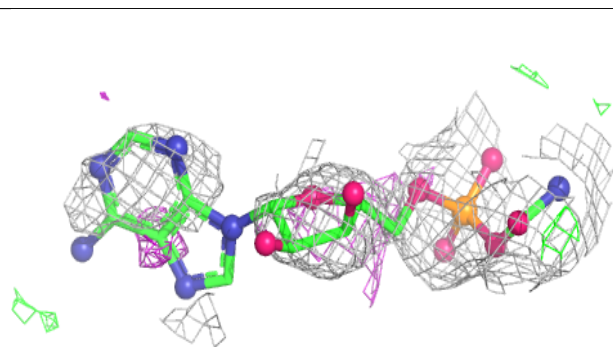
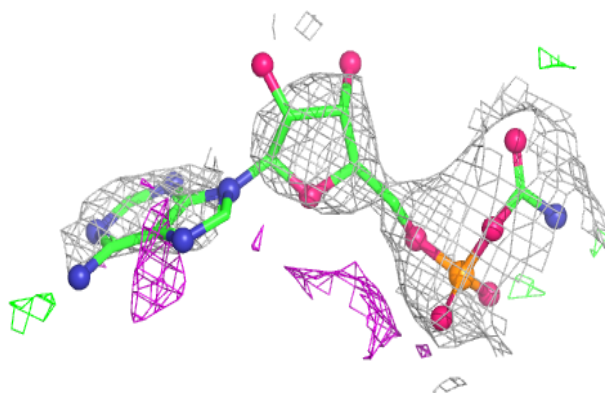
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CA0	B	602	26/26	0.86	0.15	84,120,138,141	0
3	CA0	C	602	26/26	0.87	0.14	103,127,143,156	0
3	CA0	D	602	26/26	0.89	0.14	71,108,130,133	0
3	CA0	A	602	26/26	0.90	0.12	55,83,97,100	0
2	MG	C	601	1/1	0.94	0.12	29,29,29,29	0
2	MG	B	601	1/1	0.99	0.04	27,27,27,27	0
2	MG	A	601	1/1	0.99	0.03	22,22,22,22	0
2	MG	D	601	1/1	1.00	0.02	22,22,22,22	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.

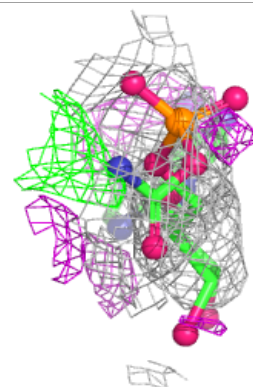
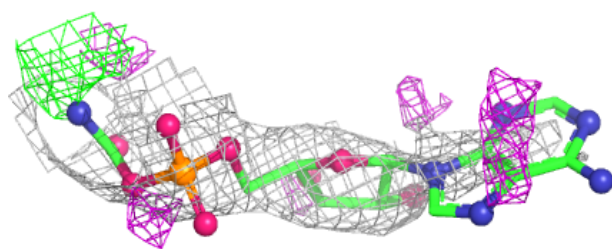
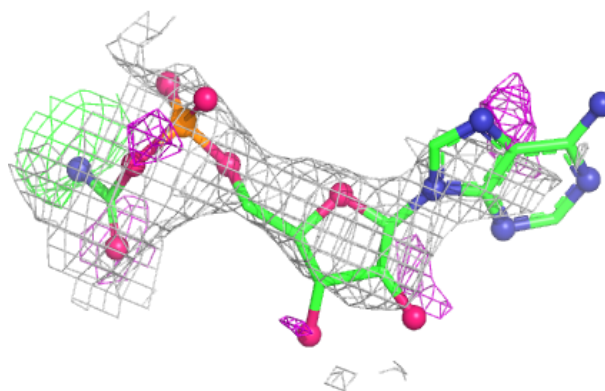
Electron density around CA0 B 602:

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

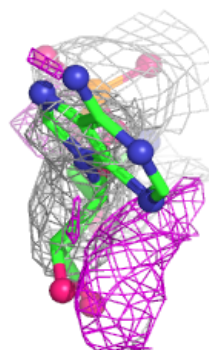
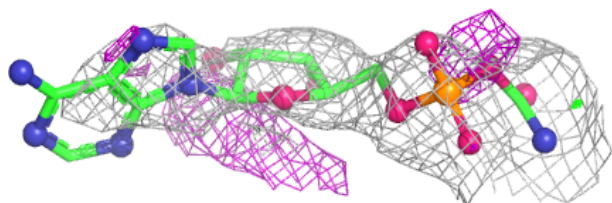
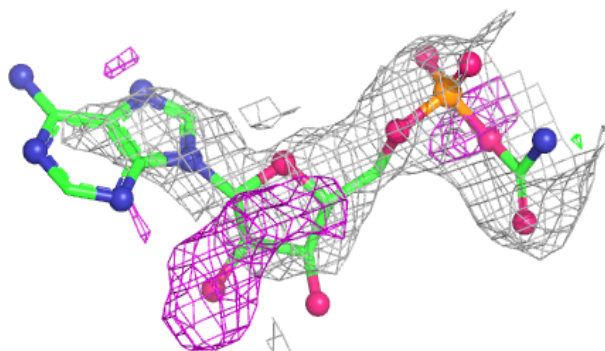


Electron density around CA0 C 602:

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

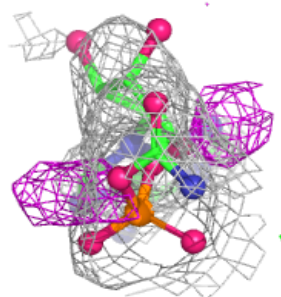
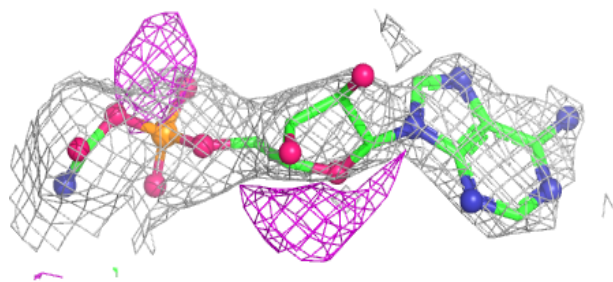
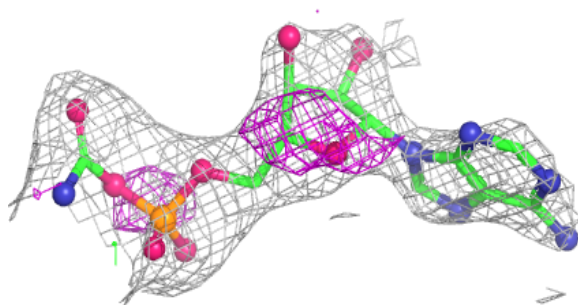
**Electron density around CA0 D 602:**

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



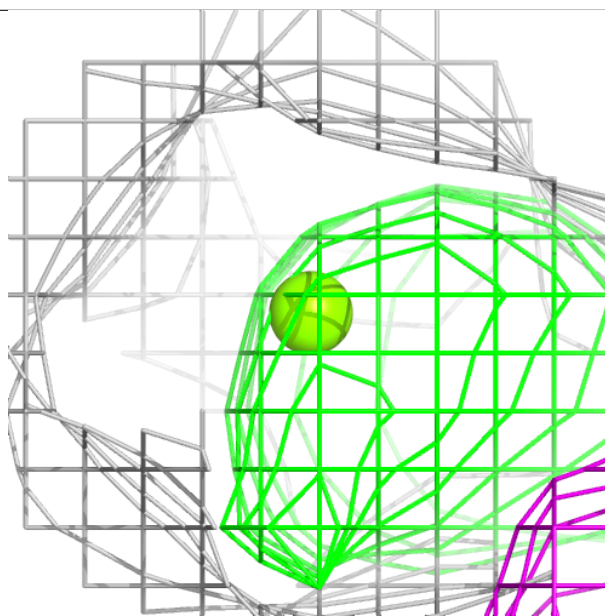
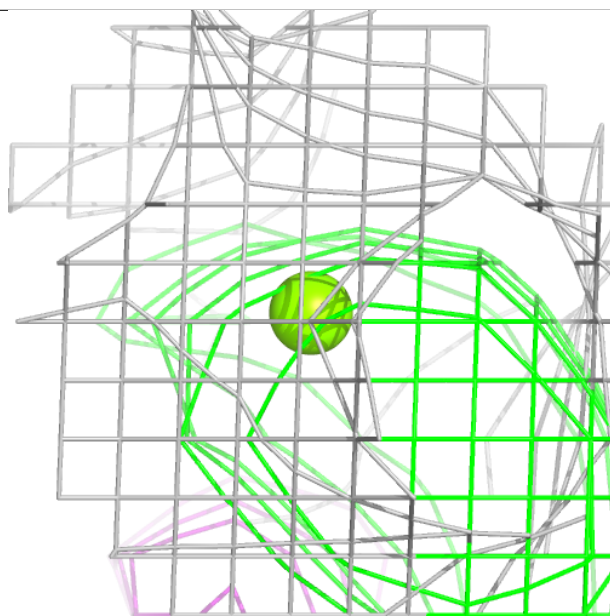
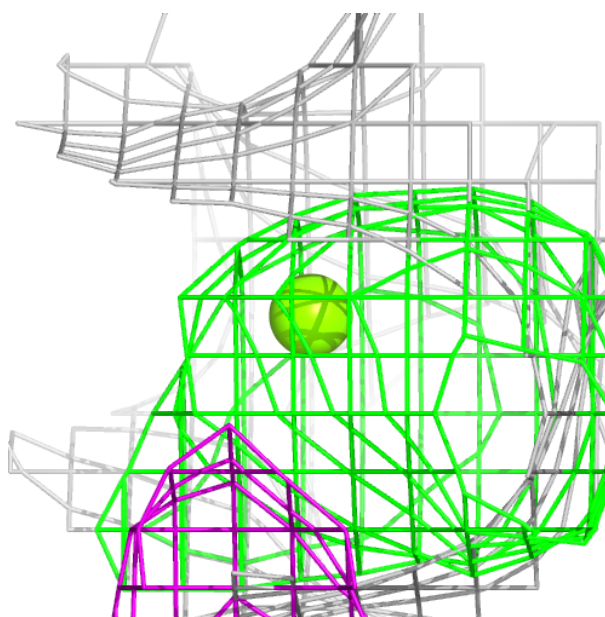
Electron density around CA0 A 602:

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



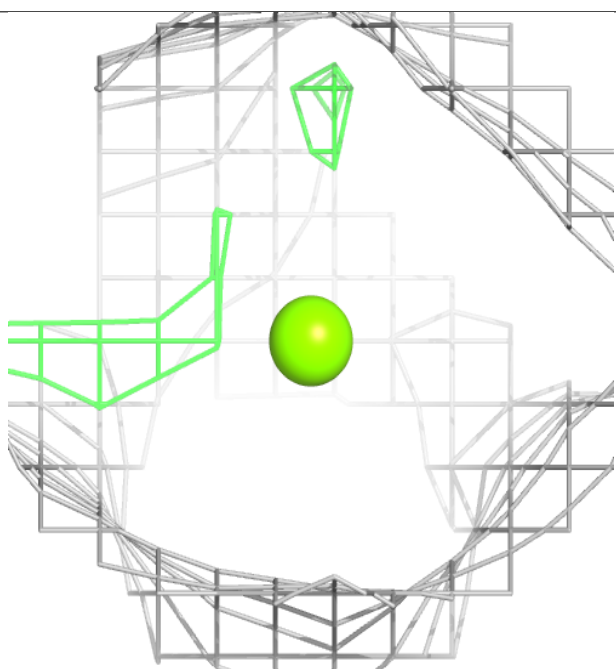
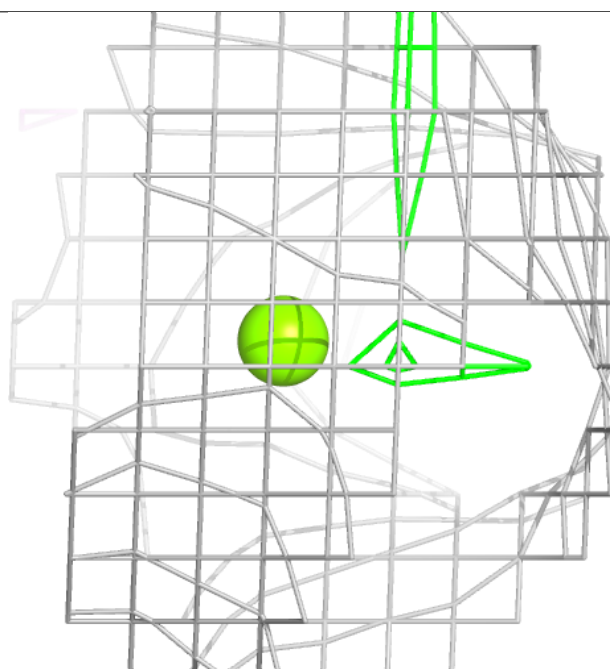
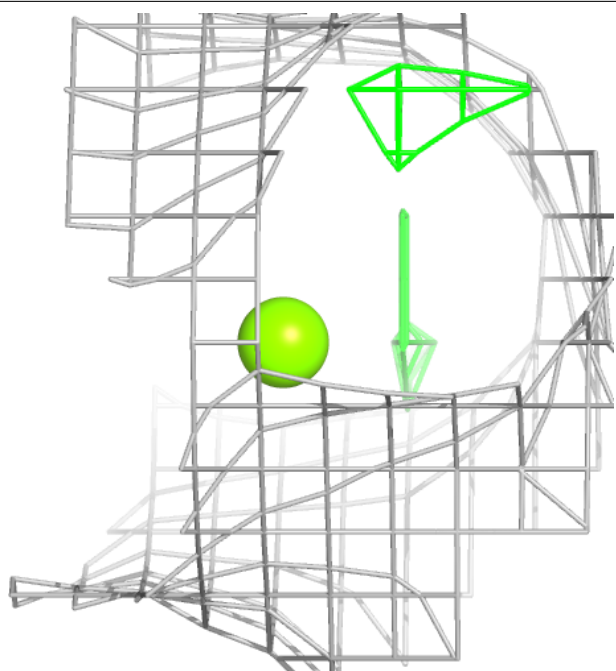
Electron density around MG C 601:

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



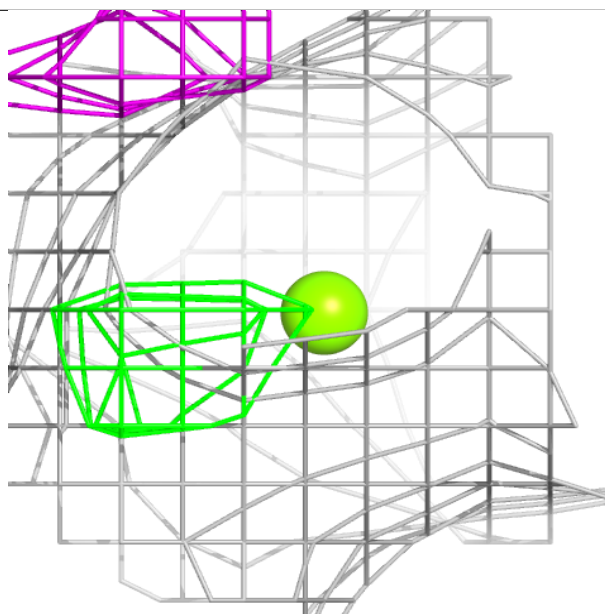
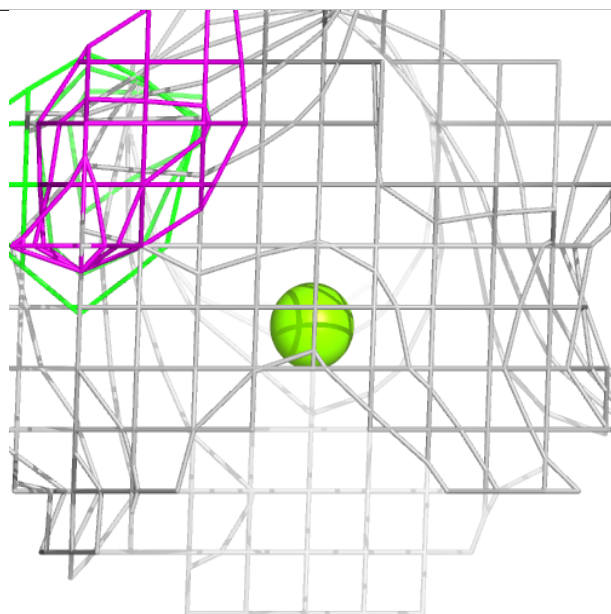
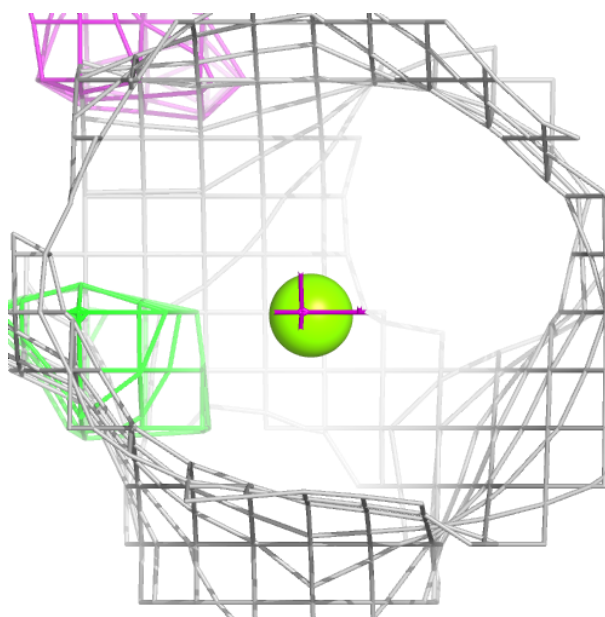
Electron density around MG B 601:

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



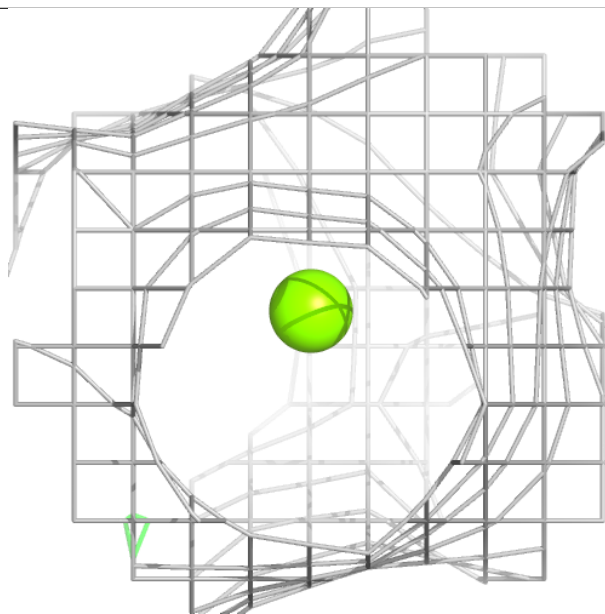
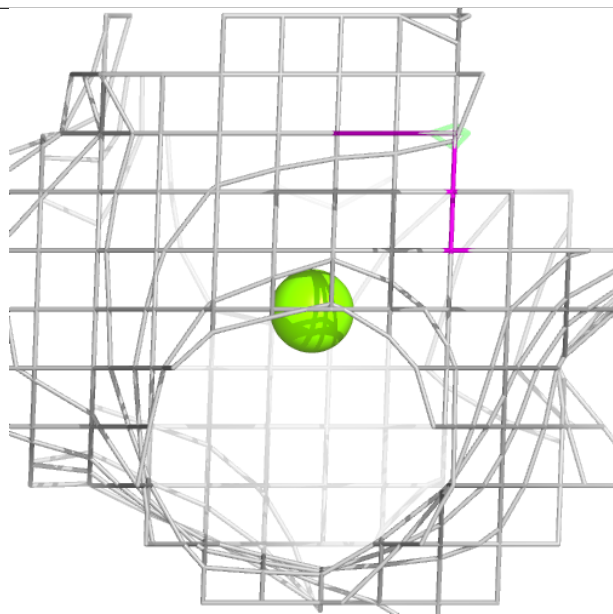
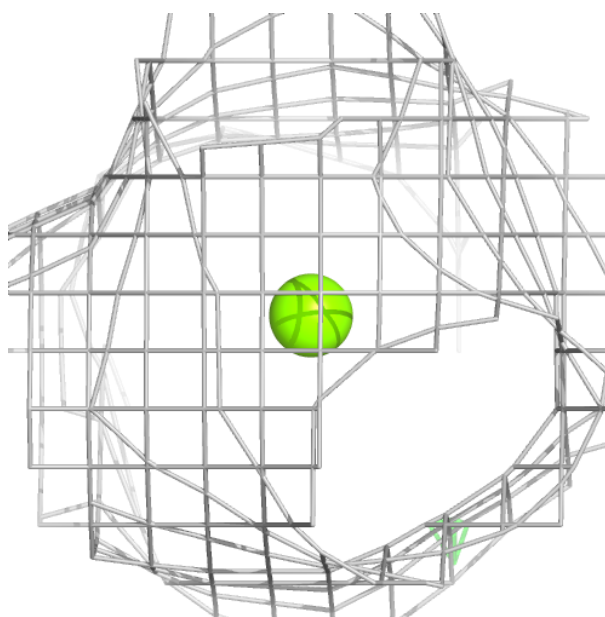
Electron density around MG A 601:

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



Electron density around MG D 601:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.