Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 06:45 PM JST

PDB ID	:	5XT3
Title	:	The catalytic domain of GdpP with c-di-GMP
Authors	:	Wang, F.; Gu, L.
Deposited on	:	2017-06-16
Resolution	:	2.59 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 (i) 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 (i)) were used in the production of this report:

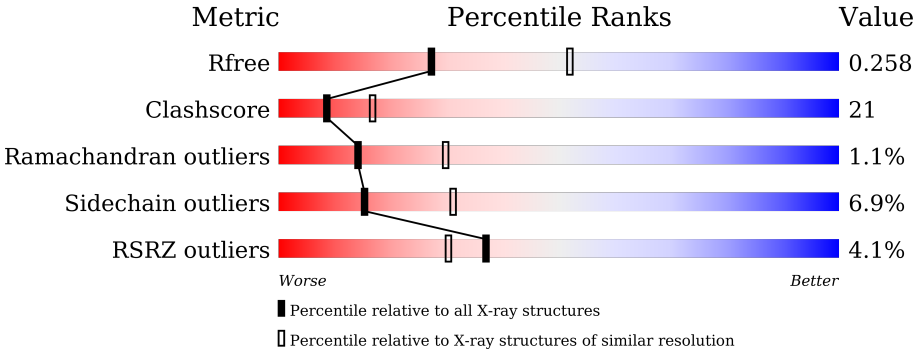
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	339	4% 62% 31% 5% •
1	B	339	4% 65% 31% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5416 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 Phosphodiesterase acting on cyclic dinucleotides.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	332	2593	1617	459	508	9	0	0	0
1	B	333	2596	1619	459	509	9	0	0	0

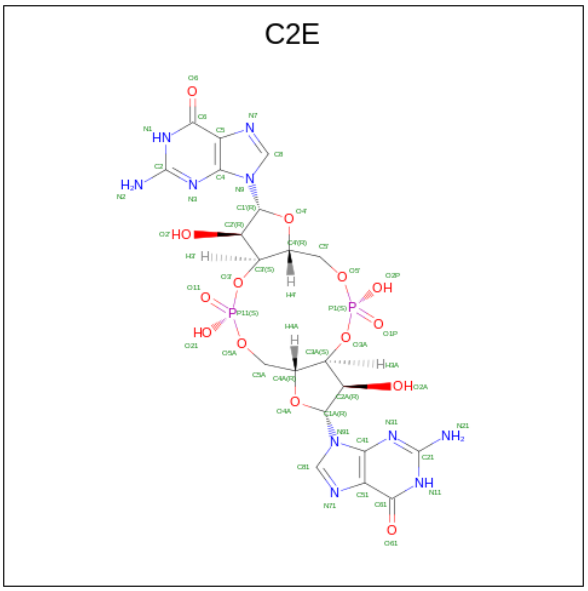
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	313	GLY	-	expression tag	UNP A0A0U1MUE2
A	314	SER	-	expression tag	UNP A0A0U1MUE2
A	315	MET	-	expression tag	UNP A0A0U1MUE2
B	350	GLY	-	expression tag	UNP A0A0U1MUE2
B	351	SER	-	expression tag	UNP A0A0U1MUE2
B	352	MET	-	expression tag	UNP A0A0U1MUE2

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
2	A	2	2	2	0	0
2	B	1	1	1	0	0

- Molecule 3 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidooctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (three-letter code: C2E) (formula: $C_{20}H_{24}N_{10}O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	46	20	10	14	2	0	0
			Total	C	N	O	P		
3	B	1	46	20	10	14	2	0	0

- Molecule 4 is water.

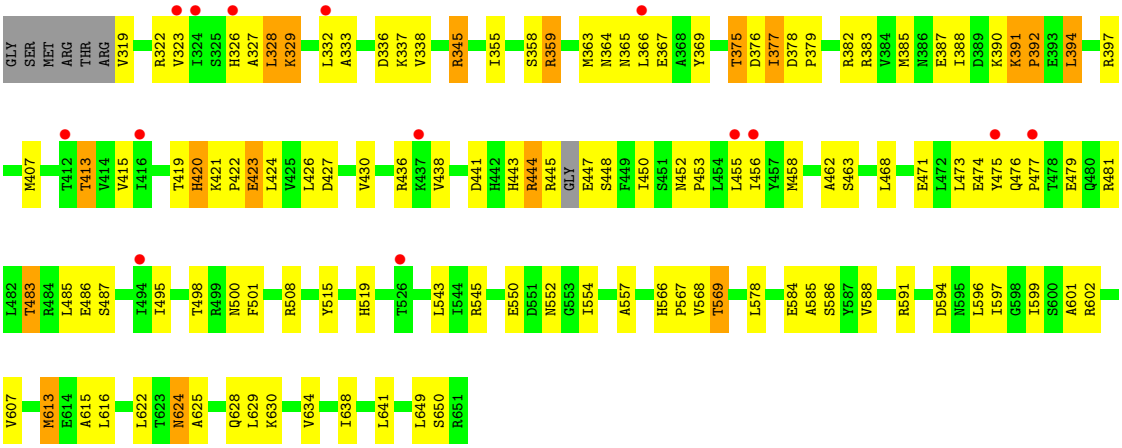
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	73	73	73	0	0
			Total	O		
4	B	59	59	59	0	0

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.

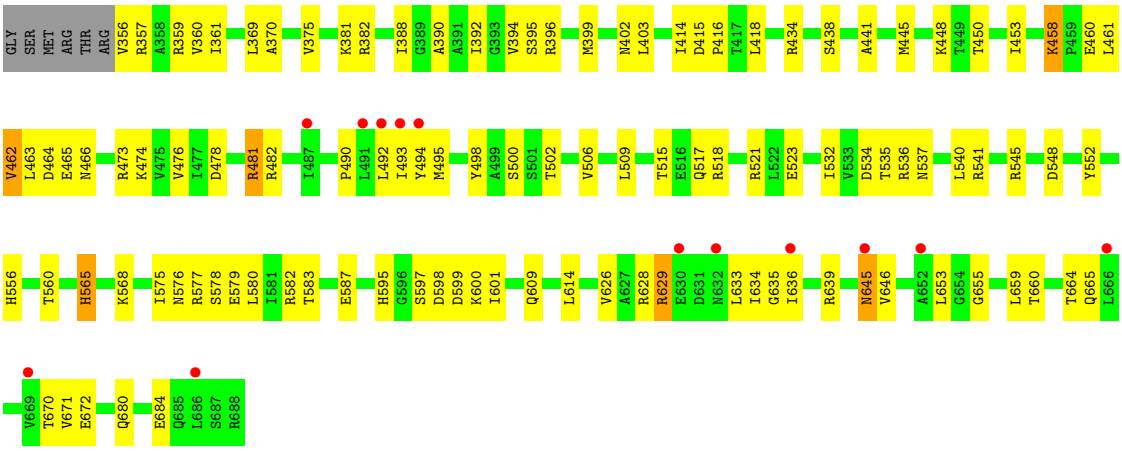
• Molecule 1: Phosphodiesterase acting on cyclic dinucleotides

Chain A:



• Molecule 1: Phosphodiesterase acting on cyclic dinucleotides

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.37Å 117.04Å 130.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.51 – 2.59 43.51 – 2.59	Depositor EDS
% Data completeness (in resolution range)	96.5 (43.51-2.59) 99.8 (43.51-2.59)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.28 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.207 , 0.262 0.204 , 0.258	Depositor DCC
R_{free} test set	1342 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	52.7	Xtriage
Anisotropy	0.856	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5416	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MN, C2E

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	0.39	0/2626	0.57	0/3558
1	B	0.36	0/2630	0.55	0/3564
All	All	0.38	0/5256	0.56	0/7122

There are no bond length outliers.

There are no bond angle outliers.

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	2593	0	2614	133	0
1	B	2596	0	2617	83	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	46	0	21	3	0
3	B	46	0	21	2	0
4	A	73	0	0	5	0
4	B	59	0	0	4	0
All	All	5416	0	5273	218	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 21.

All (218) 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:345:ARG:HH21	1:A:376:ASP:HA	1.10	1.12
1:A:359:ARG:HH11	1:A:359:ARG:HG2	1.08	1.11
1:A:328:LEU:HD21	1:A:455:LEU:HD13	1.25	1.07
1:B:583:THR:HG21	1:B:595:HIS:H	1.30	0.94
1:A:483:THR:HG22	1:A:486:GLU:OE1	1.70	0.92
1:B:633:LEU:HD21	1:B:665:GLN:HB3	1.49	0.91
1:A:345:ARG:NH2	1:A:376:ASP:HA	1.90	0.87
1:A:359:ARG:O	1:A:359:ARG:HD3	1.73	0.86
1:A:359:ARG:HG2	1:A:359:ARG:NH1	1.88	0.86
1:A:566:HIS:ND1	1:A:568:VAL:HG22	1.93	0.83
1:B:626:VAL:HG22	1:B:636:ILE:HG12	1.60	0.83
1:A:377:ILE:HD11	1:A:382:ARG:NE	1.94	0.82
1:A:328:LEU:HD21	1:A:455:LEU:CD1	2.11	0.80
1:A:483:THR:HG23	1:A:486:GLU:H	1.47	0.79
1:A:413:THR:HG23	1:A:436:ARG:HE	1.50	0.76
1:B:583:THR:CG2	1:B:595:HIS:H	1.99	0.75
1:A:456:ILE:HG22	1:A:458:MET:HG2	1.67	0.74
1:A:596:LEU:HD21	1:A:628:GLN:HB3	1.69	0.73
1:B:415:ASP:HB2	1:B:416:PRO:HD2	1.71	0.71
3:A:703:C2E:O5'	3:A:703:C2E:H4A	1.90	0.70
1:B:492:LEU:HD23	1:B:493:ILE:N	2.07	0.70
1:A:328:LEU:HD11	1:A:455:LEU:HD22	1.74	0.69
1:A:378:ASP:HB2	1:A:379:PRO:HD2	1.74	0.69
1:A:328:LEU:CD2	1:A:455:LEU:HD13	2.13	0.69
1:A:483:THR:HG22	1:A:486:GLU:CD	2.13	0.69
1:B:600:LYS:O	1:B:628:ARG:HB3	1.92	0.69
1:A:624:ASN:ND2	3:A:703:C2E:H5'2	2.09	0.68
1:B:646:VAL:HG22	1:B:659:LEU:O	1.95	0.67
1:A:363:MET:HE1	1:A:473:LEU:HD22	1.76	0.67
1:B:476:VAL:HB	1:B:493:ILE:HD13	1.77	0.67
1:B:680:GLN:O	1:B:684:GLU:HG3	1.95	0.66
1:A:391:LYS:H	1:A:392:PRO:HD3	1.59	0.66
1:B:580:LEU:O	1:B:583:THR:HG22	1.96	0.66
1:B:515:THR:HB	1:B:518:ARG:NH1	2.12	0.65
1:B:500:SER:O	1:B:541:ARG:NH2	2.30	0.64
1:B:458:LYS:HB3	1:B:461:LEU:HD13	1.80	0.64
1:A:377:ILE:HD11	1:A:382:ARG:CZ	2.28	0.64
1:A:390:LYS:HG3	1:A:391:LYS:HG3	1.80	0.64
1:A:322:ARG:HA	1:A:475:TYR:CZ	2.32	0.63
1:A:359:ARG:HD3	1:A:359:ARG:C	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:LYS:O	1:A:390:LYS:HD3	1.98	0.63
1:A:450:ILE:HG22	1:A:453:PRO:HG3	1.81	0.62
1:A:359:ARG:HH11	1:A:359:ARG:CG	1.95	0.62
1:A:329:LYS:HG2	1:A:476:GLN:HE21	1.64	0.62
1:A:390:LYS:HE2	1:A:390:LYS:HA	1.79	0.62
1:A:359:ARG:O	1:A:363:MET:HG3	1.99	0.62
1:B:629:ARG:HD2	1:B:633:LEU:HD22	1.82	0.61
3:B:702:C2E:H3'	3:B:702:C2E:H8	1.82	0.61
1:A:566:HIS:CE1	1:A:568:VAL:HG22	2.36	0.61
1:B:458:LYS:HG2	1:B:460:GLU:OE1	2.00	0.60
1:B:639:ARG:HA	1:B:660:THR:O	2.00	0.60
1:A:329:LYS:HB2	1:A:364:ASN:OD1	2.00	0.60
1:A:345:ARG:HH21	1:A:376:ASP:CA	2.01	0.60
1:A:420:HIS:HE1	1:A:444:ARG:O	1.84	0.60
1:B:628:ARG:HA	1:B:634:ILE:HD13	1.84	0.60
1:A:422:PRO:HG3	1:A:450:ILE:HD12	1.85	0.59
1:B:633:LEU:HD23	1:B:634:ILE:N	2.18	0.58
1:A:377:ILE:O	1:A:377:ILE:HG13	2.04	0.58
1:A:388:ILE:O	1:A:392:PRO:HD2	2.04	0.57
1:A:602:ARG:NH1	1:A:624:ASN:ND2	2.53	0.56
1:B:672:GLU:CD	1:B:672:GLU:H	2.08	0.56
1:A:345:ARG:NH2	1:A:375:THR:O	2.39	0.56
1:A:456:ILE:CG2	1:A:458:MET:HG2	2.36	0.56
1:B:579:GLU:HB2	1:B:582:ARG:HH21	1.70	0.56
1:B:521:ARG:HH11	1:B:521:ARG:HG2	1.71	0.55
1:B:356:VAL:HG22	1:B:359:ARG:CZ	2.36	0.55
1:B:476:VAL:HB	1:B:493:ILE:CD1	2.36	0.55
1:B:369:LEU:HD22	1:B:375:VAL:HG22	1.88	0.55
1:B:545:ARG:HA	1:B:548:ASP:OD1	2.07	0.55
1:A:378:ASP:HB2	1:A:379:PRO:CD	2.37	0.54
1:A:599:ILE:CG2	1:A:613:MET:HE1	2.37	0.54
1:A:622:LEU:HD23	1:A:622:LEU:C	2.28	0.54
1:B:579:GLU:CB	1:B:582:ARG:HH21	2.20	0.54
3:B:702:C2E:O5'	3:B:702:C2E:H4A	2.06	0.54
1:B:434:ARG:NH2	1:B:523:GLU:OE1	2.31	0.54
1:A:415:VAL:HG13	1:A:438:VAL:HG13	1.88	0.54
1:A:427:ASP:OD1	1:A:430:VAL:HG23	2.08	0.54
1:A:332:LEU:HB3	1:A:366:LEU:HD13	1.90	0.53
1:A:420:HIS:CD2	1:A:421:LYS:HD3	2.43	0.53
1:A:345:ARG:HA	1:A:345:ARG:NE	2.24	0.53
1:A:415:VAL:HG22	1:A:438:VAL:CG1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:VAL:HG12	1:A:367:GLU:O	2.10	0.52
1:A:591:ARG:HG3	1:A:591:ARG:HH11	1.75	0.52
1:B:599:ASP:OD1	1:B:599:ASP:N	2.42	0.52
1:A:622:LEU:HD23	1:A:622:LEU:O	2.09	0.52
1:B:629:ARG:HB3	1:B:633:LEU:HD22	1.90	0.52
1:A:596:LEU:HD23	1:A:597:ILE:N	2.24	0.52
1:A:566:HIS:HB3	1:A:569:THR:HG23	1.91	0.52
1:B:490:PRO:HG3	1:B:493:ILE:HD11	1.91	0.51
1:A:462:ALA:HB2	1:A:468:LEU:HD21	1.93	0.51
1:A:624:ASN:HD21	3:A:703:C2E:H5'2	1.74	0.51
1:B:575:ILE:O	1:B:578:SER:HB3	2.10	0.51
1:A:615:ALA:HB1	4:A:836:HOH:O	2.10	0.51
1:B:473:ARG:HH11	1:B:473:ARG:HG2	1.75	0.51
1:B:552:TYR:O	1:B:556:HIS:HD2	1.93	0.51
1:A:390:LYS:NZ	4:A:803:HOH:O	2.33	0.51
1:B:653:LEU:O	1:B:664:THR:HG21	2.10	0.51
1:B:464:ASP:OD2	1:B:466:ASN:HB2	2.12	0.50
1:A:364:ASN:N	1:A:364:ASN:HD22	2.08	0.50
1:B:370:ALA:HA	1:B:403:LEU:HD21	1.94	0.50
1:A:421:LYS:HE2	1:A:424:LEU:HD11	1.92	0.50
1:B:521:ARG:HG2	1:B:521:ARG:NH1	2.26	0.50
1:B:357:ARG:O	1:B:361:ILE:HG12	2.11	0.50
4:A:834:HOH:O	1:B:577:ARG:HD2	2.11	0.50
1:A:355:ILE:O	1:A:358:SER:HB3	2.12	0.49
1:A:363:MET:HE1	1:A:473:LEU:CD2	2.41	0.49
1:B:388:ILE:O	1:B:392:ILE:HG13	2.12	0.49
1:B:517:GLN:O	1:B:517:GLN:HG2	2.11	0.49
1:B:576:ASN:O	1:B:579:GLU:HG2	2.12	0.49
1:B:396:ARG:NH1	1:B:517:GLN:HG2	2.26	0.49
1:A:345:ARG:HG2	1:A:345:ARG:HH11	1.77	0.49
1:A:591:ARG:HG3	1:A:591:ARG:NH1	2.28	0.49
1:A:394:LEU:O	1:A:397:ARG:HG2	2.12	0.49
1:A:471:GLU:OE1	1:A:508:ARG:NH2	2.46	0.49
1:B:448:LYS:NZ	1:B:448:LYS:HB3	2.27	0.49
1:B:565:HIS:C	1:B:565:HIS:CD2	2.85	0.49
1:A:422:PRO:HD2	1:A:423:GLU:OE1	2.13	0.48
1:B:518:ARG:HG2	1:B:556:HIS:CE1	2.48	0.48
1:A:550:GLU:HB2	1:A:552:ASN:OD1	2.12	0.48
1:B:481:ARG:HD2	4:B:839:HOH:O	2.12	0.48
1:A:387:GLU:O	1:A:392:PRO:HD3	2.14	0.48
1:A:629:LEU:HA	4:A:822:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:LEU:O	1:B:568:LYS:HE2	2.12	0.48
1:A:328:LEU:N	1:A:328:LEU:HD23	2.29	0.48
1:A:388:ILE:O	1:A:392:PRO:CD	2.61	0.48
1:B:494:TYR:CE2	1:B:509:LEU:HD21	2.49	0.48
1:B:478:ASP:HB3	1:B:495:MET:HE3	1.96	0.48
1:B:634:ILE:HD12	1:B:671:VAL:HG23	1.96	0.48
1:A:624:ASN:HD22	1:A:625:ALA:N	2.12	0.47
1:A:359:ARG:NH1	1:A:359:ARG:CG	2.64	0.47
1:A:394:LEU:HD11	1:A:486:GLU:HG3	1.96	0.47
1:B:381:LYS:HG2	1:B:463:LEU:HA	1.97	0.47
1:B:645:ASN:HA	1:B:659:LEU:HD12	1.96	0.47
1:A:337:LYS:HE3	1:A:407:MET:O	2.15	0.47
1:A:383:ARG:CZ	4:A:843:HOH:O	2.63	0.47
1:A:452:ASN:N	1:A:453:PRO:HD3	2.29	0.47
1:B:395:SER:O	1:B:399:MET:HG3	2.15	0.47
1:A:421:LYS:HE2	1:A:424:LEU:CD1	2.45	0.47
1:A:500:ASN:O	1:A:501:PHE:HB2	2.14	0.47
1:A:391:LYS:N	1:A:392:PRO:HD3	2.30	0.46
1:A:392:PRO:HG3	1:A:485:LEU:HD23	1.96	0.46
1:A:441:ASP:OD2	1:A:443:HIS:HD2	1.98	0.46
1:B:453:ILE:HD12	1:B:462:VAL:CG2	2.45	0.46
1:A:455:LEU:HG	1:A:456:ILE:N	2.29	0.46
1:A:599:ILE:HB	1:A:613:MET:HE1	1.95	0.46
1:B:478:ASP:HB3	1:B:495:MET:CE	2.46	0.46
1:A:566:HIS:ND1	1:A:567:PRO:HD2	2.31	0.46
1:B:655:GLY:HA3	1:B:664:THR:OG1	2.16	0.46
1:A:326:HIS:O	1:A:329:LYS:HG3	2.15	0.45
1:A:336:ASP:OD1	1:A:336:ASP:N	2.48	0.45
1:B:536:ARG:HG3	1:B:540:LEU:HD12	1.97	0.45
1:B:664:THR:HG22	1:B:665:GLN:N	2.30	0.45
1:A:543:LEU:O	1:A:557:ALA:HB1	2.17	0.45
1:A:345:ARG:HG2	1:A:345:ARG:NH1	2.30	0.45
1:A:333:ALA:HA	1:A:366:LEU:HD21	1.99	0.45
1:B:597:SER:HB2	4:B:813:HOH:O	2.16	0.45
1:A:328:LEU:O	1:A:332:LEU:HD13	2.18	0.44
1:A:392:PRO:HG3	1:A:485:LEU:CD2	2.47	0.44
1:A:420:HIS:HD2	1:A:421:LYS:HD3	1.80	0.44
1:B:369:LEU:HD22	1:B:375:VAL:CG2	2.47	0.44
1:A:391:LYS:H	1:A:392:PRO:CD	2.28	0.44
1:B:587:GLU:OE1	1:B:587:GLU:HA	2.17	0.44
1:B:356:VAL:HG22	1:B:359:ARG:NH2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:THR:HB	1:B:518:ARG:HH12	1.81	0.44
1:A:329:LYS:O	1:A:333:ALA:HB2	2.18	0.44
1:A:367:GLU:HG2	1:A:369:TYR:CE1	2.53	0.44
1:B:498:TYR:HB2	4:B:826:HOH:O	2.17	0.44
1:A:377:ILE:HD11	1:A:382:ARG:HE	1.79	0.44
1:B:414:ILE:HA	1:B:418:LEU:HD23	1.99	0.44
1:B:595:HIS:HA	1:B:626:VAL:O	2.18	0.44
1:A:634:VAL:O	1:A:638:ILE:HG13	2.19	0.43
1:B:502:THR:O	1:B:506:VAL:HG23	2.19	0.43
1:B:545:ARG:NH2	4:B:804:HOH:O	2.52	0.43
1:A:377:ILE:HD13	1:A:382:ARG:HA	2.00	0.43
1:A:515:TYR:CE1	1:A:519:HIS:HE1	2.37	0.43
1:A:421:LYS:HG2	1:A:448:SER:OG	2.18	0.42
1:A:602:ARG:NH1	1:A:624:ASN:HD21	2.17	0.42
1:B:598:ASP:OD1	1:B:628:ARG:NH2	2.52	0.42
1:A:594:ASP:N	1:A:594:ASP:OD1	2.52	0.42
1:A:588:VAL:O	1:A:599:ILE:HA	2.18	0.42
1:B:626:VAL:HA	1:B:635:GLY:O	2.19	0.42
1:A:327:ALA:C	1:A:328:LEU:HD23	2.40	0.42
1:A:474:GLU:O	1:A:475:TYR:CG	2.73	0.42
1:A:328:LEU:CD2	1:A:328:LEU:N	2.81	0.42
1:A:377:ILE:CD1	1:A:382:ARG:HA	2.49	0.42
1:B:390:ALA:O	1:B:394:VAL:HG23	2.19	0.42
1:A:585:ALA:HB2	1:A:607:VAL:HB	2.00	0.42
1:A:388:ILE:HA	1:A:392:PRO:HG3	2.01	0.42
1:A:363:MET:CE	1:A:476:GLN:HB2	2.50	0.41
1:A:388:ILE:HG23	1:A:394:LEU:HB3	2.02	0.41
1:B:460:GLU:H	1:B:460:GLU:CD	2.24	0.41
1:A:326:HIS:HA	1:A:329:LYS:HG3	2.00	0.41
1:B:474:LYS:HB2	1:B:474:LYS:HE3	1.78	0.41
1:A:444:ARG:HD2	1:A:445:ARG:O	2.20	0.41
1:B:482:ARG:HE	1:B:482:ARG:HB3	1.64	0.41
1:A:616:LEU:HD11	1:A:641:LEU:HA	2.02	0.41
1:B:614:LEU:HD23	1:B:614:LEU:HA	1.92	0.41
1:A:363:MET:C	1:A:364:ASN:HD22	2.23	0.41
1:B:441:ALA:O	1:B:445:MET:HG3	2.20	0.41
1:A:421:LYS:HA	1:A:422:PRO:HD3	1.91	0.41
1:A:463:SER:HB2	1:A:498:THR:HG22	2.02	0.41
1:A:515:TYR:CZ	1:A:519:HIS:CE1	3.09	0.41
1:B:598:ASP:CG	1:B:628:ARG:HH21	2.24	0.41
1:A:554:ILE:HD11	1:A:649:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:SER:HB2	1:B:535:THR:CG2	2.50	0.41
1:B:532:ILE:HD12	1:B:537:ASN:HD22	1.86	0.41
1:A:359:ARG:NH1	1:A:486:GLU:OE1	2.53	0.41
1:A:568:VAL:HG23	1:A:569:THR:N	2.36	0.41
1:B:577:ARG:HE	1:B:609:GLN:HB3	1.85	0.41
1:A:463:SER:HB2	1:A:498:THR:CG2	2.50	0.40
1:A:586:SER:O	1:A:601:ALA:HA	2.20	0.40
1:A:385:MET:HE3	1:A:385:MET:HB2	1.92	0.40
1:B:356:VAL:O	1:B:360:VAL:HG23	2.22	0.40
1:A:388:ILE:O	1:A:392:PRO:HG2	2.22	0.40
1:A:329:LYS:HG2	1:A:476:GLN:NE2	2.35	0.40
1:A:391:LYS:N	1:A:392:PRO:CD	2.85	0.40
1:A:624:ASN:HD22	1:A:624:ASN:C	2.24	0.40
1:A:495:ILE:HD13	1:A:495:ILE:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	328/339 (97%)	309 (94%)	13 (4%)	6 (2%)	8 16
1	B	331/339 (98%)	309 (93%)	21 (6%)	1 (0%)	41 64
All	All	659/678 (97%)	618 (94%)	34 (5%)	7 (1%)	14 30

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	392	PRO
1	A	479	GLU
1	A	365	ASN
1	B	402	ASN

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Mol	Chain	Res	Type
1	A	477	PRO
1	A	391	LYS
1	A	545	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/289 (98%)	259 (91%)	25 (9%)	10	19
1	B	283/289 (98%)	269 (95%)	14 (5%)	25	48
All	All	567/578 (98%)	528 (93%)	39 (7%)	15	31

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	VAL
1	A	323	VAL
1	A	328	LEU
1	A	329	LYS
1	A	345	ARG
1	A	359	ARG
1	A	375	THR
1	A	377	ILE
1	A	394	LEU
1	A	413	THR
1	A	419	THR
1	A	420	HIS
1	A	423	GLU
1	A	426	LEU
1	A	444	ARG
1	A	447	GLU
1	A	481	ARG
1	A	483	THR
1	A	487	SER
1	A	569	THR

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Mol	Chain	Res	Type
1	A	584	GLU
1	A	613	MET
1	A	624	ASN
1	A	630	LYS
1	A	650	SER
1	B	382	ARG
1	B	438	SER
1	B	450	THR
1	B	458	LYS
1	B	462	VAL
1	B	465	GLU
1	B	481	ARG
1	B	534	ASP
1	B	560	THR
1	B	565	HIS
1	B	601	ILE
1	B	629	ARG
1	B	645	ASN
1	B	670	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	326	HIS
1	A	364	ASN
1	A	443	HIS
1	A	476	GLN
1	A	480	GLN
1	A	519	HIS
1	A	624	ASN
1	B	556	HIS
1	B	564	GLN
1	B	565	HIS
1	B	645	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	C2E	B	702	-	44,52,52	2.98	16 (36%)	52,82,82	1.55	12 (23%)
3	C2E	A	703	-	44,52,52	3.00	18 (40%)	52,82,82	1.51	10 (19%)

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	C2E	B	702	-	-	11/22/62/62	0/6/7/7
3	C2E	A	703	-	-	10/22/62/62	0/6/7/7

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	C2E	O61-C61	9.00	1.41	1.23
3	A	703	C2E	O61-C61	8.98	1.41	1.23
3	A	703	C2E	O6-C6	7.27	1.38	1.23
3	B	702	C2E	O6-C6	7.08	1.37	1.23
3	A	703	C2E	C2'-C3'	-6.42	1.38	1.52
3	B	702	C2E	C2'-C3'	-6.33	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703	C2E	C21-N21	6.16	1.48	1.34
3	B	702	C2E	C21-N21	5.83	1.48	1.34
3	B	702	C2E	C2-N2	5.69	1.47	1.34
3	A	703	C2E	C2-N2	5.60	1.47	1.34
3	B	702	C2E	O4A-C4A	4.96	1.56	1.45
3	A	703	C2E	O4A-C4A	4.60	1.55	1.45
3	A	703	C2E	C3'-C4'	-3.76	1.42	1.52
3	B	702	C2E	C2'-C1'	-3.59	1.48	1.53
3	B	702	C2E	C3'-C4'	-3.57	1.43	1.52
3	A	703	C2E	C2A-C3A	-3.52	1.45	1.52
3	B	702	C2E	C5-C6	-3.47	1.40	1.47
3	B	702	C2E	O2A-C2A	-3.44	1.34	1.43
3	A	703	C2E	C5A-C4A	-3.41	1.41	1.51
3	A	703	C2E	C2'-C1'	-3.36	1.48	1.53
3	B	702	C2E	C51-C61	-3.34	1.40	1.47
3	B	702	C2E	C5A-C4A	-3.34	1.41	1.51
3	A	703	C2E	O2A-C2A	-3.29	1.35	1.43
3	A	703	C2E	C51-C61	-3.24	1.40	1.47
3	B	702	C2E	C2A-C3A	-3.20	1.45	1.52
3	A	703	C2E	C5-C6	-3.11	1.41	1.47
3	B	702	C2E	C2A-C1A	-2.54	1.49	1.53
3	A	703	C2E	C2A-C1A	-2.43	1.50	1.53
3	B	702	C2E	C3A-C4A	-2.28	1.46	1.52
3	A	703	C2E	C3A-C4A	-2.27	1.46	1.52
3	A	703	C2E	C61-N11	-2.16	1.34	1.37
3	A	703	C2E	O4'-C4'	-2.08	1.40	1.45
3	A	703	C2E	O5A-C5A	-2.08	1.36	1.44
3	B	702	C2E	O5A-C5A	-2.06	1.36	1.44

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	702	C2E	C5-C6-N1	3.51	120.15	113.95
3	A	703	C2E	C5-C6-N1	3.35	119.86	113.95
3	A	703	C2E	C8-N7-C5	3.33	109.34	102.99
3	A	703	C2E	C81-N71-C51	3.16	109.02	102.99
3	B	702	C2E	O5'-C5'-C4'	3.08	119.60	108.99
3	A	703	C2E	C2-N1-C6	-2.99	119.60	125.10
3	B	702	C2E	C8-N7-C5	2.95	108.61	102.99
3	B	702	C2E	O5A-C5A-C4A	2.95	119.15	108.99
3	B	702	C2E	C81-N71-C51	2.94	108.59	102.99
3	A	703	C2E	C51-C61-N11	2.91	119.10	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	703	C2E	O5'-C5'-C4'	2.89	118.94	108.99
3	B	702	C2E	C51-C61-N11	2.86	119.00	113.95
3	B	702	C2E	C2-N1-C6	-2.79	119.97	125.10
3	B	702	C2E	C21-N11-C61	-2.40	120.67	125.10
3	B	702	C2E	O61-C61-C51	-2.37	119.75	124.37
3	B	702	C2E	O4'-C1'-C2'	-2.32	103.53	106.93
3	A	703	C2E	O5A-C5A-C4A	2.22	116.65	108.99
3	B	702	C2E	O21-P11-O3'	2.14	115.24	106.78
3	A	703	C2E	C21-N11-C61	-2.14	121.15	125.10
3	B	702	C2E	O6-C6-C5	-2.12	120.22	124.37
3	A	703	C2E	O3'-P11-O11	-2.08	101.66	109.47
3	A	703	C2E	O21-P11-O3'	2.07	114.95	106.78

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	702	C2E	C5'-O5'-P1-O1P
3	B	702	C2E	C4A-C3A-O3A-P1
3	A	703	C2E	O4'-C4'-C5'-O5'
3	A	703	C2E	C4A-C3A-O3A-P1
3	B	702	C2E	C4'-C3'-O3'-P11
3	B	702	C2E	C2'-C3'-O3'-P11
3	B	702	C2E	C5'-O5'-P1-O3A
3	A	703	C2E	C2'-C3'-O3'-P11
3	A	703	C2E	C3'-C4'-C5'-O5'
3	B	702	C2E	C2A-C3A-O3A-P1
3	B	702	C2E	C4A-C5A-O5A-P11
3	A	703	C2E	C3'-O3'-P11-O11
3	A	703	C2E	C4A-C5A-O5A-P11
3	A	703	C2E	C3'-O3'-P11-O5A
3	B	702	C2E	O4'-C4'-C5'-O5'
3	B	702	C2E	C5A-O5A-P11-O21
3	B	702	C2E	C3'-O3'-P11-O5A
3	A	703	C2E	C5'-O5'-P1-O3A
3	A	703	C2E	C4'-C3'-O3'-P11
3	B	702	C2E	C3'-O3'-P11-O11
3	A	703	C2E	C5'-O5'-P1-O1P

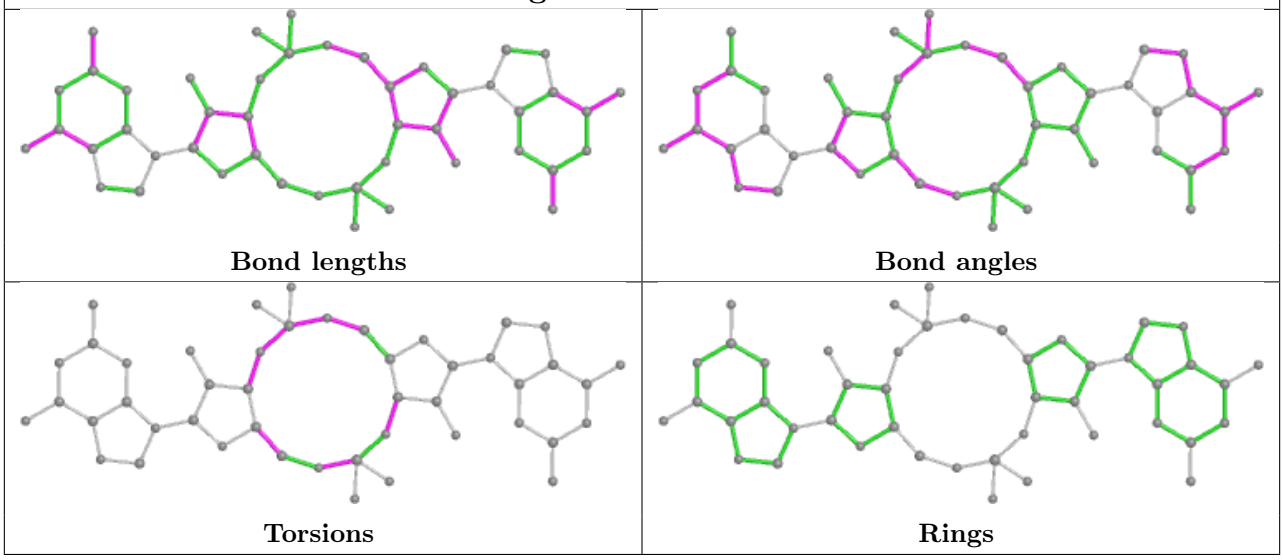
There are no ring outliers.

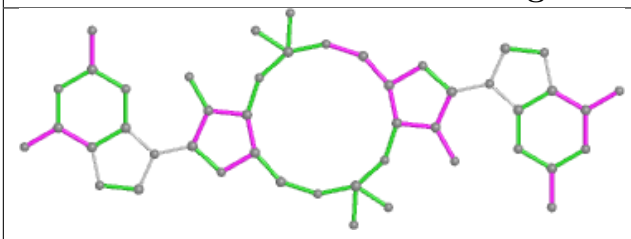
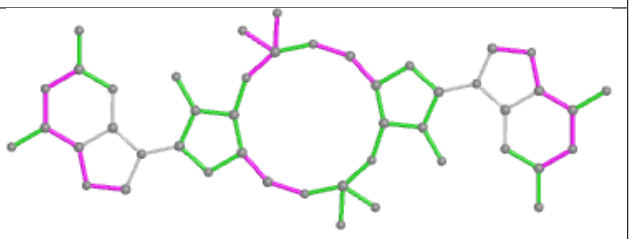
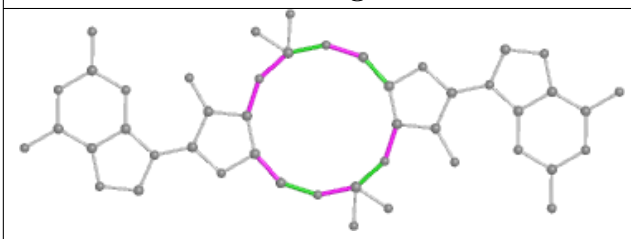
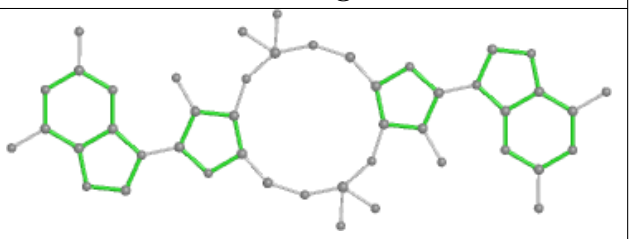
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	C2E	2	0
3	A	703	C2E	3	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 then 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 C2E B 702



Ligand C2E A 703	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	332/339 (97%)	0.51	14 (4%)	36	29	41, 61, 92, 109	0
1	B	333/339 (98%)	0.48	13 (3%)	39	32	42, 65, 92, 118	0
All	All	665/678 (98%)	0.49	27 (4%)	37	30	41, 62, 92, 118	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	669	VAL	4.5
1	B	666	LEU	4.1
1	A	323	VAL	3.9
1	A	455	LEU	3.6
1	A	366	LEU	3.2
1	A	324	ILE	2.8
1	A	326	HIS	2.7
1	B	494	TYR	2.5
1	B	492	LEU	2.5
1	B	491	LEU	2.5
1	B	487	ILE	2.3
1	B	632	ASN	2.3
1	A	456	ILE	2.3
1	B	686	LEU	2.3
1	B	636	ILE	2.3
1	B	630	GLU	2.3
1	A	412	THR	2.3
1	A	477	PRO	2.2
1	A	416	ILE	2.2
1	A	332	LEU	2.2
1	A	437	LYS	2.2
1	B	652	ALA	2.2
1	B	493	ILE	2.1
1	B	645	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	526	THR	2.0
1	A	494	ILE	2.0
1	A	475	TYR	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 monosaccharides in this entry.

6.4 Ligands (i)

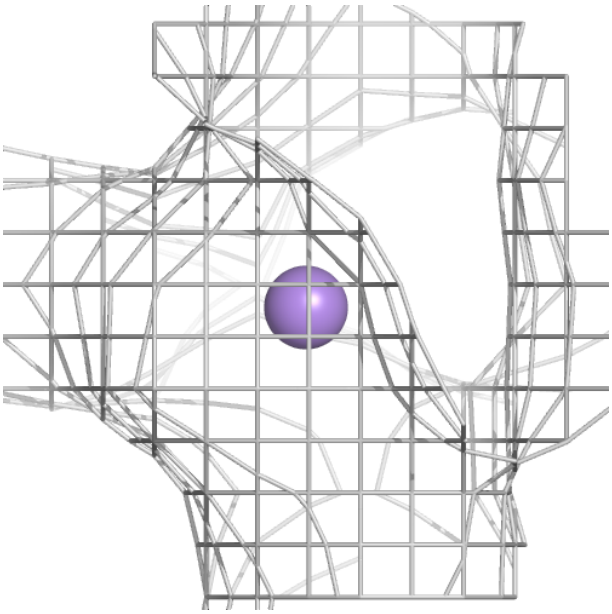
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

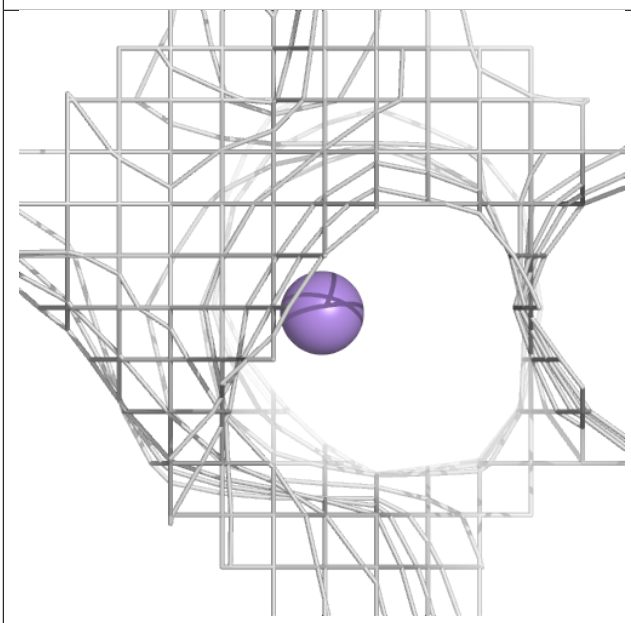
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MN	A	702	1/1	0.88	0.07	95,95,95,95	0
3	C2E	B	702	46/46	0.88	0.17	91,104,115,119	0
3	C2E	A	703	46/46	0.93	0.16	60,72,79,82	0
2	MN	A	701	1/1	0.98	0.16	71,71,71,71	0
2	MN	B	701	1/1	0.98	0.16	59,59,59,59	0

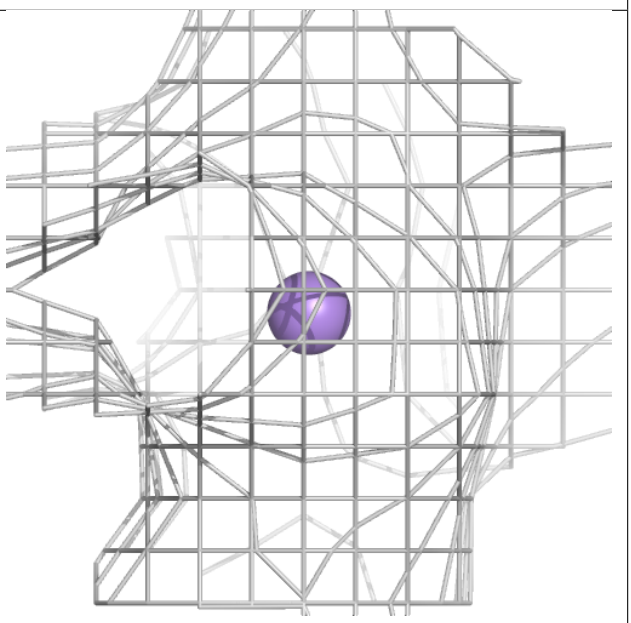
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MN A 702:

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

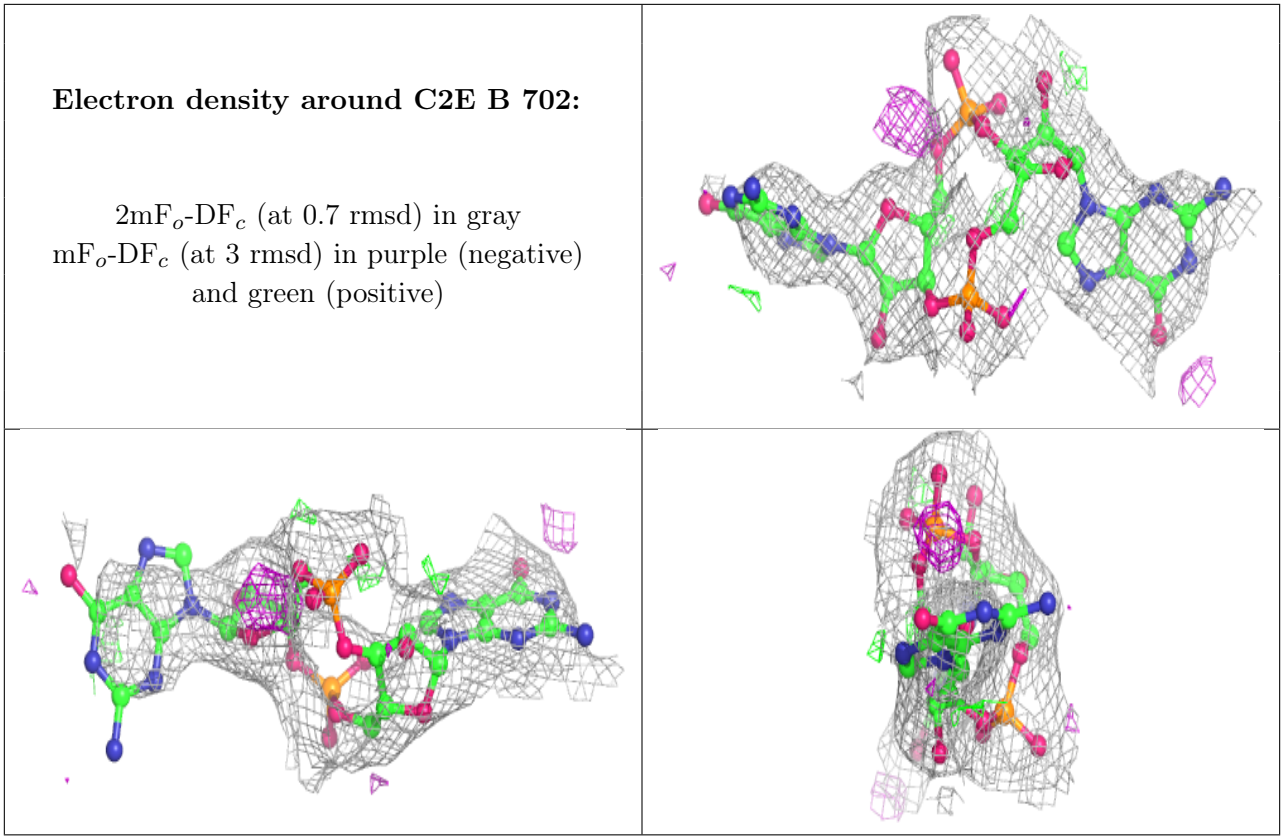






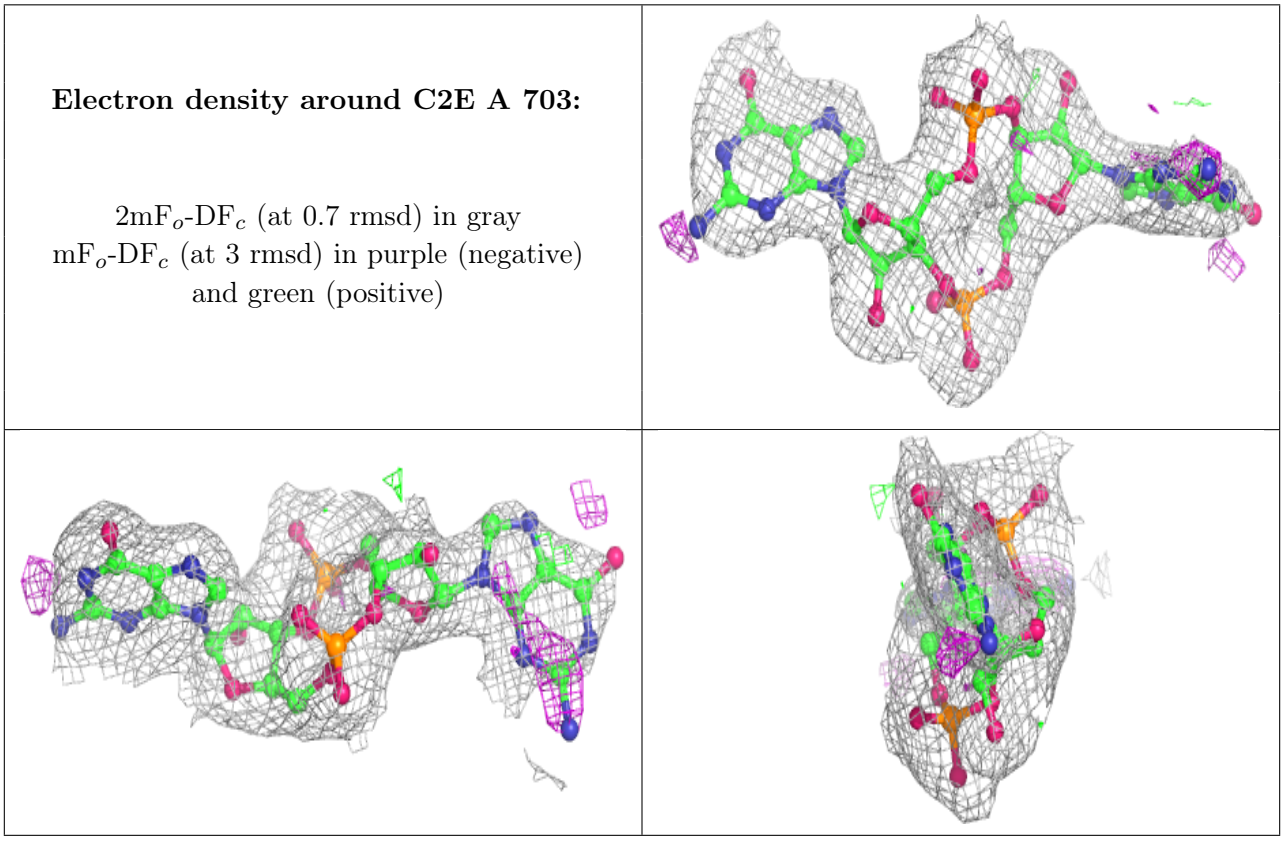
Electron density around C2E B 702:

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



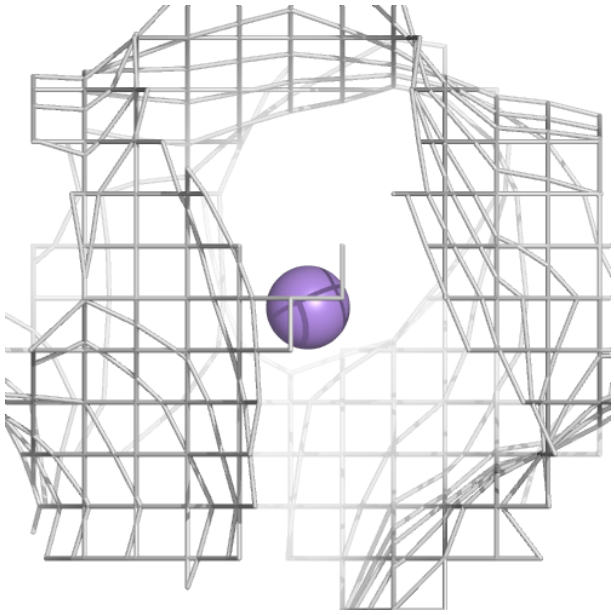
Electron density around C2E A 703:

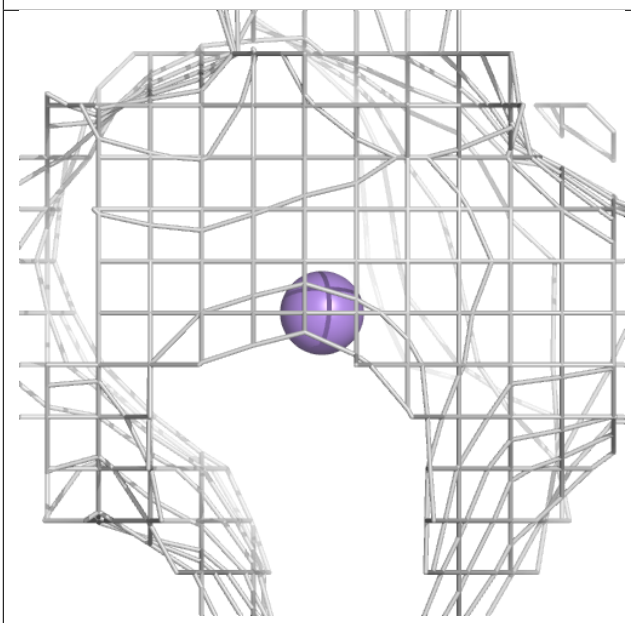
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

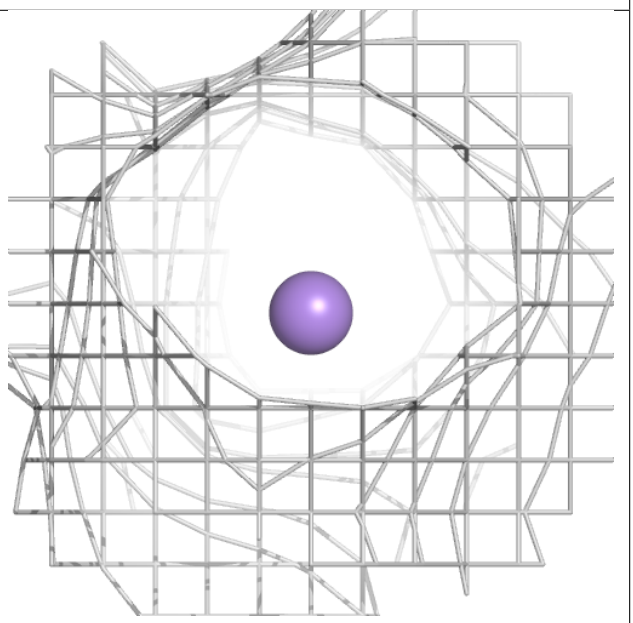


Electron density around MN A 701:

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

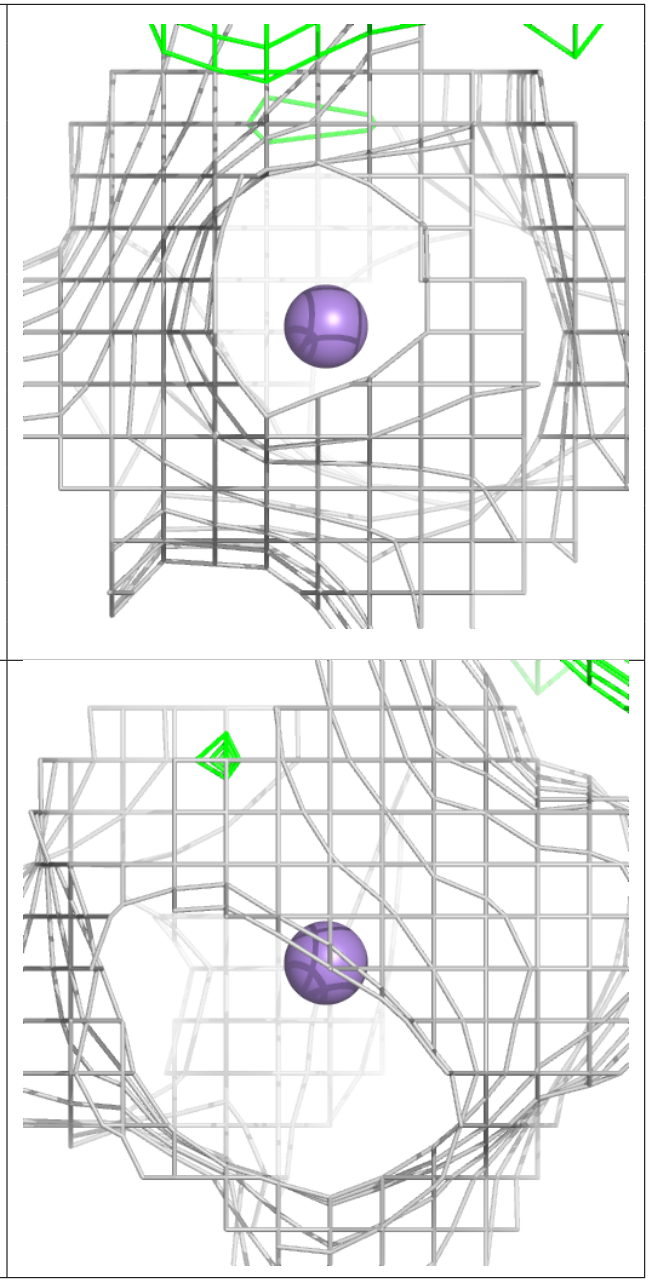






Electron density around MN B 701:

$2mF_o$-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.