



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:55 PM UTC

PDB ID : 3BRE / pdb_00003bre
Title : Crystal Structure of P.aeruginosa PA3702
Authors : De, N.; Pirruccello, M.; Krasteva, P.V.; Bae, N.; Raghavan, R.V.; Sondermann, H.
Deposited on : 2007-12-21
Resolution : 2.40 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

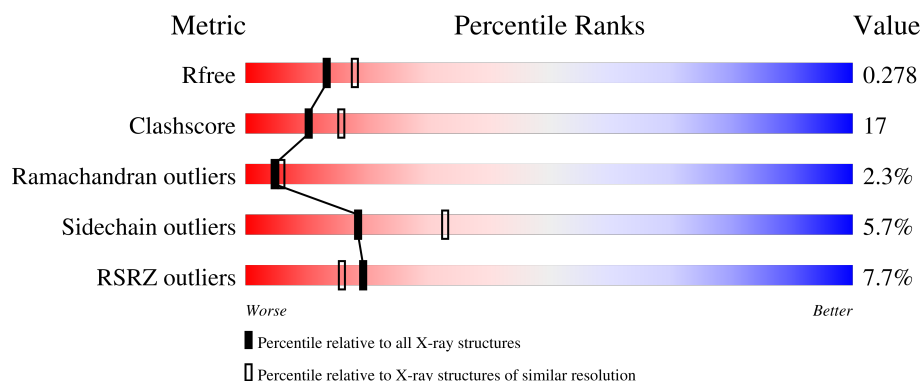
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	358	 6% 55% 31% 10%
1	B	358	 8% 66% 22% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5182 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 Probable two-component response regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2485	1546	451	477	11			
1	B	328	Total	C	N	O	S	0	0	0
			2511	1563	456	482	10			

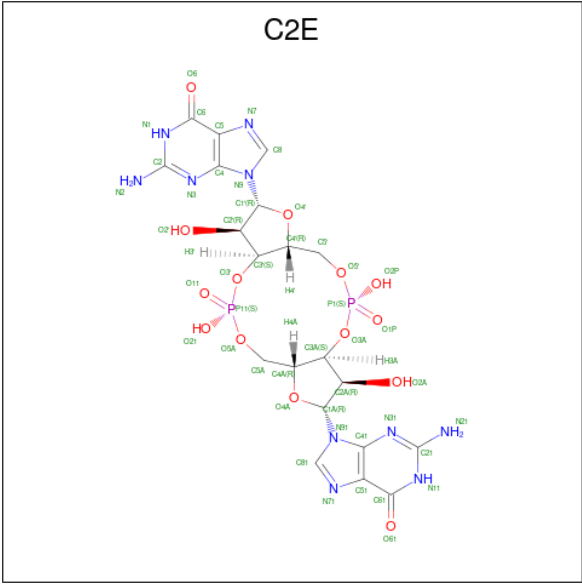
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	348	ALA	-	expression tag	UNP Q9HXT9
A	349	ALA	-	expression tag	UNP Q9HXT9
A	350	ALA	-	expression tag	UNP Q9HXT9
A	351	LEU	-	expression tag	UNP Q9HXT9
A	352	GLU	-	expression tag	UNP Q9HXT9
A	353	HIS	-	expression tag	UNP Q9HXT9
A	354	HIS	-	expression tag	UNP Q9HXT9
A	355	HIS	-	expression tag	UNP Q9HXT9
A	356	HIS	-	expression tag	UNP Q9HXT9
A	357	HIS	-	expression tag	UNP Q9HXT9
A	358	HIS	-	expression tag	UNP Q9HXT9
B	348	ALA	-	expression tag	UNP Q9HXT9
B	349	ALA	-	expression tag	UNP Q9HXT9
B	350	ALA	-	expression tag	UNP Q9HXT9
B	351	LEU	-	expression tag	UNP Q9HXT9
B	352	GLU	-	expression tag	UNP Q9HXT9
B	353	HIS	-	expression tag	UNP Q9HXT9
B	354	HIS	-	expression tag	UNP Q9HXT9
B	355	HIS	-	expression tag	UNP Q9HXT9
B	356	HIS	-	expression tag	UNP Q9HXT9
B	357	HIS	-	expression tag	UNP Q9HXT9
B	358	HIS	-	expression tag	UNP Q9HXT9

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 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) (CCD ID: C2E) (formula: C₂₀H₂₄N₁₀O₁₄P₂).



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

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.51Å 72.75Å 106.09Å 90.00° 110.79° 90.00°	Depositor
Resolution (Å)	33.78 – 2.40 33.78 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.5 (33.78-2.40) 91.5 (33.78-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.39Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.242 , 0.278 0.242 , 0.278	Depositor DCC
R_{free} test set	2935 reflections (7.32%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5182	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% 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: C2E, MG

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	0.50	0/2522	1.02	15/3412 (0.4%)
1	B	0.51	0/2549	1.01	9/3452 (0.3%)
All	All	0.50	0/5071	1.01	24/6864 (0.3%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	VAL	N-CA-C	-9.28	101.16	110.62
1	B	281	LEU	N-CA-C	-8.11	102.01	112.23
1	B	182	ARG	N-CA-C	7.22	119.23	111.36
1	B	171	MET	N-CA-C	6.99	120.29	111.69
1	A	289	ARG	CA-C-N	6.79	128.33	119.84
1	A	289	ARG	C-N-CA	6.79	128.33	119.84
1	A	208	ILE	N-CA-C	6.77	117.39	107.37
1	B	39	ALA	N-CA-C	-6.63	105.49	113.97
1	A	304	VAL	N-CA-C	-6.58	97.32	107.71
1	B	340	PRO	N-CA-CB	6.46	110.10	103.00
1	A	38	LEU	N-CA-C	-6.29	105.24	113.17
1	B	208	ILE	N-CA-C	5.78	116.19	107.75
1	A	281	LEU	N-CA-C	-5.64	105.89	112.89
1	A	334	VAL	N-CA-C	5.58	115.93	108.11
1	A	290	PRO	N-CA-C	5.45	123.70	112.47
1	A	96	ILE	N-CA-C	5.45	116.32	108.48
1	B	249	ARG	N-CA-C	-5.34	101.08	109.25
1	A	51	ASP	CA-C-N	5.31	125.12	119.28
1	A	51	ASP	C-N-CA	5.31	125.12	119.28
1	A	182	ARG	N-CA-C	5.20	116.63	111.07
1	A	106	THR	N-CA-C	-5.13	106.70	113.12
1	B	123	LEU	N-CA-C	5.10	121.08	109.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	ASP	N-CA-C	-5.07	101.70	109.76
1	A	65	THR	N-CA-C	-5.04	107.19	113.38

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	2485	0	2484	105	0
1	B	2511	0	2498	73	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	92	0	44	1	0
3	B	92	0	44	0	0
All	All	5182	0	5070	174	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 17.

All (174) 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:227:GLU:HG3	1:A:230:ARG:HH12	1.31	0.96
1:A:275:ARG:O	1:A:278:VAL:HG12	1.78	0.84
1:A:119:TYR:O	1:A:120:LEU:HD23	1.78	0.83
1:A:96:ILE:H	1:A:117:ASN:HD22	1.25	0.82
1:A:101:THR:HG23	1:A:102:LYS:H	1.47	0.79
1:A:268:ARG:HD2	1:A:336:LEU:HD21	1.65	0.79
1:A:339:GLN:HE21	1:A:339:GLN:HA	1.50	0.76
1:A:338:GLU:O	1:A:339:GLN:HB2	1.84	0.76
1:A:174:ASP:OD2	1:A:177:THR:HB	1.85	0.75
1:A:208:ILE:HG23	1:A:298:ILE:HG12	1.68	0.75
1:A:311:THR:O	1:A:314:VAL:HG12	1.88	0.73
1:A:278:VAL:HG11	1:A:296:VAL:HG22	1.69	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:MET:HG3	1:B:30:ILE:N	2.04	0.71
1:B:103:GLU:CD	1:B:105:PRO:HD2	2.16	0.71
1:B:52:PRO:HG3	1:B:73:MET:CE	2.20	0.71
1:A:22:LEU:HD12	1:A:62:ILE:HD11	1.73	0.70
1:B:103:GLU:HG2	1:B:105:PRO:CD	2.20	0.70
1:B:311:THR:O	1:B:314:VAL:HG12	1.92	0.70
1:A:135:TYR:OH	1:B:136:HIS:HD2	1.75	0.69
1:A:177:THR:HG23	1:A:233:ALA:HB1	1.76	0.68
1:B:13:ALA:N	1:B:14:PRO:HD2	2.08	0.68
1:A:60:ASN:HD21	1:A:88:ASN:ND2	1.93	0.67
1:A:95:PRO:HA	1:A:117:ASN:ND2	2.10	0.67
1:A:288:PRO:O	1:A:289:ARG:HG2	1.95	0.66
1:A:73:MET:HE3	1:A:76:VAL:HG23	1.78	0.66
1:A:339:GLN:HE21	1:A:339:GLN:CA	2.10	0.65
1:B:103:GLU:HG2	1:B:105:PRO:HD3	1.77	0.65
1:A:264:PRO:HG3	1:A:302:THR:HG21	1.79	0.65
1:A:223:VAL:O	1:A:227:GLU:HB2	1.97	0.64
1:B:21:VAL:HG11	1:B:38:LEU:HD23	1.79	0.64
1:B:35:ARG:O	1:B:35:ARG:HG2	1.96	0.64
1:B:137:SER:O	1:B:141:ILE:HG12	1.98	0.63
1:B:164:ASN:ND2	1:B:168:GLN:HE21	1.97	0.63
1:A:29:MET:HG3	1:A:30:ILE:N	2.13	0.63
1:A:96:ILE:N	1:A:117:ASN:HD22	1.96	0.62
1:A:177:THR:CG2	1:A:179:LEU:HG	2.30	0.62
1:A:287:GLN:C	1:A:289:ARG:H	2.07	0.61
1:A:77:ASP:OD1	1:A:80:THR:HG23	2.00	0.61
1:B:102:LYS:O	1:B:103:GLU:HB3	1.99	0.61
1:B:34:VAL:C	1:B:36:ARG:H	2.08	0.61
1:B:20:MET:HE2	1:B:45:ASP:HB2	1.83	0.60
1:A:232:VAL:O	1:A:236:ILE:HG13	2.01	0.60
1:B:21:VAL:HG23	1:B:66:VAL:HG13	1.82	0.60
1:B:104:GLU:H	1:B:105:PRO:HD3	1.66	0.60
1:A:177:THR:HG22	1:A:179:LEU:H	1.67	0.59
1:A:287:GLN:C	1:A:289:ARG:N	2.58	0.59
1:B:52:PRO:HG3	1:B:73:MET:SD	2.43	0.59
1:B:118:ASP:OD1	1:B:132:ARG:HD3	2.02	0.59
1:A:177:THR:HG23	1:A:233:ALA:CB	2.33	0.58
1:B:21:VAL:HG11	1:B:38:LEU:CD2	2.33	0.58
1:A:177:THR:HG21	1:A:179:LEU:HD12	1.86	0.58
1:B:103:GLU:O	1:B:104:GLU:HG3	2.03	0.58
1:B:104:GLU:H	1:B:105:PRO:CD	2.17	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ASP:CG	1:A:80:THR:HG23	2.29	0.57
1:A:22:LEU:C	1:A:22:LEU:HD23	2.29	0.57
1:B:259:LEU:HD13	1:B:270:LEU:HD12	1.86	0.57
1:B:234:GLY:HA2	1:B:237:ARG:HH12	1.71	0.56
1:B:68:LEU:HD23	1:B:97:ILE:HB	1.88	0.56
1:A:339:GLN:HA	1:A:339:GLN:NE2	2.17	0.56
1:B:20:MET:HE2	1:B:45:ASP:CB	2.36	0.56
1:A:215:SER:O	1:A:219:THR:HG22	2.06	0.56
1:A:177:THR:HG22	1:A:179:LEU:HG	1.89	0.55
1:A:190:GLU:CG	1:A:194:ARG:HH12	2.19	0.55
1:B:287:GLN:HG3	1:B:288:PRO:HA	1.89	0.54
1:A:219:THR:HG23	1:A:220:PHE:CD2	2.42	0.54
1:A:39:ALA:C	1:A:41:GLU:H	2.16	0.54
1:B:172:ASN:CB	1:B:184:HIS:HB2	2.38	0.53
1:A:210:VAL:HA	1:A:296:VAL:HG12	1.90	0.53
1:B:20:MET:HB3	1:B:64:PRO:HA	1.89	0.53
1:A:101:THR:HG23	1:A:102:LYS:N	2.21	0.53
1:A:174:ASP:OD2	1:A:249:ARG:HD3	2.08	0.53
1:A:120:LEU:HD11	1:A:132:ARG:HD2	1.90	0.52
1:B:104:GLU:N	1:B:105:PRO:CD	2.73	0.52
1:A:33:ALA:HB3	1:A:123:LEU:CD1	2.40	0.52
1:A:129:LEU:O	1:A:133:ILE:HG13	2.10	0.52
1:B:100:SER:O	1:B:122:LYS:HG2	2.10	0.52
1:B:104:GLU:O	1:B:106:THR:N	2.43	0.52
1:A:89:PRO:HA	1:A:92:ARG:HD3	1.91	0.51
1:B:103:GLU:HG2	1:B:105:PRO:HD2	1.89	0.51
1:A:227:GLU:HG3	1:A:230:ARG:NH1	2.14	0.51
1:B:103:GLU:CG	1:B:105:PRO:HD2	2.40	0.51
1:A:73:MET:HE1	1:A:81:LEU:CD1	2.41	0.51
1:B:52:PRO:HB2	1:B:76:VAL:HG21	1.93	0.51
1:A:96:ILE:H	1:A:117:ASN:ND2	2.04	0.50
1:B:30:ILE:HD13	1:B:122:LYS:HD2	1.93	0.50
3:A:360:C2E:H512	3:A:360:C2E:H5'2	1.94	0.50
1:A:89:PRO:HA	1:A:92:ARG:CD	2.42	0.50
1:A:128:GLU:HG3	1:B:112:PHE:CD1	2.47	0.50
1:B:42:ALA:C	1:B:44:ILE:H	2.20	0.50
1:B:264:PRO:HA	1:B:302:THR:HG21	1.92	0.49
1:A:27:GLN:HG3	1:A:30:ILE:HD12	1.94	0.49
1:A:32:GLU:OE2	1:A:35:ARG:HD2	2.13	0.49
1:B:52:PRO:HG3	1:B:73:MET:HE2	1.95	0.49
1:A:135:TYR:CZ	1:B:136:HIS:HD2	2.30	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:GLN:O	1:A:289:ARG:N	2.46	0.49
1:B:79:LEU:HD21	1:B:111:ALA:HA	1.95	0.49
1:B:58:VAL:O	1:B:62:ILE:HG23	2.13	0.49
1:B:172:ASN:HB2	1:B:184:HIS:CG	2.47	0.49
1:A:264:PRO:HG3	1:A:302:THR:CG2	2.43	0.48
1:B:25:ASP:OD2	1:B:122:LYS:HE2	2.13	0.48
1:A:20:MET:HG3	1:A:64:PRO:HA	1.95	0.48
1:A:47:HIS:CD2	1:A:62:ILE:HG21	2.49	0.48
1:A:146:ARG:HD2	1:A:146:ARG:C	2.38	0.48
1:A:270:LEU:O	1:A:274:VAL:HG23	2.14	0.48
1:B:237:ARG:CZ	1:B:237:ARG:HB3	2.44	0.48
1:A:190:GLU:HG2	1:A:194:ARG:NH1	2.29	0.47
1:A:159:GLN:NE2	1:B:160:LEU:HD13	2.29	0.47
1:B:213:PHE:CE1	1:B:229:LEU:HD13	2.49	0.47
1:A:303:LEU:HD11	1:A:318:MET:SD	2.55	0.47
1:A:30:ILE:CD1	1:A:122:LYS:HD3	2.45	0.47
1:B:79:LEU:CD2	1:B:111:ALA:HA	2.45	0.47
1:A:77:ASP:OD1	1:A:80:THR:CG2	2.62	0.47
1:A:95:PRO:HA	1:A:117:ASN:HD22	1.78	0.46
1:B:19:VAL:HB	1:B:44:ILE:HB	1.97	0.46
1:B:180:SER:OG	1:B:184:HIS:HD2	1.99	0.46
1:B:68:LEU:HD21	1:B:97:ILE:HD12	1.98	0.46
1:A:140:TYR:O	1:A:144:GLN:HG2	2.15	0.46
1:A:285:HIS:CD2	1:A:288:PRO:HD3	2.50	0.46
1:B:34:VAL:C	1:B:36:ARG:N	2.73	0.46
1:A:60:ASN:HD21	1:A:88:ASN:HD22	1.63	0.46
1:A:73:MET:HE1	1:A:81:LEU:HD11	1.97	0.46
1:A:103:GLU:O	1:A:103:GLU:HG3	2.16	0.45
1:A:102:LYS:O	1:A:104:GLU:HG3	2.16	0.45
1:B:13:ALA:N	1:B:14:PRO:CD	2.76	0.45
1:B:68:LEU:CD2	1:B:97:ILE:HD12	2.46	0.45
1:B:121:VAL:O	1:B:122:LYS:C	2.59	0.45
1:A:135:TYR:OH	1:B:136:HIS:CD2	2.63	0.45
1:A:54:GLN:O	1:A:58:VAL:HG23	2.17	0.44
1:B:208:ILE:HG23	1:B:296:VAL:CG1	2.47	0.44
1:B:304:VAL:O	1:B:305:PRO:C	2.61	0.44
1:A:86:ARG:HH22	1:A:117:ASN:HD21	1.65	0.44
1:A:172:ASN:HA	1:A:181:ASN:HD21	1.83	0.44
1:B:103:GLU:O	1:B:104:GLU:CG	2.65	0.44
1:A:330:GLY:O	1:A:331:ARG:HB2	2.18	0.44
1:A:313:ARG:O	1:A:317:GLU:HG3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:MET:CG	1:A:64:PRO:HA	2.48	0.43
1:B:150:TYR:O	1:B:154:ARG:HG3	2.19	0.43
1:B:330:GLY:O	1:B:331:ARG:HB2	2.19	0.43
1:A:82:LEU:HD12	1:A:82:LEU:O	2.19	0.43
1:B:41:GLU:O	1:B:44:ILE:HG23	2.19	0.43
1:B:101:THR:C	1:B:103:GLU:H	2.27	0.43
1:B:259:LEU:CD1	1:B:270:LEU:HD12	2.47	0.43
1:A:273:LYS:O	1:A:277:THR:HG23	2.18	0.43
1:A:288:PRO:O	1:A:289:ARG:CG	2.66	0.43
1:B:174:ASP:OD2	1:B:249:ARG:HD3	2.18	0.43
1:A:25:ASP:OD2	1:A:122:LYS:HE2	2.19	0.42
1:B:88:ASN:HB3	1:B:91:THR:OG1	2.19	0.42
1:B:125:ASP:O	1:B:127:ILE:N	2.52	0.42
1:A:82:LEU:HD13	1:A:96:ILE:HD13	2.01	0.42
1:A:89:PRO:HA	1:A:92:ARG:HG2	2.01	0.42
1:A:339:GLN:CA	1:A:339:GLN:NE2	2.80	0.42
1:B:331:ARG:O	1:B:332:ASN:C	2.63	0.42
1:A:268:ARG:CD	1:A:336:LEU:HD21	2.40	0.42
1:A:273:LYS:HG3	1:A:276:ARG:HH22	1.85	0.42
1:A:69:GLN:O	1:A:98:VAL:HA	2.20	0.42
1:A:227:GLU:HA	1:A:230:ARG:NH1	2.34	0.42
1:A:234:GLY:O	1:A:238:GLU:HG3	2.20	0.42
1:A:190:GLU:CG	1:A:194:ARG:NH1	2.83	0.42
1:A:287:GLN:O	1:A:288:PRO:C	2.62	0.41
1:B:296:VAL:HG12	1:B:298:ILE:HG13	2.01	0.41
1:A:118:ASP:OD1	1:A:136:HIS:HE1	2.03	0.41
1:A:29:MET:HG3	1:A:30:ILE:H	1.83	0.41
1:A:177:THR:CG2	1:A:233:ALA:HB1	2.49	0.41
1:B:71:LEU:HD13	1:B:107:VAL:HG11	2.01	0.41
1:A:69:GLN:NE2	1:A:81:LEU:HD12	2.35	0.41
1:A:211:ASP:OD1	1:A:331:ARG:HD3	2.21	0.41
1:A:336:LEU:HD12	1:A:336:LEU:N	2.36	0.41
1:B:64:PRO:HG2	1:B:94:ILE:HD13	2.03	0.41
1:A:30:ILE:HD13	1:A:122:LYS:HD3	2.02	0.41
1:B:30:ILE:HD13	1:B:122:LYS:CE	2.51	0.41
1:A:212:TYR:CD1	1:A:288:PRO:HG3	2.56	0.41
1:A:126:ALA:O	1:A:130:VAL:HG13	2.20	0.40
1:A:194:ARG:HG3	1:A:194:ARG:HH11	1.86	0.40
1:A:288:PRO:O	1:A:289:ARG:CB	2.70	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	320/358 (89%)	296 (92%)	15 (5%)	9 (3%)	4	3
1	B	326/358 (91%)	302 (93%)	18 (6%)	6 (2%)	6	9
All	All	646/716 (90%)	598 (93%)	33 (5%)	15 (2%)	5	6

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	ARG
1	A	310	GLN
1	B	104	GLU
1	B	105	PRO
1	B	126	ALA
1	A	37	SER
1	A	122	LYS
1	A	290	PRO
1	A	309	GLY
1	B	122	LYS
1	B	35	ARG
1	A	40	SER
1	A	123	LEU
1	A	105	PRO
1	B	44	ILE

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	264/291 (91%)	246 (93%)	18 (7%)	14	25
1	B	264/291 (91%)	252 (96%)	12 (4%)	24	42
All	All	528/582 (91%)	498 (94%)	30 (6%)	18	33

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ILE
1	A	88	ASN
1	A	96	ILE
1	A	101	THR
1	A	161	LEU
1	A	165	LEU
1	A	168	GLN
1	A	176	LEU
1	A	215	SER
1	A	227	GLU
1	A	237	ARG
1	A	250	TYR
1	A	290	PRO
1	A	302	THR
1	A	325	GLN
1	A	336	LEU
1	A	337	MET
1	A	339	GLN
1	B	20	MET
1	B	44	ILE
1	B	60	ASN
1	B	67	ILE
1	B	103	GLU
1	B	105	PRO
1	B	183	ARG
1	B	215	SER
1	B	229	LEU
1	B	253	GLU
1	B	296	VAL
1	B	302	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	54	GLN
1	A	60	ASN
1	A	117	ASN
1	A	136	HIS
1	A	159	GLN
1	A	184	HIS
1	A	202	GLN
1	A	285	HIS
1	A	310	GLN
1	A	329	ASN
1	A	339	GLN
1	B	136	HIS
1	B	164	ASN
1	B	168	GLN
1	B	172	ASN
1	B	184	HIS
1	B	202	GLN
1	B	325	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 6 ligands modelled in this entry, 2 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	C2E	A	360	-	52,52,52	1.22	4 (7%)	78,82,82	1.85	15 (19%)
3	C2E	B	360	-	52,52,52	1.27	4 (7%)	78,82,82	1.79	14 (17%)
3	C2E	A	361	-	52,52,52	1.25	5 (9%)	78,82,82	1.80	15 (19%)
3	C2E	B	361	-	52,52,52	1.24	4 (7%)	78,82,82	1.80	15 (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	A	360	-	-	0/30/62/62	0/6/7/7
3	C2E	B	360	-	-	0/30/62/62	0/6/7/7
3	C2E	A	361	-	-	0/30/62/62	0/6/7/7
3	C2E	B	361	-	-	0/30/62/62	0/6/7/7

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	361	C2E	C5-C4	3.71	1.49	1.38
3	B	360	C2E	C5-C4	3.68	1.48	1.38
3	B	361	C2E	C5-C4	3.65	1.48	1.38
3	B	360	C2E	C51-C41	3.61	1.48	1.38
3	A	360	C2E	C5-C4	3.56	1.48	1.38
3	A	360	C2E	C51-C41	3.50	1.48	1.38
3	B	361	C2E	C51-C41	3.48	1.48	1.38
3	A	361	C2E	C51-C41	3.43	1.48	1.38
3	B	361	C2E	C5-N7	-2.87	1.33	1.39
3	B	361	C2E	C51-N71	-2.75	1.33	1.39
3	A	361	C2E	C5-N7	-2.69	1.33	1.39
3	B	360	C2E	C51-N71	-2.65	1.33	1.39
3	A	360	C2E	C5-N7	-2.61	1.33	1.39
3	B	360	C2E	C5-N7	-2.46	1.34	1.39
3	A	360	C2E	C51-N71	-2.39	1.34	1.39
3	A	361	C2E	C51-N71	-2.36	1.34	1.39
3	A	361	C2E	C21-N31	2.00	1.38	1.33

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	361	C2E	C5-C4-N3	-5.70	119.32	128.39
3	B	360	C2E	C5-C4-N3	-5.70	119.32	128.39
3	A	361	C2E	C5-C4-N3	-5.61	119.46	128.39
3	A	360	C2E	C5-C4-N3	-5.53	119.59	128.39
3	A	360	C2E	C51-C41-N31	-5.38	119.83	128.39
3	B	361	C2E	C51-C41-N31	-5.35	119.88	128.39
3	B	360	C2E	C51-C41-N31	-5.29	119.98	128.39
3	A	361	C2E	C51-C41-N31	-5.24	120.06	128.39
3	A	360	C2E	C2-N3-C4	5.22	121.29	112.30
3	B	360	C2E	C2-N3-C4	5.09	121.07	112.30
3	A	360	C2E	C21-N31-C41	4.91	120.76	112.30
3	A	361	C2E	C2-N3-C4	4.87	120.69	112.30
3	B	361	C2E	C2-N3-C4	4.82	120.60	112.30
3	B	361	C2E	C21-N31-C41	4.72	120.43	112.30
3	A	361	C2E	C21-N31-C41	4.70	120.39	112.30
3	B	360	C2E	C21-N31-C41	4.61	120.23	112.30
3	B	361	C2E	N9-C4-N3	4.28	134.51	125.95
3	A	361	C2E	N9-C4-N3	4.25	134.45	125.95
3	B	360	C2E	N9-C4-N3	4.18	134.31	125.95
3	A	360	C2E	N9-C4-N3	4.06	134.08	125.95
3	A	360	C2E	C61-C51-N71	4.01	137.59	130.29
3	B	361	C2E	N91-C41-N31	3.93	133.81	125.95
3	A	361	C2E	N91-C41-N31	3.89	133.73	125.95
3	B	360	C2E	C61-C51-N71	3.74	137.09	130.29
3	B	360	C2E	N91-C41-N31	3.67	133.30	125.95
3	B	361	C2E	C61-C51-N71	3.54	136.74	130.29
3	A	361	C2E	C61-C51-N71	3.48	136.62	130.29
3	A	360	C2E	N91-C41-N31	3.46	132.88	125.95
3	A	360	C2E	C6-C5-N7	3.39	136.46	130.29
3	B	360	C2E	C6-C5-N7	3.36	136.40	130.29
3	A	361	C2E	C3'-C2'-C1'	3.32	107.18	99.89
3	A	361	C2E	C6-C5-N7	3.30	136.29	130.29
3	B	361	C2E	C3'-C2'-C1'	3.17	106.86	99.89
3	B	361	C2E	C6-C5-N7	3.11	135.95	130.29
3	A	360	C2E	C3'-C2'-C1'	3.04	106.58	99.89
3	B	360	C2E	C3'-C2'-C1'	2.92	106.30	99.89
3	A	360	C2E	C41-C51-N71	-2.90	106.07	110.67
3	B	361	C2E	C3A-C2A-C1A	2.87	106.20	99.89
3	B	360	C2E	C3A-C2A-C1A	2.86	106.18	99.89
3	A	361	C2E	C3A-C2A-C1A	2.78	106.01	99.89
3	A	361	C2E	C41-C51-N71	-2.75	106.31	110.67
3	A	360	C2E	C3A-C2A-C1A	2.72	105.86	99.89
3	B	360	C2E	C41-C51-N71	-2.65	106.48	110.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	361	C2E	C41-C51-N71	-2.57	106.60	110.67
3	A	360	C2E	C4-C5-N7	-2.34	106.96	110.67
3	A	360	C2E	C2A-C3A-C4A	-2.25	99.29	103.24
3	B	361	C2E	C4-C5-N7	-2.23	107.14	110.67
3	B	360	C2E	C4-C5-N7	-2.22	107.15	110.67
3	A	361	C2E	O6-C6-C5	-2.22	120.67	126.53
3	A	361	C2E	C4-C5-N7	-2.19	107.20	110.67
3	B	360	C2E	C5-C6-N1	2.18	118.81	113.25
3	B	361	C2E	O6-C6-C5	-2.17	120.80	126.53
3	A	360	C2E	O6-C6-C5	-2.16	120.83	126.53
3	A	361	C2E	C5-C6-N1	2.13	118.67	113.25
3	B	360	C2E	O6-C6-C5	-2.12	120.92	126.53
3	B	361	C2E	C2'-C3'-C4'	-2.12	99.52	103.24
3	A	360	C2E	C2'-C3'-C4'	-2.10	99.56	103.24
3	B	361	C2E	C5-C6-N1	2.05	118.47	113.25
3	A	361	C2E	C2'-C3'-C4'	-2.00	99.73	103.24

There are no chirality outliers.

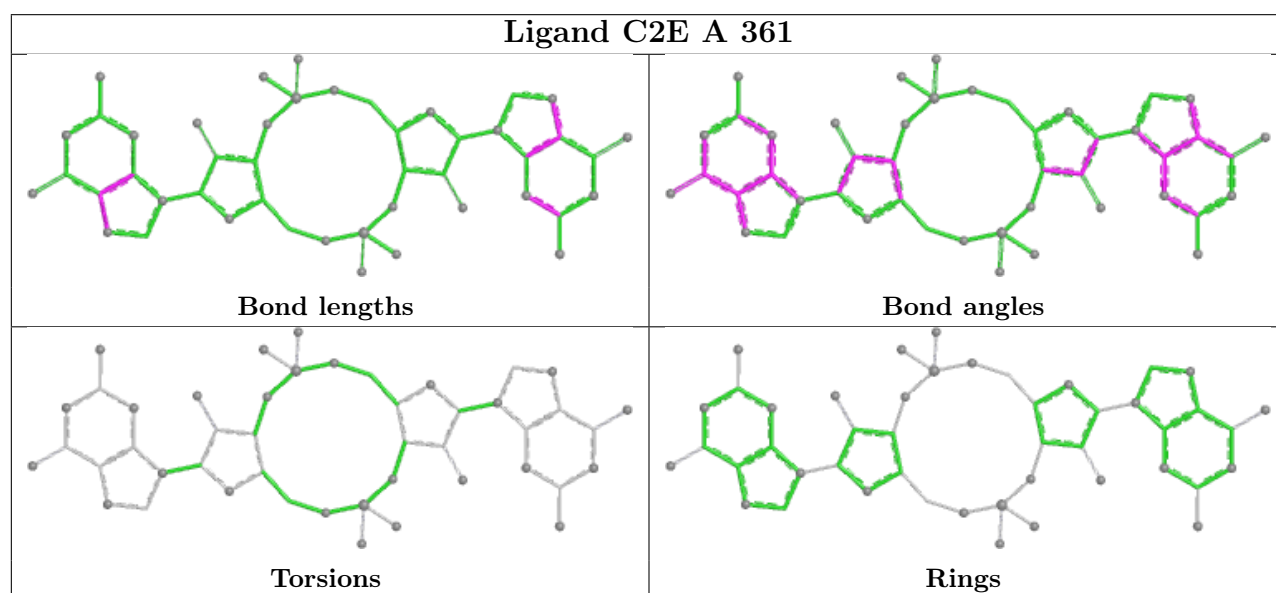
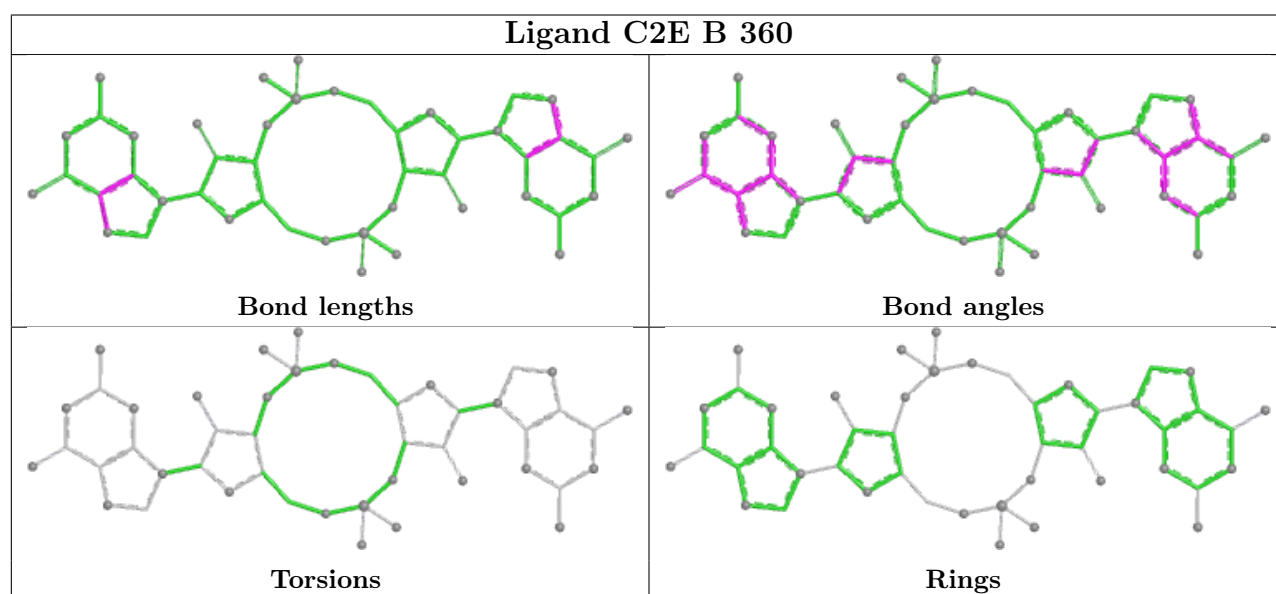
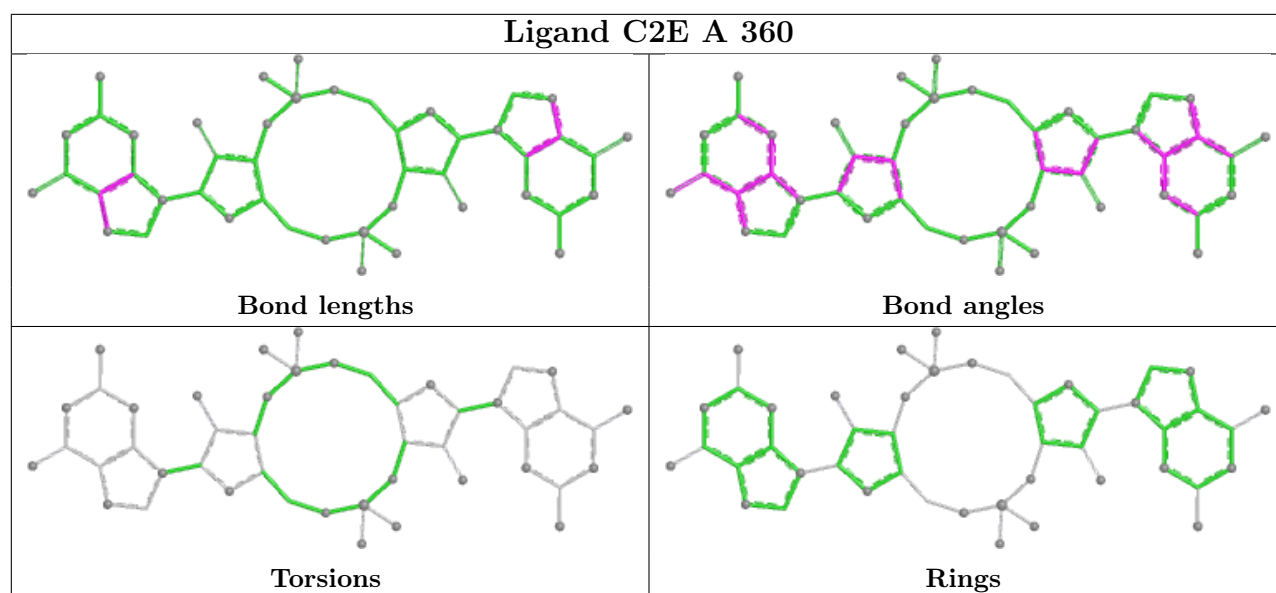
There are no torsion outliers.

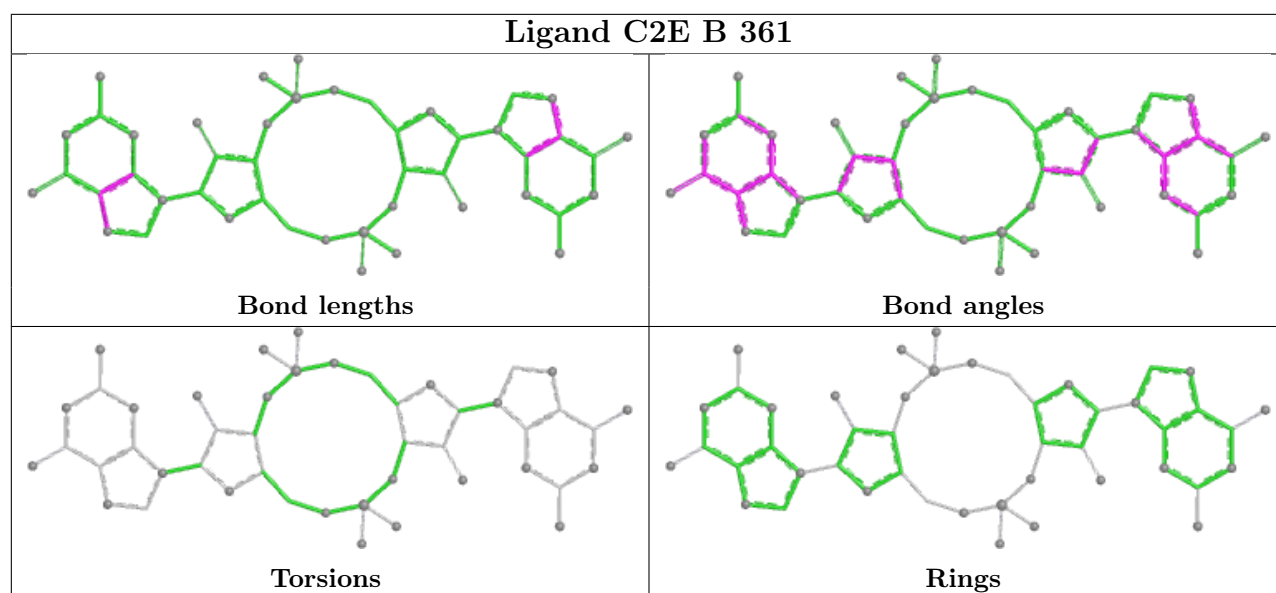
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	360	C2E	1	0

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





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	322/358 (89%)	0.66	22 (6%) 23 20	41, 66, 94, 107	0
1	B	328/358 (91%)	0.76	28 (8%) 16 13	42, 64, 102, 112	0
All	All	650/716 (90%)	0.71	50 (7%) 19 16	41, 65, 98, 112	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	ALA	5.3
1	B	13	ALA	4.4
1	B	339	GLN	4.1
1	B	308	GLY	3.7
1	B	105	PRO	3.7
1	B	338	GLU	3.7
1	B	29	MET	3.6
1	A	288	PRO	3.4
1	B	127	ILE	3.4
1	B	340	PRO	3.4
1	A	101	THR	3.3
1	B	106	THR	3.3
1	B	307	GLY	3.3
1	A	336	LEU	3.3
1	A	222	HIS	3.2
1	B	107	VAL	3.1
1	B	15	LEU	3.1
1	A	50	SER	3.1
1	B	309	GLY	3.0
1	A	46	PHE	3.0
1	B	42	ALA	3.0
1	B	28	ALA	3.0
1	B	39	ALA	3.0
1	B	126	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	123	LEU	2.9
1	B	222	HIS	2.8
1	B	46	PHE	2.6
1	B	101	THR	2.6
1	B	38	LEU	2.5
1	B	102	LYS	2.5
1	A	44	ILE	2.4
1	B	108	LYS	2.4
1	A	29	MET	2.4
1	A	324	TYR	2.2
1	A	287	GLN	2.2
1	A	289	ARG	2.2
1	A	339	GLN	2.2
1	B	30	ILE	2.2
1	B	337	MET	2.1
1	B	44	ILE	2.1
1	B	48	PHE	2.1
1	A	27	GLN	2.1
1	A	38	LEU	2.1
1	A	102	LYS	2.1
1	A	43	GLY	2.0
1	A	91	THR	2.0
1	A	47	HIS	2.0
1	B	220	PHE	2.0
1	A	214	LYS	2.0
1	A	337	MET	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](#)

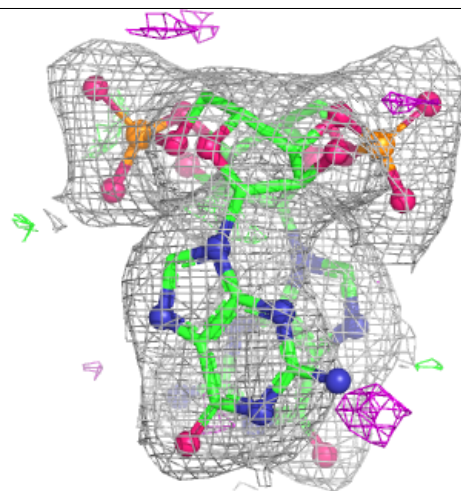
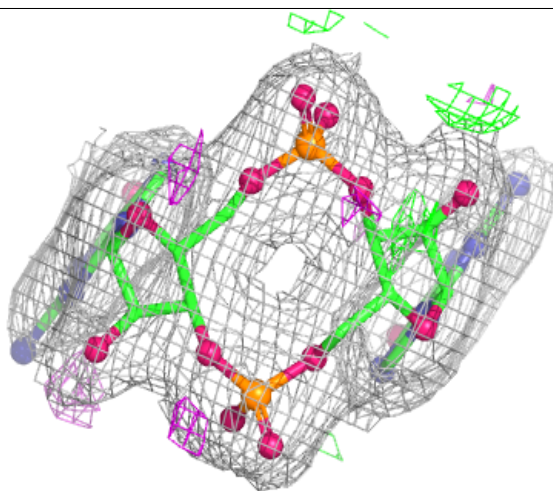
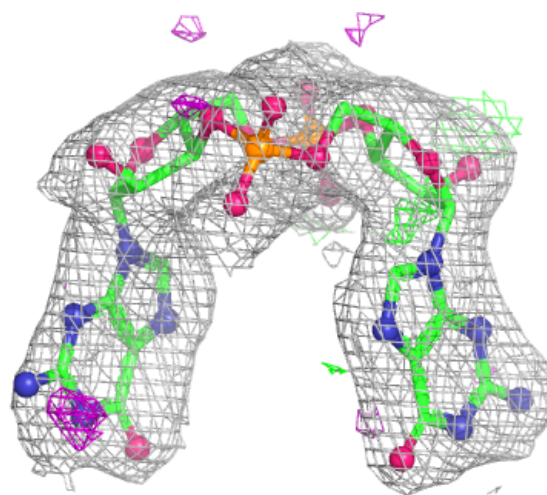
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	359	1/1	0.85	0.21	71,71,71,71	0
2	MG	A	359	1/1	0.88	0.15	76,76,76,76	0
3	C2E	B	360	46/46	0.93	0.10	50,63,66,67	0
3	C2E	B	361	46/46	0.94	0.08	52,59,66,69	0
3	C2E	A	360	46/46	0.95	0.08	44,55,60,60	0
3	C2E	A	361	46/46	0.96	0.07	40,50,53,54	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.

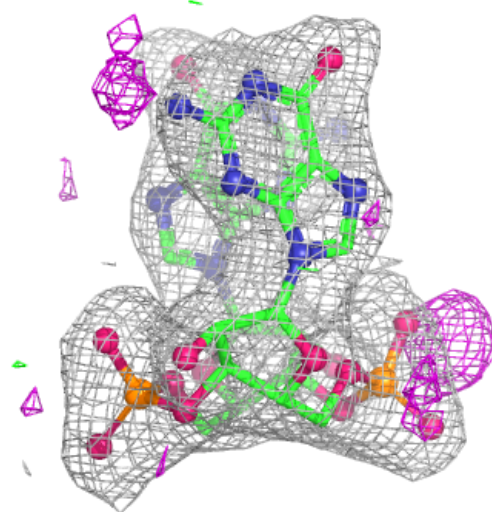
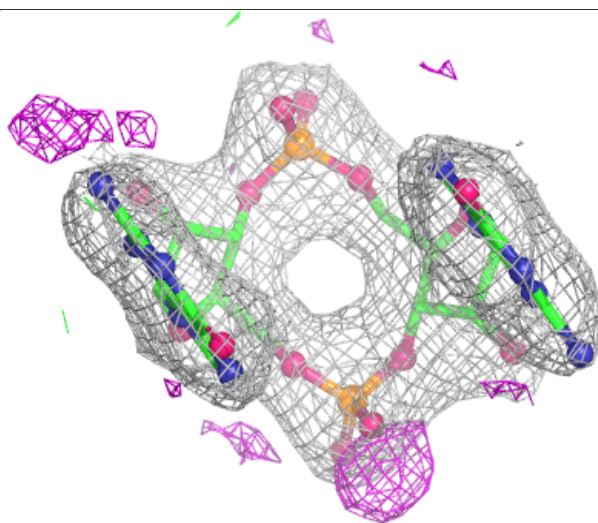
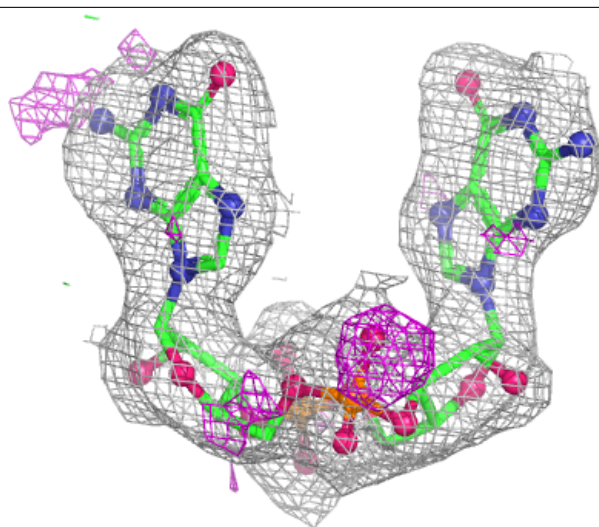
Electron density around C2E B 360:

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



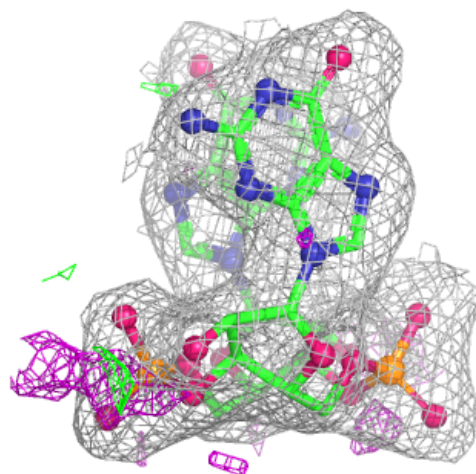
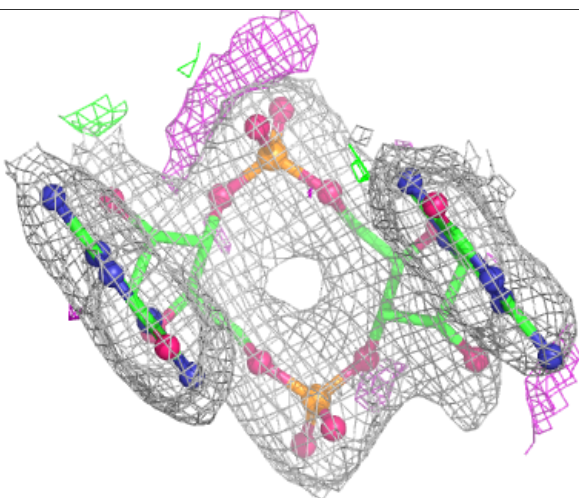
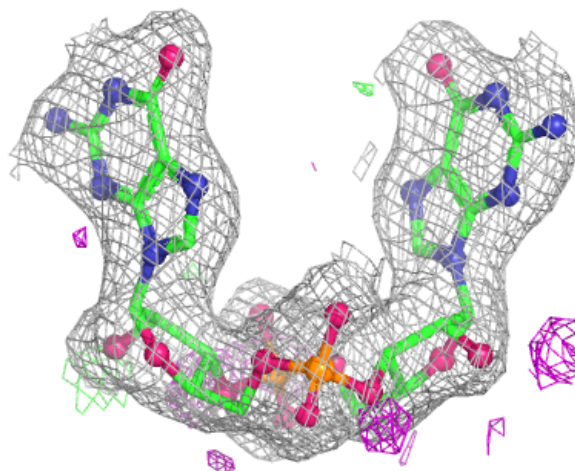
Electron density around C2E B 361:

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



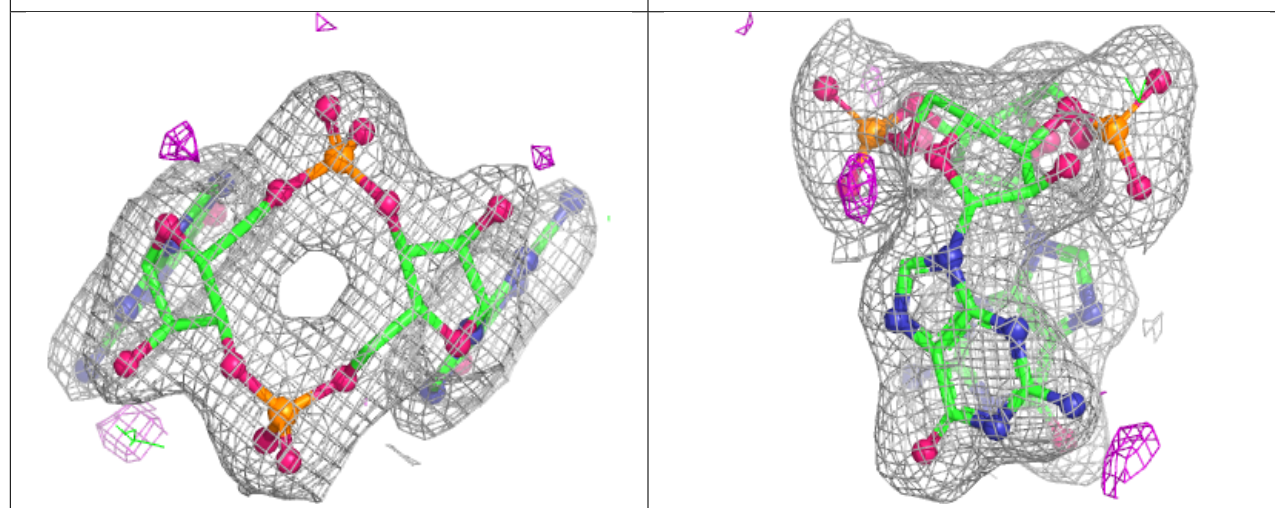
Electron density around C2E A 360:

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



Electron density around C2E A 361:

$2mF_o-DF_c$ (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.