



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:36 PM UTC

PDB ID : 2C47 / pdb_00002c47
Title : Structure of casein kinase 1 gamma 2
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Eswaran, J.; Amos, A.; Ball, L.; von Delft, F.; Bullock, A.; Debreczeni,
J.; Turnbull, A.; Sundstrom, M.; Weigelt, J.; Arrowsmith, C.; Edwards, A.;
Knapp, S.
Deposited on : 2005-10-16
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](#) ①) were used in the production of this report:

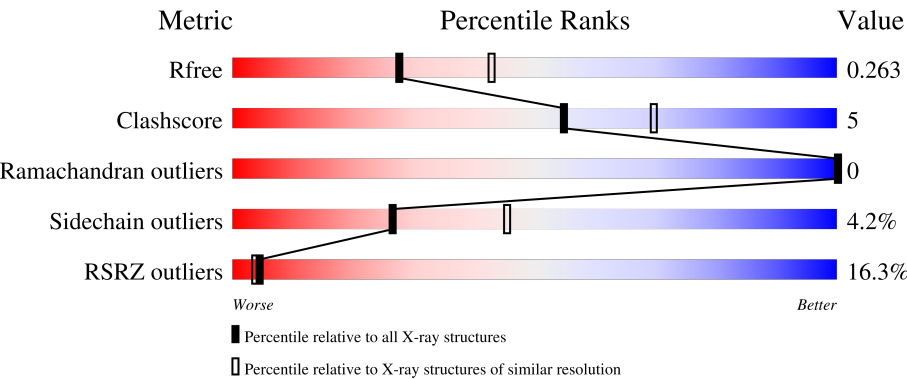
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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	313	3% 82% 10% • 8%
1	B	313	10% 82% 10% 7%
1	C	313	27% 80% 9% • 10%
1	D	313	20% 79% 12% • 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9545 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.

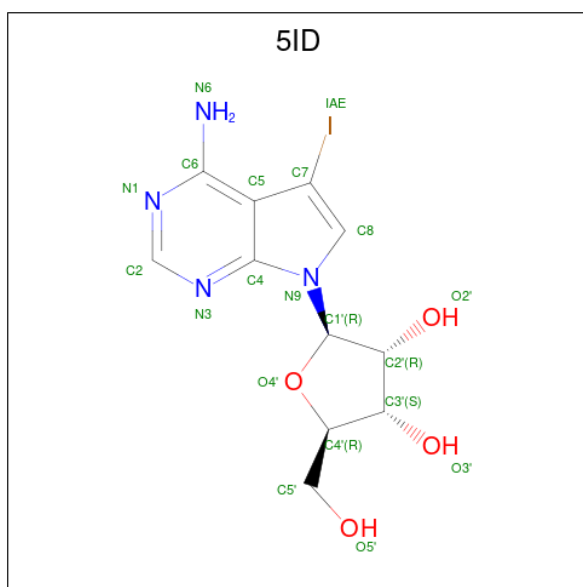
- Molecule 1 is a protein called CASEIN KINASE 1 GAMMA 2 ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	1	0
			2366	1539	392	425	10			
1	B	290	Total	C	N	O	S	0	1	0
			2376	1542	399	425	10			
1	C	283	Total	C	N	O	S	0	0	0
			2219	1440	366	403	10			
1	D	291	Total	C	N	O	S	0	0	0
			2295	1498	375	411	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	SER	-	expression tag	UNP P78368
A	42	MET	-	expression tag	UNP P78368
B	41	SER	-	expression tag	UNP P78368
B	42	MET	-	expression tag	UNP P78368
C	41	SER	-	expression tag	UNP P78368
C	42	MET	-	expression tag	UNP P78368
D	41	SER	-	expression tag	UNP P78368
D	42	MET	-	expression tag	UNP P78368

- Molecule 2 is (2R,3R,4S,5R)-2-(4-AMINO-5-iodo-7H-PYRROLO[2,3-D]PYRIMIDIN-7-YL)-5-(HYDROXYMETHYL)TETRAHYDROFURAN-3,4-DIOL (CCD ID: 5ID) (formula: C₁₁H₁₃IN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 20	C 11	I 1	N 4	O 4	0	0
2	B	1	Total 20	C 11	I 1	N 4	O 4	0	0
2	C	1	Total 20	C 11	I 1	N 4	O 4	0	0
2	D	1	Total 20	C 11	I 1	N 4	O 4	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	64	Total	O	0	0
			64	64		
4	B	81	Total	O	0	0
			81	81		
4	C	31	Total	O	0	0
			31	31		

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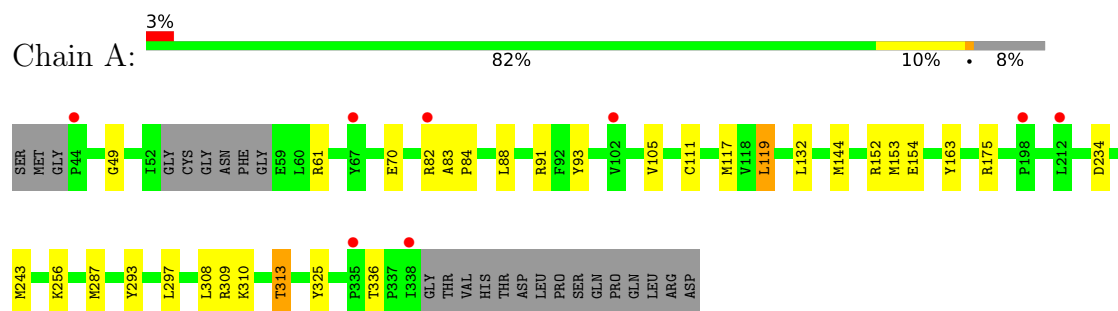
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	31	Total	O	0	0
			31	31		

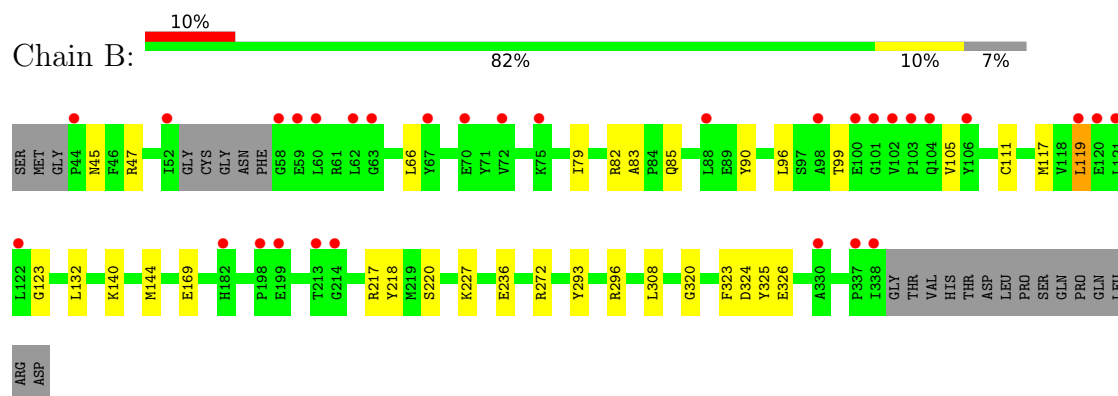
3 Residue-property plots [i](#)

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.

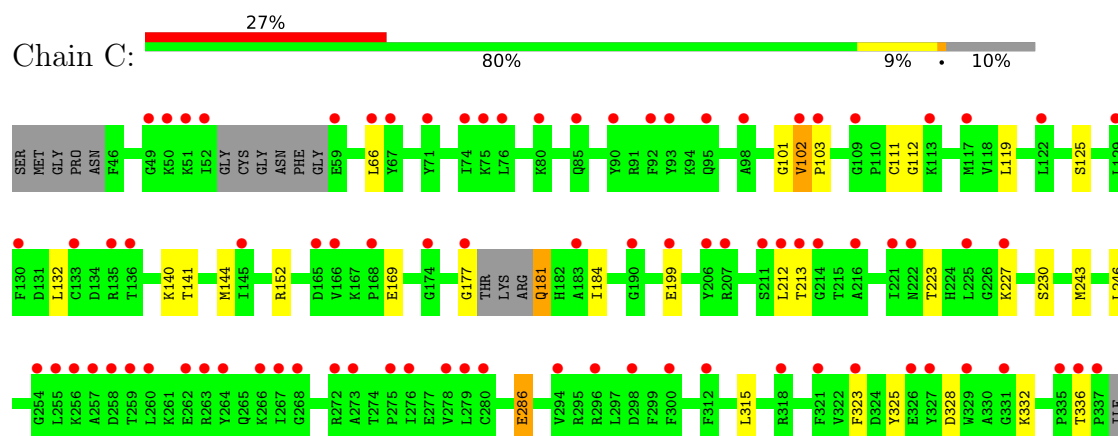
• Molecule 1: CASEIN KINASE 1 GAMMA 2 ISOFORM



• Molecule 1: CASEIN KINASE 1 GAMMA 2 ISOFORM

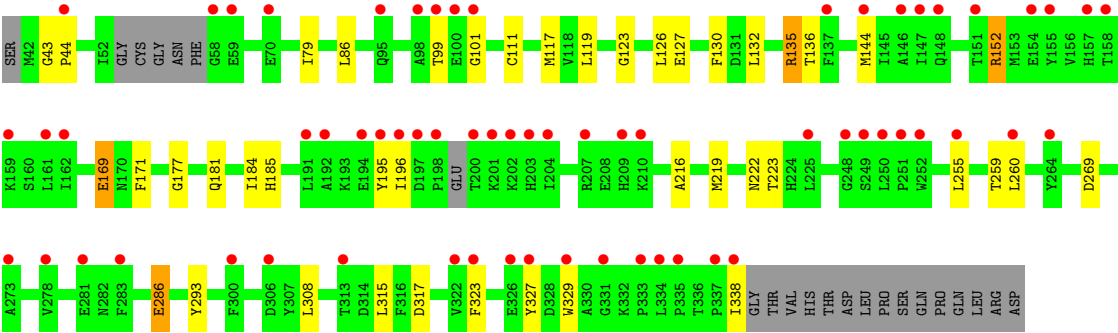
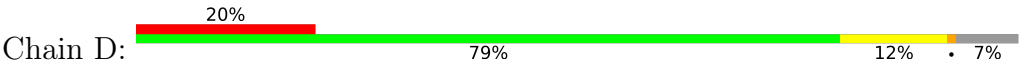


• Molecule 1: CASEIN KINASE 1 GAMMA 2 ISOFORM



GLY
THR
VAL
HIS
THR
ASP
LEU
PRO
SER
GLN
PRO
GLN
LEU
ARG
ASP

● Molecule 1: CASEIN KINASE 1 GAMMA 2 ISOFORM



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.96Å 97.09Å 185.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.40) 99.2 (50.00-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.208 , 0.257 0.216 , 0.263	Depositor DCC
R_{free} test set	3383 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 73.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9545	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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: CSD, MG, 5ID

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	0.74	0/2425	0.86	0/3284
1	B	0.87	0/2434	0.95	4/3292 (0.1%)
1	C	0.65	0/2267	0.83	0/3074
1	D	0.72	1/2349 (0.0%)	0.88	2/3189 (0.1%)
All	All	0.75	1/9475 (0.0%)	0.88	6/12839 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	269	ASP	CG-OD2	9.36	1.43	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	324	ASP	CB-CA-C	-5.55	98.70	110.31
1	B	123	GLY	CA-C-N	5.44	125.75	119.92
1	B	123	GLY	C-N-CA	5.44	125.75	119.92
1	B	45	ASN	N-CA-C	5.32	118.13	109.24
1	D	123	GLY	CA-C-N	5.06	125.33	119.92
1	D	123	GLY	C-N-CA	5.06	125.33	119.92

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	2366	0	2307	23	0
1	B	2376	0	2337	16	0
1	C	2219	0	2099	20	0
1	D	2295	0	2172	28	0
2	A	20	0	13	0	0
2	B	20	0	13	3	0
2	C	20	0	13	3	0
2	D	20	0	13	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	64	0	0	2	0
4	B	81	0	0	3	0
4	C	31	0	0	1	0
4	D	31	0	0	1	0
All	All	9545	0	8967	87	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 5.

All (87) 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:D:127:GLU:OE2	1:D:135:ARG:NH1	2.10	0.85
1:B:144:MET:HE1	1:B:325:TYR:H	1.42	0.84
1:D:152:ARG:NH1	1:D:184:ILE:O	2.14	0.80
1:D:222:ASN:CB	4:D:2017:HOH:O	2.32	0.77
1:C:144:MET:HE1	1:C:325:TYR:H	1.49	0.77
1:A:93:TYR:CD1	1:A:117:MET:HE1	2.23	0.74
1:B:105:VAL:HG12	1:B:119:LEU:HD23	1.70	0.73
1:A:153:MET:HE1	1:A:163:TYR:HB2	1.72	0.71
1:D:152:ARG:HH11	1:D:152:ARG:HG2	1.58	0.69
1:A:297:LEU:O	4:A:2058:HOH:O	2.11	0.68
1:A:153:MET:HE1	1:A:163:TYR:CB	2.23	0.68
1:A:93:TYR:HD1	1:A:117:MET:HE1	1.61	0.66
1:C:177:GLY:C	1:C:181:GLN:OE1	2.38	0.65
1:C:286:GLU:HG3	1:C:315:LEU:HD22	1.78	0.65
1:A:310:LYS:HA	1:A:313:THR:HG22	1.80	0.64
1:B:144:MET:HE3	1:B:323:PHE:HA	1.80	0.63
1:A:153:MET:HE2	1:A:234:ASP:CG	2.26	0.61
1:A:153:MET:HE2	1:A:234:ASP:OD2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:GLU:CG	1:C:315:LEU:HD22	2.32	0.60
1:C:112:GLY:HA3	1:D:259:THR:HG23	1.83	0.59
2:B:1300:5ID:H5'2	4:B:2030:HOH:O	2.03	0.57
1:C:102:VAL:HG12	1:C:103:PRO:HD2	1.87	0.57
1:C:169:GLU:O	2:C:1300:5ID:H5'1	2.05	0.57
1:D:101:GLY:HA3	1:D:152:ARG:HD2	1.89	0.55
2:C:1300:5ID:H2'	2:C:1300:5ID:N3	2.21	0.55
1:C:141:THR:HG21	1:C:328:ASP:H	1.72	0.54
1:B:105:VAL:CG1	1:B:119:LEU:HD23	2.37	0.54
1:D:195:TYR:CD2	1:D:196:ILE:HD12	2.44	0.52
1:C:140:LYS:O	1:C:144:MET:HG3	2.09	0.52
1:A:153:MET:HE2	1:A:234:ASP:CB	2.41	0.51
1:D:286:GLU:HG2	1:D:315:LEU:HD22	1.93	0.51
1:B:82:ARG:O	1:B:83:ALA:HB3	2.10	0.51
1:C:101:GLY:HA3	1:C:152:ARG:HD2	1.92	0.51
1:D:195:TYR:CE2	1:D:196:ILE:CD1	2.94	0.51
1:D:286:GLU:CG	1:D:315:LEU:HD22	2.42	0.50
1:D:259:THR:HG22	1:D:260:LEU:N	2.27	0.49
1:A:293:TYR:CD1	1:A:308:LEU:HD21	2.47	0.49
1:C:243:MET:CE	1:C:246:LEU:HD12	2.42	0.48
1:A:153:MET:HE1	1:A:163:TYR:HB3	1.94	0.48
1:C:144:MET:HE3	1:C:323:PHE:HA	1.96	0.48
1:A:119:LEU:N	1:A:119:LEU:HD23	2.29	0.47
1:D:130:PHE:CE2	1:D:135:ARG:HG3	2.49	0.47
1:C:243:MET:HE1	1:C:246:LEU:HD12	1.95	0.47
1:B:47:ARG:HG3	1:B:66:LEU:HD21	1.97	0.47
1:A:154:GLU:OE1	1:A:309:ARG:NH2	2.45	0.46
1:B:90:TYR:HB2	1:B:117:MET:HE2	1.97	0.46
1:A:83:ALA:N	1:A:84:PRO:HD3	2.30	0.46
1:D:144:MET:CE	1:D:323:PHE:HA	2.45	0.46
1:B:144:MET:HE2	1:B:323:PHE:CD2	2.51	0.46
1:A:153:MET:HE2	1:A:234:ASP:HB3	1.98	0.45
1:C:141:THR:HG21	1:C:328:ASP:N	2.30	0.45
1:D:293:TYR:CD1	1:D:308:LEU:HD21	2.52	0.45
1:A:144:MET:HE1	1:A:325:TYR:H	1.82	0.45
1:D:126:LEU:HD21	1:D:184:ILE:HD12	1.99	0.45
1:A:256:LYS:NZ	4:A:2046:HOH:O	2.50	0.45
1:D:43:GLY:N	1:D:44:PRO:CD	2.80	0.44
1:D:216:ALA:HA	1:D:219:MET:SD	2.57	0.44
1:C:230:SER:HB2	4:C:2011:HOH:O	2.19	0.43
1:B:217:ARG:HD2	1:B:218:TYR:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:SER:HB3	2:C:1300:5ID:H5'1	2.00	0.43
1:D:144:MET:HE2	1:D:323:PHE:HA	1.99	0.43
1:D:86:LEU:HD11	1:D:117:MET:HE2	2.00	0.43
1:C:112:GLY:HA3	1:D:259:THR:CG2	2.48	0.42
1:A:243:MET:HE1	1:A:287:MET:SD	2.58	0.42
1:C:212:LEU:HD21	1:C:223:THR:O	2.19	0.42
4:B:2079:HOH:O	1:C:199:GLU:CB	2.67	0.42
1:A:49:GLY:O	1:A:61:ARG:HD2	2.20	0.42
1:B:96:LEU:O	1:B:99:THR:HG22	2.20	0.42
2:B:1300:5ID:C5'	4:B:2030:HOH:O	2.65	0.41
1:D:327:TYR:CD1	1:D:329:TRP:CZ2	3.08	0.41
1:A:82:ARG:O	1:A:83:ALA:HB3	2.20	0.41
1:A:105:VAL:HG11	1:A:117:MET:CE	2.51	0.41
1:A:243:MET:HE1	1:A:287:MET:CG	2.51	0.41
1:B:140:LYS:O	1:B:144:MET:HG3	2.21	0.41
1:D:259:THR:HG22	1:D:260:LEU:H	1.85	0.41
1:B:119:LEU:HD13	2:B:1300:5ID:IAE	2.91	0.41
1:B:220:SER:HB2	1:B:236:GLU:CD	2.45	0.41
1:D:127:GLU:HG2	1:D:169:GLU:OE1	2.21	0.41
1:A:88:LEU:O	1:A:91:ARG:HB2	2.21	0.41
1:B:47:ARG:CG	1:B:66:LEU:HD21	2.51	0.41
1:B:293:TYR:CD1	1:B:308:LEU:HD21	2.56	0.41
1:B:320:GLY:HA3	1:C:199:GLU:O	2.21	0.41
1:D:152:ARG:HD3	1:D:152:ARG:HA	1.84	0.41
1:D:177:GLY:H	1:D:181:GLN:NE2	2.19	0.41
1:D:327:TYR:CG	1:D:329:TRP:CZ2	3.09	0.40
1:D:171:PHE:HA	1:D:185:HIS:O	2.21	0.40
1:D:219:MET:HE2	1:D:223:THR:HG22	2.04	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	285/313 (91%)	277 (97%)	8 (3%)	0	100	100
1	B	286/313 (91%)	282 (99%)	4 (1%)	0	100	100
1	C	276/313 (88%)	273 (99%)	3 (1%)	0	100	100
1	D	284/313 (91%)	279 (98%)	5 (2%)	0	100	100
All	All	1131/1252 (90%)	1111 (98%)	20 (2%)	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	245/277 (88%)	238 (97%)	7 (3%)	37	60
1	B	248/277 (90%)	239 (96%)	9 (4%)	31	52
1	C	217/277 (78%)	206 (95%)	11 (5%)	21	37
1	D	224/277 (81%)	212 (95%)	12 (5%)	20	35
All	All	934/1108 (84%)	895 (96%)	39 (4%)	26	45

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

Mol	Chain	Res	Type
1	A	70	GLU
1	A	119	LEU
1	A	132	LEU
1	A	152	ARG
1	A	175	ARG
1	A	313	THR
1	A	336	THR
1	B	79	ILE
1	B	85	GLN
1	B	119	LEU
1	B	132	LEU
1	B	169	GLU
1	B	227	LYS

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Mol	Chain	Res	Type
1	B	272	ARG
1	B	296	ARG
1	B	326	GLU
1	C	66	LEU
1	C	102	VAL
1	C	119	LEU
1	C	132	LEU
1	C	181	GLN
1	C	184	ILE
1	C	213	THR
1	C	227	LYS
1	C	286	GLU
1	C	332	LYS
1	C	336	THR
1	D	79	ILE
1	D	99	THR
1	D	119	LEU
1	D	132	LEU
1	D	135	ARG
1	D	136	THR
1	D	152	ARG
1	D	169	GLU
1	D	255	LEU
1	D	286	GLU
1	D	317	ASP
1	D	338	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	209	HIS
1	A	229	GLN
1	B	104	GLN
1	B	229	GLN
1	C	229	GLN
1	D	87	HIS
1	D	181	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	D	111	1	4,7,8	17.39	1 (25%)	1,8,10	4.42	1 (100%)
1	CSD	B	111	1	4,7,8	18.51	1 (25%)	1,8,10	8.37	1 (100%)
1	CSD	A	111	1	4,7,8	17.48	1 (25%)	1,8,10	9.44	1 (100%)
1	CSD	C	111	1	4,7,8	18.10	1 (25%)	1,8,10	3.51	1 (100%)

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
1	CSD	D	111	1	-	2/2/6/8	-
1	CSD	B	111	1	-	2/2/6/8	-
1	CSD	A	111	1	-	2/2/6/8	-
1	CSD	C	111	1	-	2/2/6/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111	CSD	OD1-SG	36.97	1.81	1.47
1	C	111	CSD	OD1-SG	36.18	1.80	1.47
1	A	111	CSD	OD1-SG	34.91	1.79	1.47
1	D	111	CSD	OD1-SG	34.69	1.79	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	CSD	OD1-SG-CB	9.44	122.98	105.60
1	B	111	CSD	OD1-SG-CB	8.37	121.03	105.60
1	D	111	CSD	OD1-SG-CB	4.42	113.75	105.60
1	C	111	CSD	OD1-SG-CB	3.51	112.06	105.60

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	111	CSD	N-CA-CB-SG
1	A	111	CSD	CA-CB-SG-OD1
1	B	111	CSD	N-CA-CB-SG
1	B	111	CSD	CA-CB-SG-OD1
1	C	111	CSD	N-CA-CB-SG
1	C	111	CSD	CA-CB-SG-OD1
1	D	111	CSD	N-CA-CB-SG
1	D	111	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

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
2	5ID	B	1300	-	21,22,22	1.23	2 (9%)	28,33,33	2.45	9 (32%)
2	5ID	A	1300	-	21,22,22	1.32	3 (14%)	28,33,33	2.31	6 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	5ID	C	1300	-	21,22,22	1.28	3 (14%)	28,33,33	3.04	13 (46%)
2	5ID	D	1300	-	21,22,22	1.13	1 (4%)	28,33,33	2.30	8 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5ID	B	1300	-	-	3/6/22/22	0/3/3/3
2	5ID	A	1300	-	-	1/6/22/22	0/3/3/3
2	5ID	C	1300	-	-	3/6/22/22	0/3/3/3
2	5ID	D	1300	-	-	3/6/22/22	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1300	5ID	O4'-C1'	3.59	1.50	1.42
2	A	1300	5ID	C1'-N9	2.85	1.54	1.46
2	C	1300	5ID	C8-N9	-2.65	1.33	1.38
2	A	1300	5ID	O4'-C1'	2.64	1.48	1.42
2	A	1300	5ID	C8-N9	-2.64	1.33	1.38
2	D	1300	5ID	O4'-C1'	2.61	1.48	1.42
2	B	1300	5ID	C1'-N9	2.43	1.53	1.46
2	B	1300	5ID	C5'-C4'	2.30	1.59	1.51
2	C	1300	5ID	C1'-N9	2.30	1.52	1.46

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1300	5ID	C5-C4-N3	-9.06	117.35	126.97
2	A	1300	5ID	C5-C4-N3	-7.84	118.65	126.97
2	B	1300	5ID	C5-C4-N3	-7.62	118.89	126.97
2	D	1300	5ID	C5-C4-N3	-7.62	118.89	126.97
2	D	1300	5ID	C6-C5-C4	5.66	119.98	115.74
2	C	1300	5ID	O4'-C1'-N9	5.12	117.92	108.09
2	A	1300	5ID	C6-C5-C4	4.98	119.47	115.74
2	C	1300	5ID	O4'-C4'-C5'	4.70	119.16	109.22
2	C	1300	5ID	C6-C5-C4	4.67	119.24	115.74
2	C	1300	5ID	N3-C2-N1	-4.46	121.83	128.58
2	B	1300	5ID	C6-C5-C4	4.37	119.02	115.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1300	5ID	C2-N3-C4	4.24	122.18	111.83
2	A	1300	5ID	N3-C2-N1	-4.21	122.21	128.58
2	B	1300	5ID	O4'-C4'-C5'	3.98	117.63	109.22
2	B	1300	5ID	N3-C2-N1	-3.87	122.72	128.58
2	C	1300	5ID	N3-C4-N9	3.83	133.69	127.17
2	C	1300	5ID	C2'-C3'-C4'	-3.79	95.28	102.61
2	A	1300	5ID	C2-N3-C4	3.64	120.71	111.83
2	D	1300	5ID	N3-C2-N1	-3.45	123.35	128.58
2	B	1300	5ID	C2-N3-C4	3.41	120.16	111.83
2	C	1300	5ID	C1'-N9-C8	-3.10	122.21	125.72
2	D	1300	5ID	C2-N3-C4	3.04	119.26	111.83
2	D	1300	5ID	N3-C4-N9	3.03	132.32	127.17
2	A	1300	5ID	N3-C4-N9	3.02	132.30	127.17
2	B	1300	5ID	C3'-C2'-C1'	2.89	106.93	101.46
2	C	1300	5ID	C4'-O4'-C1'	-2.71	103.49	109.47
2	C	1300	5ID	O4'-C4'-C3'	-2.62	99.95	105.15
2	B	1300	5ID	N3-C4-N9	2.52	131.45	127.17
2	B	1300	5ID	C5'-C4'-C3'	-2.36	109.52	115.10
2	D	1300	5ID	C3'-C2'-C1'	2.32	105.85	101.46
2	D	1300	5ID	C5'-C4'-C3'	-2.30	109.67	115.10
2	A	1300	5ID	C2'-C1'-N9	-2.25	107.72	113.30
2	D	1300	5ID	O4'-C4'-C5'	2.20	113.86	109.22
2	C	1300	5ID	C2'-C1'-N9	-2.10	108.08	113.30
2	C	1300	5ID	C3'-C2'-C1'	-2.05	97.58	101.46
2	B	1300	5ID	C2-N1-C6	2.01	122.03	118.73

There are no chirality outliers.

All (10) torsion outliers are listed below:

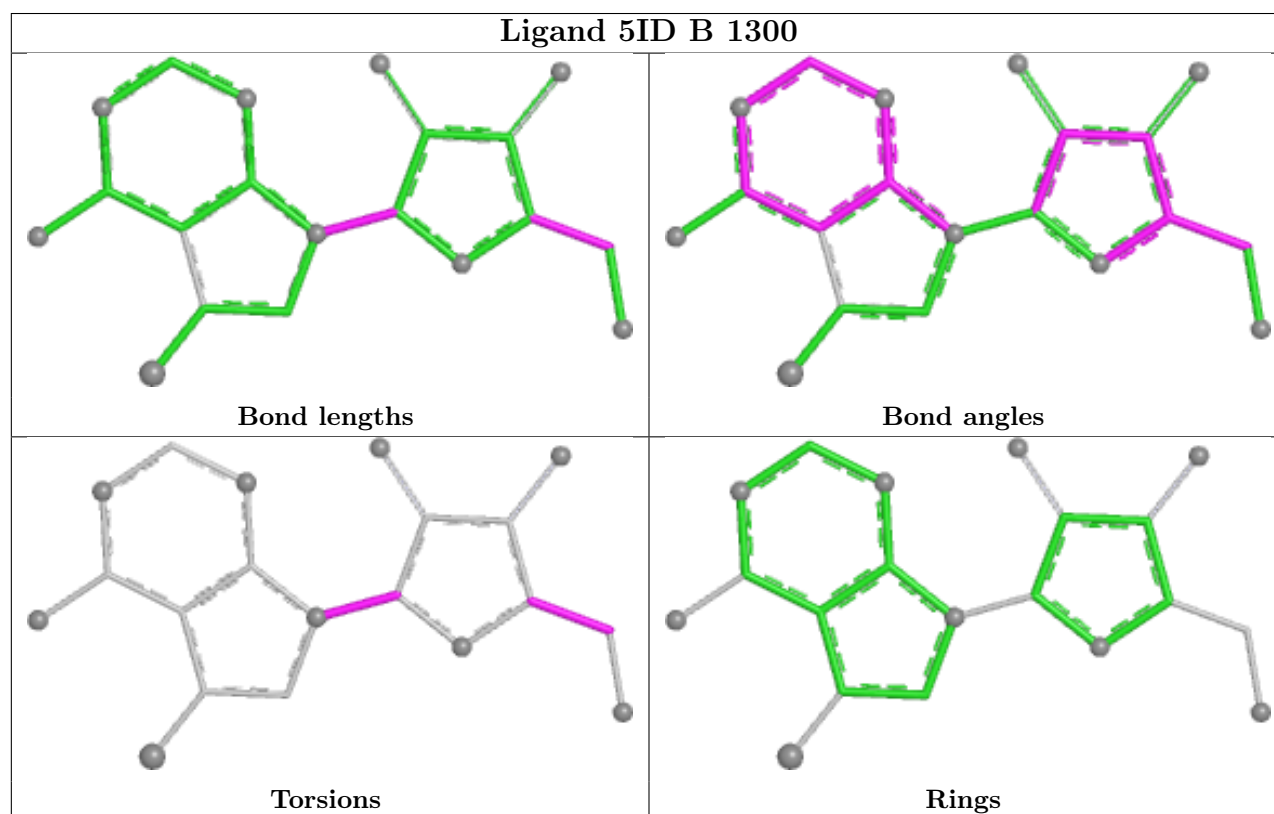
Mol	Chain	Res	Type	Atoms
2	C	1300	5ID	C2'-C1'-N9-C8
2	C	1300	5ID	C2'-C1'-N9-C4
2	B	1300	5ID	C3'-C4'-C5'-O5'
2	B	1300	5ID	O4'-C4'-C5'-O5'
2	D	1300	5ID	O4'-C4'-C5'-O5'
2	D	1300	5ID	C3'-C4'-C5'-O5'
2	B	1300	5ID	O4'-C1'-N9-C8
2	D	1300	5ID	O4'-C1'-N9-C8
2	C	1300	5ID	O4'-C4'-C5'-O5'
2	A	1300	5ID	O4'-C1'-N9-C8

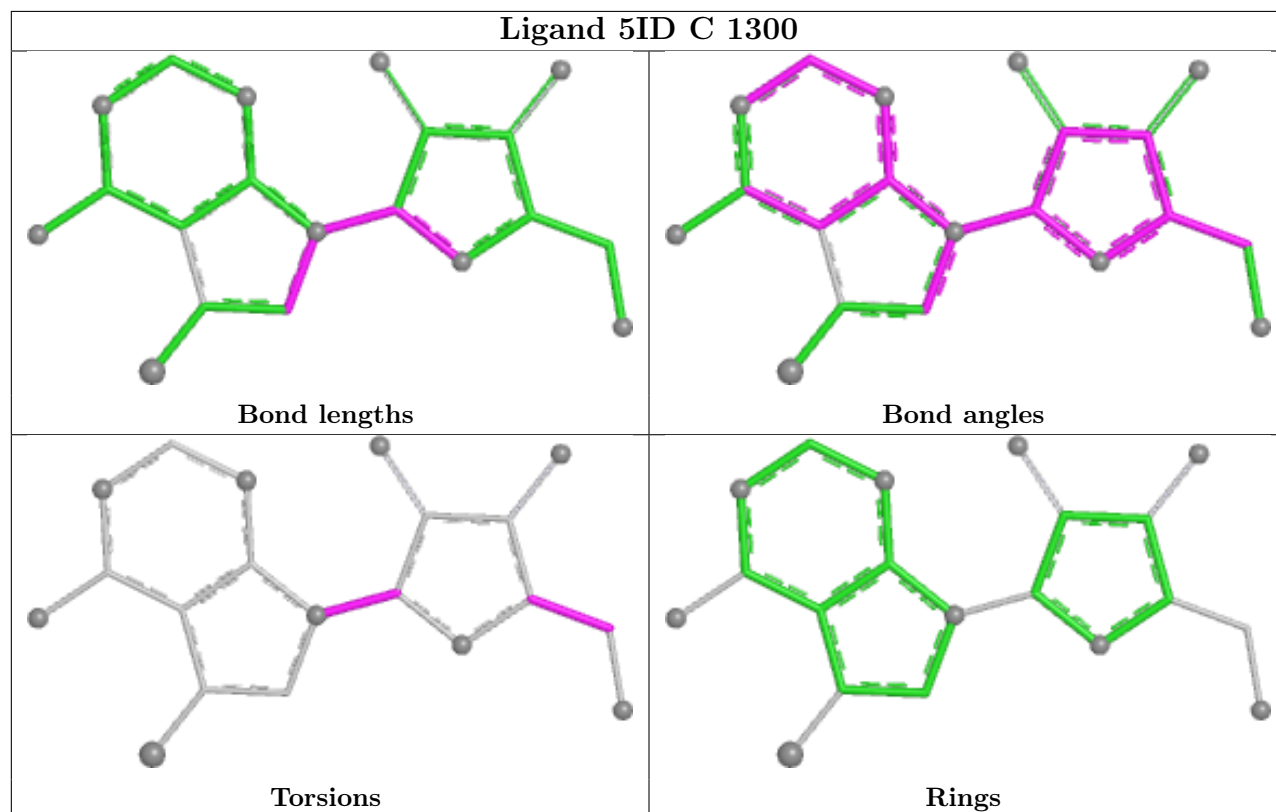
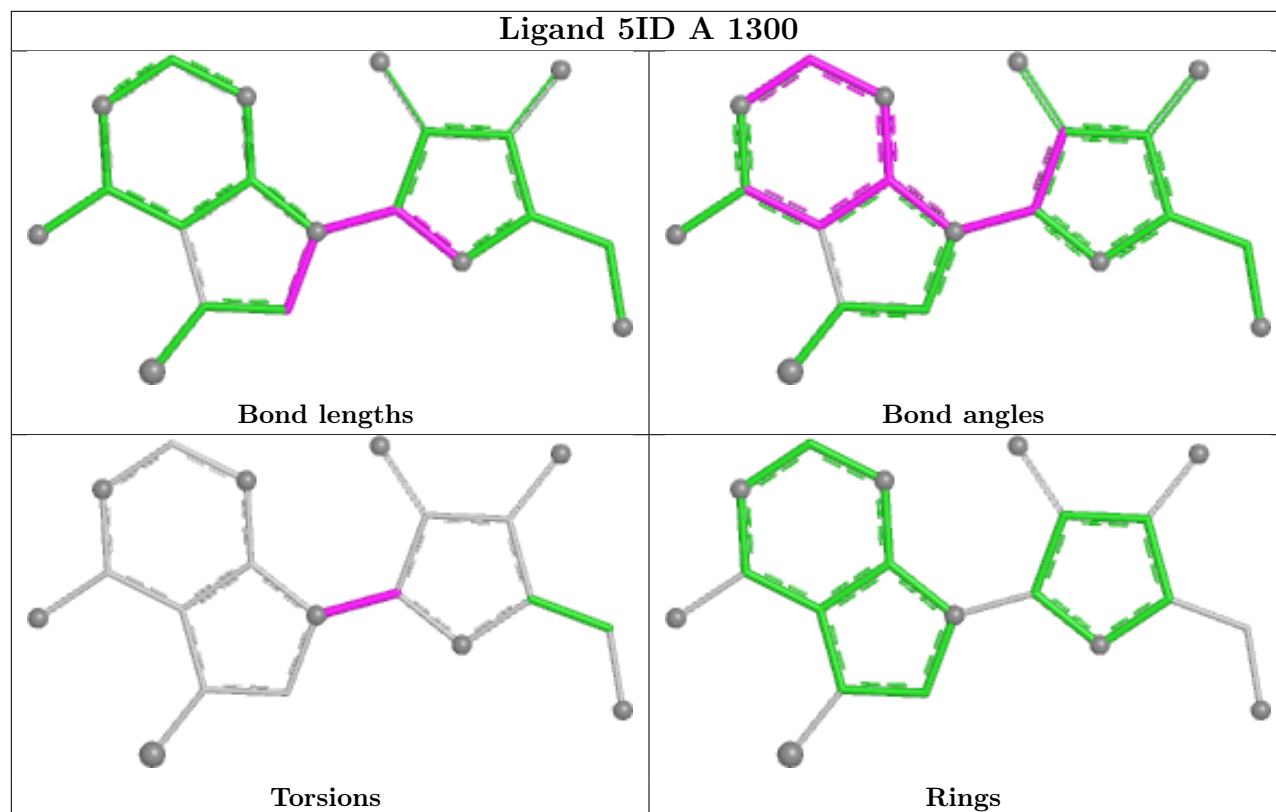
There are no ring outliers.

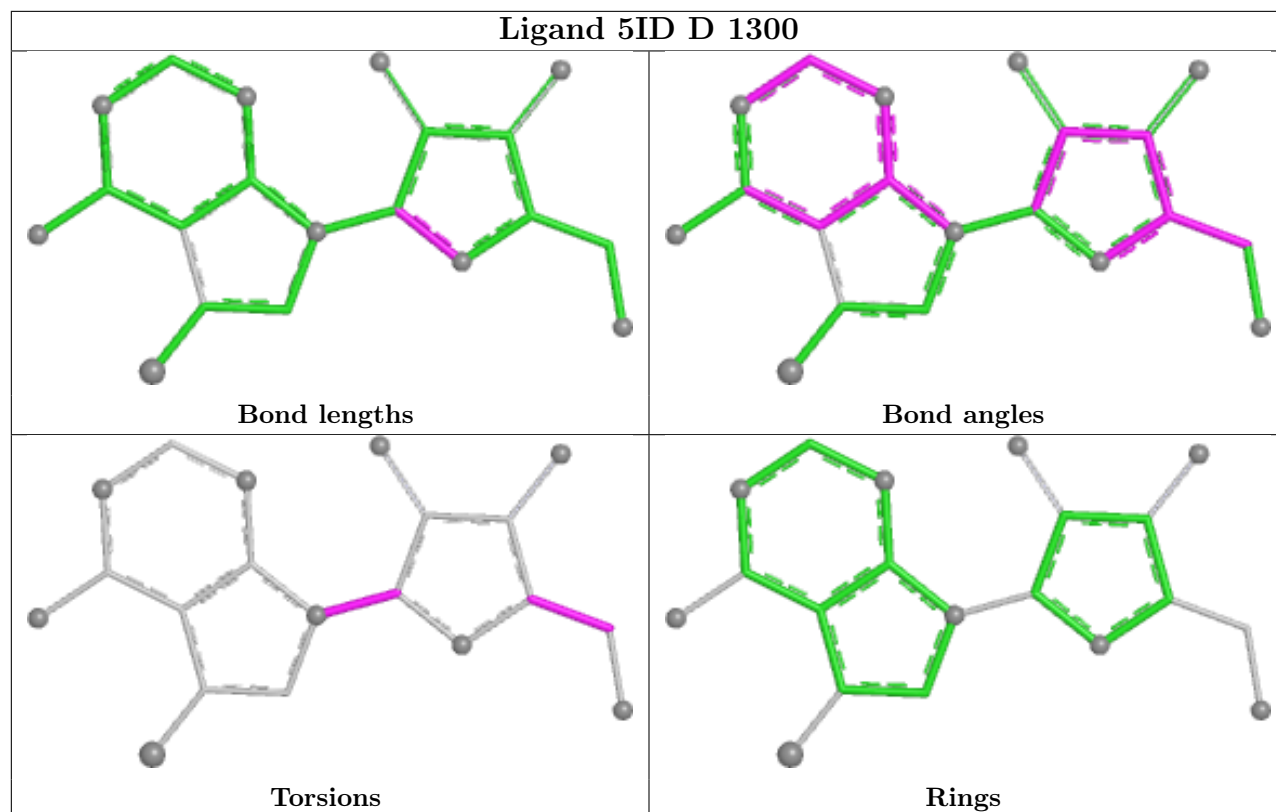
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1300	5ID	3	0
2	C	1300	5ID	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 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	288/313 (92%)	0.61	8 (2%) 55 51	33, 61, 76, 91	1 (0%)
1	B	289/313 (92%)	0.74	31 (10%) 11 8	35, 61, 76, 93	1 (0%)
1	C	282/313 (90%)	1.62	84 (29%) 1 1	51, 61, 75, 80	0
1	D	290/313 (92%)	1.41	64 (22%) 2 2	51, 61, 74, 88	0
All	All	1149/1252 (91%)	1.09	187 (16%) 4 4	33, 61, 76, 93	2 (0%)

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	338	ILE	6.9
1	B	101	GLY	5.0
1	D	197	ASP	4.5
1	C	59	GLU	4.5
1	D	200	THR	4.4
1	D	326	GLU	4.3
1	D	196	ILE	4.2
1	C	259	THR	4.2
1	A	338	ILE	4.1
1	D	337	PRO	4.0
1	A	44	PRO	3.8
1	C	136	THR	3.8
1	C	329	TRP	3.8
1	D	100	GLU	3.7
1	B	44	PRO	3.7
1	D	251	PRO	3.7
1	C	212	LEU	3.6
1	B	338	ILE	3.6
1	D	155	TYR	3.6
1	D	95	GLN	3.6
1	D	255	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	52	ILE	3.5
1	B	213	THR	3.4
1	C	335	PRO	3.4
1	C	312	PHE	3.4
1	D	58	GLY	3.4
1	C	337	PRO	3.4
1	C	221	ILE	3.4
1	C	199	GLU	3.3
1	B	102	VAL	3.3
1	C	275	PRO	3.3
1	D	323	PHE	3.3
1	D	248	GLY	3.2
1	B	104	GLN	3.2
1	C	66	LEU	3.2
1	D	334	LEU	3.2
1	C	266	LYS	3.1
1	C	76	LEU	3.1
1	D	249	SER	3.1
1	C	207	ARG	3.1
1	C	257	ALA	3.1
1	C	75	LYS	3.0
1	C	133	CYS	3.0
1	D	194	GLU	2.9
1	C	263	ARG	2.9
1	D	161	LEU	2.9
1	C	258	ASP	2.9
1	B	67	TYR	2.9
1	D	70	GLU	2.9
1	D	158	THR	2.9
1	D	202	LYS	2.9
1	A	67	TYR	2.9
1	D	195	TYR	2.9
1	D	203	HIS	2.9
1	C	130	PHE	2.9
1	C	190	GLY	2.9
1	C	211	SER	2.8
1	D	99	THR	2.8
1	D	225	LEU	2.8
1	D	201	LYS	2.8
1	D	98	ALA	2.8
1	C	166	VAL	2.8
1	D	151	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	85	GLN	2.8
1	C	214	GLY	2.8
1	D	101	GLY	2.8
1	D	192	ALA	2.8
1	C	273	ALA	2.7
1	D	283	PHE	2.7
1	C	272	ARG	2.7
1	D	281	GLU	2.7
1	C	331	GLY	2.7
1	C	145	ILE	2.7
1	C	276	ILE	2.7
1	D	335	PRO	2.7
1	C	102	VAL	2.7
1	B	122	LEU	2.7
1	D	147	ILE	2.7
1	D	198	PRO	2.7
1	D	210	LYS	2.6
1	C	95	GLN	2.6
1	C	122	LEU	2.6
1	C	213	THR	2.6
1	C	71	TYR	2.6
1	D	157	HIS	2.6
1	B	214	GLY	2.6
1	C	323	PHE	2.6
1	D	322	VAL	2.6
1	B	52	ILE	2.5
1	D	137	PHE	2.5
1	D	250	LEU	2.5
1	B	70	GLU	2.5
1	C	113	LYS	2.5
1	C	278	VAL	2.5
1	D	146	ALA	2.5
1	B	121	LEU	2.5
1	D	159	LYS	2.5
1	C	49	GLY	2.5
1	D	264	TYR	2.5
1	D	162	ILE	2.5
1	D	252	TRP	2.5
1	C	280	CYS	2.4
1	D	333	PRO	2.4
1	B	63	GLY	2.4
1	C	336	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	58	GLY	2.4
1	C	80	LYS	2.4
1	D	331	GLY	2.4
1	C	74	ILE	2.4
1	C	327	TYR	2.4
1	C	135	ARG	2.4
1	C	225	LEU	2.4
1	C	92	PHE	2.4
1	D	300	PHE	2.4
1	B	60	LEU	2.4
1	C	260	LEU	2.4
1	D	44	PRO	2.3
1	C	262	GLU	2.3
1	C	279	LEU	2.3
1	D	204	ILE	2.3
1	C	51	LYS	2.3
1	C	256	LYS	2.3
1	B	106	TYR	2.3
1	C	206	TYR	2.3
1	B	198	PRO	2.3
1	C	177	GLY	2.3
1	B	182	HIS	2.3
1	B	120	GLU	2.3
1	B	330	ALA	2.3
1	C	103	PRO	2.3
1	C	168	PRO	2.3
1	C	216	ALA	2.3
1	C	296	ARG	2.3
1	B	119	LEU	2.3
1	C	255	LEU	2.3
1	D	329	TRP	2.3
1	D	144	MET	2.3
1	C	183	ALA	2.2
1	C	254	GLY	2.2
1	C	165	ASP	2.2
1	D	306	ASP	2.2
1	D	59	GLU	2.2
1	D	154	GLU	2.2
1	C	227	LYS	2.2
1	C	268	GLY	2.2
1	D	260	LEU	2.2
1	B	100	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	50	LYS	2.2
1	C	129	LEU	2.2
1	C	300	PHE	2.2
1	C	98	ALA	2.2
1	D	273	ALA	2.2
1	C	109	GLY	2.2
1	C	267	ILE	2.2
1	A	335	PRO	2.2
1	B	75	LYS	2.2
1	D	278	VAL	2.1
1	B	62	LEU	2.1
1	D	191	LEU	2.1
1	C	67	TYR	2.1
1	C	326	GLU	2.1
1	B	103	PRO	2.1
1	B	72	VAL	2.1
1	C	174	GLY	2.1
1	C	321	PHE	2.1
1	C	222	ASN	2.1
1	B	88	LEU	2.1
1	D	207	ARG	2.1
1	C	264	TYR	2.1
1	B	337	PRO	2.1
1	D	148	GLN	2.1
1	B	98	ALA	2.1
1	A	82	ARG	2.1
1	D	327	TYR	2.1
1	D	209	HIS	2.1
1	B	59	GLU	2.0
1	C	117	MET	2.0
1	A	102	VAL	2.0
1	C	294	VAL	2.0
1	C	318	ARG	2.0
1	A	212	LEU	2.0
1	B	199	GLU	2.0
1	D	313	THR	2.0
1	A	198	PRO	2.0
1	C	298	ASP	2.0
1	C	90	TYR	2.0
1	C	93	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSD	D	111	8/9	0.84	0.15	27,35,43,54	0
1	CSD	B	111	8/9	0.85	0.12	29,35,47,51	0
1	CSD	C	111	8/9	0.88	0.14	31,34,47,53	0
1	CSD	A	111	8/9	0.88	0.13	31,35,50,55	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

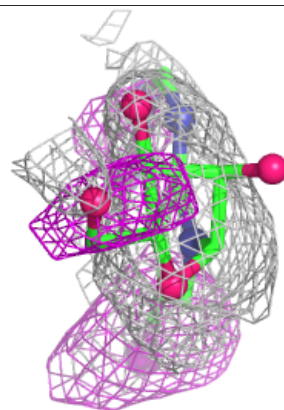
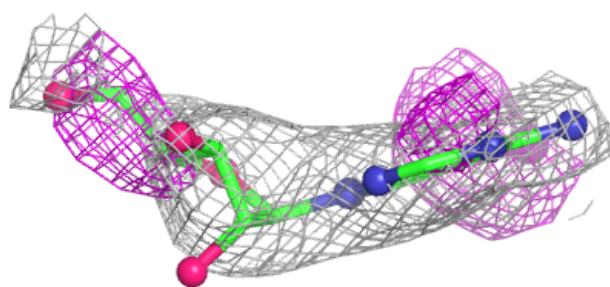
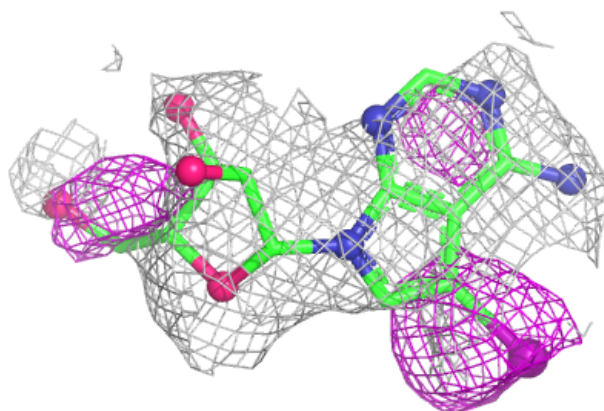
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	5ID	C	1300	20/20	0.92	0.15	79,108,127,128	0
3	MG	C	1301	1/1	0.93	0.08	33,33,33,33	0
2	5ID	A	1300	20/20	0.98	0.13	41,49,64,70	0
2	5ID	D	1300	20/20	0.98	0.13	32,55,75,83	0
3	MG	B	1301	1/1	0.98	0.09	32,32,32,32	0
2	5ID	B	1300	20/20	0.98	0.11	25,40,50,65	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.

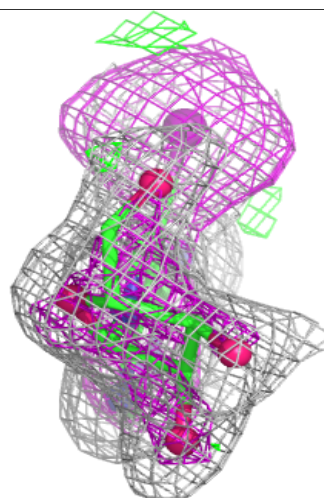
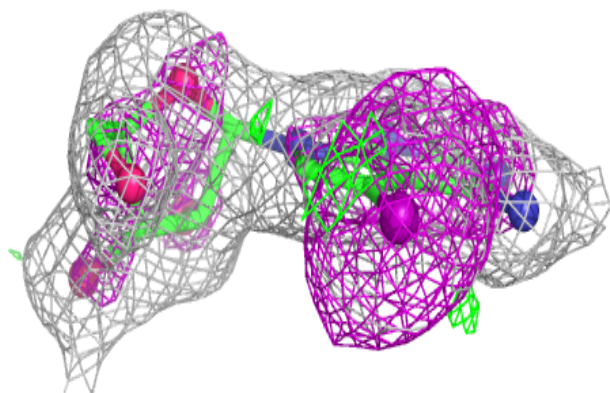
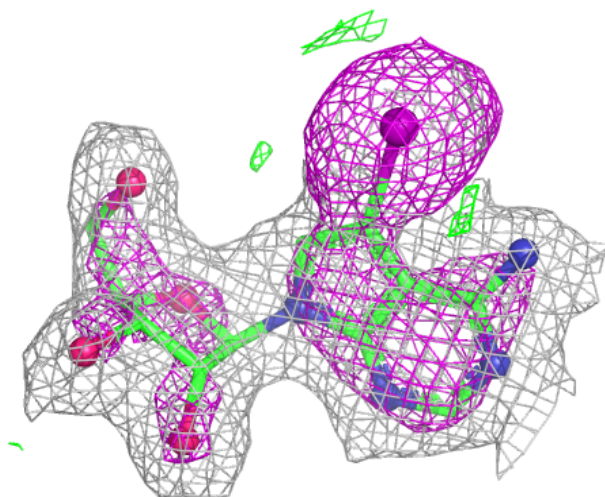
Electron density around 5ID C 1300:

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



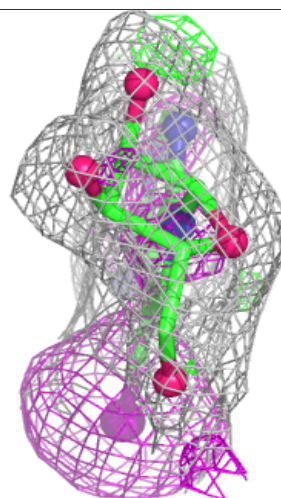
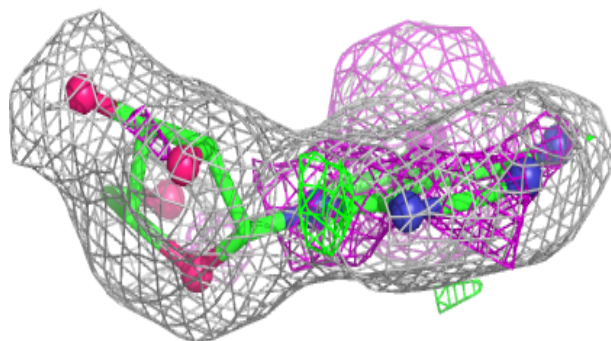
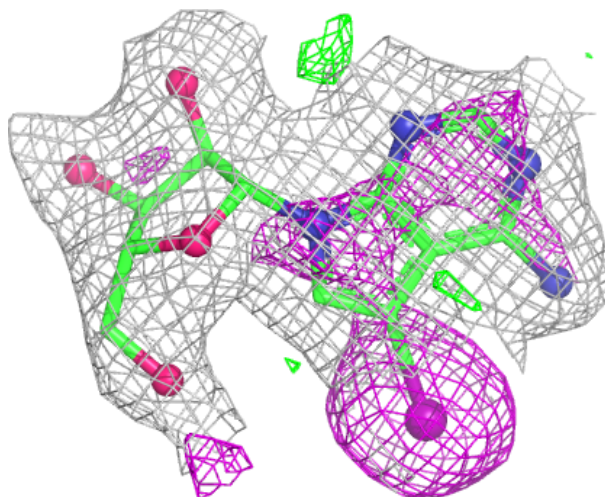
Electron density around 5ID A 1300:

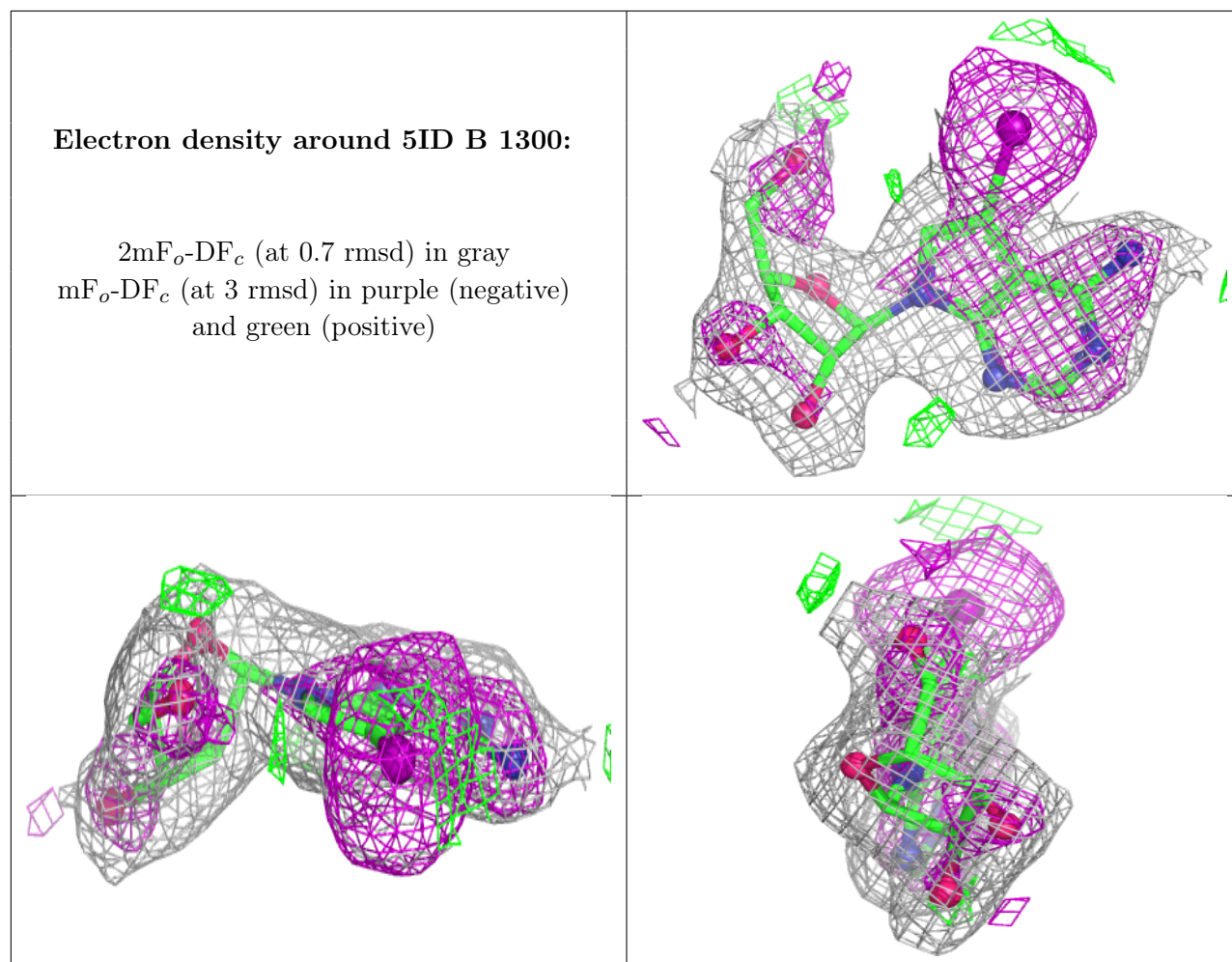
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 5ID D 1300:

$2mF_o-DF_c$ (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.