



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:44 PM UTC

PDB ID : 6ZRH / pdb_00006zrh
Title : Crystal structure of OXA-10loop24 in complex with ertapenem
Authors : Tassone, G.; Di Pisa, F.; Benvenuti, M.; De Luca, F.; Pozzi, C.; Mangani, S.;
Docquier, J.D.
Deposited on : 2020-07-13
Resolution : 1.88 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

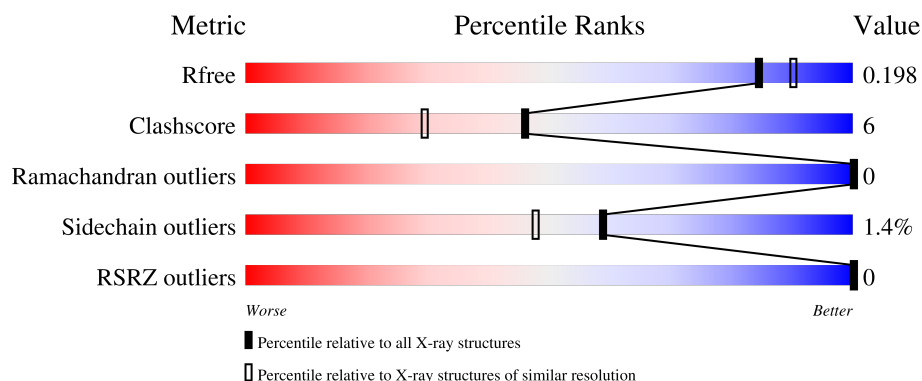
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	243	 88% 11% .
1	B	243	 86% 14%
1	C	243	 88% 11% .
1	D	243	 91% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	B	302	-	-	X	-
3	EDO	C	302	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9014 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 Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	11	0
			1960	1256	327	370	7			
1	B	243	Total	C	N	O	S	0	7	0
			1954	1253	325	369	7			
1	C	242	Total	C	N	O	S	0	4	0
			1932	1238	323	364	7			
1	D	243	Total	C	N	O	S	0	4	0
			1930	1238	318	367	7			

There are 36 discrepancies between the modelled and reference sequences:

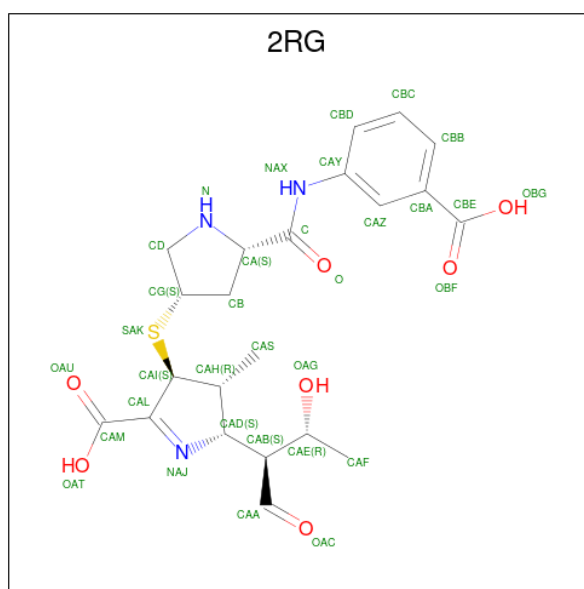
Chain	Residue	Modelled	Actual	Comment	Reference
A	208	TRP	PHE	conflict	UNP Q7BNC2
A	?	-	SER	deletion	UNP Q7BNC2
A	210	MET	VAL	conflict	UNP Q7BNC2
A	212	VAL	THR	conflict	UNP Q7BNC2
A	?	-	GLU	deletion	UNP Q7BNC2
A	?	-	SER	deletion	UNP Q7BNC2
A	213	THR	ASN	conflict	UNP Q7BNC2
A	215	GLN	GLY	conflict	UNP Q7BNC2
A	217	GLY	ALA	conflict	UNP Q7BNC2
B	208	TRP	PHE	conflict	UNP Q7BNC2
B	?	-	SER	deletion	UNP Q7BNC2
B	210	MET	VAL	conflict	UNP Q7BNC2
B	212	VAL	THR	conflict	UNP Q7BNC2
B	?	-	GLU	deletion	UNP Q7BNC2
B	?	-	SER	deletion	UNP Q7BNC2
B	213	THR	ASN	conflict	UNP Q7BNC2
B	215	GLN	GLY	conflict	UNP Q7BNC2
B	217	GLY	ALA	conflict	UNP Q7BNC2
C	208	TRP	PHE	conflict	UNP Q7BNC2
C	?	-	SER	deletion	UNP Q7BNC2
C	210	MET	VAL	conflict	UNP Q7BNC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	212	VAL	THR	conflict	UNP Q7BNC2
C	?	-	GLU	deletion	UNP Q7BNC2
C	?	-	SER	deletion	UNP Q7BNC2
C	213	THR	ASN	conflict	UNP Q7BNC2
C	215	GLN	GLY	conflict	UNP Q7BNC2
C	217	GLY	ALA	conflict	UNP Q7BNC2
D	208	TRP	PHE	conflict	UNP Q7BNC2
D	?	-	SER	deletion	UNP Q7BNC2
D	210	MET	VAL	conflict	UNP Q7BNC2
D	212	VAL	THR	conflict	UNP Q7BNC2
D	?	-	GLU	deletion	UNP Q7BNC2
D	?	-	SER	deletion	UNP Q7BNC2
D	213	THR	ASN	conflict	UNP Q7BNC2
D	215	GLN	GLY	conflict	UNP Q7BNC2
D	217	GLY	ALA	conflict	UNP Q7BNC2

- Molecule 2 is (2S,3R,4S)-4-((3S,5S)-5-[(3-carboxyphenyl)carbamoyl]pyrrolidin-3-yl)sulfany 1)-2-[(1S,2R)-1-formyl-2-hydroxypropyl]-3-methyl-3,4-dihydro-2H-pyrrole-5-carboxylic acid (CCD ID: 2RG) (formula: C₂₂H₂₇N₃O₇S) (labeled as "Ligand of Interest" by depositor).



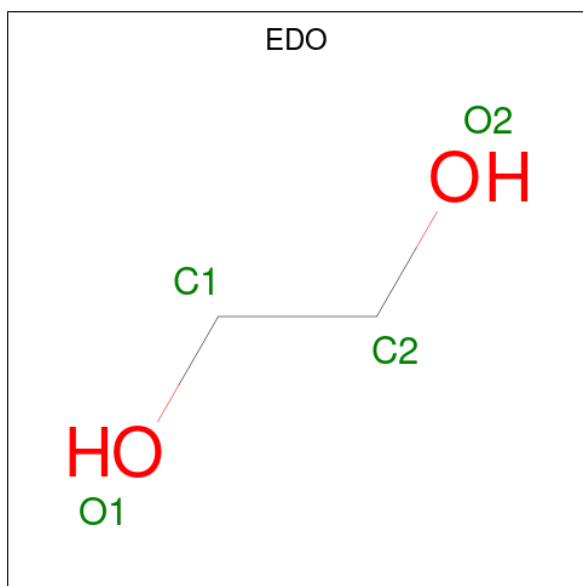
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			17	11	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			17	11	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			33	22	3	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	S	0	0
			33	22	3	7	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	246	Total O 247 247	0	2
4	B	251	Total O 254 254	0	4
4	C	298	Total O 301 301	0	5
4	D	276	Total O 280 280	0	6

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.

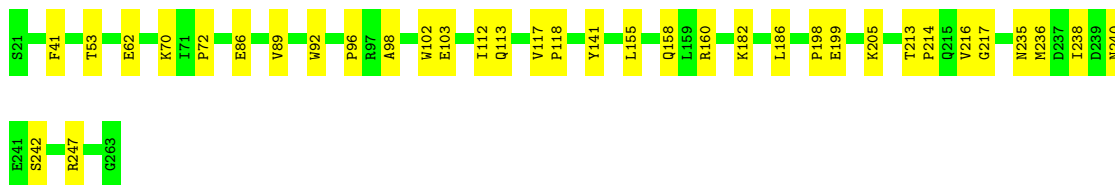
- Molecule 1: Beta-lactamase

Chain A: 



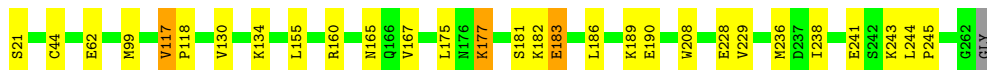
- Molecule 1: Beta-lactamase

Chain B: 



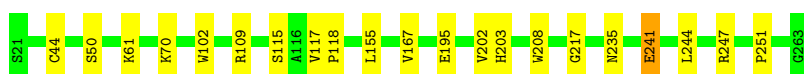
- Molecule 1: Beta-lactamase

Chain C: 



- Molecule 1: Beta-lactamase

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	80.93Å 80.93Å 152.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.73 – 1.88 35.73 – 1.88	Depositor EDS
% Data completeness (in resolution range)	91.1 (35.73-1.88) 91.1 (35.73-1.88)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.167 , 0.198 0.168 , 0.198	Depositor DCC
R_{free} test set	4204 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l 0.477 for h,-h-k,-l 0.023 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9014	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: KCX, 2RG, EDO

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	0.63	0/2010	1.11	3/2722 (0.1%)
1	B	0.66	0/1996	1.16	4/2699 (0.1%)
1	C	0.67	0/1970	1.09	3/2664 (0.1%)
1	D	0.69	2/1971 (0.1%)	1.10	1/2668 (0.0%)
All	All	0.66	2/7947 (0.0%)	1.12	11/10753 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	203	HIS	CE1-NE2	5.84	1.38	1.32
1	D	109	ARG	C-O	-5.34	1.17	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	VAL	CA-C-N	-7.23	117.05	122.33
1	A	216	VAL	C-N-CA	-7.23	117.05	122.33
1	A	26	THR	CB-CA-C	-6.68	99.32	110.68
1	D	241	GLU	CB-CG-CD	6.33	123.36	112.60
1	B	216	VAL	CA-C-N	-6.17	117.82	122.33
1	B	216	VAL	C-N-CA	-6.17	117.82	122.33
1	B	247	ARG	CB-CA-C	-6.16	100.57	110.79
1	C	117	VAL	CB-CA-C	-5.61	108.37	113.70
1	C	117	VAL	N-CA-CB	5.54	114.23	110.52
1	B	247	ARG	CB-CG-CD	-5.46	98.73	111.30
1	C	165	ASN	CA-CB-CG	5.08	117.68	112.60

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	1960	0	1924	16	0
1	B	1954	0	1916	28	0
1	C	1932	0	1913	26	0
1	D	1930	0	1898	16	0
2	A	17	0	12	2	0
2	B	17	0	12	2	0
2	C	33	0	24	9	0
2	D	33	0	24	7	0
3	A	4	0	6	0	0
3	B	8	0	12	7	0
3	C	24	0	36	4	0
3	D	20	0	30	0	0
4	A	247	0	0	4	0
4	B	254	0	0	6	0
4	C	301	0	0	4	0
4	D	280	0	0	2	0
All	All	9014	0	7807	92	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 6.

All (92) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:THR:HG22	4:B:582:HOH:O	1.59	1.03
1:B:182[A]:LYS:HE3	4:B:573:HOH:O	1.63	0.97
1:D:208:TRP:CH2	1:D:241:GLU:HG3	2.03	0.94
1:C:208:TRP:CH2	1:C:241:GLU:HG2	2.05	0.91
3:B:302:EDO:H12	4:B:412:HOH:O	1.83	0.79
1:C:183[A]:GLU:CD	1:C:183[A]:GLU:H	1.92	0.77
1:A:101:GLN:HB2	4:A:455:HOH:O	1.88	0.74
1:C:243:LYS:HE3	4:C:545:HOH:O	1.91	0.70
1:C:175:LEU:CD1	1:C:177:LYS:HE2	2.23	0.69
1:C:190:GLU:HB3	3:C:302:EDO:H12	1.77	0.67
1:C:99:MET:HE1	2:C:301:2RG:HD	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:302:EDO:H21	4:B:466:HOH:O	1.98	0.62
1:C:175:LEU:HD12	1:C:177:LYS:HE2	1.80	0.61
1:A:236:MET:HE2	1:A:238:ILE:HD13	1.81	0.61
1:D:117[B]:VAL:HG22	1:D:118:PRO:HD3	1.81	0.61
1:A:176:ASN:ND2	1:A:182[A]:LYS:HE3	2.16	0.61
1:B:86[B]:GLU:OE2	1:C:186:LEU:HD21	2.00	0.60
1:D:102:TRP:CH2	1:D:117[A]:VAL:HG23	2.35	0.60
1:D:117[B]:VAL:CG1	2:D:301:2RG:HAE	2.32	0.60
2:D:301:2RG:OAU	2:D:301:2RG:HDA	2.01	0.60
1:C:190:GLU:CB	3:C:302:EDO:H12	2.32	0.58
1:B:86[B]:GLU:OE2	1:C:182:LYS:HE3	2.04	0.58
1:B:155:LEU:HD22	2:B:301:2RG:HAF	1.86	0.58
1:A:198:PRO:HD2	4:A:479:HOH:O	2.04	0.57
1:C:155:LEU:CD2	2:C:301:2RG:HAF	2.36	0.56
2:C:301:2RG:HASB	2:C:301:2RG:OAG	2.06	0.55
1:A:182[A]:LYS:HD3	4:D:640:HOH:O	2.07	0.54
1:B:89:VAL:HG11	3:B:303:EDO:H21	1.88	0.54
1:B:205:LYS:HA	3:B:302:EDO:H22	1.87	0.54
1:C:241:GLU:HG3	4:C:602:HOH:O	2.07	0.54
1:B:158:GLN:HG2	4:B:502:HOH:O	2.08	0.54
1:B:96:PRO:HA	1:B:103:GLU:OE2	2.09	0.53
1:D:44:CYS:SG	1:D:167:VAL:HG11	2.48	0.53
1:B:240:ASN:OD1	1:B:242:SER:HB2	2.08	0.53
1:D:208:TRP:HH2	1:D:241:GLU:HG3	1.69	0.53
1:C:236:MET:HE2	1:C:238:ILE:HD13	1.91	0.53
2:C:301:2RG:HB	4:C:583:HOH:O	2.10	0.50
1:D:195[B]:GLU:HB2	1:D:202:VAL:HB	1.93	0.50
1:A:72:PRO:HG3	1:A:141:TYR:CE1	2.46	0.50
1:A:244:LEU:HD22	1:A:247:ARG:HD3	1.93	0.49
1:B:213:THR:HA	1:B:214:PRO:C	2.37	0.49
1:D:155:LEU:CD2	2:D:301:2RG:HAF	2.42	0.49
1:C:44:CYS:SG	1:C:167:VAL:HG11	2.52	0.49
1:A:96:PRO:HA	1:A:103:GLU:OE1	2.12	0.48
1:C:117:VAL:CG2	2:C:301:2RG:HAE	2.43	0.48
1:B:112:ILE:O	1:B:205:LYS:HE2	2.14	0.48
1:A:35:GLU:HB2	4:A:530:HOH:O	2.14	0.48
1:A:256:GLU:HG3	1:A:261[A]:ILE:HG13	1.97	0.47
1:A:122:GLN:OE1	1:A:125[B]:ARG:NH2	2.37	0.47
1:B:102:TRP:CH2	1:B:117:VAL:HG23	2.49	0.47
1:B:113:GLN:HA	3:B:302:EDO:H11	1.97	0.46
1:C:117:VAL:N	1:C:118:PRO:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:TRP:CE3	1:D:244:LEU:HD11	2.51	0.46
1:A:155:LEU:CD2	2:A:301:2RG:HAF	2.46	0.46
2:D:301:2RG:NAJ	4:D:402:HOH:O	2.36	0.45
1:B:198:PRO:CB	2:C:301:2RG:HBC	2.46	0.45
1:B:236:MET:HE2	1:B:238:ILE:HD13	1.98	0.45
1:C:228:GLU:HG3	1:C:229:VAL:N	2.31	0.45
1:A:155:LEU:HD22	2:A:301:2RG:HAF	1.99	0.45
1:C:130:VAL:O	1:C:134:LYS:HG3	2.16	0.45
1:B:72:PRO:HG3	1:B:141:TYR:CE1	2.51	0.45
1:B:117:VAL:N	1:B:118:PRO:HD2	2.31	0.45
1:B:155:LEU:CD2	2:B:301:2RG:HAF	2.45	0.45
1:D:117[B]:VAL:HG12	2:D:301:2RG:HAE	1.99	0.45
3:B:302:EDO:C2	4:B:466:HOH:O	2.61	0.45
1:D:247:ARG:O	1:D:251:PRO:HG2	2.17	0.45
1:A:137:LYS:HB2	4:A:476:HOH:O	2.16	0.45
2:C:301:2RG:CAM	2:C:301:2RG:HG	2.47	0.45
1:C:117:VAL:HG22	2:C:301:2RG:HAE	1.99	0.44
1:D:155:LEU:HD21	2:D:301:2RG:HAF	2.00	0.44
1:C:244:LEU:N	1:C:245:PRO:CD	2.80	0.44
1:C:189:LYS:NZ	4:C:402[B]:HOH:O	2.26	0.43
1:B:217:GLY:O	1:B:235:ASN:HA	2.18	0.43
1:D:117[B]:VAL:CG2	1:D:118:PRO:HD3	2.45	0.43
1:B:98:ALA:HB3	1:B:102:TRP:CZ3	2.53	0.43
1:B:198:PRO:HD2	1:B:199:GLU:OE1	2.19	0.43
1:A:117:VAL:N	1:A:118:PRO:HD2	2.34	0.43
1:B:186:LEU:HD23	3:C:302:EDO:H22	2.01	0.42
1:B:198:PRO:HB2	2:C:301:2RG:CBC	2.47	0.42
1:B:41:PHE:O	1:B:53:THR:HA	2.19	0.42
1:B:62:GLU:HB3	1:B:160:ARG:HB3	2.02	0.42
1:D:117[B]:VAL:CG1	2:D:301:2RG:CAE	2.98	0.41
1:B:92:TRP:CH2	1:B:103:GLU:HB3	2.56	0.41
1:B:89:VAL:HG11	3:B:303:EDO:C2	2.50	0.41
1:C:190:GLU:OE1	3:C:302:EDO:H21	2.21	0.41
1:D:117[A]:VAL:HB	1:D:118:PRO:HD3	2.03	0.41
1:A:217:GLY:O	1:A:235:ASN:HA	2.21	0.41
1:C:62:GLU:HB3	1:C:160:ARG:HB3	2.03	0.41
1:C:181:SER:HB2	1:C:183[A]:GLU:OE1	2.20	0.40
1:D:217:GLY:O	1:D:235:ASN:HA	2.21	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	249/243 (102%)	242 (97%)	7 (3%)	0	100	100
1	B	246/243 (101%)	237 (96%)	9 (4%)	0	100	100
1	C	242/243 (100%)	234 (97%)	8 (3%)	0	100	100
1	D	244/243 (100%)	234 (96%)	10 (4%)	0	100	100
All	All	981/972 (101%)	947 (96%)	34 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	209/207 (101%)	204 (98%)	5 (2%)	43	27
1	B	206/207 (100%)	206 (100%)	0	100	100
1	C	207/207 (100%)	203 (98%)	4 (2%)	50	36
1	D	205/207 (99%)	202 (98%)	3 (2%)	57	46
All	All	827/828 (100%)	815 (98%)	12 (2%)	59	46

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	THR
1	A	33	SER

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Mol	Chain	Res	Type
1	A	115	SER
1	A	152	LYS
1	A	244	LEU
1	C	21	SER
1	C	177	LYS
1	C	183[A]	GLU
1	C	183[B]	GLU
1	D	50	SER
1	D	61	LYS
1	D	115	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	GLN
1	B	25	ASN
1	B	38	ASN
1	D	87	HIS

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	KCX	C	70	1	10,11,12	0.76	0	6,12,14	0.56	0
1	KCX	B	70	1	10,11,12	2.22	2 (20%)	6,12,14	2.33	1 (16%)
1	KCX	A	70	1	10,11,12	1.09	1 (10%)	6,12,14	0.70	0
1	KCX	D	70	1	10,11,12	1.78	2 (20%)	6,12,14	3.21	1 (16%)

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	KCX	C	70	1	-	0/9/10/12	-
1	KCX	B	70	1	-	0/9/10/12	-
1	KCX	A	70	1	-	1/9/10/12	-
1	KCX	D	70	1	-	0/9/10/12	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	70	KCX	OQ1-CX	6.42	1.33	1.21
1	D	70	KCX	OQ1-CX	4.56	1.30	1.21
1	A	70	KCX	CX-NZ	3.22	1.40	1.35
1	D	70	KCX	CX-NZ	2.55	1.39	1.35
1	B	70	KCX	CX-NZ	2.10	1.38	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	70	KCX	OQ1-CX-NZ	-7.82	113.04	124.92
1	B	70	KCX	OQ1-CX-NZ	-5.63	116.37	124.92

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	70	KCX	C-CA-CB-CG

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](#)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	2RG	B	301	1	15,17,35	1.77	4 (26%)	8,24,50	2.26	3 (37%)
3	EDO	C	303	-	3,3,3	0.49	0	2,2,2	0.49	0
3	EDO	C	306	-	3,3,3	0.23	0	2,2,2	0.82	0
3	EDO	C	302	-	3,3,3	0.55	0	2,2,2	0.92	0
3	EDO	C	304	-	3,3,3	0.18	0	2,2,2	0.49	0
2	2RG	A	301	1	15,17,35	1.55	2 (13%)	8,24,50	2.09	3 (37%)
3	EDO	D	303	-	3,3,3	0.55	0	2,2,2	0.77	0
3	EDO	D	302	-	3,3,3	0.21	0	2,2,2	0.68	0
3	EDO	C	307	-	3,3,3	0.22	0	2,2,2	0.41	0
3	EDO	D	305	-	3,3,3	0.17	0	2,2,2	0.95	0
3	EDO	C	305	-	3,3,3	0.43	0	2,2,2	0.98	0
2	2RG	D	301	1	32,35,35	0.94	4 (12%)	27,50,50	0.87	1 (3%)
3	EDO	D	304	-	3,3,3	0.12	0	2,2,2	0.29	0
2	2RG	C	301	1	32,35,35	1.11	4 (12%)	27,50,50	0.86	1 (3%)
3	EDO	B	303	-	3,3,3	0.14	0	2,2,2	0.28	0
3	EDO	D	306	-	3,3,3	0.28	0	2,2,2	0.13	0
3	EDO	A	302	-	3,3,3	0.41	0	2,2,2	0.59	0
3	EDO	B	302	-	3,3,3	0.26	0	2,2,2	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2RG	B	301	1	-	0/12/32/55	0/1/1/3
3	EDO	C	303	-	-	0/1/1/1	-
3	EDO	C	306	-	-	0/1/1/1	-
3	EDO	C	302	-	-	1/1/1/1	-
3	EDO	C	304	-	-	0/1/1/1	-
2	2RG	A	301	1	-	0/12/32/55	0/1/1/3
3	EDO	D	303	-	-	0/1/1/1	-
3	EDO	D	302	-	-	0/1/1/1	-
3	EDO	C	307	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	305	-	-	1/1/1/1	-
3	EDO	C	305	-	-	1/1/1/1	-
2	2RG	D	301	1	-	3/26/55/55	0/3/3/3
3	EDO	D	304	-	-	0/1/1/1	-
2	2RG	C	301	1	-	1/26/55/55	0/3/3/3
3	EDO	B	303	-	-	0/1/1/1	-
3	EDO	D	306	-	-	1/1/1/1	-
3	EDO	A	302	-	-	0/1/1/1	-
3	EDO	B	302	-	-	1/1/1/1	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	2RG	CAI-SAK	4.68	1.87	1.82
2	A	301	2RG	CAI-SAK	4.55	1.86	1.82
2	C	301	2RG	CAD-NAJ	3.63	1.51	1.47
2	C	301	2RG	CAL-NAJ	3.13	1.30	1.28
2	B	301	2RG	CAM-CAL	2.66	1.53	1.48
2	B	301	2RG	CAD-NAJ	2.47	1.50	1.47
2	A	301	2RG	OAT-CAM	-2.38	1.24	1.30
2	D	301	2RG	OAT-CAM	-2.37	1.24	1.30
2	C	301	2RG	OAT-CAM	-2.33	1.24	1.30
2	D	301	2RG	CAM-CAL	2.28	1.52	1.48
2	D	301	2RG	CAL-NAJ	2.26	1.30	1.28
2	B	301	2RG	OAT-CAM	-2.25	1.24	1.30
2	D	301	2RG	CAD-NAJ	2.18	1.50	1.47
2	C	301	2RG	CAI-CAH	-2.01	1.53	1.55

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	2RG	CG-SAK-CAI	4.21	109.94	102.36
2	B	301	2RG	CG-SAK-CAI	4.00	109.56	102.36
2	D	301	2RG	OAC-CAA-CAB	-3.31	117.36	125.27
2	B	301	2RG	OAC-CAA-CAB	-3.10	117.88	125.27
2	B	301	2RG	OAU-CAM-CAL	-3.06	117.02	121.13
2	C	301	2RG	OAC-CAA-CAB	-3.02	118.07	125.27
2	A	301	2RG	OAC-CAA-CAB	-2.73	118.75	125.27
2	A	301	2RG	CAB-CAD-NAJ	-2.25	107.76	111.95

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	2RG	CA-C-NAX-CAY
2	D	301	2RG	O-C-NAX-CAY
3	B	302	EDO	O1-C1-C2-O2
3	C	305	EDO	O1-C1-C2-O2
2	C	301	2RG	CAH-CAI-SAK-CG
2	D	301	2RG	CAH-CAI-SAK-CG
3	D	306	EDO	O1-C1-C2-O2
3	D	305	EDO	O1-C1-C2-O2
3	C	302	EDO	O1-C1-C2-O2

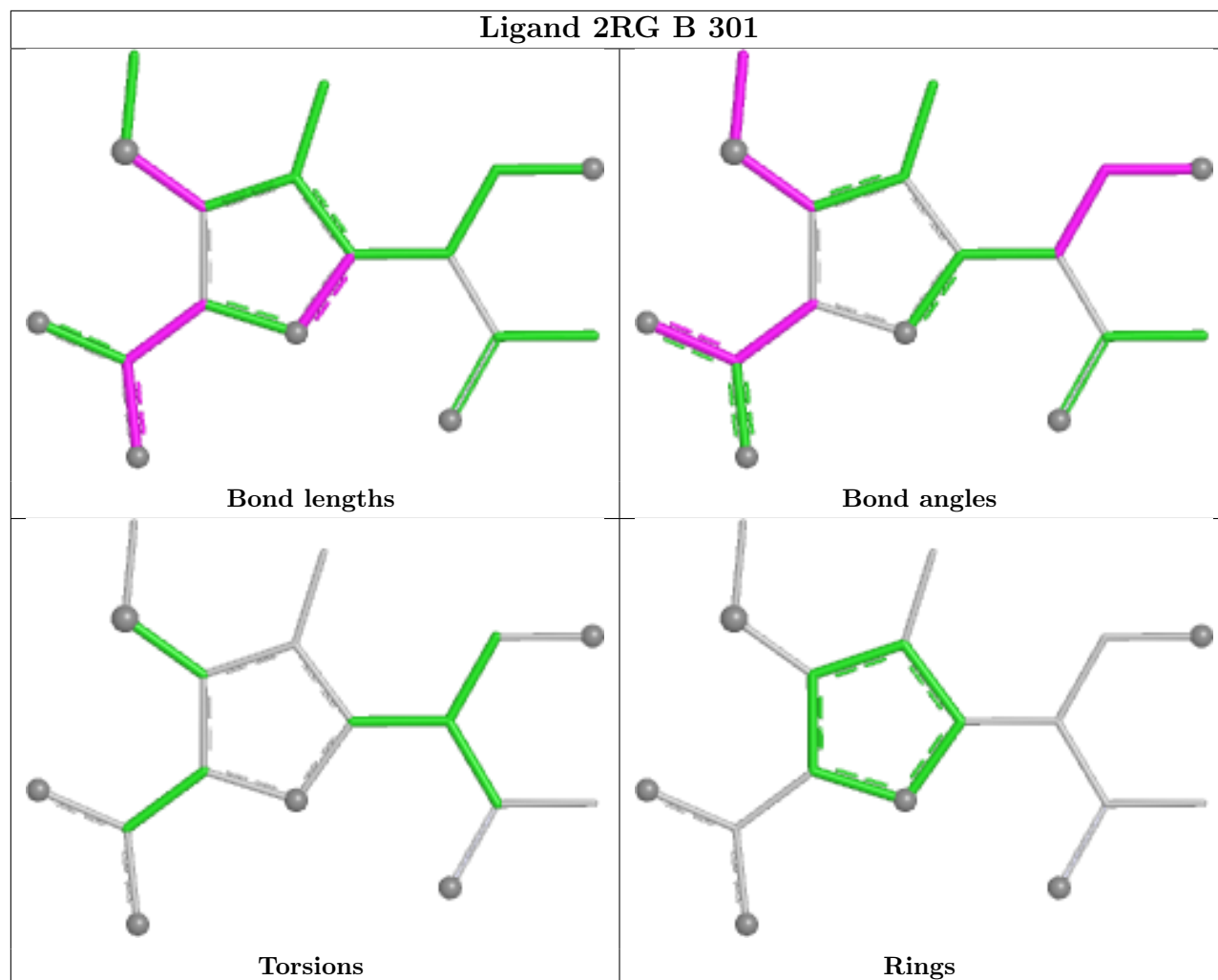
There are no ring outliers.

7 monomers are involved in 31 short contacts:

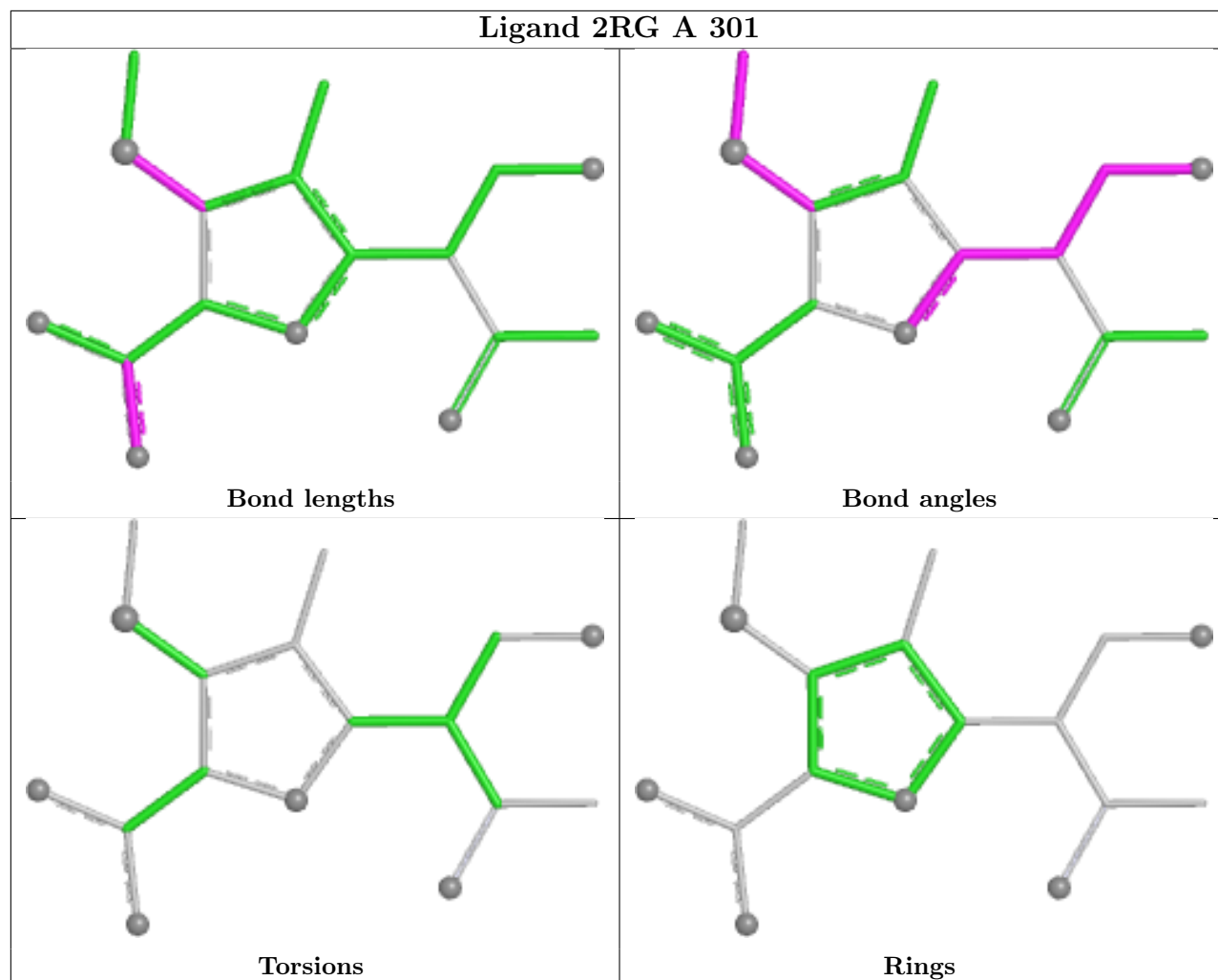
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	2RG	2	0
3	C	302	EDO	4	0
2	A	301	2RG	2	0
2	D	301	2RG	7	0
2	C	301	2RG	9	0
3	B	303	EDO	2	0
3	B	302	EDO	5	0

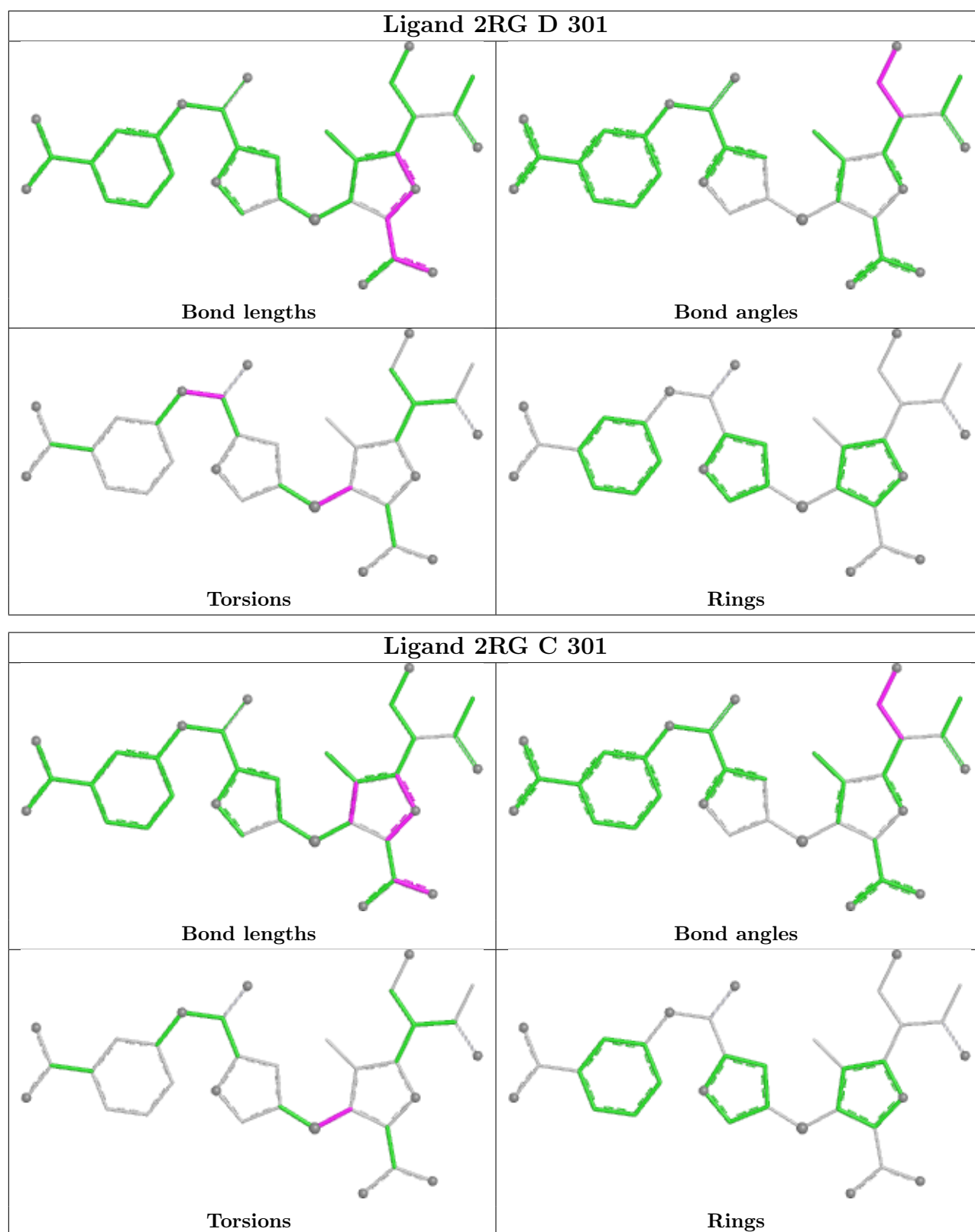
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand 2RG B 301



Ligand 2RG A 301





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	241/243 (99%)	-1.54	0 100 100	7, 16, 35, 47	14 (5%)
1	B	242/243 (99%)	-1.54	0 100 100	7, 17, 37, 50	10 (4%)
1	C	241/243 (99%)	-1.62	0 100 100	8, 16, 29, 43	8 (3%)
1	D	242/243 (99%)	-1.61	0 100 100	9, 16, 31, 48	6 (2%)
All	All	966/972 (99%)	-1.58	0 100 100	7, 16, 35, 50	38 (3%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
1	KCX	A	70	12/13	0.99	0.02	10,12,19,21	0
1	KCX	B	70	12/13	0.99	0.02	9,12,21,22	0
1	KCX	C	70	12/13	0.99	0.02	10,11,13,14	0
1	KCX	D	70	12/13	1.00	0.02	9,10,13,15	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

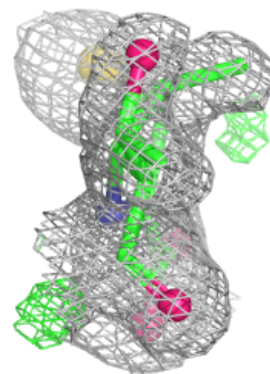
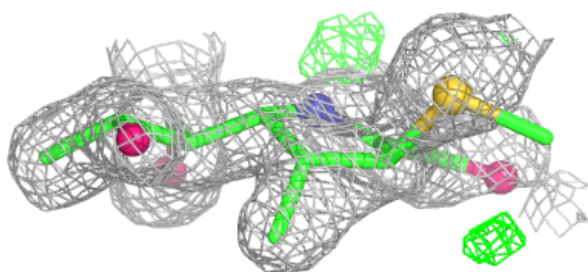
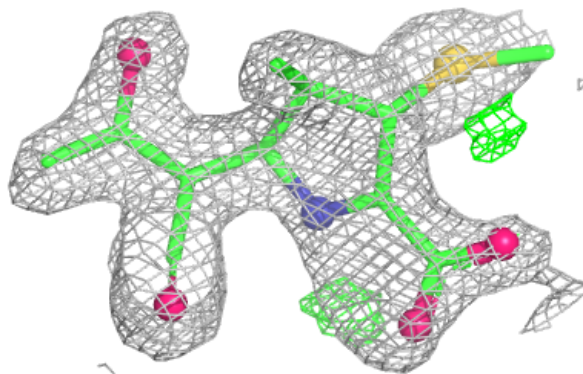
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	2RG	A	301	17/33	0.98	0.06	17,40,63,74	0
2	2RG	B	301	17/33	0.98	0.06	17,39,61,71	0
2	2RG	C	301	33/33	0.99	0.05	19,42,69,72	0
2	2RG	D	301	33/33	0.99	0.05	16,39,83,88	0
3	EDO	A	302	4/4	0.99	0.03	25,35,39,52	0
3	EDO	B	302	4/4	0.99	0.04	31,32,34,42	0
3	EDO	B	303	4/4	0.99	0.05	32,35,37,39	0
3	EDO	C	302	4/4	0.99	0.06	23,26,29,30	0
3	EDO	C	303	4/4	0.99	0.04	24,31,34,45	0
3	EDO	C	304	4/4	0.99	0.03	22,23,25,26	0
3	EDO	C	305	4/4	0.99	0.04	29,29,36,37	0
3	EDO	C	306	4/4	0.99	0.05	21,27,32,42	0
3	EDO	C	307	4/4	0.99	0.04	33,35,36,39	0
3	EDO	D	302	4/4	0.99	0.05	20,23,30,37	0
3	EDO	D	303	4/4	0.99	0.05	22,32,37,50	0
3	EDO	D	304	4/4	0.99	0.04	30,41,44,50	0
3	EDO	D	305	4/4	0.99	0.04	32,36,37,38	0
3	EDO	D	306	4/4	0.99	0.04	38,41,43,46	0

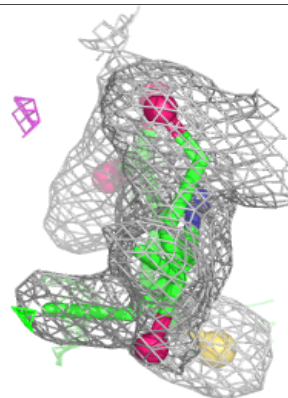
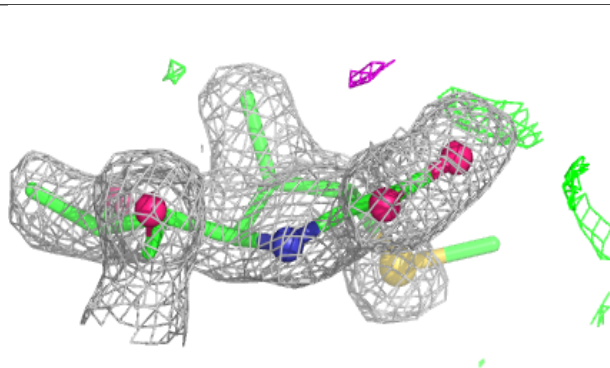
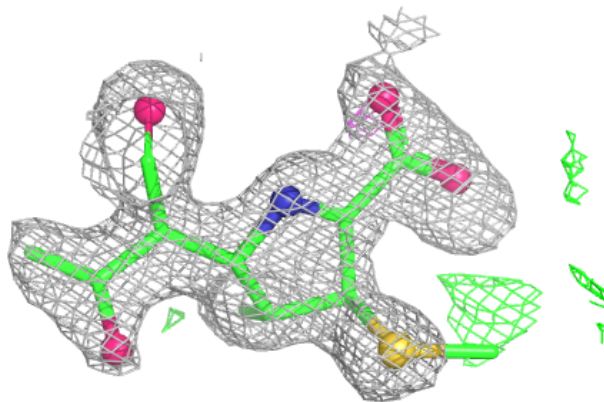
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2RG A 301:

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

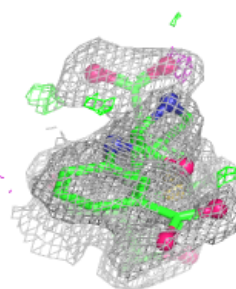
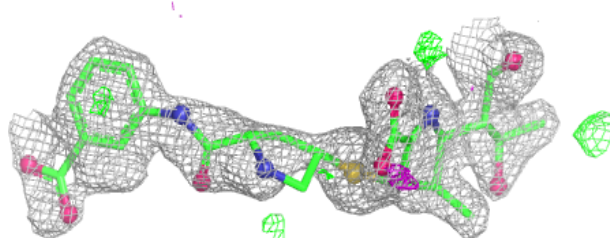
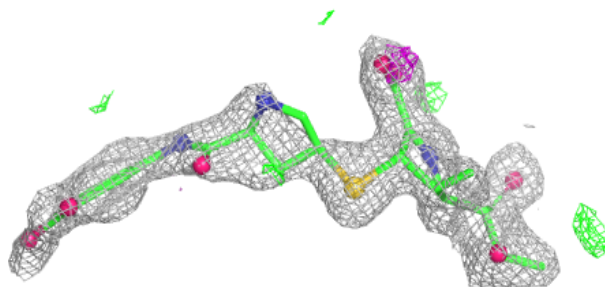
**Electron density around 2RG B 301:**

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

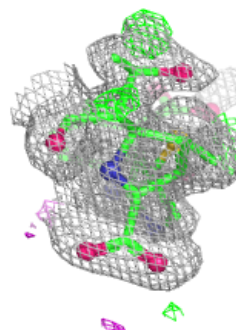
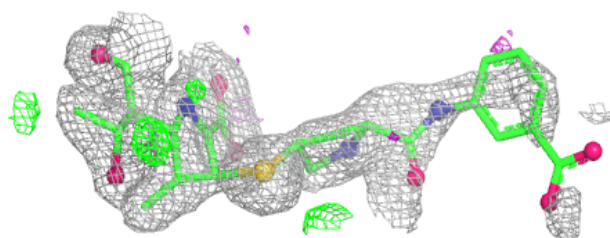
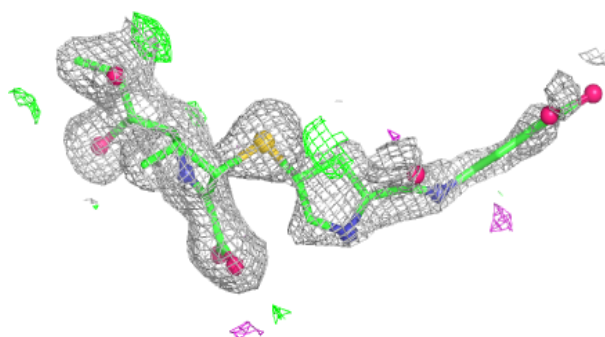


Electron density around 2RG C 301:

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

**Electron density around 2RG D 301:**

$2mF_o-DF_c$ (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.