



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:28 AM UTC

PDB ID : 2O3R / pdb_00002o3r
Title : Structural Basis for Formation and Hydrolysis of Calcium Messenger Cyclic ADP-ribose by Human CD38
Authors : Liu, Q.; Kriksunov, I.A.; Graeff, R.; Lee, H.C.; Hao, Q.
Deposited on : 2006-12-01
Resolution : 1.75 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

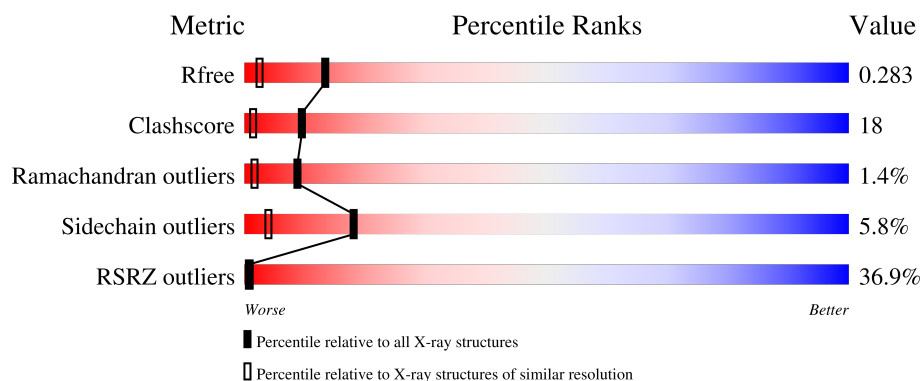
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	262	
1	B	262	

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
2	CXR	A	301	X	-	-	-
2	CXR	B	301	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4484 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.

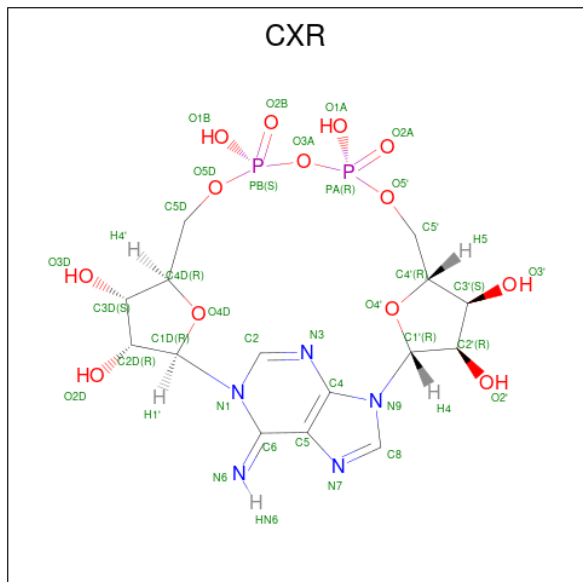
- Molecule 1 is a protein called ADP-ribosyl cyclase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total 2007	C 1265	N 351	O 375	S 16	0	0	0
1	B	252	Total 2007	C 1265	N 351	O 375	S 16	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	LYS	-	cloning artifact	UNP P28907
A	40	ARG	-	cloning artifact	UNP P28907
A	41	GLU	-	cloning artifact	UNP P28907
A	42	ALA	-	cloning artifact	UNP P28907
A	43	GLU	-	cloning artifact	UNP P28907
A	44	ALA	-	cloning artifact	UNP P28907
A	49	THR	GLN	engineered mutation	UNP P28907
A	100	ASP	ASN	engineered mutation	UNP P28907
A	164	ASP	ASN	engineered mutation	UNP P28907
A	209	ASP	ASN	engineered mutation	UNP P28907
A	219	ASP	ASN	engineered mutation	UNP P28907
A	226	ASP	GLU	engineered mutation	UNP P28907
B	39	LYS	-	cloning artifact	UNP P28907
B	40	ARG	-	cloning artifact	UNP P28907
B	41	GLU	-	cloning artifact	UNP P28907
B	42	ALA	-	cloning artifact	UNP P28907
B	43	GLU	-	cloning artifact	UNP P28907
B	44	ALA	-	cloning artifact	UNP P28907
B	49	THR	GLN	engineered mutation	UNP P28907
B	100	ASP	ASN	engineered mutation	UNP P28907
B	164	ASP	ASN	engineered mutation	UNP P28907
B	209	ASP	ASN	engineered mutation	UNP P28907
B	219	ASP	ASN	engineered mutation	UNP P28907
B	226	ASP	GLU	engineered mutation	UNP P28907

- Molecule 2 is CYCLIC ADENOSINE DIPHOSPHATE-RIBOSE (CCD ID: CXR) (formula: $C_{15}H_{21}N_5O_{13}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
2	B	1	Total	C	N	O	P	0	0
			35	15	5	13	2		

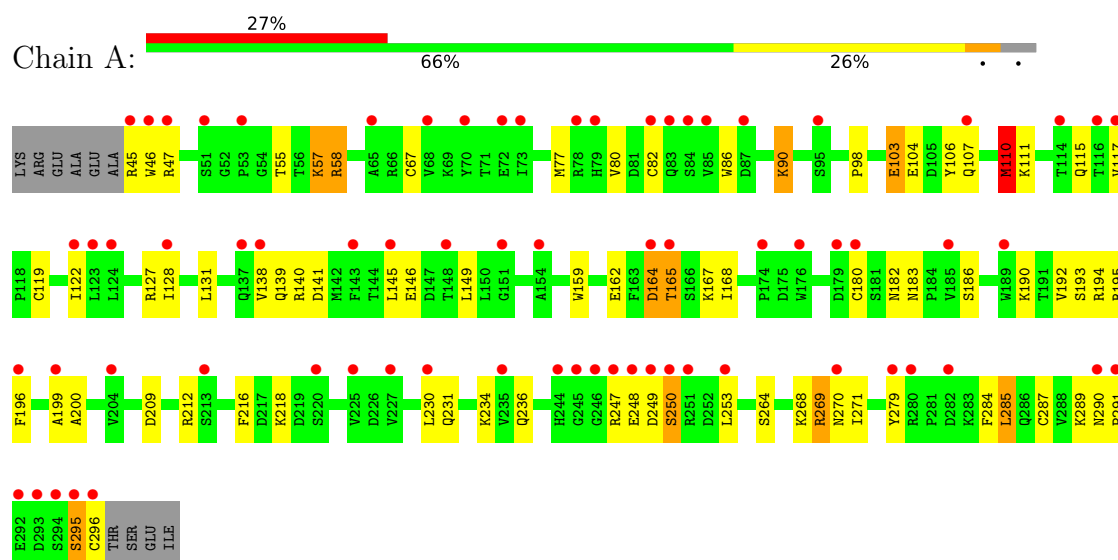
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	223	Total	O	0	0
			223	223		
3	B	177	Total	O	0	0
			177	177		

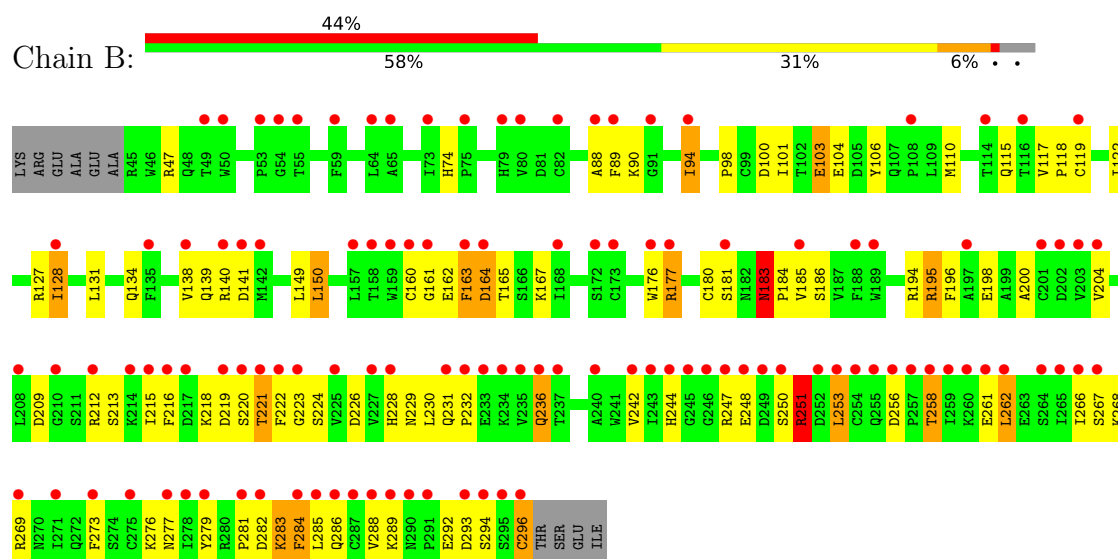
3 Residue-property plots

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: ADP-ribosyl cyclase 1



• Molecule 1: ADP-ribosyl cyclase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.72Å 53.00Å 65.94Å 104.96° 91.22° 94.57°	Depositor
Resolution (Å)	20.00 – 1.75 20.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.75) 94.5 (20.00-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.183 , 0.229 0.251 , 0.283	Depositor DCC
R_{free} test set	2631 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 64.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4484	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% 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: CXR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.63	16/2057 (0.8%)	1.45	14/2784 (0.5%)
1	B	1.63	25/2057 (1.2%)	1.45	15/2784 (0.5%)
All	All	1.63	41/4114 (1.0%)	1.45	29/5568 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	PHE	C-N	10.16	1.47	1.33
1	B	283	LYS	CD-CE	9.99	1.82	1.52
1	B	101	ILE	N-CA	9.41	1.57	1.46
1	A	234	LYS	N-CA	8.84	1.57	1.46
1	B	101	ILE	CA-CB	-8.82	1.43	1.54
1	B	286	GLN	CA-C	8.34	1.63	1.52
1	A	110	MET	CG-SD	-7.61	1.61	1.80
1	B	283	LYS	C-O	7.38	1.32	1.24
1	B	161	GLY	CA-C	7.29	1.59	1.51
1	B	164	ASP	CA-C	7.03	1.62	1.52
1	B	164	ASP	N-CA	-6.97	1.37	1.46
1	B	251	ARG	CZ-NH1	6.96	1.42	1.32
1	B	277	ASN	CG-OD1	6.85	1.36	1.23
1	B	163	PHE	CB-CG	-6.79	1.35	1.50
1	B	150	LEU	N-CA	6.74	1.54	1.46
1	A	200	ALA	CA-CB	-6.74	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	GLN	C-O	6.68	1.31	1.24
1	A	193	SER	N-CA	6.64	1.54	1.46
1	B	284	PHE	C-O	6.60	1.31	1.24
1	B	185	VAL	CA-CB	-6.55	1.46	1.54
1	B	284	PHE	C-N	6.51	1.42	1.33
1	B	163	PHE	N-CA	-6.42	1.38	1.46
1	B	103	GLU	N-CA	6.38	1.54	1.46
1	A	253	LEU	C-O	-6.33	1.15	1.24
1	A	146	GLU	N-CA	6.27	1.54	1.46
1	A	159	TRP	N-CA	6.02	1.53	1.45
1	B	296	CYS	C-O	6.00	1.35	1.23
1	B	160	CYS	C-O	5.76	1.30	1.23
1	A	196	PHE	N-CA	5.67	1.53	1.46
1	B	94	ILE	CA-CB	5.67	1.60	1.54
1	A	140	ARG	CA-C	-5.66	1.46	1.53
1	B	276	LYS	CE-NZ	5.62	1.66	1.49
1	B	292	GLU	C-O	5.43	1.30	1.24
1	B	196	PHE	CA-C	-5.41	1.46	1.52
1	B	253	LEU	C-O	5.33	1.30	1.24
1	B	183	ASN	CG-ND2	-5.24	1.22	1.33
1	A	192	VAL	CA-CB	5.22	1.61	1.54
1	A	231	GLN	N-CA	5.22	1.52	1.46
1	A	271	ILE	CA-CB	5.16	1.61	1.54
1	A	106	TYR	C-O	-5.14	1.17	1.24
1	A	230	LEU	N-CA	5.08	1.52	1.46

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ARG	NE-CZ-NH2	-11.69	108.68	119.20
1	A	269	ARG	NE-CZ-NH1	10.81	132.31	121.50
1	B	231	GLN	CA-C-N	10.44	130.21	119.56
1	B	231	GLN	C-N-CA	10.44	130.21	119.56
1	B	164	ASP	N-CA-CB	-8.50	97.31	110.06
1	A	269	ARG	CD-NE-CZ	8.25	135.94	124.40
1	B	161	GLY	N-CA-C	-8.03	103.16	112.79
1	B	163	PHE	N-CA-C	-7.16	103.51	111.82
1	A	90	LYS	CB-CA-C	-7.16	98.91	110.79
1	A	80	VAL	N-CA-C	6.16	116.97	108.84
1	B	163	PHE	CA-C-N	6.01	128.62	120.38
1	B	163	PHE	C-N-CA	6.01	128.62	120.38
1	B	213	SER	N-CA-C	-6.00	104.08	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	ILE	N-CA-C	5.88	117.04	108.58
1	A	141	ASP	N-CA-C	-5.86	105.02	111.82
1	B	140	ARG	N-CA-C	-5.78	106.31	113.19
1	B	283	LYS	O-C-N	5.75	128.30	122.09
1	B	262	LEU	N-CA-C	-5.64	106.94	113.88
1	A	290	ASN	CA-C-N	5.59	125.52	119.76
1	A	290	ASN	C-N-CA	5.59	125.52	119.76
1	A	269	ARG	CG-CD-NE	-5.53	99.83	112.00
1	B	119	CYS	N-CA-C	5.32	117.83	111.71
1	A	138	VAL	O-C-N	5.28	127.39	121.90
1	A	77	MET	N-CA-C	5.23	118.52	112.97
1	B	88	ALA	N-CA-C	5.20	117.03	111.36
1	B	89	PHE	N-CA-C	-5.12	105.61	111.14
1	A	165	THR	CA-C-N	-5.04	114.61	122.73
1	A	165	THR	C-N-CA	-5.04	114.61	122.73
1	A	145	LEU	N-CA-CB	-5.01	102.50	110.22

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	164	ASP	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2007	0	1915	58	0
1	B	2007	0	1915	92	0
2	A	35	0	18	0	0
2	B	35	0	19	7	0
3	A	223	0	0	18	0
3	B	177	0	0	16	0
All	All	4484	0	3867	142	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 18.

All (142) 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:283:LYS:CD	1:B:283:LYS:CE	1.82	1.56
1:B:221:THR:HG21	2:B:301:CXR:C5D	1.71	1.20
1:B:221:THR:CG2	2:B:301:CXR:H12	1.78	1.13
1:A:270:ASN:HB2	3:A:523:HOH:O	1.53	1.06
1:A:165:THR:HG23	1:A:167:LYS:H	1.19	1.05
1:B:221:THR:HG21	2:B:301:CXR:H12	1.06	1.04
1:B:195:ARG:HG3	1:B:195:ARG:HH11	1.20	1.04
1:B:176:TRP:HD1	1:B:177:ARG:HG3	1.26	0.97
1:B:266:ILE:HD11	1:B:273:PHE:HB2	1.49	0.91
1:A:269:ARG:HD2	3:B:413:HOH:O	1.70	0.91
1:B:74:HIS:HD2	3:B:437:HOH:O	1.55	0.89
1:B:165:THR:HG23	1:B:167:LYS:H	1.40	0.86
1:B:115:GLN:HE22	1:B:149:LEU:H	1.30	0.80
1:A:269:ARG:HD3	1:B:100:ASP:CG	2.07	0.79
1:A:115:GLN:HE22	1:A:149:LEU:H	1.29	0.79
1:B:74:HIS:CD2	3:B:437:HOH:O	2.34	0.79
1:B:177:ARG:CB	1:B:177:ARG:HH11	1.95	0.79
1:B:103:GLU:CD	1:B:194:ARG:HH21	1.93	0.76
1:A:291:PRO:CA	3:A:449:HOH:O	2.34	0.76
1:B:177:ARG:NH1	1:B:177:ARG:HB3	2.00	0.75
1:B:198:GLU:HG3	1:B:229:ASN:HB3	1.68	0.75
1:B:177:ARG:HH11	1:B:177:ARG:HB3	1.52	0.74
1:B:221:THR:HG21	2:B:301:CXR:H11	1.69	0.73
1:A:268:LYS:HD2	1:B:163:PHE:HE1	1.54	0.73
1:B:195:ARG:HG3	1:B:195:ARG:NH1	1.98	0.71
1:B:236:GLN:HB3	3:B:365:HOH:O	1.92	0.70
1:B:244:HIS:HB2	1:B:279:TYR:O	1.92	0.70
1:B:176:TRP:CD1	1:B:177:ARG:HG3	2.18	0.69
1:A:270:ASN:CG	3:A:461:HOH:O	2.34	0.69
1:A:295:SER:C	1:A:296:CYS:SG	2.76	0.69
1:A:268:LYS:CD	1:B:163:PHE:HE1	2.06	0.68
1:A:270:ASN:HB2	3:A:522:HOH:O	1.91	0.68
1:A:268:LYS:HD2	1:B:163:PHE:CE1	2.28	0.68
1:B:162:GLU:HB2	1:B:165:THR:HG22	1.75	0.67
1:B:195:ARG:N	1:B:195:ARG:HD2	2.10	0.67
1:A:122:ILE:CD1	3:A:444:HOH:O	2.43	0.66
1:A:199:ALA:HB3	3:A:444:HOH:O	1.94	0.66
1:A:122:ILE:HD11	3:A:444:HOH:O	1.96	0.65
1:B:138:VAL:CG1	1:B:289:LYS:HA	2.26	0.65
1:A:110:MET:SD	1:A:195:ARG:HD2	2.37	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:THR:HG23	1:A:167:LYS:N	2.03	0.65
1:A:119:CYS:HB3	3:A:357:HOH:O	1.98	0.63
1:B:228:HIS:HD2	1:B:269:ARG:HH21	1.47	0.63
1:A:268:LYS:CD	1:B:163:PHE:CE1	2.82	0.62
1:B:90:LYS:HG2	1:B:94:ILE:HG13	1.81	0.62
1:A:183:ASN:ND2	1:A:186:SER:H	1.98	0.62
1:B:283:LYS:CE	1:B:283:LYS:CG	2.75	0.62
1:A:270:ASN:CB	3:A:522:HOH:O	2.47	0.61
1:B:138:VAL:HG13	1:B:289:LYS:HA	1.82	0.61
1:A:285:LEU:HD13	1:A:289:LYS:HE3	1.83	0.61
1:B:283:LYS:CD	1:B:283:LYS:NZ	2.64	0.60
1:A:269:ARG:HD3	1:B:100:ASP:CB	2.30	0.60
1:A:162:GLU:HB2	1:A:165:THR:HG22	1.83	0.60
1:A:269:ARG:HD3	1:B:100:ASP:HB3	1.84	0.60
1:B:209:ASP:OD2	1:B:212:ARG:NE	2.32	0.60
1:A:209:ASP:HB3	1:A:212:ARG:HG3	1.84	0.59
1:B:251:ARG:HD3	1:B:251:ARG:H	1.67	0.59
1:B:222:PHE:HA	1:B:226:ASP:HB2	1.84	0.59
1:B:195:ARG:NH1	3:B:416:HOH:O	2.36	0.58
1:A:57:LYS:C	1:A:58:ARG:HG2	2.28	0.58
2:B:301:CXR:O5D	2:B:301:CXR:H3	2.03	0.58
1:B:221:THR:HB	2:B:301:CXR:O2B	2.04	0.57
1:B:139:GLN:C	1:B:141:ASP:H	2.12	0.57
1:A:164:ASP:OD2	1:A:164:ASP:N	2.38	0.57
1:B:216:PHE:HB3	1:B:258:THR:O	2.04	0.57
1:B:253:LEU:HD22	3:B:445:HOH:O	2.04	0.56
1:B:244:HIS:NE2	1:B:279:TYR:HD1	2.03	0.56
1:B:228:HIS:HD2	1:B:269:ARG:NH2	2.04	0.55
1:B:104:GLU:HG3	3:B:415:HOH:O	2.06	0.55
1:B:266:ILE:HD11	1:B:273:PHE:CB	2.30	0.55
1:A:182:ASN:HB2	3:A:505:HOH:O	2.06	0.55
1:A:194:ARG:CZ	3:A:435:HOH:O	2.55	0.54
1:A:57:LYS:O	1:A:58:ARG:HG2	2.08	0.54
1:A:165:THR:CG2	1:A:167:LYS:H	2.08	0.53
1:A:162:GLU:OE2	1:A:165:THR:HG21	2.09	0.53
1:A:127:ARG:HB3	1:A:212:ARG:NE	2.24	0.53
1:B:183:ASN:ND2	1:B:186:SER:H	2.06	0.53
1:A:115:GLN:NE2	1:A:149:LEU:H	2.04	0.53
1:B:220:SER:O	1:B:223:GLY:N	2.42	0.52
1:A:98:PRO:O	1:A:183:ASN:HA	2.10	0.52
1:B:177:ARG:CB	1:B:177:ARG:NH1	2.64	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ARG:CZ	3:B:442:HOH:O	2.56	0.52
1:B:293:ASP:H	1:B:296:CYS:HB2	1.73	0.52
1:A:104:GLU:HG2	3:A:456:HOH:O	2.09	0.52
1:B:47:ARG:NE	3:B:442:HOH:O	2.42	0.52
1:B:244:HIS:CE1	1:B:279:TYR:CD1	2.98	0.52
1:A:128:ILE:HG23	1:A:128:ILE:O	2.08	0.51
1:B:221:THR:HG22	3:B:390:HOH:O	2.11	0.51
1:B:98:PRO:O	1:B:183:ASN:HA	2.11	0.50
1:B:228:HIS:CD2	1:B:269:ARG:HH21	2.28	0.50
1:B:279:TYR:O	1:B:281:PRO:HD3	2.11	0.50
1:B:261:GLU:HG3	1:B:261:GLU:O	2.13	0.49
1:B:216:PHE:CD2	1:B:262:LEU:HB2	2.47	0.49
1:A:122:ILE:HD13	3:A:444:HOH:O	2.11	0.48
1:B:215:ILE:HD12	1:B:256:ASP:CG	2.39	0.48
1:B:127:ARG:HE	1:B:212:ARG:HH11	1.61	0.48
1:A:55:THR:HG21	1:A:168:ILE:HG21	1.95	0.48
1:A:268:LYS:HD3	1:B:163:PHE:CE1	2.48	0.47
1:B:176:TRP:CD1	1:B:176:TRP:C	2.89	0.47
1:B:128:ILE:HB	1:B:209:ASP:HB2	1.96	0.47
1:B:296:CYS:HA	3:B:434:HOH:O	2.13	0.47
1:A:183:ASN:HD21	1:A:186:SER:H	1.60	0.47
1:A:249:ASP:CA	1:A:279:TYR:CD1	2.97	0.47
1:A:86:TRP:CE2	1:A:90:LYS:HG3	2.50	0.47
1:B:221:THR:HG22	2:B:301:CXR:H12	1.86	0.46
1:A:57:LYS:H	1:A:57:LYS:HG3	1.25	0.46
1:B:115:GLN:NE2	1:B:149:LEU:H	2.08	0.46
1:B:139:GLN:C	1:B:141:ASP:N	2.72	0.46
1:B:141:ASP:HB3	3:B:401:HOH:O	2.15	0.46
1:B:200:ALA:HB1	1:B:204:VAL:HG22	1.98	0.46
1:A:107:GLN:HA	1:A:110:MET:HG3	1.98	0.46
1:B:106:TYR:O	1:B:110:MET:HG2	2.16	0.46
1:B:244:HIS:NE2	1:B:279:TYR:CD1	2.83	0.45
1:B:266:ILE:HG13	1:B:267:SER:N	2.32	0.45
1:A:117:VAL:HG12	3:A:415:HOH:O	2.15	0.45
1:B:176:TRP:CH2	3:B:409:HOH:O	2.69	0.45
1:A:216:PHE:CE2	1:A:218:LYS:HG2	2.52	0.44
1:B:176:TRP:CZ3	1:B:181:SER:HB2	2.52	0.44
1:B:195:ARG:HD2	1:B:195:ARG:H	1.79	0.44
1:B:244:HIS:CG	1:B:279:TYR:HA	2.53	0.44
1:A:67:CYS:C	1:A:82:CYS:SG	3.01	0.44
1:A:103:GLU:HG2	3:A:320:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LYS:NZ	3:A:375:HOH:O	2.48	0.43
1:B:103:GLU:CD	1:B:194:ARG:NH2	2.69	0.43
1:B:134:GLN:OE1	1:B:285:LEU:HD11	2.18	0.43
1:A:55:THR:HG21	1:A:168:ILE:CG2	2.49	0.42
1:A:47:ARG:O	1:A:47:ARG:HG2	2.18	0.42
1:B:117:VAL:O	1:B:118:PRO:C	2.61	0.42
1:A:180:CYS:HB2	3:A:505:HOH:O	2.20	0.42
1:B:228:HIS:CE1	3:B:456:HOH:O	2.73	0.42
1:A:287:CYS:HB3	1:A:296:CYS:HB3	1.80	0.41
1:B:176:TRP:HD1	1:B:177:ARG:CG	2.13	0.41
1:A:45:ARG:HB2	1:A:46:TRP:H	1.75	0.41
1:B:110:MET:CE	1:B:150:LEU:HD13	2.51	0.41
1:B:180:CYS:HB2	3:B:325:HOH:O	2.21	0.41
1:B:244:HIS:CD2	1:B:250:SER:HB2	2.56	0.41
1:B:284:PHE:O	1:B:288:VAL:HG23	2.21	0.40
1:A:264:SER:CB	1:B:163:PHE:HZ	2.34	0.40
1:A:295:SER:CA	3:A:341:HOH:O	2.69	0.40
1:B:176:TRP:CZ3	3:B:409:HOH:O	2.58	0.40
1:B:230:LEU:O	1:B:232:PRO:HD3	2.21	0.40
1:B:127:ARG:NE	1:B:212:ARG:HH11	2.18	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	250/262 (95%)	235 (94%)	11 (4%)	4 (2%)	7	1
1	B	250/262 (95%)	233 (93%)	14 (6%)	3 (1%)	10	2
All	All	500/524 (95%)	468 (94%)	25 (5%)	7 (1%)	9	2

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	GLU
1	A	295	SER
1	B	248	GLU
1	A	250	SER
1	A	247	ARG
1	B	294	SER
1	B	247	ARG

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	223/241 (92%)	213 (96%)	10 (4%)	24	7
1	B	223/241 (92%)	207 (93%)	16 (7%)	13	2
All	All	446/482 (92%)	420 (94%)	26 (6%)	18	4

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LYS
1	A	58	ARG
1	A	103	GLU
1	A	110	MET
1	A	111	LYS
1	A	131	LEU
1	A	164	ASP
1	A	236	GLN
1	A	250	SER
1	A	285	LEU
1	B	128	ILE
1	B	131	LEU
1	B	177	ARG
1	B	183	ASN
1	B	184	PRO
1	B	195	ARG
1	B	218	LYS

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Mol	Chain	Res	Type
1	B	219	ASP
1	B	221	THR
1	B	224	SER
1	B	236	GLN
1	B	242	VAL
1	B	251	ARG
1	B	258	THR
1	B	268	LYS
1	B	282	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	83	GLN
1	A	107	GLN
1	A	115	GLN
1	A	134	GLN
1	A	139	GLN
1	A	171	GLN
1	A	183	ASN
1	B	83	GLN
1	B	115	GLN
1	B	171	GLN
1	B	183	ASN
1	B	228	HIS
1	B	286	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 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	CXR	B	301	-	38,39,39	3.29	17 (44%)	55,62,62	2.18	13 (23%)
2	CXR	A	301	-	38,39,39	2.35	19 (50%)	55,62,62	1.84	10 (18%)

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	CXR	B	301	-	1/1/10/10	3/26/58/58	0/3/5/5
2	CXR	A	301	-	1/1/10/10	0/26/58/58	0/3/5/5

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	CXR	C6-N6	10.28	1.52	1.28
2	A	301	CXR	C8-N7	6.35	1.50	1.32
2	B	301	CXR	C2-N1	6.28	1.51	1.36
2	B	301	CXR	C5-N7	-5.78	1.27	1.39
2	B	301	CXR	O2D-C2D	5.52	1.56	1.43
2	B	301	CXR	C5-C4	5.09	1.52	1.38
2	B	301	CXR	PB-O3A	4.95	1.64	1.59
2	B	301	CXR	C5-C6	-4.60	1.31	1.43
2	A	301	CXR	O2D-C2D	4.55	1.54	1.43
2	B	301	CXR	C2D-C3D	-4.53	1.41	1.53
2	B	301	CXR	PA-O3A	4.38	1.64	1.59
2	B	301	CXR	C1'-N9	4.04	1.59	1.47
2	A	301	CXR	O4'-C1'	3.98	1.51	1.42
2	A	301	CXR	O4D-C1D	3.45	1.50	1.42
2	A	301	CXR	PB-O3A	3.33	1.63	1.59
2	A	301	CXR	C5-N7	-3.30	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	CXR	PA-O5'	3.21	1.72	1.59
2	A	301	CXR	C6-N6	2.99	1.35	1.28
2	B	301	CXR	O4'-C4'	2.91	1.51	1.45
2	B	301	CXR	C8-N7	2.89	1.40	1.32
2	A	301	CXR	C2-N3	2.74	1.35	1.30
2	A	301	CXR	C5-C4	2.70	1.46	1.38
2	B	301	CXR	PB-O5D	2.68	1.69	1.59
2	A	301	CXR	O3D-C3D	2.67	1.49	1.43
2	B	301	CXR	O4'-C1'	2.65	1.48	1.42
2	B	301	CXR	C4-N3	-2.65	1.30	1.35
2	A	301	CXR	C4-N3	2.63	1.41	1.35
2	A	301	CXR	C2D-C3D	-2.61	1.46	1.53
2	A	301	CXR	O5'-C5'	-2.49	1.35	1.44
2	B	301	CXR	C4-N9	-2.49	1.31	1.38
2	A	301	CXR	PA-O2A	2.49	1.59	1.50
2	A	301	CXR	O4'-C4'	2.36	1.50	1.45
2	A	301	CXR	C5-C6	-2.33	1.37	1.43
2	A	301	CXR	PA-O3A	2.32	1.62	1.59
2	B	301	CXR	O3'-C3'	2.23	1.48	1.43
2	A	301	CXR	PB-O1B	-2.11	1.45	1.55

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	CXR	N1-C2-N3	-7.87	116.23	125.84
2	A	301	CXR	C5-C4-N3	-6.66	117.47	127.27
2	B	301	CXR	C2-N3-C4	6.23	124.75	112.53
2	B	301	CXR	C3'-C2'-C1'	5.37	111.62	101.46
2	A	301	CXR	N9-C8-N7	-4.44	105.17	113.40
2	B	301	CXR	C5-C4-N3	-4.14	121.17	127.27
2	A	301	CXR	N9-C4-N3	3.74	135.43	126.90
2	B	301	CXR	O2'-C2'-C3'	-3.33	101.14	111.82
2	A	301	CXR	O1B-PB-O2B	3.33	127.92	112.44
2	B	301	CXR	O1A-PA-O3A	-3.23	98.54	107.27
2	A	301	CXR	C2'-C3'-C4'	3.22	108.83	102.61
2	A	301	CXR	C2-N3-C4	3.14	118.69	112.53
2	A	301	CXR	C8-N9-C4	3.03	111.70	106.03
2	B	301	CXR	O4'-C4'-C5'	2.88	118.56	109.33
2	B	301	CXR	N9-C4-N3	2.88	133.45	126.90
2	B	301	CXR	O4'-C1'-N9	-2.67	102.30	108.36
2	B	301	CXR	N9-C8-N7	-2.62	108.54	113.40
2	A	301	CXR	O2'-C2'-C1'	-2.59	101.19	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	CXR	C8-N7-C5	2.50	108.72	104.26
2	A	301	CXR	C2D-C1D-N1	2.40	119.94	113.25
2	A	301	CXR	O4D-C1D-C2D	-2.33	101.64	106.62
2	B	301	CXR	O1B-PB-O2B	2.17	122.56	112.44
2	B	301	CXR	C5'-C4'-C3'	-2.17	107.42	115.21

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	301	CXR	C3'
2	B	301	CXR	C3'

All (3) torsion outliers are listed below:

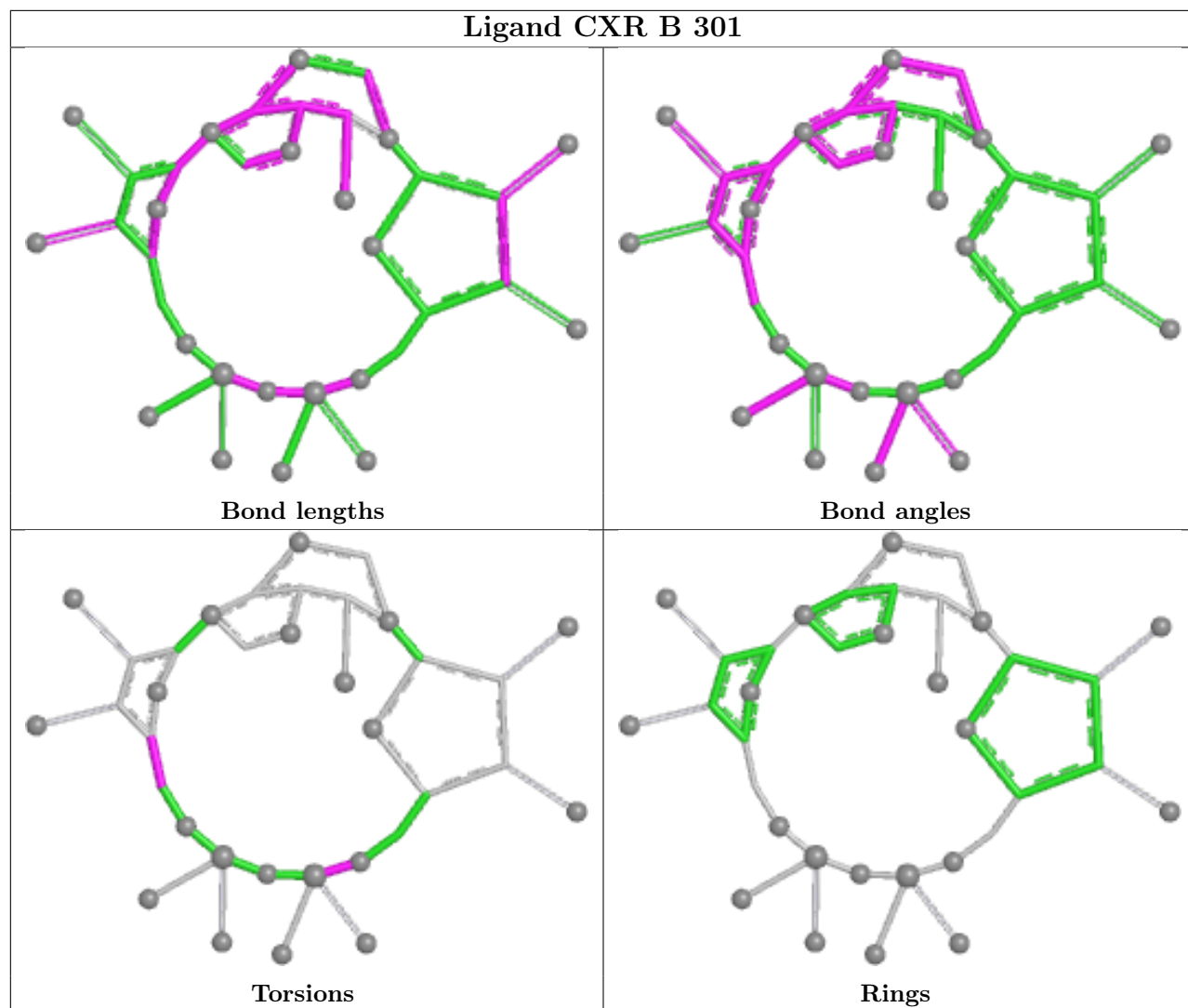
Mol	Chain	Res	Type	Atoms
2	B	301	CXR	O4'-C4'-C5'-O5'
2	B	301	CXR	C3'-C4'-C5'-O5'
2	B	301	CXR	C5D-O5D-PB-O2B

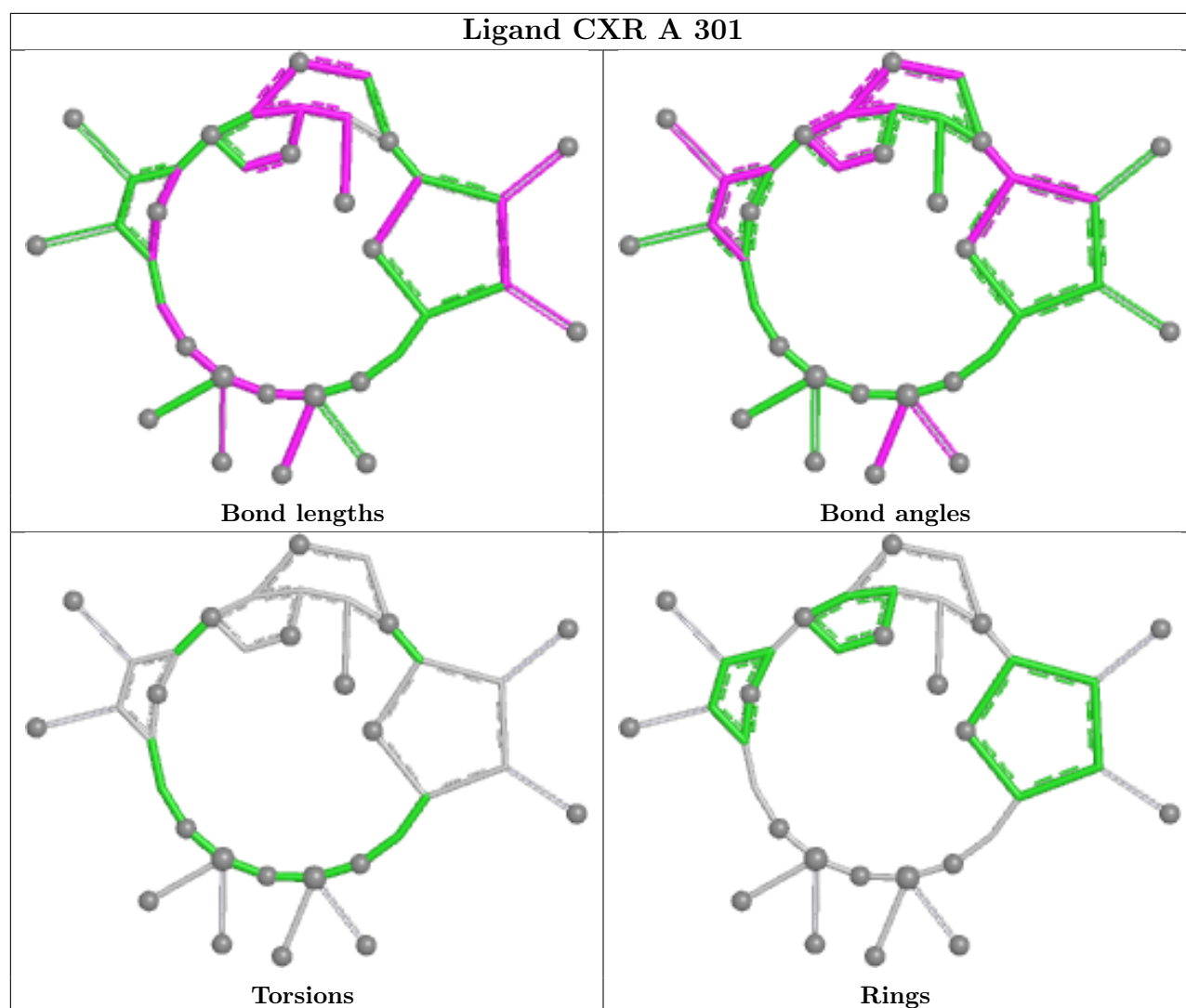
There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	CXR	7	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	252/262 (96%)	1.71	70 (27%) 1 1	36, 43, 60, 71	0
1	B	252/262 (96%)	2.12	116 (46%) 0 0	33, 47, 69, 78	0
All	All	504/524 (96%)	1.91	186 (36%) 1 1	33, 44, 67, 78	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	ASP	7.9
1	A	248	GLU	7.1
1	A	296	CYS	6.3
1	B	296	CYS	6.0
1	B	265	ILE	5.8
1	B	254	CYS	5.4
1	B	253	LEU	5.4
1	A	46	TRP	5.3
1	B	287	CYS	5.3
1	B	259	ILE	5.1
1	B	295	SER	5.1
1	A	176	TRP	4.9
1	B	258	THR	4.9
1	B	225	VAL	4.7
1	B	275	CYS	4.6
1	A	291	PRO	4.5
1	B	291	PRO	4.5
1	B	266	ILE	4.5
1	B	279	TYR	4.4
1	B	284	PHE	4.4
1	A	165	THR	4.3
1	B	255	GLN	4.2
1	B	237	THR	4.2
1	B	236	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	249	ASP	4.1
1	B	271	ILE	4.1
1	B	278	ILE	4.0
1	B	203	VAL	4.0
1	B	264	SER	3.9
1	B	246	GLY	3.9
1	B	201	CYS	3.9
1	A	180	CYS	3.9
1	B	281	PRO	3.9
1	B	294	SER	3.7
1	B	219	ASP	3.7
1	A	68	VAL	3.7
1	B	285	LEU	3.7
1	B	290	ASN	3.7
1	B	293	ASP	3.7
1	B	244	HIS	3.6
1	B	221	THR	3.6
1	B	260	LYS	3.6
1	B	267	SER	3.6
1	B	235	VAL	3.6
1	B	257	PRO	3.5
1	A	250	SER	3.5
1	A	293	ASP	3.5
1	A	294	SER	3.5
1	B	159	TRP	3.5
1	A	292	GLU	3.5
1	B	73	ILE	3.4
1	B	289	LYS	3.4
1	A	246	GLY	3.3
1	B	157	LEU	3.3
1	B	277	ASN	3.3
1	A	227	VAL	3.2
1	A	51	SER	3.2
1	B	164	ASP	3.2
1	B	54	GLY	3.1
1	B	248	GLU	3.1
1	A	279	TYR	3.1
1	A	295	SER	3.1
1	B	176	TRP	3.1
1	B	141	ASP	3.1
1	B	185	VAL	3.0
1	B	233	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	55	THR	3.0
1	B	208	LEU	3.0
1	B	223	GLY	3.0
1	B	286	GLN	2.9
1	B	250	SER	2.9
1	A	164	ASP	2.9
1	B	135	PHE	2.9
1	B	242	VAL	2.9
1	A	84	SER	2.9
1	A	79	HIS	2.8
1	A	143	PHE	2.8
1	A	245	GLY	2.8
1	B	262	LEU	2.8
1	A	45	ARG	2.8
1	B	282	ASP	2.8
1	B	222	PHE	2.8
1	A	73	ILE	2.8
1	B	273	PHE	2.7
1	B	232	PRO	2.7
1	B	243	ILE	2.7
1	A	95	SER	2.7
1	A	199	ALA	2.7
1	A	114	THR	2.7
1	B	64	LEU	2.7
1	B	197	ALA	2.7
1	A	247	ARG	2.6
1	B	91	GLY	2.6
1	A	117	VAL	2.6
1	B	204	VAL	2.6
1	B	231	GLN	2.6
1	A	270	ASN	2.6
1	B	59	PHE	2.6
1	B	128	ILE	2.6
1	B	240	ALA	2.6
1	B	210	GLY	2.6
1	B	269	ARG	2.6
1	A	82	CYS	2.6
1	B	79	HIS	2.6
1	B	215	ILE	2.6
1	A	290	ASN	2.6
1	B	228	HIS	2.5
1	A	213	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	235	VAL	2.5
1	A	251	ARG	2.5
1	B	80	VAL	2.5
1	B	288	VAL	2.5
1	B	158	THR	2.5
1	B	220	SER	2.5
1	B	261	GLU	2.5
1	B	216	PHE	2.5
1	A	204	VAL	2.5
1	A	225	VAL	2.5
1	B	114	THR	2.5
1	B	189	TRP	2.5
1	B	119	CYS	2.5
1	B	252	ASP	2.5
1	A	148	THR	2.5
1	A	124	LEU	2.4
1	B	163	PHE	2.4
1	B	65	ALA	2.4
1	A	128	ILE	2.4
1	B	202	ASP	2.4
1	B	82	CYS	2.4
1	A	145	LEU	2.4
1	B	50	TRP	2.4
1	B	245	GLY	2.4
1	A	138	VAL	2.4
1	A	196	PHE	2.4
1	B	138	VAL	2.4
1	A	78	ARG	2.3
1	B	94	ILE	2.3
1	B	161	GLY	2.3
1	B	75	PRO	2.3
1	B	49	THR	2.3
1	A	154	ALA	2.3
1	A	83	GLN	2.3
1	B	177	ARG	2.3
1	B	108	PRO	2.3
1	A	116	THR	2.3
1	A	87	ASP	2.3
1	B	142	MET	2.3
1	A	230	LEU	2.2
1	B	234	LYS	2.2
1	B	188	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	70	TYR	2.2
1	A	107	GLN	2.2
1	A	65	ALA	2.2
1	B	160	CYS	2.2
1	B	217	ASP	2.2
1	B	168	ILE	2.2
1	B	247	ARG	2.2
1	A	174	PRO	2.2
1	B	53	PRO	2.2
1	B	227	VAL	2.2
1	A	282	ASP	2.2
1	A	189	TRP	2.2
1	A	253	LEU	2.2
1	B	89	PHE	2.2
1	A	53	PRO	2.2
1	B	172	SER	2.2
1	B	181	SER	2.2
1	A	85	VAL	2.1
1	A	72	GLU	2.1
1	B	140	ARG	2.1
1	A	220	SER	2.1
1	B	256	ASP	2.1
1	A	122	ILE	2.1
1	B	212	ARG	2.1
1	A	137	GLN	2.1
1	A	179	ASP	2.1
1	A	47	ARG	2.1
1	B	173	CYS	2.1
1	A	123	LEU	2.1
1	A	280	ARG	2.1
1	B	116	THR	2.1
1	A	244	HIS	2.1
1	B	214	LYS	2.1
1	A	151	GLY	2.0
1	B	88	ALA	2.0
1	A	185	VAL	2.0

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

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](#)

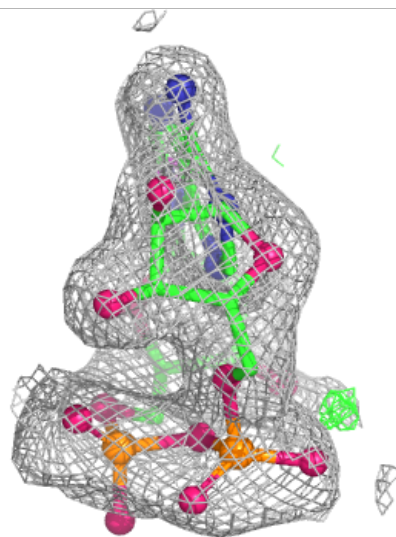
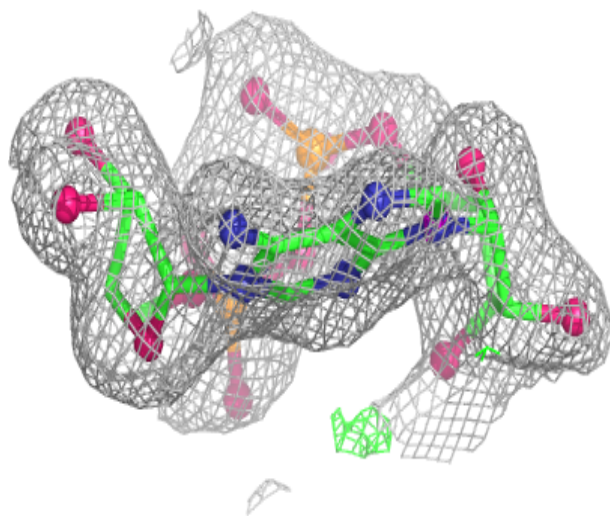
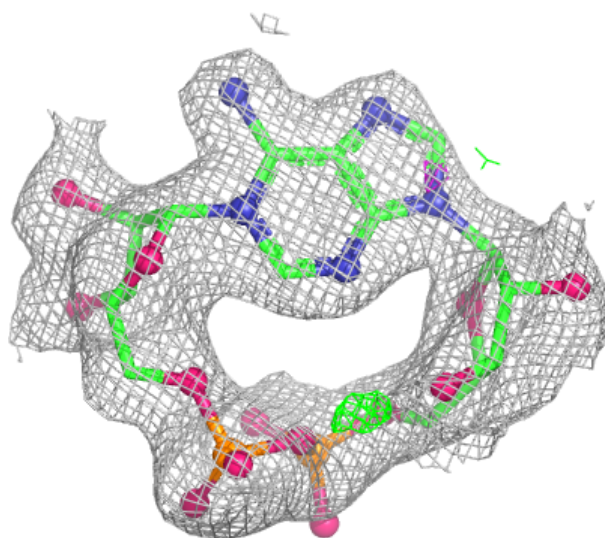
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	CXR	B	301	35/35	0.89	0.12	33,45,69,71	0
2	CXR	A	301	35/35	0.91	0.11	30,36,53,60	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.

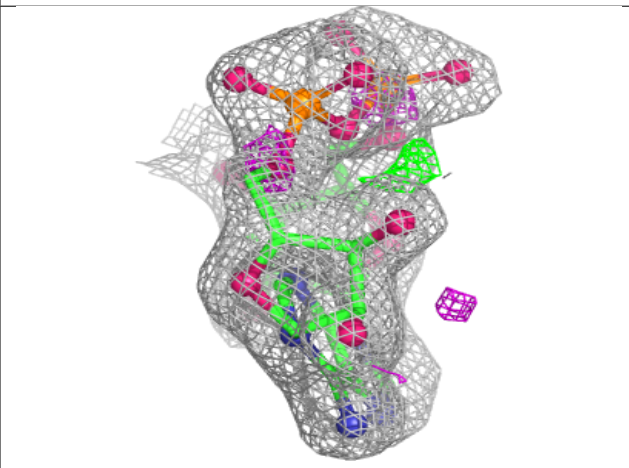
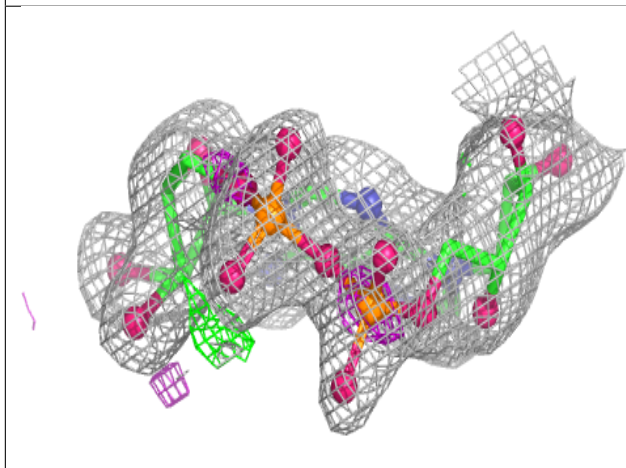
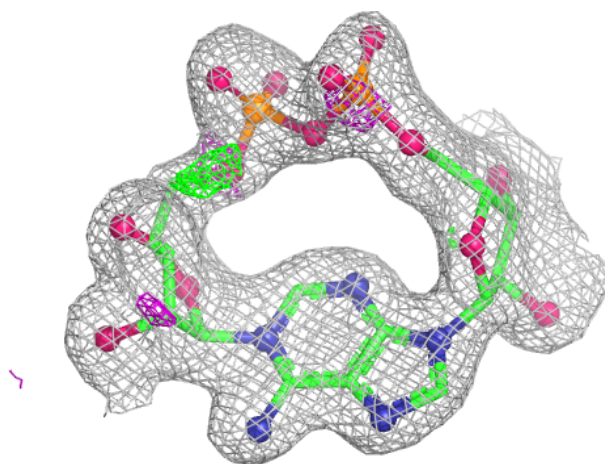
Electron density around CXR B 301:

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



Electron density around CXR 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.