



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 08:10 AM EDT

PDB ID : 2O3S / pdb_00002o3s
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 : 1.50 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

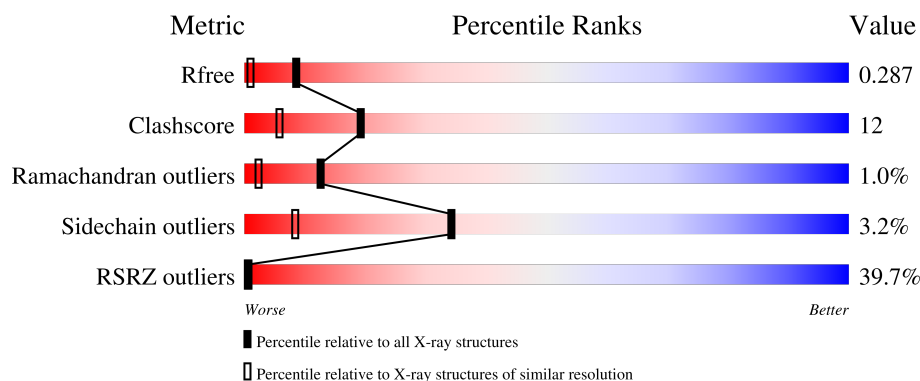
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	22% 81% 13% • •
1	B	262	55% 74% 20% • •

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 4808 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	C	N	O	S	0	0	0
			2038	1286	352	384	16			
1	B	252	Total	C	N	O	S	0	0	0
			2038	1286	352	384	16			

There are 26 discrepancies between the modelled and reference sequences:

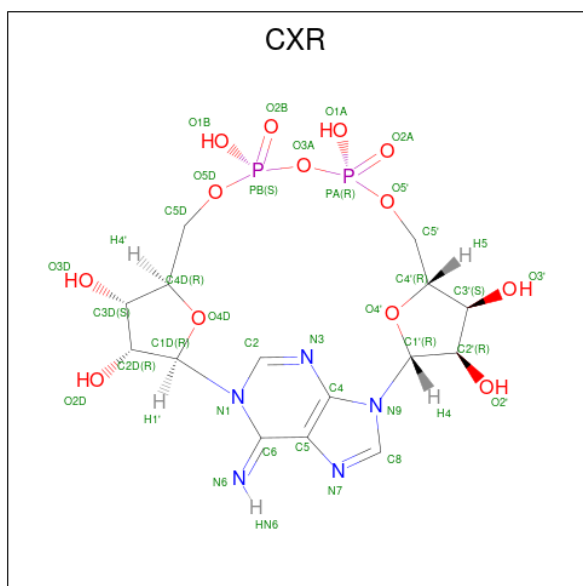
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	LYS	-	cloning artifact	UNP P28907
A	40	ARG	-	cloning artifact	UNP P28907
A	41	GLU	-	cloning artifact	UNP P28907
A	42	ALA	-	cloning artifact	UNP P28907
A	43	GLU	-	cloning artifact	UNP P28907
A	44	ALA	-	cloning artifact	UNP P28907
A	45	PHE	ARG	engineered mutation	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	GLY	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	45	PHE	ARG	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	226	GLY	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		

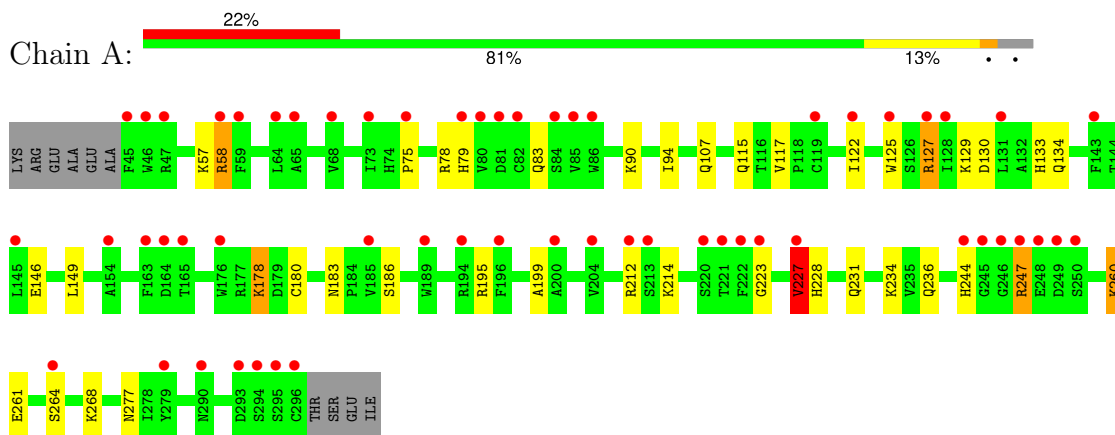
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	386	Total	O	0	0
			386	386		
3	B	276	Total	O	0	0
			276	276		

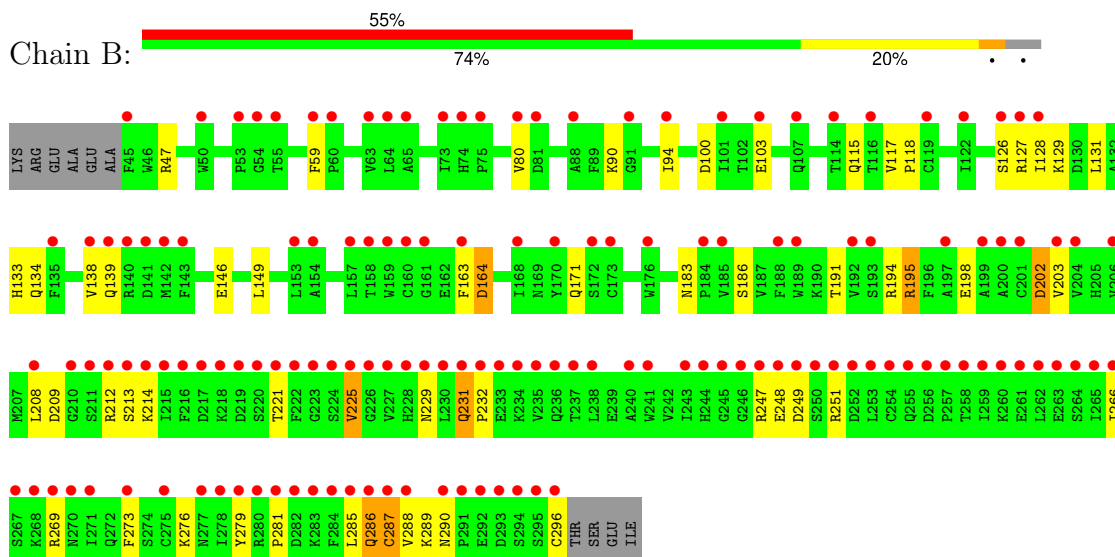
3 Residue-property plots [i](#)

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: 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	42.35Å 53.79Å 66.83Å 104.97° 91.71° 95.04°	Depositor
Resolution (Å)	20.00 – 1.50 20.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	86.7 (20.00-1.50) 86.6 (20.00-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.3.0017	Depositor
R, R_{free}	0.189 , 0.238 0.254 , 0.287	Depositor DCC
R_{free} test set	3852 reflections (4.28%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 64.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4808	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.41% 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	1.23	2/2090 (0.1%)	1.02	1/2832 (0.0%)
1	B	1.07	4/2090 (0.2%)	1.00	7/2832 (0.2%)
All	All	1.15	6/4180 (0.1%)	1.01	8/5664 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	202	ASP	C-N	9.97	1.46	1.33
1	B	202	ASP	C-O	7.02	1.32	1.24
1	A	227	VAL	CA-CB	5.88	1.61	1.54
1	B	59	PHE	CA-C	5.55	1.58	1.52
1	A	234	LYS	N-CA	5.41	1.53	1.46
1	B	287	CYS	CB-SG	5.18	1.98	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	248	GLU	CB-CA-C	-8.24	107.07	116.63
1	A	178	LYS	N-CA-C	6.39	118.33	111.36
1	B	164	ASP	N-CA-C	6.03	123.65	110.80
1	B	231	GLN	CA-C-N	5.91	125.59	119.56
1	B	231	GLN	C-N-CA	5.91	125.59	119.56
1	B	290	ASN	CA-C-N	5.81	125.48	119.56
1	B	290	ASN	C-N-CA	5.81	125.48	119.56
1	B	129	LYS	N-CA-C	5.04	116.46	111.07

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	2038	0	1957	47	0
1	B	2038	0	1959	52	0
2	A	35	0	18	0	0
2	B	35	0	19	3	0
3	A	386	0	0	22	0
3	B	276	0	0	8	0
All	All	4808	0	3953	94	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 12.

All (94) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ARG:HH11	1:A:58:ARG:HG2	1.03	1.18
1:B:195:ARG:HH11	1:B:195:ARG:HG2	0.95	1.11
1:A:268:LYS:HD3	1:B:163:PHE:HE1	1.12	1.05
1:A:268:LYS:HD3	1:B:163:PHE:CE1	1.91	1.05
1:B:195:ARG:HG2	1:B:195:ARG:NH1	1.74	0.93
1:B:287:CYS:HG	1:B:296:CYS:HG	0.95	0.88
1:A:58:ARG:HH11	1:A:58:ARG:CG	1.84	0.87
1:A:58:ARG:HG2	1:A:58:ARG:NH1	1.85	0.84
1:A:115:GLN:HE22	1:A:149:LEU:H	1.26	0.82
1:A:228:HIS:HD2	1:B:100:ASP:OD1	1.62	0.82
1:B:131:LEU:O	1:B:131:LEU:HD23	1.82	0.80
1:B:115:GLN:HE22	1:B:149:LEU:H	1.28	0.79
1:A:268:LYS:CD	1:B:163:PHE:CE1	2.66	0.78
1:A:231:GLN:HG3	3:A:665:HOH:O	1.84	0.77
1:B:195:ARG:HH11	1:B:195:ARG:CG	1.88	0.76
1:A:127:ARG:HB3	1:A:212:ARG:HE	1.50	0.74
1:A:268:LYS:CD	1:B:163:PHE:HE1	1.96	0.73
1:A:260:LYS:NZ	3:A:675:HOH:O	2.24	0.71
1:A:261:GLU:HG3	3:A:679:HOH:O	1.90	0.70
1:A:79:HIS:CE1	3:A:608:HOH:O	2.47	0.67
1:A:199:ALA:HB3	3:A:538:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ILE:HD11	1:B:273:PHE:HB2	1.81	0.61
1:B:134:GLN:HE21	1:B:285:LEU:HD11	1.67	0.59
1:A:228:HIS:CD2	1:B:100:ASP:OD1	2.52	0.58
1:A:75:PRO:O	1:A:78:ARG:HG2	2.04	0.58
1:B:183:ASN:ND2	1:B:186:SER:H	2.02	0.58
1:B:139:GLN:HE21	1:B:288:VAL:HG13	1.70	0.57
1:B:90:LYS:CG	1:B:94:ILE:HG13	2.36	0.56
1:A:180:CYS:HB2	3:A:426:HOH:O	2.05	0.55
1:A:183:ASN:ND2	1:A:186:SER:H	2.05	0.55
1:B:118:PRO:HG2	3:B:435:HOH:O	2.06	0.55
1:B:269:ARG:HH11	1:B:269:ARG:HB3	1.71	0.55
1:A:57:LYS:HG3	3:A:516:HOH:O	2.06	0.54
1:A:134:GLN:CD	3:A:666:HOH:O	2.50	0.54
1:B:90:LYS:HG2	1:B:94:ILE:HG13	1.90	0.54
1:A:195:ARG:NH1	3:A:367:HOH:O	2.39	0.54
1:A:261:GLU:HA	3:A:679:HOH:O	2.08	0.54
1:A:90:LYS:CG	1:A:94:ILE:HG13	2.38	0.53
1:B:131:LEU:HD23	1:B:131:LEU:C	2.33	0.53
1:B:221:THR:HG21	2:B:301:CXR:H12	1.89	0.53
1:A:125:TRP:CH2	1:A:129:LYS:HB2	2.44	0.53
1:B:212:ARG:C	1:B:214:LYS:H	2.16	0.53
1:B:232:PRO:HD3	1:B:269:ARG:HH12	1.73	0.53
1:B:195:ARG:HD3	3:B:431:HOH:O	2.08	0.53
1:B:47:ARG:HH11	1:B:47:ARG:HG2	1.73	0.52
1:A:90:LYS:HG3	1:A:94:ILE:HG13	1.92	0.51
1:B:115:GLN:NE2	1:B:149:LEU:H	2.04	0.51
3:A:679:HOH:O	1:B:163:PHE:HE2	1.93	0.50
1:B:171:GLN:NE2	3:B:563:HOH:O	2.44	0.50
1:B:47:ARG:HG2	1:B:47:ARG:NH1	2.27	0.50
1:A:214:LYS:NZ	3:A:501:HOH:O	2.45	0.50
2:B:301:CXR:H4'	3:B:575:HOH:O	2.13	0.49
1:A:57:LYS:HG2	3:A:620:HOH:O	2.12	0.49
1:B:195:ARG:NH1	1:B:195:ARG:CG	2.56	0.49
1:B:209:ASP:OD2	1:B:212:ARG:HG2	2.12	0.49
1:B:212:ARG:C	1:B:214:LYS:N	2.70	0.49
1:A:58:ARG:CG	1:A:58:ARG:NH1	2.56	0.48
1:B:194:ARG:HG3	1:B:229:ASN:ND2	2.28	0.48
1:B:171:GLN:NE2	3:B:365:HOH:O	2.45	0.48
1:A:236:GLN:HG2	3:A:376:HOH:O	2.13	0.48
1:B:198:GLU:HG3	1:B:229:ASN:HB3	1.96	0.47
1:A:133:HIS:HE1	1:A:146:GLU:OE1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ARG:CB	1:A:212:ARG:HE	2.24	0.47
1:B:90:LYS:HD2	3:B:565:HOH:O	2.14	0.47
1:B:183:ASN:HD21	1:B:186:SER:H	1.63	0.47
1:A:244:HIS:HE1	1:A:277:ASN:OD1	1.98	0.46
1:B:279:TYR:O	1:B:281:PRO:HD3	2.16	0.46
1:A:83:GLN:NE2	3:A:674:HOH:O	2.40	0.45
1:A:122:ILE:CD1	3:A:538:HOH:O	2.63	0.45
1:B:126:SER:HB3	1:B:208:LEU:HD23	1.99	0.45
1:A:247:ARG:HD3	1:A:247:ARG:HA	1.77	0.44
1:B:133:HIS:CE1	1:B:146:GLU:HB2	2.53	0.44
1:B:133:HIS:HE1	1:B:146:GLU:OE1	2.00	0.43
1:B:47:ARG:HD2	3:B:529:HOH:O	2.18	0.43
1:A:115:GLN:NE2	1:A:149:LEU:H	2.04	0.43
2:B:301:CXR:H3	2:B:301:CXR:C5D	2.49	0.43
1:B:209:ASP:HB3	1:B:212:ARG:HG2	2.00	0.43
1:A:78:ARG:NH1	3:A:491:HOH:O	2.52	0.42
1:A:122:ILE:HD11	3:A:538:HOH:O	2.19	0.42
1:B:286:GLN:HG3	3:B:495:HOH:O	2.18	0.42
1:A:183:ASN:HD21	1:A:186:SER:H	1.65	0.42
1:B:287:CYS:CB	1:B:296:CYS:HG	2.32	0.42
1:A:264:SER:HB2	1:B:163:PHE:HZ	1.85	0.42
1:B:231:GLN:HA	1:B:232:PRO:HD3	1.90	0.42
1:B:138:VAL:HG11	1:B:289:LYS:HA	2.03	0.41
1:A:90:LYS:HG2	1:A:94:ILE:HG13	2.02	0.41
1:A:223:GLY:O	1:A:227:VAL:CG1	2.69	0.41
1:A:236:GLN:CG	3:A:376:HOH:O	2.67	0.41
1:B:103:GLU:HG3	1:B:191:THR:HG23	2.01	0.41
1:B:221:THR:O	1:B:225:VAL:HB	2.21	0.41
1:A:178:LYS:HG3	3:A:387:HOH:O	2.20	0.40
1:B:202:ASP:HB3	1:B:203:VAL:H	1.57	0.40
1:A:107:GLN:HG2	3:A:609:HOH:O	2.20	0.40
1:A:228:HIS:HE1	3:A:324:HOH:O	2.03	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%)	237 (95%)	12 (5%)	1 (0%)	30	12
1	B	250/262 (95%)	229 (92%)	17 (7%)	4 (2%)	7	1
All	All	500/524 (95%)	466 (93%)	29 (6%)	5 (1%)	12	2

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	247	ARG
1	B	225	VAL
1	B	213	SER
1	B	247	ARG
1	B	249	ASP

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	231/240 (96%)	225 (97%)	6 (3%)	40	13
1	B	231/240 (96%)	222 (96%)	9 (4%)	28	5
All	All	462/480 (96%)	447 (97%)	15 (3%)	34	8

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ARG
1	A	117	VAL
1	A	127	ARG
1	A	130	ASP
1	A	227	VAL
1	A	260	LYS
1	B	80	VAL

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Mol	Chain	Res	Type
1	B	117	VAL
1	B	127	ARG
1	B	128	ILE
1	B	164	ASP
1	B	195	ARG
1	B	251	ARG
1	B	276	LYS
1	B	286	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	115	GLN
1	A	133	HIS
1	A	134	GLN
1	A	183	ASN
1	A	228	HIS
1	A	236	GLN
1	A	244	HIS
1	A	286	GLN
1	A	290	ASN
1	B	74	HIS
1	B	83	GLN
1	B	115	GLN
1	B	133	HIS
1	B	134	GLN
1	B	139	GLN
1	B	171	GLN
1	B	183	ASN
1	B	229	ASN
1	B	244	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	2.20	11 (28%)	55,62,62	1.57	8 (14%)
2	CXR	A	301	-	38,39,39	2.09	9 (23%)	55,62,62	1.70	11 (20%)

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	7/26/58/58	0/3/5/5
2	CXR	A	301	-	1/1/10/10	1/26/58/58	0/3/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	CXR	PA-O3A	8.57	1.68	1.59
2	B	301	CXR	C2-N1	5.88	1.50	1.36
2	B	301	CXR	C6-N6	5.65	1.41	1.28
2	B	301	CXR	C5-C4	4.35	1.50	1.38
2	B	301	CXR	O4'-C1'	3.78	1.50	1.42
2	B	301	CXR	C2-N3	3.35	1.36	1.30
2	B	301	CXR	C5-N7	-3.35	1.32	1.39
2	A	301	CXR	C2-N3	3.15	1.36	1.30
2	B	301	CXR	PA-O3A	-3.04	1.56	1.59
2	A	301	CXR	O4'-C4'	2.97	1.51	1.45
2	A	301	CXR	C2-N1	2.96	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	CXR	C8-N7	2.88	1.40	1.32
2	A	301	CXR	O3'-C3'	2.77	1.49	1.43
2	A	301	CXR	PB-O2B	2.77	1.60	1.50
2	A	301	CXR	O3D-C3D	2.61	1.49	1.43
2	A	301	CXR	O2D-C2D	2.41	1.48	1.43
2	A	301	CXR	C6-N6	2.40	1.33	1.28
2	B	301	CXR	O4'-C4'	2.29	1.50	1.45
2	B	301	CXR	O3'-C3'	2.24	1.48	1.43
2	B	301	CXR	O2D-C2D	2.05	1.48	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	CXR	C5-C4-N3	-5.72	118.85	127.27
2	B	301	CXR	N1-C2-N3	-4.03	120.91	125.84
2	B	301	CXR	C2-N3-C4	4.00	120.37	112.53
2	A	301	CXR	C2-N3-C4	3.86	120.09	112.53
2	B	301	CXR	N1-C6-N6	3.85	125.68	119.16
2	B	301	CXR	C5-C4-N3	-3.47	122.16	127.27
2	A	301	CXR	N9-C4-N3	3.07	133.89	126.90
2	B	301	CXR	C3'-C2'-C1'	2.95	107.04	101.46
2	A	301	CXR	O3'-C3'-C4'	2.94	119.52	111.08
2	A	301	CXR	O2'-C2'-C3'	-2.88	102.60	111.82
2	B	301	CXR	N9-C4-N3	2.80	133.28	126.90
2	A	301	CXR	N9-C8-N7	-2.66	108.47	113.40
2	A	301	CXR	N1-C2-N3	-2.65	122.59	125.84
2	B	301	CXR	C2'-C3'-C4'	2.38	107.21	102.61
2	A	301	CXR	O4'-C1'-N9	-2.32	103.10	108.36
2	A	301	CXR	C2'-C3'-C4'	2.31	107.08	102.61
2	B	301	CXR	O2'-C2'-C3'	-2.29	104.46	111.82
2	A	301	CXR	O1B-PB-O2B	2.08	122.13	112.44
2	A	301	CXR	O1A-PA-O3A	2.06	112.84	107.27

All (2) chirality outliers are listed below:

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

All (8) torsion outliers are listed below:

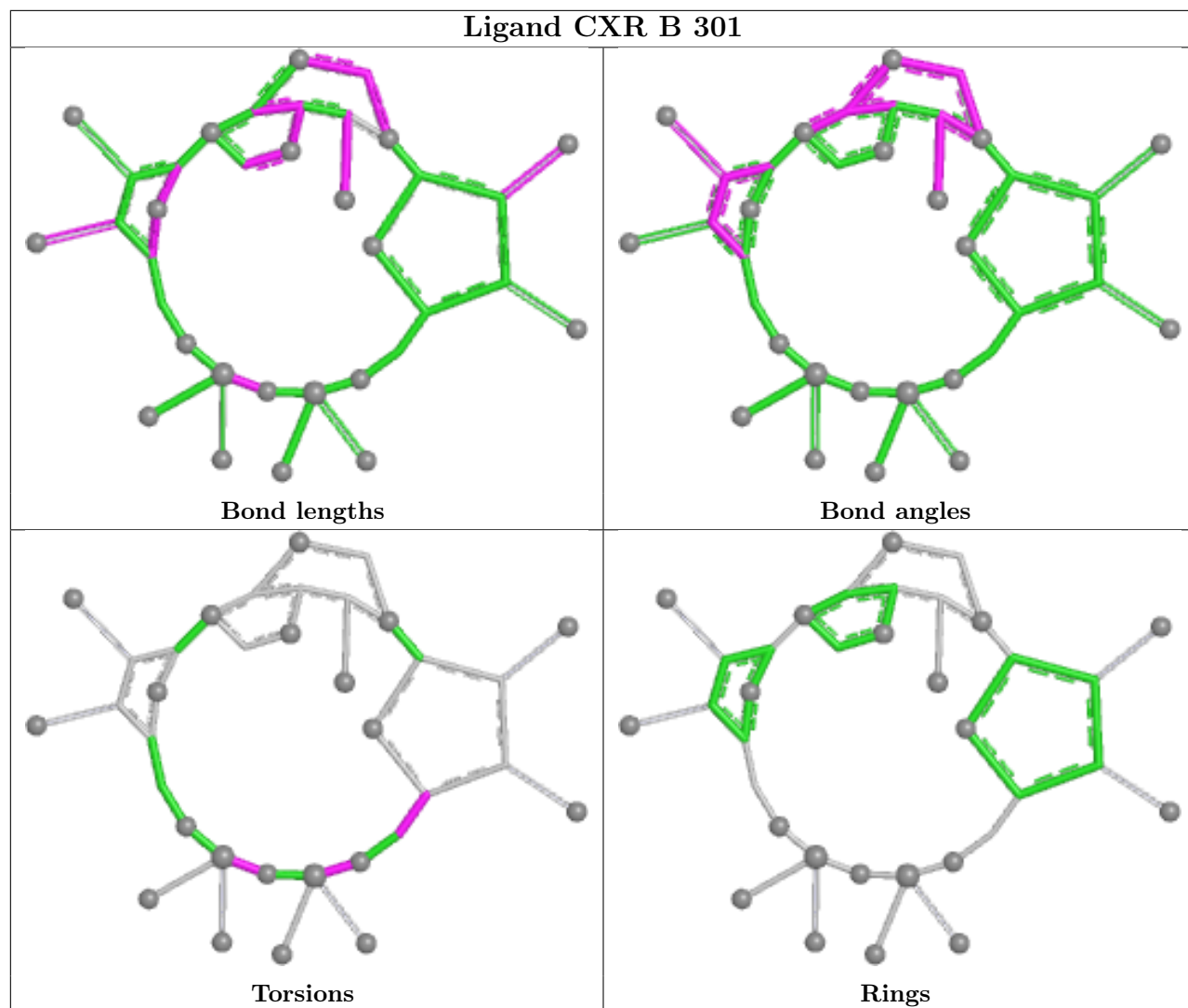
Mol	Chain	Res	Type	Atoms
2	B	301	CXR	C5D-O5D-PB-O2B
2	B	301	CXR	C5D-O5D-PB-O3A
2	B	301	CXR	C5D-O5D-PB-O1B
2	B	301	CXR	C3D-C4D-C5D-O5D
2	B	301	CXR	O4D-C4D-C5D-O5D
2	A	301	CXR	C3'-C4'-C5'-O5'
2	B	301	CXR	PB-O3A-PA-O2A
2	B	301	CXR	PB-O3A-PA-O1A

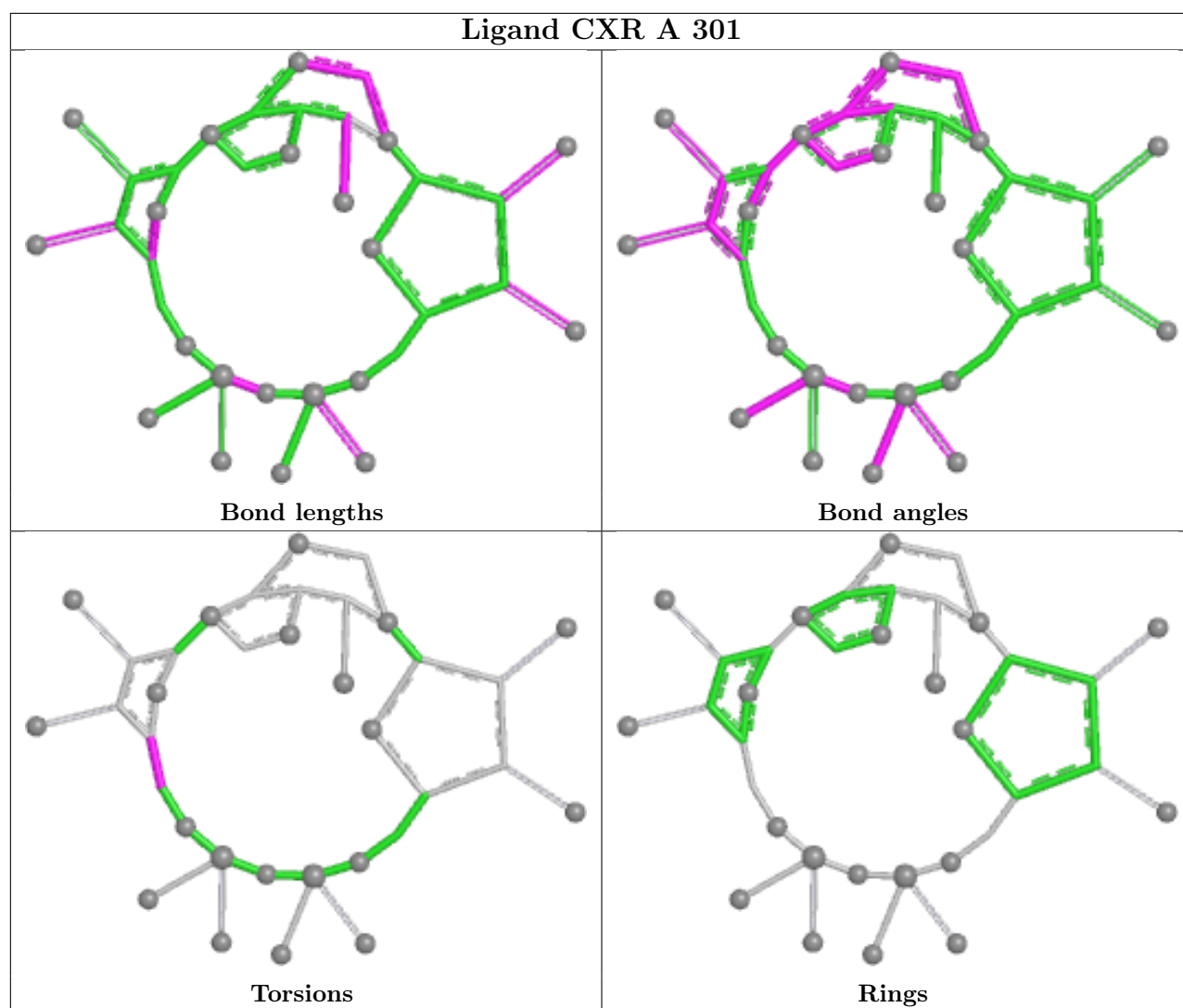
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	CXR	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	252/262 (96%)	1.62	57 (22%) 2 2	28, 34, 47, 64	0
1	B	252/262 (96%)	2.29	143 (56%) 0 0	26, 38, 64, 71	0
All	All	504/524 (96%)	1.95	200 (39%) 1 0	26, 35, 57, 71	0

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	ASP	6.9
1	B	259	ILE	6.2
1	B	296	CYS	6.2
1	B	225	VAL	6.1
1	A	246	GLY	6.1
1	A	248	GLU	6.0
1	B	215	ILE	5.5
1	B	284	PHE	5.1
1	B	266	ILE	5.0
1	B	262	LEU	4.7
1	B	271	ILE	4.7
1	B	226	GLY	4.7
1	B	73	ILE	4.5
1	B	265	ILE	4.5
1	B	254	CYS	4.5
1	B	249	ASP	4.5
1	A	164	ASP	4.4
1	A	79	HIS	4.4
1	B	258	THR	4.3
1	A	227	VAL	4.3
1	A	295	SER	4.3
1	B	236	GLN	4.3
1	B	219	ASP	4.2
1	B	246	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	163	PHE	4.2
1	B	273	PHE	4.2
1	A	247	ARG	4.2
1	B	201	CYS	4.0
1	B	255	GLN	4.0
1	A	250	SER	3.9
1	A	80	VAL	3.8
1	B	227	VAL	3.8
1	B	275	CYS	3.8
1	B	247	ARG	3.8
1	B	222	PHE	3.8
1	B	224	SER	3.8
1	B	292	GLU	3.8
1	B	270	ASN	3.7
1	B	80	VAL	3.7
1	B	281	PRO	3.7
1	B	244	HIS	3.7
1	B	287	CYS	3.7
1	B	159	TRP	3.7
1	B	235	VAL	3.6
1	A	47	ARG	3.6
1	B	223	GLY	3.6
1	B	213	SER	3.6
1	B	295	SER	3.6
1	A	81	ASP	3.5
1	A	294	SER	3.5
1	A	221	THR	3.5
1	B	237	THR	3.5
1	B	285	LEU	3.4
1	B	199	ALA	3.4
1	B	279	TYR	3.4
1	B	267	SER	3.4
1	B	206	VAL	3.4
1	A	290	ASN	3.4
1	B	294	SER	3.3
1	B	50	TRP	3.3
1	B	141	ASP	3.3
1	B	260	LYS	3.3
1	B	253	LEU	3.3
1	B	217	ASP	3.3
1	B	283	LYS	3.3
1	B	185	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	240	ALA	3.3
1	B	291	PRO	3.2
1	B	245	GLY	3.2
1	A	46	TRP	3.2
1	B	138	VAL	3.2
1	B	59	PHE	3.2
1	A	165	THR	3.2
1	B	203	VAL	3.1
1	B	234	LYS	3.1
1	B	228	HIS	3.1
1	B	184	PRO	3.1
1	B	210	GLY	3.1
1	B	214	LYS	3.1
1	B	238	LEU	3.1
1	B	264	SER	3.1
1	B	282	ASP	3.1
1	A	128	ILE	3.1
1	B	221	THR	3.0
1	A	176	TRP	3.0
1	B	231	GLN	3.0
1	A	213	SER	3.0
1	B	204	VAL	3.0
1	A	245	GLY	3.0
1	A	194	ARG	3.0
1	B	212	ARG	2.9
1	B	278	ILE	2.9
1	B	157	LEU	2.9
1	B	119	CYS	2.9
1	B	192	VAL	2.9
1	B	200	ALA	2.9
1	B	216	PHE	2.9
1	B	293	ASP	2.9
1	B	63	VAL	2.9
1	B	160	CYS	2.9
1	B	268	LYS	2.9
1	A	45	PHE	2.8
1	B	229	ASN	2.8
1	B	220	SER	2.8
1	B	197	ALA	2.8
1	A	73	ILE	2.8
1	A	122	ILE	2.8
1	B	107	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	293	ASP	2.8
1	B	91	GLY	2.8
1	B	64	LEU	2.8
1	B	55	THR	2.7
1	A	222	PHE	2.7
1	B	122	ILE	2.7
1	A	75	PRO	2.7
1	B	257	PRO	2.7
1	A	58	ARG	2.7
1	B	135	PHE	2.7
1	B	188	PHE	2.7
1	B	248	GLU	2.7
1	B	53	PRO	2.6
1	B	161	GLY	2.6
1	B	170	TYR	2.6
1	B	252	ASP	2.6
1	A	264	SER	2.6
1	B	280	ARG	2.6
1	A	244	HIS	2.6
1	B	168	ILE	2.6
1	A	163	PHE	2.6
1	A	68	VAL	2.6
1	B	232	PRO	2.6
1	B	256	ASP	2.6
1	A	82	CYS	2.5
1	A	296	CYS	2.5
1	A	143	PHE	2.5
1	B	54	GLY	2.5
1	B	250	SER	2.5
1	B	208	LEU	2.5
1	B	263	GLU	2.5
1	B	116	THR	2.5
1	B	88	ALA	2.5
1	B	101	ILE	2.5
1	B	233	GLU	2.5
1	A	145	LEU	2.5
1	B	286	GLN	2.4
1	B	290	ASN	2.4
1	B	261	GLU	2.4
1	B	243	ILE	2.4
1	B	269	ARG	2.4
1	B	128	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	139	GLN	2.4
1	A	220	SER	2.4
1	B	103	GLU	2.4
1	B	143	PHE	2.4
1	B	176	TRP	2.3
1	B	74	HIS	2.3
1	A	212	ARG	2.3
1	A	84	SER	2.3
1	A	196	PHE	2.3
1	A	127	ARG	2.3
1	B	173	CYS	2.3
1	A	189	TRP	2.3
1	B	189	TRP	2.3
1	A	119	CYS	2.3
1	B	127	ARG	2.3
1	A	125	TRP	2.3
1	B	60	PRO	2.2
1	B	140	ARG	2.2
1	B	158	THR	2.2
1	B	172	SER	2.2
1	A	86	TRP	2.2
1	A	64	LEU	2.2
1	B	142	MET	2.2
1	B	114	THR	2.2
1	A	131	LEU	2.2
1	A	154	ALA	2.2
1	A	279	TYR	2.2
1	B	65	ALA	2.2
1	B	81	ASP	2.2
1	A	85	VAL	2.2
1	B	288	VAL	2.2
1	B	153	LEU	2.1
1	B	75	PRO	2.1
1	B	241	TRP	2.1
1	A	185	VAL	2.1
1	B	251	ARG	2.1
1	A	65	ALA	2.1
1	B	154	ALA	2.1
1	B	277	ASN	2.1
1	B	218	LYS	2.1
1	B	45	PHE	2.1
1	B	126	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	204	VAL	2.1
1	A	59	PHE	2.0
1	B	94	ILE	2.0
1	B	211	SER	2.0
1	A	223	GLY	2.0
1	A	200	ALA	2.0
1	B	230	LEU	2.0
1	B	193	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

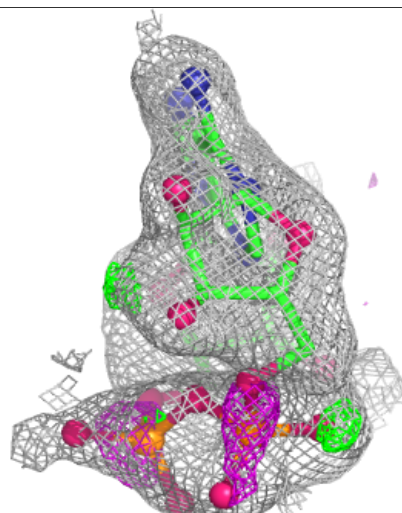
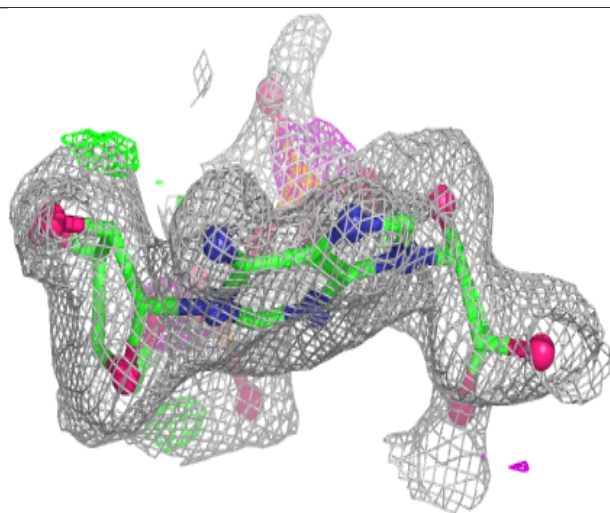
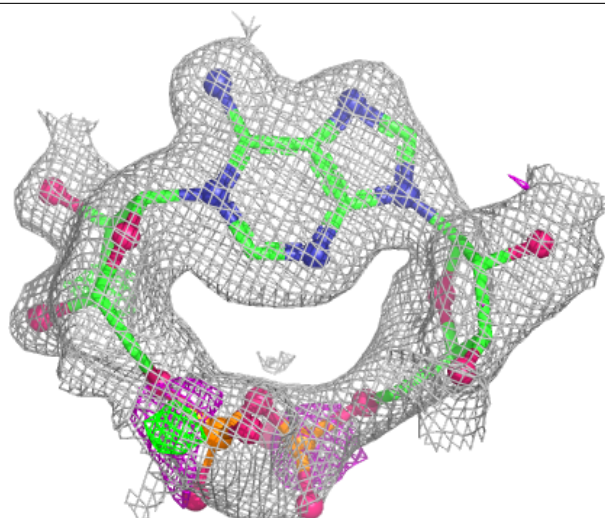
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CXR	B	301	35/35	0.79	0.14	30,44,62,64	0
2	CXR	A	301	35/35	0.92	0.11	21,26,39,42	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.

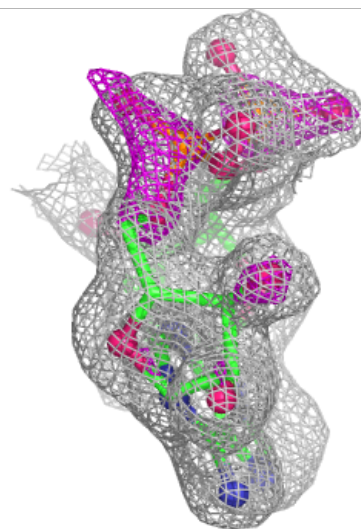
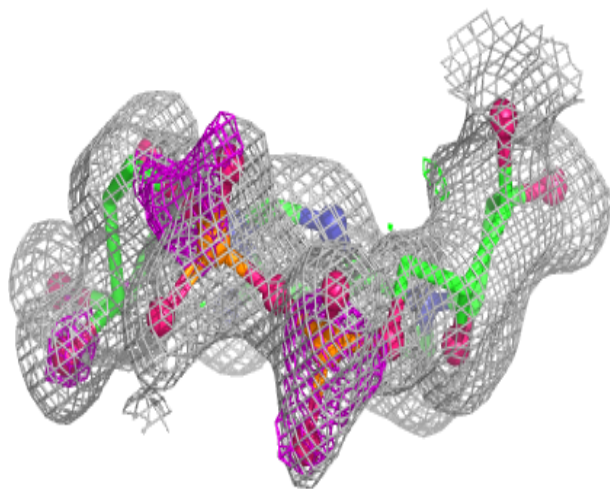
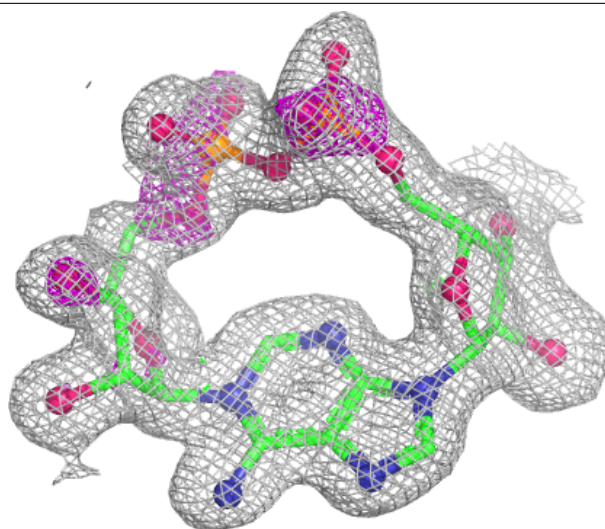
Electron density around CXR B 301:

$2mF_o-DF_c$ (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.