



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:28 AM UTC

PDB ID : 7FTG / pdb_00007ftg
Title : Crystal Structure of human cyclic GMP-AMP synthase in complex with cGAMP
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Deposited on : 2023-02-08
Resolution : 1.73 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

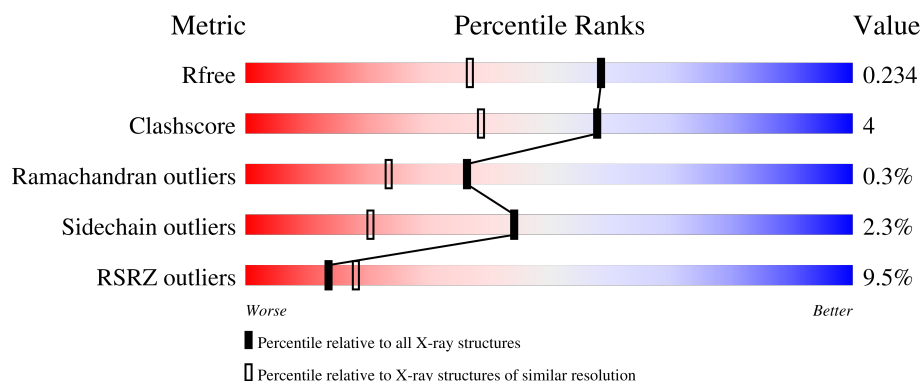
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	362	12% 84% 13% ..
1	B	362	6% 86% 11% .

2 Entry composition [i](#)

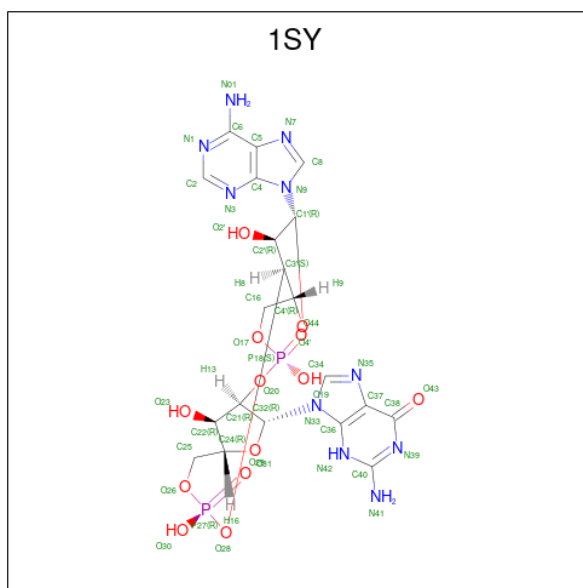
There are 4 unique types of molecules in this entry. The entry contains 6286 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cyclic GMP-AMP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	1	0
			2897	1855	495	531	16			
1	B	353	Total	C	N	O	S	0	1	0
			2908	1861	500	531	16			

- Molecule 2 is cGAMP (CCD ID: 1SY) (formula: $C_{20}H_{24}N_{10}O_{13}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Zn 1	0	0
3	B	1	Total 1	Zn 1	0	0

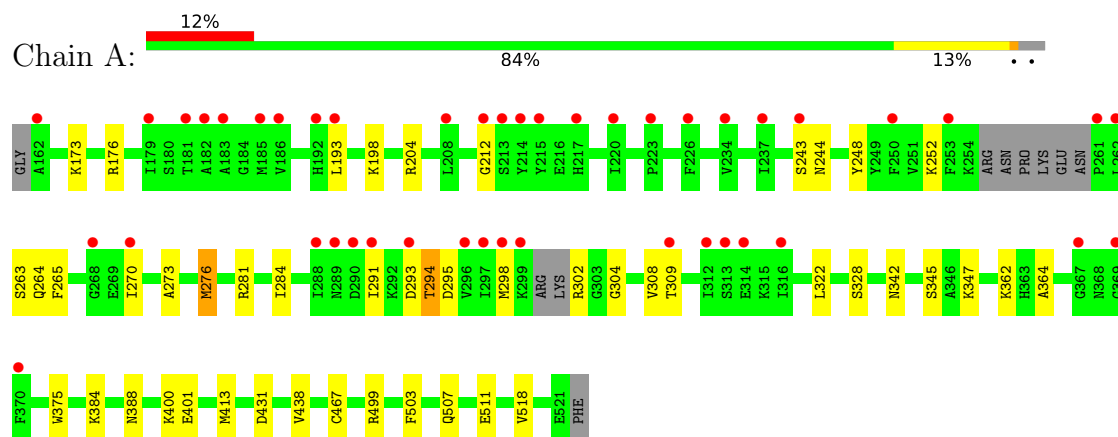
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	190	Total 190	O 190	0	0
4	B	199	Total 199	O 199	0	0

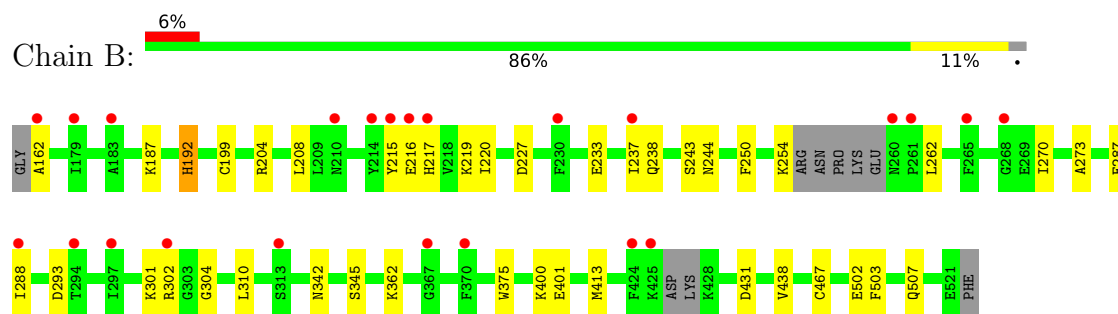
3 Residue-property plots

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: Cyclic GMP-AMP synthase



• Molecule 1: Cyclic GMP-AMP synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.09Å 118.34Å 125.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.89 – 1.73 44.89 – 1.73	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.89-1.73) 96.3 (44.89-1.73)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 1.73Å)	Xtriage
Refinement program	PHENIX 1.11_2558	Depositor
R, R_{free}	0.192 , 0.230 0.197 , 0.234	Depositor DCC
R_{free} test set	3659 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.8	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	0.97	EDS
Total number of atoms	6286	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 73.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8186e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 1SY, ZN

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	0.28	0/2956	0.50	0/3961
1	B	0.30	0/2967	0.51	0/3976
All	All	0.29	0/5923	0.50	0/7937

There are no bond length outliers.

There are no bond angle outliers.

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	2897	0	2937	29	0
1	B	2908	0	2951	24	0
2	A	45	0	22	0	0
2	B	45	0	22	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	190	0	0	4	0
4	B	199	0	0	3	0
All	All	6286	0	5932	53	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 4.

All (53) 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:302:ARG:HH22	1:B:431:ASP:HB3	1.24	1.01
1:A:243:SER:OG	1:A:244:ASN:N	2.18	0.77
1:B:243:SER:OG	1:B:244:ASN:N	2.16	0.75
1:B:288:ILE:HD11	1:B:310:LEU:HD22	1.68	0.74
1:B:238:GLN:HG3	1:B:254:LYS:HB3	1.71	0.73
1:A:212:GLY:O	1:A:384:LYS:NZ	2.22	0.71
1:A:413[B]:MET:HE2	1:A:438:VAL:HG13	1.73	0.68
1:A:400:LYS:NZ	1:A:401:GLU:OE1	2.26	0.68
1:B:413[B]:MET:HE2	1:B:438:VAL:HG13	1.80	0.64
1:A:302:ARG:NH2	1:A:431:ASP:O	2.35	0.60
1:A:198:LYS:HA	1:A:204:ARG:HA	1.88	0.55
1:A:347:LYS:NZ	4:A:706:HOH:O	2.38	0.54
1:B:215:TYR:HD1	1:B:216:GLU:H	1.57	0.52
1:B:162:ALA:N	4:B:1206:HOH:O	2.42	0.52
1:B:502:GLU:OE1	4:B:1201:HOH:O	2.18	0.52
1:A:503:PHE:O	1:A:507:GLN:HG2	2.10	0.51
1:A:265:PHE:CD2	1:A:276:MET:HG2	2.46	0.50
1:B:400:LYS:NZ	1:B:401:GLU:OE1	2.40	0.49
1:A:248:TYR:CG	1:A:364:ALA:HB2	2.48	0.48
1:A:511:GLU:OE2	1:A:518:VAL:HG13	2.14	0.48
1:B:342:ASN:HB2	4:B:1219:HOH:O	2.13	0.48
1:A:248:TYR:HE2	1:A:362:LYS:HG3	1.79	0.48
1:B:187:LYS:HE2	1:B:217:HIS:HD2	1.79	0.48
1:A:413[B]:MET:SD	1:A:467:CYS:HB3	2.54	0.47
1:B:192:HIS:HB3	1:B:287:GLU:OE2	2.14	0.47
1:B:413[B]:MET:HB3	1:B:438:VAL:HG13	1.96	0.47
1:B:208:LEU:HD12	1:B:217:HIS:HB3	1.97	0.47
1:B:250:PHE:HB3	1:B:270:ILE:HD12	1.97	0.47
1:A:173:LYS:HD2	1:A:176:ARG:HH11	1.78	0.47
1:A:294:THR:HG22	1:A:295:ASP:H	1.81	0.46
1:A:264:GLN:NE2	4:A:705:HOH:O	2.36	0.46
1:A:304:GLY:O	1:A:362:LYS:HD2	2.15	0.45
1:A:252:LYS:HG2	1:A:270:ILE:HD13	1.99	0.45
1:B:413[B]:MET:SD	1:B:467:CYS:HB3	2.56	0.45
1:B:302:ARG:H	1:B:302:ARG:HG3	1.48	0.45
1:B:413[B]:MET:HB3	1:B:438:VAL:CG1	2.48	0.44
1:B:219:LYS:HB3	1:B:227:ASP:HB3	2.00	0.44
1:A:413[B]:MET:HB3	1:A:438:VAL:HG13	2.01	0.43
1:A:276:MET:HE2	1:A:276:MET:HB3	1.77	0.42
1:B:288:ILE:HD11	1:B:310:LEU:CD2	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:GLY:O	1:B:362:LYS:HD2	2.19	0.42
1:A:499:ARG:HG3	4:A:853:HOH:O	2.19	0.42
1:B:273:ALA:HA	1:B:375:TRP:CZ2	2.55	0.42
1:B:503:PHE:O	1:B:507:GLN:HG2	2.20	0.42
1:A:273:ALA:HA	1:A:375:TRP:CZ2	2.55	0.42
1:A:281:ARG:HH11	1:A:308:VAL:HG22	1.84	0.41
1:A:511:GLU:CD	1:A:518:VAL:HG13	2.45	0.41
1:A:384:LYS:HE3	1:A:388:ASN:ND2	2.35	0.41
1:A:291:ILE:HG12	1:A:293:ASP:H	1.86	0.41
1:B:187:LYS:HE3	1:B:215:TYR:CD2	2.56	0.41
1:A:193:LEU:HD21	1:A:284:ILE:HG23	2.03	0.41
1:A:342:ASN:HB2	4:A:721:HOH:O	2.20	0.41
1:A:276:MET:HE2	1:A:322:LEU:HD21	2.02	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	347/362 (96%)	333 (96%)	13 (4%)	1 (0%)	36	23
1	B	348/362 (96%)	335 (96%)	12 (3%)	1 (0%)	36	23
All	All	695/724 (96%)	668 (96%)	25 (4%)	2 (0%)	36	23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	345	SER
1	B	345	SER

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	326/334 (98%)	320 (98%)	6 (2%)	51	30
1	B	327/334 (98%)	318 (97%)	9 (3%)	38	15
All	All	653/668 (98%)	638 (98%)	15 (2%)	44	20

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

Mol	Chain	Res	Type
1	A	263	SER
1	A	276	MET
1	A	294	THR
1	A	298	MET
1	A	309	THR
1	A	328	SER
1	B	192	HIS
1	B	199	CYS
1	B	204	ARG
1	B	220	ILE
1	B	233	GLU
1	B	237	ILE
1	B	262	LEU
1	B	293	ASP
1	B	301	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	HIS
1	A	264	GLN
1	A	429	HIS
1	A	514	ASN
1	B	217	HIS
1	B	494	ASN
1	B	514	ASN

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 ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	1SY	A	601	-	51,51,51	2.70	19 (37%)	70,80,80	2.12	18 (25%)
2	1SY	B	1101	-	51,51,51	2.66	19 (37%)	70,80,80	2.03	15 (21%)

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	1SY	A	601	-	-	7/30/62/62	0/6/7/7
2	1SY	B	1101	-	-	6/30/62/62	0/6/7/7

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	1SY	C36-N42	7.06	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	1SY	C36-N42	6.41	1.48	1.37
2	B	1101	1SY	C36-N33	-6.27	1.30	1.37
2	A	601	1SY	C36-N33	-5.92	1.31	1.37
2	B	1101	1SY	C6-N01	5.86	1.49	1.34
2	A	601	1SY	C40-N41	5.84	1.47	1.34
2	A	601	1SY	C6-N01	5.69	1.48	1.34
2	B	1101	1SY	C40-N41	5.59	1.47	1.34
2	A	601	1SY	P18-O20	5.05	1.74	1.59
2	B	1101	1SY	P18-O20	4.82	1.73	1.59
2	B	1101	1SY	C38-N39	4.58	1.45	1.38
2	A	601	1SY	C38-N39	4.47	1.45	1.38
2	A	601	1SY	C21-C32	-4.44	1.42	1.53
2	A	601	1SY	P27-O28	4.22	1.72	1.59
2	B	1101	1SY	C21-C32	-4.17	1.42	1.53
2	B	1101	1SY	C40-N39	4.12	1.43	1.33
2	B	1101	1SY	P27-O28	4.11	1.71	1.59
2	A	601	1SY	C3'-C4'	-4.02	1.42	1.52
2	A	601	1SY	P18-O17	3.94	1.74	1.59
2	B	1101	1SY	C3'-C4'	-3.91	1.42	1.52
2	A	601	1SY	C40-N39	3.84	1.42	1.33
2	B	1101	1SY	P18-O17	3.46	1.73	1.59
2	A	601	1SY	C40-N42	2.88	1.44	1.37
2	B	1101	1SY	C40-N42	2.71	1.44	1.37
2	A	601	1SY	P27-O26	2.70	1.70	1.59
2	B	1101	1SY	P27-O26	2.70	1.69	1.59
2	A	601	1SY	C38-C37	2.66	1.52	1.45
2	A	601	1SY	O31-C32	2.60	1.48	1.42
2	B	1101	1SY	O31-C32	2.52	1.47	1.42
2	B	1101	1SY	C8-N7	2.51	1.36	1.31
2	A	601	1SY	C8-N7	2.45	1.36	1.31
2	A	601	1SY	C22-C21	-2.43	1.47	1.53
2	B	1101	1SY	C22-C21	-2.33	1.47	1.53
2	B	1101	1SY	C38-C37	2.28	1.51	1.45
2	B	1101	1SY	C5-N7	-2.21	1.35	1.39
2	B	1101	1SY	C8-N9	-2.19	1.33	1.37
2	A	601	1SY	C5-C4	-2.10	1.35	1.39
2	A	601	1SY	C25-C24	-2.05	1.45	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	1SY	N3-C2-N1	-6.13	119.31	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	1SY	N9-C8-N7	-6.00	105.42	113.94
2	B	1101	1SY	N9-C8-N7	-5.91	105.55	113.94
2	B	1101	1SY	N3-C2-N1	-5.81	119.79	128.58
2	A	601	1SY	C4-N9-C8	5.53	111.54	105.74
2	B	1101	1SY	C4-N9-C8	5.42	111.43	105.74
2	A	601	1SY	C32-N33-C34	-4.84	112.98	126.73
2	A	601	1SY	C34-N33-C36	4.65	110.59	106.67
2	B	1101	1SY	C5-C4-N3	-4.53	120.48	126.72
2	B	1101	1SY	C37-C36-N33	4.40	108.28	106.25
2	A	601	1SY	C5-C4-N3	-4.21	120.92	126.72
2	B	1101	1SY	C32-N33-C34	-4.08	115.14	126.73
2	A	601	1SY	N33-C34-N35	-4.05	105.90	113.40
2	B	1101	1SY	C34-N33-C36	3.98	110.03	106.67
2	B	1101	1SY	N3-C4-N9	3.96	133.91	127.17
2	B	1101	1SY	N33-C34-N35	-3.76	106.42	113.40
2	A	601	1SY	N3-C4-N9	3.54	133.18	127.17
2	A	601	1SY	C37-C36-N33	3.48	107.86	106.25
2	B	1101	1SY	C5-N7-C8	3.40	108.80	103.45
2	A	601	1SY	C5-N7-C8	3.36	108.73	103.45
2	A	601	1SY	C2-N3-C4	3.34	119.98	111.83
2	B	1101	1SY	C2-N3-C4	3.18	119.59	111.83
2	A	601	1SY	C3'-C2'-C1'	2.73	105.90	99.89
2	A	601	1SY	O30-P27-O28	2.56	117.12	106.70
2	B	1101	1SY	C3'-C2'-C1'	2.36	105.07	99.89
2	B	1101	1SY	C24-O31-C32	-2.32	104.34	109.47
2	A	601	1SY	C34-N35-C37	2.29	108.35	104.26
2	A	601	1SY	O31-C32-C21	2.20	110.37	106.59
2	A	601	1SY	C24-O31-C32	-2.19	104.62	109.47
2	A	601	1SY	N42-C40-N39	-2.17	119.36	123.32
2	B	1101	1SY	O30-P27-O28	2.11	115.28	106.70
2	B	1101	1SY	C34-N35-C37	2.05	107.91	104.26
2	A	601	1SY	C4-N9-C1'	-2.00	121.95	126.63

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	1SY	C16-O17-P18-O19
2	A	601	1SY	C16-O17-P18-O20
2	A	601	1SY	C16-O17-P18-O44
2	A	601	1SY	C21-O20-P18-O17
2	B	1101	1SY	C16-O17-P18-O19

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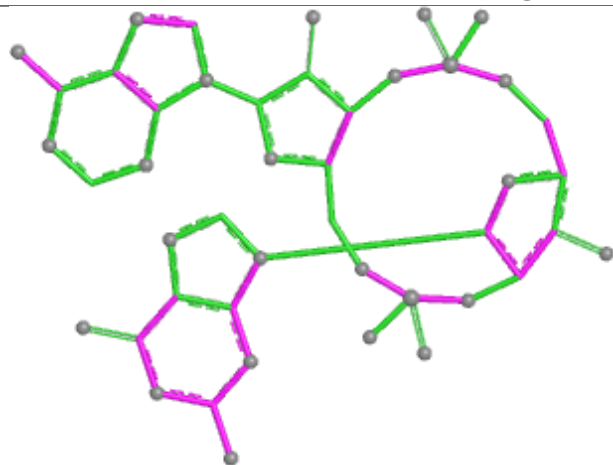
Mol	Chain	Res	Type	Atoms
2	B	1101	1SY	C16-O17-P18-O20
2	B	1101	1SY	C16-O17-P18-O44
2	A	601	1SY	C22-C24-C25-O26
2	A	601	1SY	C25-O26-P27-O29
2	B	1101	1SY	C21-O20-P18-O17
2	A	601	1SY	O31-C24-C25-O26
2	B	1101	1SY	C22-C24-C25-O26
2	B	1101	1SY	C21-O20-P18-O44

There are no ring outliers.

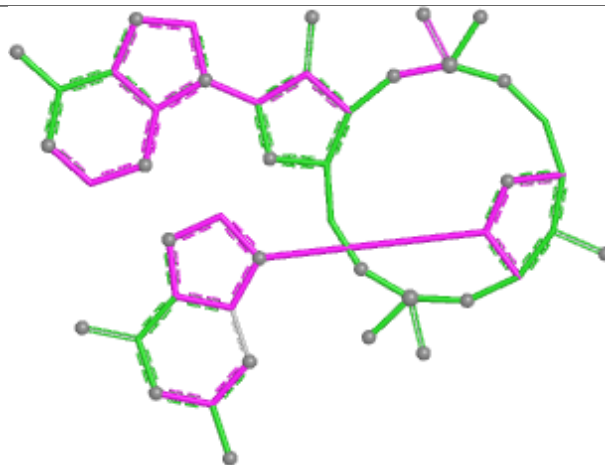
No monomer is involved in short contacts.

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.

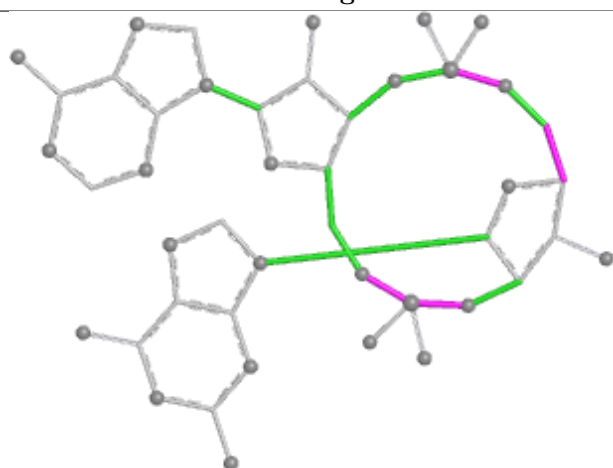
Ligand 1SY A 601



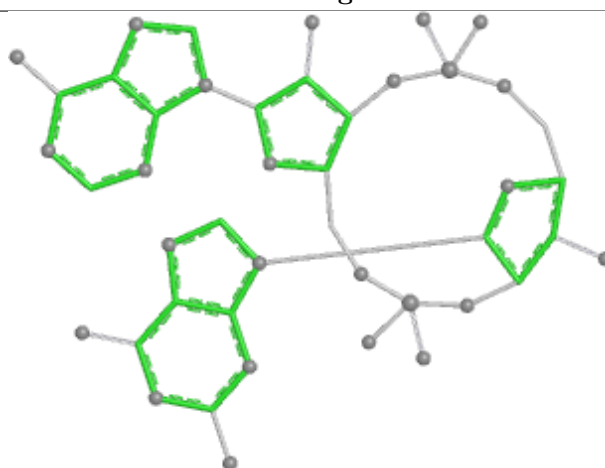
Bond lengths



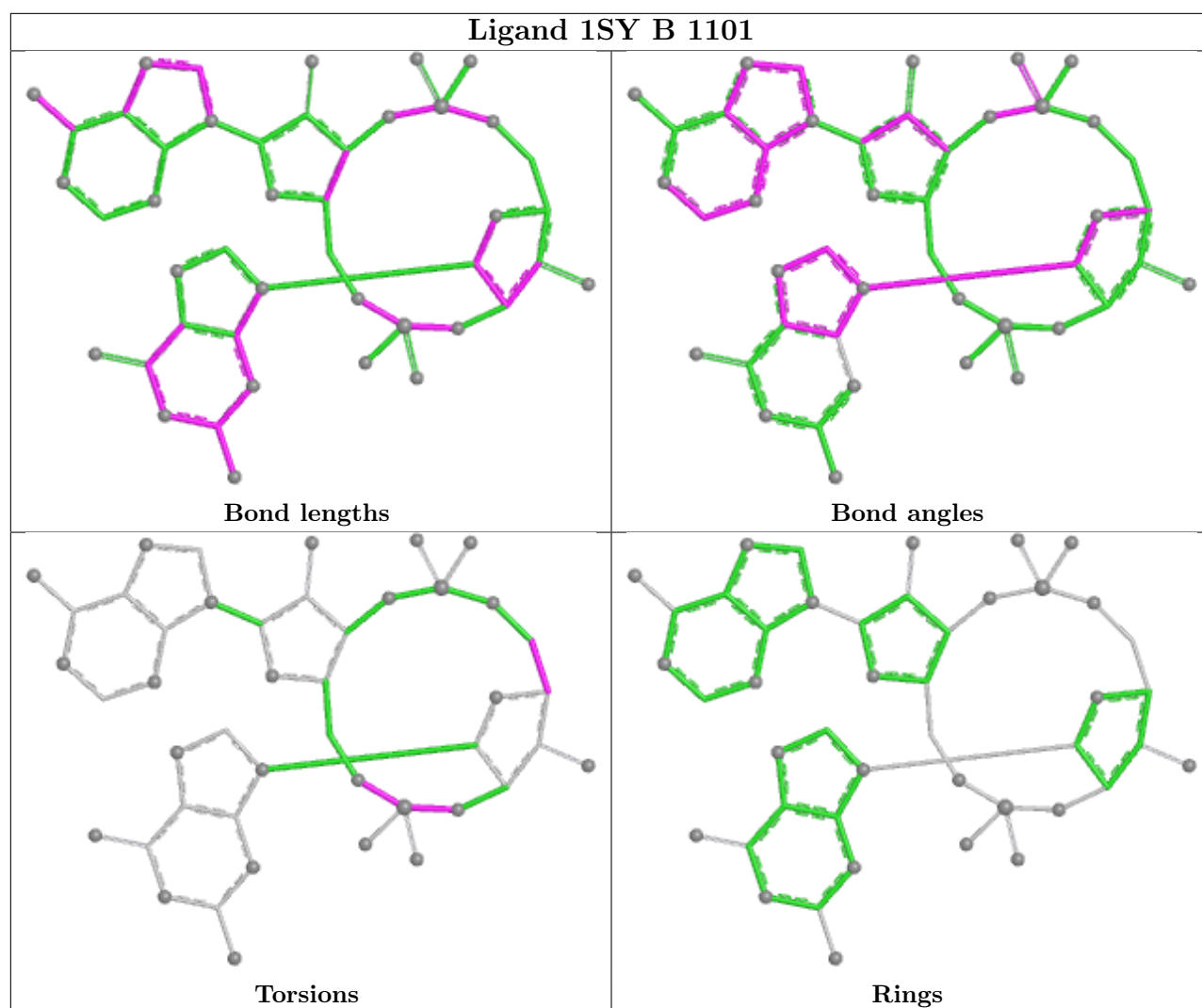
Bond angles



Torsions



Rings



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	352/362 (97%)	0.72	44 (12%) 8 10	17, 50, 112, 160	1 (0%)
1	B	353/362 (97%)	0.48	23 (6%) 25 30	17, 45, 90, 148	1 (0%)
All	All	705/724 (97%)	0.60	67 (9%) 14 18	17, 47, 104, 160	2 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	261	PRO	5.8
1	A	223	PRO	4.5
1	A	215	TYR	4.4
1	B	215	TYR	4.2
1	A	183	ALA	3.9
1	B	424	PHE	3.5
1	A	288	ILE	3.4
1	A	179	ILE	3.4
1	A	297	ILE	3.4
1	A	367	GLY	3.4
1	A	253	PHE	3.2
1	B	162	ALA	3.0
1	B	294	THR	2.9
1	A	182	ALA	2.9
1	A	268	GLY	2.9
1	A	291	ILE	2.9
1	A	226	PHE	2.8
1	A	217	HIS	2.8
1	B	217	HIS	2.8
1	B	367	GLY	2.8
1	A	370	PHE	2.8
1	A	289	ASN	2.7
1	A	212	GLY	2.7
1	B	260	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	265	PHE	2.7
1	A	186	VAL	2.7
1	B	313	SER	2.7
1	A	214	TYR	2.6
1	B	179	ILE	2.6
1	B	288	ILE	2.6
1	A	262	LEU	2.6
1	B	297	ILE	2.5
1	A	162	ALA	2.5
1	A	296	VAL	2.5
1	A	234	VAL	2.5
1	A	192	HIS	2.4
1	A	312	ILE	2.4
1	A	309	THR	2.4
1	B	268	GLY	2.3
1	B	370	PHE	2.3
1	A	270	ILE	2.3
1	A	193	LEU	2.3
1	B	230	PHE	2.3
1	B	302	ARG	2.3
1	B	425	LYS	2.3
1	B	183	ALA	2.3
1	A	250	PHE	2.3
1	A	316	ILE	2.3
1	A	369	GLY	2.3
1	A	208	LEU	2.2
1	A	220	ILE	2.2
1	B	210	ASN	2.2
1	A	313	SER	2.2
1	B	261	PRO	2.2
1	A	299	LYS	2.2
1	A	314	GLU	2.2
1	A	243	SER	2.2
1	A	298	MET	2.1
1	B	216	GLU	2.1
1	A	237	ILE	2.1
1	A	185	MET	2.1
1	A	290	ASP	2.1
1	A	181	THR	2.1
1	B	214	TYR	2.0
1	B	237	ILE	2.0
1	A	293	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	213	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](#)

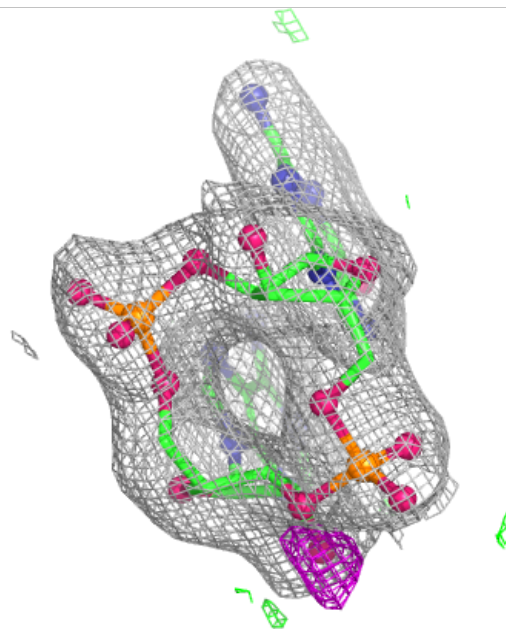
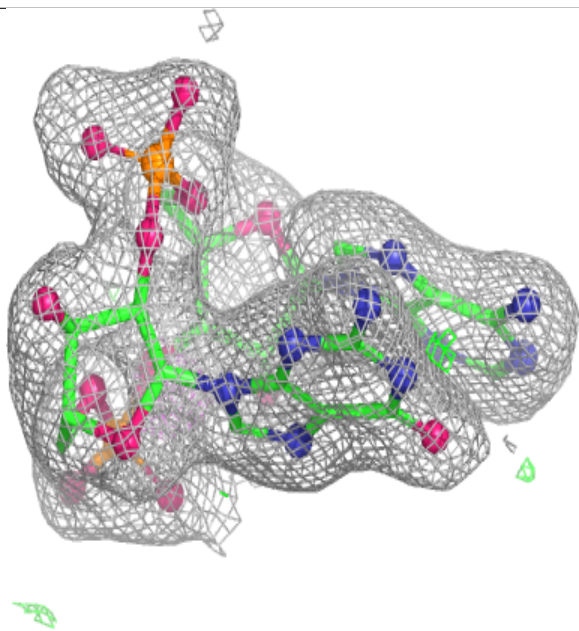
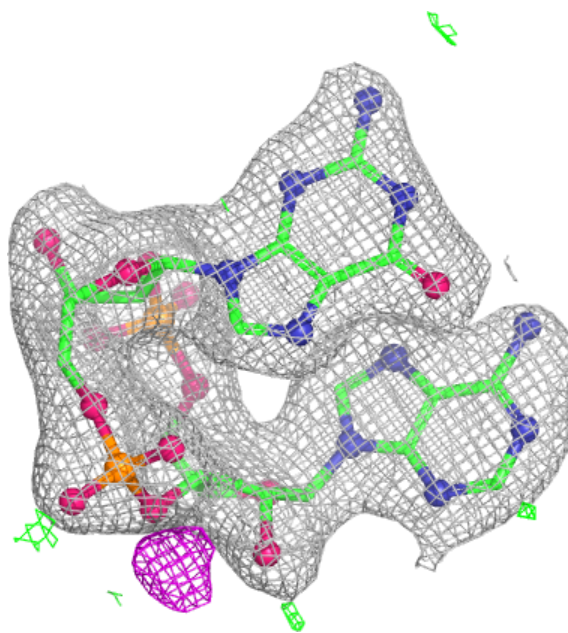
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	1SY	A	601	45/45	0.93	0.08	34,49,65,72	0
2	1SY	B	1101	45/45	0.95	0.07	31,40,48,54	0
3	ZN	A	602	1/1	0.99	0.02	28,28,28,28	0
3	ZN	B	1102	1/1	0.99	0.03	27,27,27,27	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.

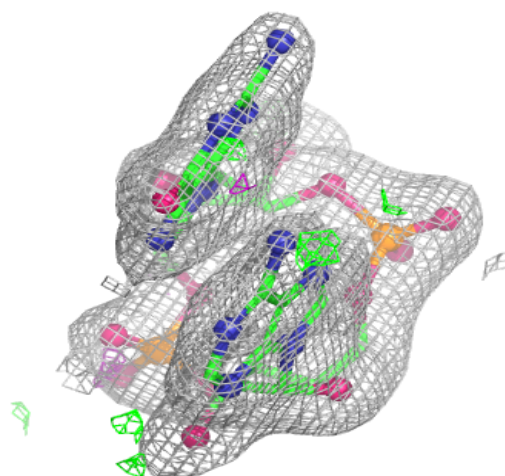
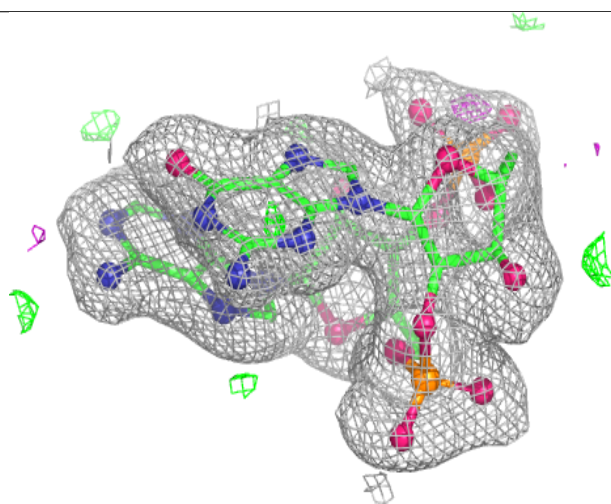
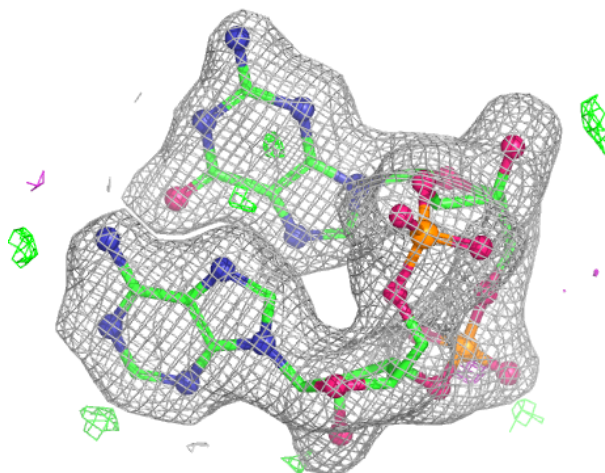
Electron density around 1SY A 601:

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



Electron density around 1SY B 1101:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.