



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:32 PM UTC

PDB ID : 5GRM / pdb_00005grm
Title : Crystal structure of rat STING in complex with cyclic GMP-AMP with 2'5' and 3'5' phosphodiester linkage (2'3'-cGAMP)
Authors : Zhang, H.; Han, M.J.; Tao, J.L.; Ye, Z.Y.; Du, X.X.; Deng, M.J.; Zhang, X.Y.; Li, L.F.; Jiang, Z.F.; Su, X.D.
Deposited on : 2016-08-11
Resolution : 1.55 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

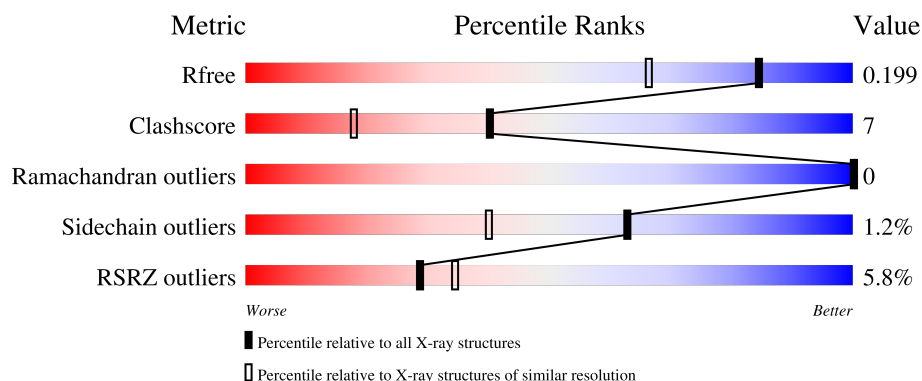
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	210	5% 40% 46% 10%
1	B	210	6% 39% 46% 6% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3473 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 Stimulator of interferon genes protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1503	945	270	279	9			
1	B	190	Total	C	N	O	S	0	0	0
			1519	951	272	287	9			

There are 46 discrepancies between the modelled and reference sequences:

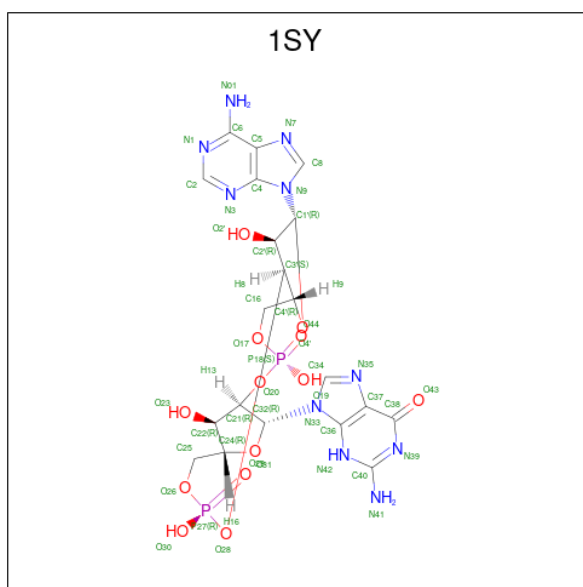
Chain	Residue	Modelled	Actual	Comment	Reference
A	132	MET	-	expression tag	UNP F1M391
A	133	GLY	-	expression tag	UNP F1M391
A	134	SER	-	expression tag	UNP F1M391
A	135	SER	-	expression tag	UNP F1M391
A	136	HIS	-	expression tag	UNP F1M391
A	137	HIS	-	expression tag	UNP F1M391
A	138	HIS	-	expression tag	UNP F1M391
A	139	HIS	-	expression tag	UNP F1M391
A	140	HIS	-	expression tag	UNP F1M391
A	141	HIS	-	expression tag	UNP F1M391
A	142	SER	-	expression tag	UNP F1M391
A	143	SER	-	expression tag	UNP F1M391
A	144	GLY	-	expression tag	UNP F1M391
A	145	GLU	-	expression tag	UNP F1M391
A	146	ASN	-	expression tag	UNP F1M391
A	147	LEU	-	expression tag	UNP F1M391
A	148	TYR	-	expression tag	UNP F1M391
A	149	PHE	-	expression tag	UNP F1M391
A	150	GLN	-	expression tag	UNP F1M391
A	151	GLY	-	expression tag	UNP F1M391
A	152	SER	-	expression tag	UNP F1M391
A	153	HIS	-	expression tag	UNP F1M391
A	154	MET	-	expression tag	UNP F1M391
B	132	MET	-	expression tag	UNP F1M391
B	133	GLY	-	expression tag	UNP F1M391

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Chain	Residue	Modelled	Actual	Comment	Reference
B	134	SER	-	expression tag	UNP F1M391
B	135	SER	-	expression tag	UNP F1M391
B	136	HIS	-	expression tag	UNP F1M391
B	137	HIS	-	expression tag	UNP F1M391
B	138	HIS	-	expression tag	UNP F1M391
B	139	HIS	-	expression tag	UNP F1M391
B	140	HIS	-	expression tag	UNP F1M391
B	141	HIS	-	expression tag	UNP F1M391
B	142	SER	-	expression tag	UNP F1M391
B	143	SER	-	expression tag	UNP F1M391
B	144	GLY	-	expression tag	UNP F1M391
B	145	GLU	-	expression tag	UNP F1M391
B	146	ASN	-	expression tag	UNP F1M391
B	147	LEU	-	expression tag	UNP F1M391
B	148	TYR	-	expression tag	UNP F1M391
B	149	PHE	-	expression tag	UNP F1M391
B	150	GLN	-	expression tag	UNP F1M391
B	151	GLY	-	expression tag	UNP F1M391
B	152	SER	-	expression tag	UNP F1M391
B	153	HIS	-	expression tag	UNP F1M391
B	154	MET	-	expression tag	UNP F1M391

- Molecule 2 is cGAMP (CCD ID: 1SY) (formula: $C_{20}H_{24}N_{10}O_{13}P_2$).



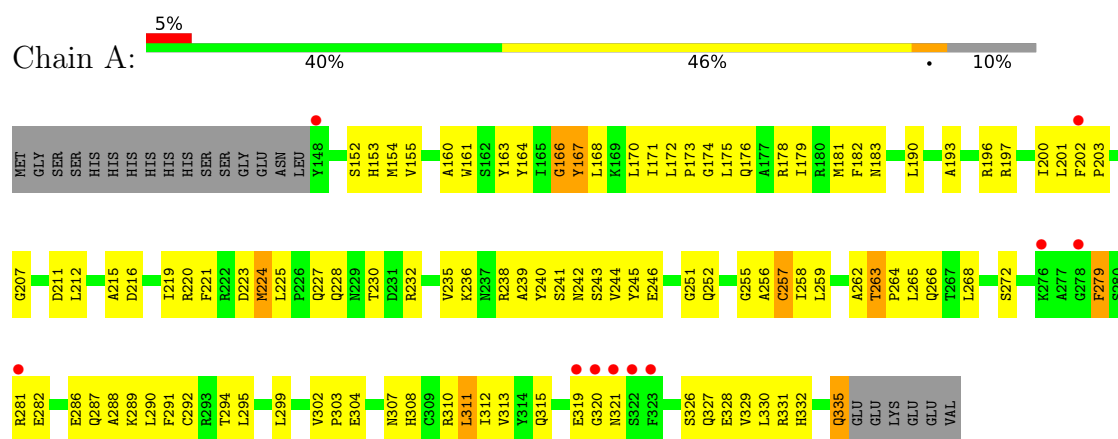
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	211	Total 211	O 211	0	0
3	B	195	Total 195	O 195	0	0

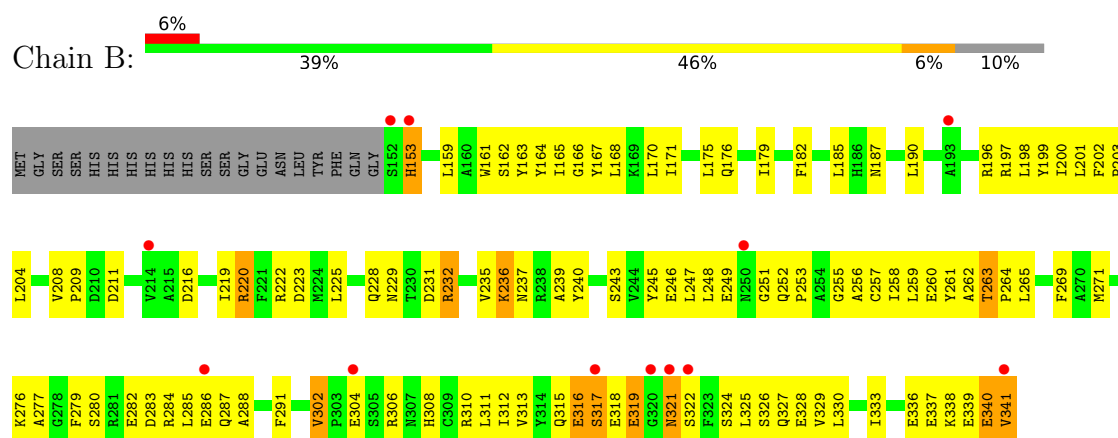
3 Residue-property plots [i](#)

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: Stimulator of interferon genes protein



- Molecule 1: Stimulator of interferon genes protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	77.20Å 77.20Å 152.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.38 – 1.55 42.38 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.38-1.55) 99.8 (42.38-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 1.55Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.181 , 0.193 (Not available) , 0.199	Depositor DCC
R_{free} test set	3407 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3473	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 4.61% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1SY

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	2.35	99/1534 (6.5%)	1.10	8/2072 (0.4%)
1	B	2.30	94/1548 (6.1%)	1.28	9/2090 (0.4%)
All	All	2.33	193/3082 (6.3%)	1.20	17/4162 (0.4%)

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 (193) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	TYR	C-O	-22.18	0.96	1.24
1	A	167	TYR	N-CA	17.89	1.69	1.46
1	A	167	TYR	C-N	12.65	1.51	1.33
1	B	255	GLY	C-O	-9.64	1.14	1.23
1	B	263	THR	C-O	-9.07	1.16	1.24
1	A	263	THR	C-O	-8.77	1.16	1.24
1	B	220	ARG	C-O	-8.65	1.14	1.24
1	B	321	ASN	CA-C	-8.32	1.40	1.52
1	A	172	LEU	C-O	-8.08	1.16	1.24
1	A	171	ILE	C-O	-7.97	1.16	1.24
1	B	175	LEU	C-O	-7.86	1.15	1.24
1	B	202	PHE	C-O	-7.85	1.15	1.24
1	A	330	LEU	C-O	-7.83	1.15	1.24
1	B	228	GLN	C-O	-7.57	1.14	1.24
1	A	235	VAL	C-O	-7.57	1.15	1.23
1	A	245	TYR	C-O	-7.51	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	201	LEU	C-O	-7.46	1.14	1.24
1	B	262	ALA	C-O	-7.40	1.15	1.24
1	A	220	ARG	C-O	-7.38	1.15	1.24
1	A	240	TYR	C-O	-7.36	1.15	1.24
1	B	324	SER	C-O	-7.32	1.15	1.24
1	B	209	PRO	C-O	-7.31	1.15	1.23
1	B	166	GLY	C-O	-7.21	1.17	1.24
1	A	225	LEU	C-O	-7.19	1.14	1.23
1	B	232	ARG	C-O	-7.13	1.15	1.24
1	A	239	ALA	C-O	-7.08	1.15	1.24
1	A	178	ARG	C-O	-7.07	1.15	1.24
1	B	245	TYR	C-O	-7.05	1.14	1.23
1	A	289	LYS	C-O	-7.05	1.15	1.24
1	B	239	ALA	C-O	-7.04	1.15	1.24
1	B	259	LEU	C-O	-7.03	1.15	1.23
1	B	310	ARG	C-O	-7.02	1.16	1.24
1	A	216	ASP	C-O	-7.02	1.15	1.24
1	A	176	GLN	C-O	-6.98	1.15	1.24
1	B	153	HIS	CA-CB	-6.96	1.44	1.53
1	A	154	MET	C-O	-6.91	1.15	1.23
1	A	313	VAL	C-O	-6.89	1.16	1.24
1	A	311	LEU	C-O	-6.84	1.15	1.24
1	A	290	LEU	C-O	-6.82	1.16	1.24
1	B	329	VAL	C-O	-6.82	1.16	1.24
1	B	279	PHE	C-O	-6.79	1.16	1.24
1	A	193	ALA	C-O	-6.76	1.16	1.24
1	A	279	PHE	C-O	-6.76	1.16	1.24
1	B	291	PHE	C-O	-6.71	1.16	1.24
1	B	216	ASP	C-O	-6.70	1.15	1.24
1	A	238	ARG	C-O	-6.62	1.16	1.23
1	B	236	LYS	C-O	-6.62	1.16	1.23
1	A	288	ALA	C-O	-6.62	1.16	1.24
1	B	336	GLU	C-O	-6.59	1.16	1.24
1	B	235	VAL	C-O	-6.55	1.16	1.23
1	A	166	GLY	C-O	-6.54	1.18	1.24
1	B	232	ARG	CZ-NH2	-6.54	1.25	1.33
1	B	280	SER	C-O	-6.52	1.15	1.23
1	B	284	ARG	C-O	-6.51	1.16	1.24
1	B	182	PHE	C-O	-6.50	1.16	1.24
1	B	243	SER	C-O	-6.48	1.16	1.24
1	B	287	GLN	C-O	-6.47	1.16	1.24
1	A	243	SER	C-O	-6.47	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	GLY	C-O	-6.46	1.16	1.23
1	B	225	LEU	C-O	-6.46	1.15	1.23
1	B	167	TYR	C-O	-6.44	1.15	1.24
1	A	310	ARG	C-O	-6.43	1.16	1.24
1	A	246	GLU	C-O	-6.39	1.16	1.23
1	A	307	ASN	C-O	-6.38	1.16	1.23
1	B	333	ILE	C-O	-6.38	1.17	1.24
1	A	241	SER	C-O	-6.38	1.15	1.23
1	A	266	GLN	C-O	-6.37	1.16	1.24
1	A	302	VAL	C-O	-6.36	1.16	1.24
1	A	326	SER	C-O	-6.33	1.16	1.24
1	B	248	LEU	C-O	-6.32	1.16	1.23
1	B	208	VAL	C-O	-6.31	1.16	1.24
1	B	170	LEU	C-O	-6.31	1.16	1.24
1	A	203	PRO	C-O	-6.31	1.17	1.23
1	B	153	HIS	CA-C	-6.30	1.45	1.53
1	B	161	TRP	C-O	-6.30	1.16	1.24
1	A	219	ILE	C-O	-6.29	1.17	1.24
1	B	321	ASN	N-CA	-6.26	1.37	1.46
1	A	227	GLN	C-O	-6.25	1.16	1.23
1	A	196	ARG	C-O	-6.24	1.15	1.24
1	A	262	ALA	C-O	-6.24	1.16	1.24
1	B	337	GLU	C-O	-6.21	1.16	1.24
1	B	282	GLU	C-O	-6.20	1.16	1.24
1	B	302	VAL	C-O	-6.20	1.16	1.24
1	B	163	TYR	C-O	-6.19	1.16	1.24
1	B	159	LEU	C-O	-6.18	1.16	1.24
1	A	230	THR	C-O	-6.17	1.17	1.23
1	B	190	LEU	C-O	-6.15	1.16	1.24
1	A	329	VAL	C-O	-6.11	1.17	1.24
1	A	303	PRO	C-O	-6.09	1.16	1.23
1	A	197	ARG	C-O	-6.07	1.16	1.23
1	A	228	GLN	C-O	-6.03	1.16	1.23
1	B	256	ALA	C-O	-6.01	1.16	1.23
1	B	240	TYR	C-O	-6.00	1.17	1.24
1	B	330	LEU	C-O	-5.99	1.16	1.24
1	B	326	SER	C-O	-5.96	1.17	1.24
1	B	283	ASP	C-O	-5.96	1.16	1.24
1	A	179	ILE	C-O	-5.95	1.17	1.24
1	A	164	TYR	C-O	-5.93	1.17	1.24
1	A	287	GLN	C-O	-5.92	1.17	1.24
1	A	265	LEU	C-O	-5.92	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	ASN	C-O	-5.92	1.16	1.23
1	B	203	PRO	C-O	-5.92	1.16	1.23
1	B	265	LEU	C-O	-5.90	1.16	1.24
1	B	223	ASP	C-O	-5.89	1.17	1.23
1	A	282	GLU	C-O	-5.88	1.17	1.24
1	A	232	ARG	C-O	-5.88	1.17	1.23
1	A	294	THR	C-O	-5.87	1.17	1.24
1	A	182	PHE	C-O	-5.87	1.17	1.24
1	A	244	VAL	C-O	-5.85	1.17	1.24
1	A	257	CYS	C-O	-5.85	1.17	1.23
1	B	185	LEU	C-O	-5.85	1.17	1.24
1	B	288	ALA	C-O	-5.84	1.17	1.24
1	A	212	LEU	C-O	-5.83	1.16	1.24
1	A	181	MET	C-O	-5.81	1.17	1.24
1	A	207	GLY	C-O	-5.81	1.16	1.23
1	A	224	MET	C-O	-5.80	1.16	1.23
1	B	260	GLU	C-O	-5.80	1.17	1.23
1	B	211	ASP	C-O	-5.76	1.17	1.24
1	A	201	LEU	C-O	-5.76	1.17	1.24
1	B	261	TYR	C-O	-5.75	1.16	1.23
1	B	312	ILE	C-O	-5.74	1.17	1.24
1	A	299	LEU	C-O	-5.73	1.16	1.24
1	B	311	LEU	C-O	-5.72	1.17	1.24
1	A	304	GLU	C-O	-5.71	1.17	1.24
1	A	312	ILE	C-O	-5.70	1.17	1.24
1	B	198	LEU	C-O	-5.70	1.17	1.24
1	B	258	ILE	C-O	-5.70	1.17	1.24
1	B	200	ILE	C-O	-5.69	1.18	1.24
1	B	269	PHE	C-O	-5.69	1.17	1.24
1	A	256	ALA	CA-CB	-5.66	1.43	1.53
1	A	160	ALA	C-O	-5.64	1.17	1.24
1	A	163	TYR	C-O	-5.62	1.17	1.24
1	A	200	ILE	C-O	-5.62	1.18	1.24
1	B	179	ILE	C-O	-5.59	1.17	1.24
1	B	321	ASN	CA-CB	5.59	1.63	1.54
1	A	292	CYS	C-O	-5.59	1.17	1.24
1	A	327	GLN	C-O	-5.57	1.17	1.24
1	A	223	ASP	C-O	-5.57	1.17	1.23
1	A	308	HIS	C-O	-5.57	1.17	1.23
1	B	286	GLU	C-O	-5.54	1.17	1.24
1	B	164	TYR	C-O	-5.53	1.17	1.24
1	B	176	GLN	C-O	-5.50	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	281	ARG	C-O	-5.49	1.17	1.24
1	B	229	ASN	C-O	-5.49	1.17	1.24
1	A	236	LYS	C-O	-5.49	1.17	1.23
1	B	162	SER	C-O	-5.49	1.17	1.24
1	B	340	GLU	CB-CG	-5.48	1.36	1.52
1	A	168	LEU	C-O	-5.47	1.17	1.24
1	A	252	GLN	C-O	-5.43	1.17	1.24
1	A	291	PHE	C-O	-5.42	1.17	1.24
1	B	339	GLU	C-O	-5.41	1.17	1.24
1	A	255	GLY	C-O	-5.40	1.18	1.23
1	A	183	ASN	C-O	-5.38	1.17	1.24
1	A	259	LEU	C-O	-5.38	1.17	1.23
1	B	306	ARG	C-O	-5.38	1.17	1.24
1	A	170	LEU	C-O	-5.36	1.17	1.24
1	A	286	GLU	C-O	-5.36	1.17	1.24
1	B	247	LEU	C-O	-5.36	1.17	1.24
1	A	190	LEU	C-O	-5.35	1.16	1.23
1	A	173	PRO	C-O	-5.33	1.17	1.24
1	A	258	ILE	C-O	-5.29	1.18	1.24
1	B	315	GLN	C-O	-5.28	1.18	1.24
1	A	153	HIS	C-O	-5.28	1.16	1.23
1	A	155	VAL	C-O	-5.28	1.18	1.24
1	B	328	GLU	C-O	-5.27	1.18	1.24
1	A	211	ASP	C-O	-5.26	1.17	1.24
1	A	328	GLU	C-O	-5.25	1.18	1.24
1	B	204	LEU	C-O	-5.24	1.17	1.24
1	B	327	GLN	C-O	-5.24	1.18	1.24
1	A	272	SER	C-O	-5.23	1.17	1.24
1	B	199	TYR	C-O	-5.23	1.17	1.24
1	A	315	GLN	C-O	-5.21	1.18	1.24
1	A	268	LEU	C-O	-5.21	1.18	1.24
1	A	331	ARG	C-O	-5.20	1.18	1.24
1	A	295	LEU	C-O	-5.19	1.18	1.24
1	B	277	ALA	C-O	-5.18	1.17	1.24
1	A	215	ALA	CA-CB	-5.18	1.45	1.53
1	B	285	LEU	C-O	-5.18	1.18	1.24
1	A	251	GLY	C-O	-5.17	1.17	1.24
1	B	165	ILE	C-O	-5.17	1.18	1.24
1	A	161	TRP	C-O	-5.14	1.18	1.24
1	A	175	LEU	C-O	-5.14	1.18	1.24
1	B	257	CYS	C-O	-5.13	1.17	1.23
1	B	249	GLU	C-O	-5.13	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	313	VAL	C-O	-5.11	1.18	1.24
1	B	171	ILE	C-O	-5.10	1.19	1.24
1	B	271	MET	C-O	-5.08	1.18	1.24
1	B	325	LEU	C-O	-5.06	1.18	1.24
1	B	219	ILE	C-O	-5.06	1.18	1.24
1	A	167	TYR	CA-C	-5.04	1.46	1.52
1	B	197	ARG	C-O	-5.04	1.17	1.24
1	B	168	LEU	C-O	-5.01	1.18	1.24
1	B	237	ASN	C-O	-5.00	1.17	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	321	ASN	N-CA-C	24.23	144.09	114.04
1	B	321	ASN	CB-CA-C	-9.66	91.95	109.15
1	B	316	GLU	N-CA-C	-8.90	97.94	110.50
1	B	321	ASN	CA-C-O	7.96	129.01	119.06
1	A	167	TYR	N-CA-CB	-7.51	97.80	110.49
1	A	320	GLY	N-CA-C	7.22	121.18	111.72
1	B	318	GLU	N-CA-C	-6.82	103.38	113.61
1	B	319	GLU	N-CA-C	6.54	119.40	111.82
1	A	224	MET	CG-SD-CE	-5.92	87.88	100.90
1	A	319	GLU	N-CA-C	5.79	120.38	112.04
1	A	167	TYR	CA-C-N	-5.67	112.23	120.29
1	A	167	TYR	C-N-CA	-5.67	112.23	120.29
1	B	251	GLY	N-CA-C	5.55	122.43	115.21
1	B	341	VAL	CB-CA-C	5.36	121.59	111.40
1	B	170	LEU	N-CA-C	5.36	117.20	111.36
1	A	152	SER	N-CA-C	5.08	116.89	111.36
1	A	167	TYR	CB-CA-C	5.00	120.38	110.42

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	319	GLU	Peptide

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	1503	0	1469	13	0
1	B	1519	0	1488	26	0
2	B	45	0	21	3	0
3	A	211	0	0	2	0
3	B	195	0	0	4	0
All	All	3473	0	2978	40	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 7.

All (40) 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:167:TYR:N	1:A:167:TYR:CA	1.69	1.52
1:B:220:ARG:HE	1:B:222:ARG:NH1	1.26	1.30
1:B:220:ARG:NE	1:B:222:ARG:HH12	1.35	1.23
1:B:220:ARG:HH21	1:B:222:ARG:HH22	1.13	0.91
1:A:167:TYR:N	1:A:167:TYR:CB	2.46	0.78
1:B:220:ARG:NE	1:B:222:ARG:NH1	2.09	0.74
2:B:401:1SY:H9	3:B:508:HOH:O	1.89	0.71
1:B:321:ASN:OD1	1:B:321:ASN:O	2.09	0.70
1:A:166:GLY:C	1:A:167:TYR:CA	2.61	0.69
1:A:202:PHE:CE1	1:A:311:LEU:HD22	2.28	0.68
1:B:220:ARG:CZ	1:B:222:ARG:HH12	2.06	0.66
1:B:220:ARG:HH21	1:B:222:ARG:NH2	1.89	0.66
1:B:316:GLU:O	1:B:317:SER:CB	2.44	0.65
1:B:220:ARG:HE	1:B:222:ARG:HH12	0.65	0.60
1:A:202:PHE:HE1	1:A:311:LEU:HD22	1.67	0.59
1:B:220:ARG:NH2	1:B:222:ARG:HH22	1.93	0.59
1:B:340:GLU:O	1:B:341:VAL:HB	2.04	0.57
1:B:316:GLU:O	1:B:317:SER:HB3	2.03	0.57
1:B:222:ARG:HE	1:B:246:GLU:CD	2.16	0.53
1:B:321:ASN:OD1	1:B:321:ASN:C	2.50	0.52
2:B:401:1SY:C4'	3:B:508:HOH:O	2.53	0.52
1:A:224:MET:HG2	3:A:457:HOH:O	2.10	0.52
2:B:401:1SY:O26	2:B:401:1SY:H21	2.11	0.51
1:B:304:GLU:O	1:B:308:HIS:HD2	1.94	0.50
1:B:196:ARG:NH2	1:B:340:GLU:OE1	2.45	0.49
1:B:338:LYS:NZ	3:B:505:HOH:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:PHE:HE1	1:B:153:HIS:NE2	2.14	0.45
1:B:276:LYS:HA	1:B:276:LYS:HD2	1.65	0.45
1:B:263:THR:N	1:B:264:PRO:CD	2.80	0.45
1:B:252:GLN:HB3	1:B:253:PRO:HD2	1.99	0.45
1:A:257:CYS:HB2	3:A:428:HOH:O	2.17	0.45
1:A:167:TYR:N	1:A:167:TYR:C	2.63	0.44
1:B:196:ARG:HH22	1:B:340:GLU:CD	2.25	0.44
1:A:332:HIS:HA	1:A:335:GLN:HG2	2.00	0.43
1:A:221:PHE:HZ	1:A:224:MET:HE2	1.83	0.43
1:B:302:VAL:O	1:B:302:VAL:HG23	2.19	0.43
1:A:263:THR:N	1:A:264:PRO:CD	2.81	0.42
1:B:231:ASP:C	1:B:232:ARG:HG2	2.45	0.42
1:B:187:ASN:N	3:B:511:HOH:O	2.52	0.41
1:A:221:PHE:CE1	1:B:236:LYS:HG3	2.56	0.41

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	186/210 (89%)	184 (99%)	2 (1%)	0	100	100
1	B	188/210 (90%)	185 (98%)	3 (2%)	0	100	100
All	All	374/420 (89%)	369 (99%)	5 (1%)	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	161/181 (89%)	159 (99%)	2 (1%)	63	40
1	B	164/181 (91%)	162 (99%)	2 (1%)	63	40
All	All	325/362 (90%)	321 (99%)	4 (1%)	63	40

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	321	ASN
1	A	335	GLN
1	B	317	SER
1	B	322	SER

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	150	GLN
1	A	266	GLN
1	B	186	HIS
1	B	227	GLN
1	B	229	ASN
1	B	273	GLN
1	B	308	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is 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	1SY	B	401	-	51,51,51	3.56	27 (52%)	70,80,80	4.34	48 (68%)

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	B	401	-	-	2/30/62/62	0/6/7/7

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	1SY	C38-N39	8.94	1.53	1.38
2	B	401	1SY	C37-C36	-8.54	1.25	1.38
2	B	401	1SY	C36-N33	-8.29	1.28	1.37
2	B	401	1SY	C2-N3	-6.61	1.22	1.33
2	B	401	1SY	O43-C38	6.20	1.35	1.23
2	B	401	1SY	C5-C6	-5.69	1.25	1.41
2	B	401	1SY	O4'-C1'	5.62	1.55	1.42
2	B	401	1SY	C16-C4'	5.58	1.68	1.51
2	B	401	1SY	O4'-C4'	-5.41	1.33	1.45
2	B	401	1SY	C40-N41	4.61	1.45	1.34
2	B	401	1SY	C5-C4	-4.60	1.30	1.39
2	B	401	1SY	C38-C37	-3.97	1.34	1.45
2	B	401	1SY	O31-C24	3.96	1.53	1.45
2	B	401	1SY	C22-C24	-3.80	1.43	1.53
2	B	401	1SY	P18-O17	3.79	1.74	1.59
2	B	401	1SY	P18-O19	-3.43	1.39	1.55
2	B	401	1SY	C8-N9	3.43	1.43	1.37
2	B	401	1SY	O20-C21	-2.89	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	1SY	C34-N33	2.80	1.43	1.37
2	B	401	1SY	C40-N39	-2.79	1.26	1.33
2	B	401	1SY	C22-C21	2.73	1.58	1.53
2	B	401	1SY	P18-O44	-2.66	1.41	1.50
2	B	401	1SY	C37-N35	2.61	1.44	1.39
2	B	401	1SY	O2'-C2'	2.60	1.49	1.43
2	B	401	1SY	C21-C32	-2.26	1.47	1.53
2	B	401	1SY	C4-N3	2.17	1.38	1.34
2	B	401	1SY	O23-C22	2.00	1.47	1.43

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	1SY	C37-C36-N33	14.48	112.95	106.25
2	B	401	1SY	N42-C40-N39	11.79	144.90	123.32
2	B	401	1SY	C5-C4-N3	11.13	142.04	126.72
2	B	401	1SY	O4'-C1'-N9	7.85	123.17	108.09
2	B	401	1SY	O43-C38-N39	-7.57	107.52	120.27
2	B	401	1SY	C38-C37-C36	7.21	128.99	118.08
2	B	401	1SY	N3-C4-N9	-6.49	116.13	127.17
2	B	401	1SY	N9-C8-N7	-6.29	105.01	113.94
2	B	401	1SY	C2-N3-C4	-6.27	96.53	111.83
2	B	401	1SY	N41-C40-N39	-6.16	107.65	119.67
2	B	401	1SY	C4-N9-C8	5.55	111.57	105.74
2	B	401	1SY	C34-N33-C36	-5.49	102.04	106.67
2	B	401	1SY	C38-N39-C40	-5.48	103.15	119.24
2	B	401	1SY	O31-C32-N33	-5.27	96.42	108.36
2	B	401	1SY	O28-C3'-C4'	5.19	128.32	110.03
2	B	401	1SY	C1'-N9-C8	-4.75	116.56	127.09
2	B	401	1SY	N41-C40-N42	-4.66	106.93	116.76
2	B	401	1SY	O31-C32-C21	-4.65	98.59	106.59
2	B	401	1SY	C2'-C1'-N9	4.47	124.41	113.30
2	B	401	1SY	O4'-C1'-C2'	-4.43	97.13	106.62
2	B	401	1SY	C22-C21-C32	4.22	110.89	102.81
2	B	401	1SY	N3-C2-N1	3.94	134.55	128.58
2	B	401	1SY	C5-C4-N9	-3.71	101.76	105.81
2	B	401	1SY	C38-C37-N35	-3.63	118.33	130.12
2	B	401	1SY	O20-P18-O44	-3.54	98.49	109.81
2	B	401	1SY	C6-C5-C4	-3.46	112.45	117.18
2	B	401	1SY	C34-N35-C37	-3.45	98.11	104.26
2	B	401	1SY	O17-C16-C4'	-3.42	97.34	108.99
2	B	401	1SY	O20-C21-C22	-3.06	100.71	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	1SY	C24-O31-C32	2.95	115.97	109.47
2	B	401	1SY	C5-N7-C8	2.82	107.88	103.45
2	B	401	1SY	C32-N33-C34	2.79	134.66	126.73
2	B	401	1SY	C4-C5-N7	2.66	113.62	110.58
2	B	401	1SY	O23-C22-C21	-2.66	103.75	111.19
2	B	401	1SY	O20-C21-C32	2.64	119.35	110.05
2	B	401	1SY	C36-C37-N35	2.63	112.68	109.26
2	B	401	1SY	O28-C3'-C2'	-2.56	102.49	111.68
2	B	401	1SY	C25-C24-C22	-2.48	106.29	115.21
2	B	401	1SY	C5-C6-N01	2.48	129.42	123.29
2	B	401	1SY	P27-O26-C25	-2.46	107.27	121.35
2	B	401	1SY	O28-P27-O29	-2.35	102.30	109.81
2	B	401	1SY	O2'-C2'-C3'	2.29	117.58	111.19
2	B	401	1SY	C2'-C3'-C4'	-2.20	99.39	103.24
2	B	401	1SY	C4-N9-C1'	2.18	131.74	126.63
2	B	401	1SY	P18-O17-C16	-2.13	109.15	121.35
2	B	401	1SY	O17-P18-O44	2.06	117.10	108.94
2	B	401	1SY	O19-P18-O20	2.05	115.06	106.70
2	B	401	1SY	C21-C32-N33	-2.02	110.40	114.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	1SY	C25-O26-P27-O29
2	B	401	1SY	C25-O26-P27-O28

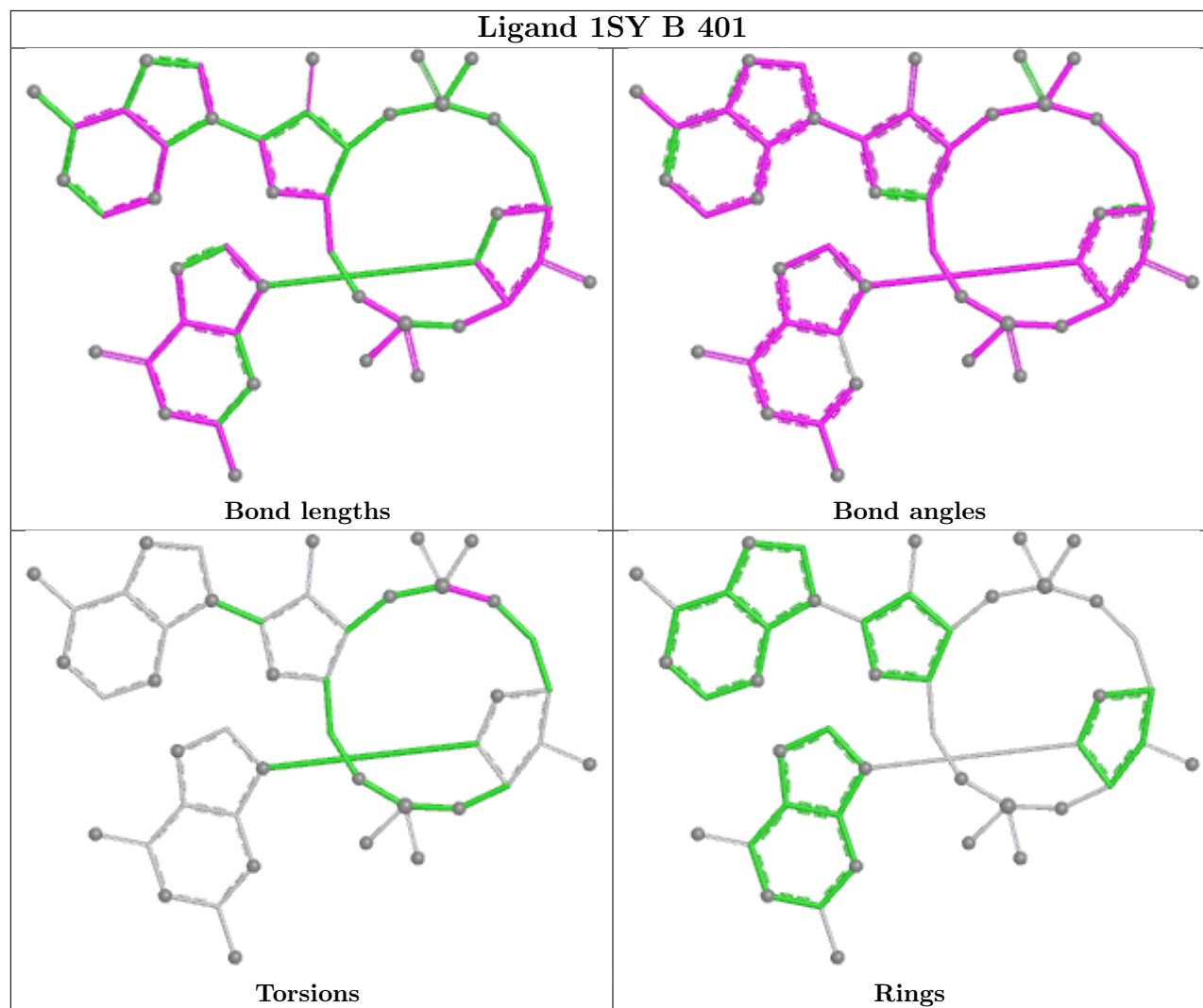
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	1SY	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	188/210 (89%)	0.17	10 (5%) 32 39	7, 15, 35, 90	0
1	B	190/210 (90%)	0.41	12 (6%) 26 31	9, 17, 42, 87	0
All	All	378/420 (90%)	0.29	22 (5%) 29 34	7, 16, 40, 90	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	153	HIS	5.7
1	A	320	GLY	5.2
1	B	341	VAL	4.3
1	B	320	GLY	4.3
1	B	152	SER	3.7
1	A	321	ASN	3.6
1	B	322	SER	3.4
1	B	317	SER	3.3
1	B	321	ASN	3.2
1	A	322	SER	3.2
1	A	148	TYR	3.2
1	B	304	GLU	3.1
1	A	276	LYS	3.0
1	A	319	GLU	2.6
1	A	278	GLY	2.4
1	A	202	PHE	2.4
1	B	214	VAL	2.3
1	B	250	ASN	2.3
1	B	286	GLU	2.3
1	A	323	PHE	2.2
1	B	193	ALA	2.1
1	A	281	ARG	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](#)

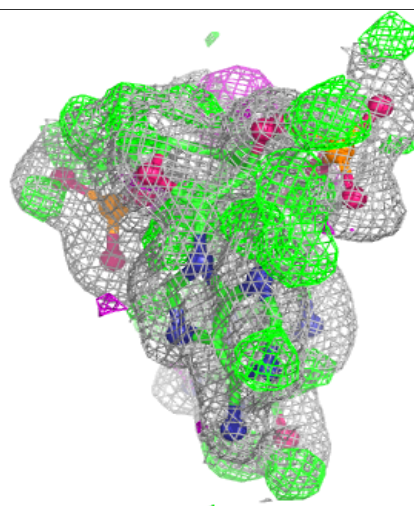
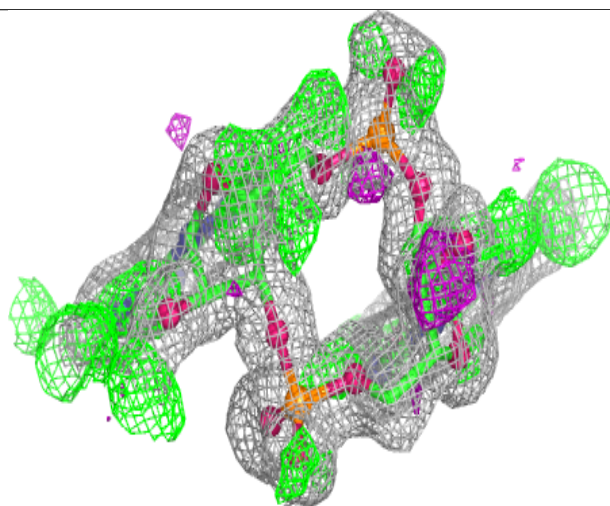
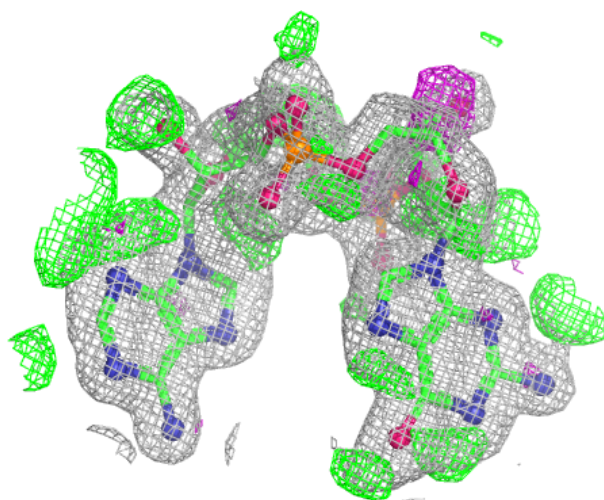
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	401	45/45	0.95	0.08	7,13,19,21	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 B 401:

$2mF_o-DF_c$ (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.