



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 02:47 AM UTC

PDB ID : 9M7A / pdb_00009m7a
Title : Crystal structure of Serine Acetyltransferase (SAT) from *Planctomyces limnophilus* in complex with its inhibitor (Cysteine)
Authors : Kumar, N.; Kumaran, S.
Deposited on : 2025-03-10
Resolution : 2.45 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

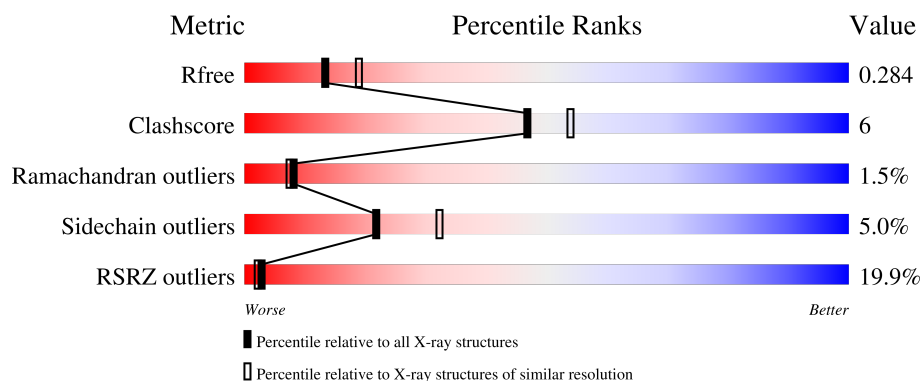
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	331	
1	B	331	
1	C	331	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7042 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 Serine O-acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	1	0
			2267	1433	409	419	6			
1	B	297	Total	C	N	O	S	0	1	0
			2327	1472	418	432	5			
1	C	300	Total	C	N	O	S	0	1	0
			2351	1484	425	436	6			

There are 60 discrepancies between the modelled and reference sequences:

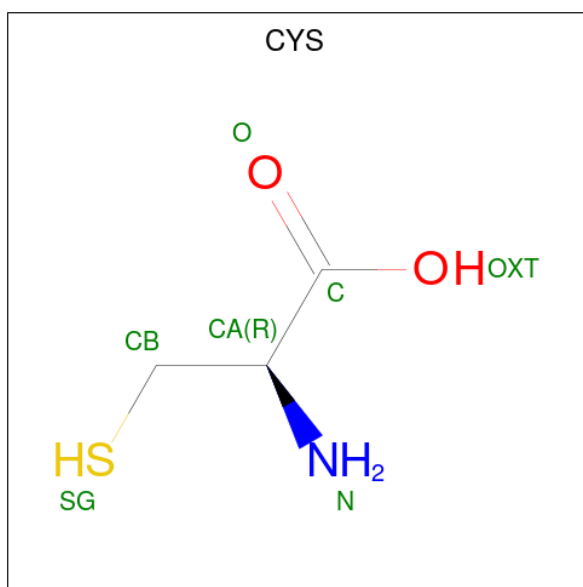
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP D5SUT9
A	-18	GLY	-	expression tag	UNP D5SUT9
A	-17	SER	-	expression tag	UNP D5SUT9
A	-16	SER	-	expression tag	UNP D5SUT9
A	-15	HIS	-	expression tag	UNP D5SUT9
A	-14	HIS	-	expression tag	UNP D5SUT9
A	-13	HIS	-	expression tag	UNP D5SUT9
A	-12	HIS	-	expression tag	UNP D5SUT9
A	-11	HIS	-	expression tag	UNP D5SUT9
A	-10	HIS	-	expression tag	UNP D5SUT9
A	-9	SER	-	expression tag	UNP D5SUT9
A	-8	SER	-	expression tag	UNP D5SUT9
A	-7	GLY	-	expression tag	UNP D5SUT9
A	-6	LEU	-	expression tag	UNP D5SUT9
A	-5	VAL	-	expression tag	UNP D5SUT9
A	-4	PRO	-	expression tag	UNP D5SUT9
A	-3	ARG	-	expression tag	UNP D5SUT9
A	-2	GLY	-	expression tag	UNP D5SUT9
A	-1	SER	-	expression tag	UNP D5SUT9
A	0	HIS	-	expression tag	UNP D5SUT9
B	-19	MET	-	expression tag	UNP D5SUT9
B	-18	GLY	-	expression tag	UNP D5SUT9
B	-17	SER	-	expression tag	UNP D5SUT9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP D5SUT9
B	-15	HIS	-	expression tag	UNP D5SUT9
B	-14	HIS	-	expression tag	UNP D5SUT9
B	-13	HIS	-	expression tag	UNP D5SUT9
B	-12	HIS	-	expression tag	UNP D5SUT9
B	-11	HIS	-	expression tag	UNP D5SUT9
B	-10	HIS	-	expression tag	UNP D5SUT9
B	-9	SER	-	expression tag	UNP D5SUT9
B	-8	SER	-	expression tag	UNP D5SUT9
B	-7	GLY	-	expression tag	UNP D5SUT9
B	-6	LEU	-	expression tag	UNP D5SUT9
B	-5	VAL	-	expression tag	UNP D5SUT9
B	-4	PRO	-	expression tag	UNP D5SUT9
B	-3	ARG	-	expression tag	UNP D5SUT9
B	-2	GLY	-	expression tag	UNP D5SUT9
B	-1	SER	-	expression tag	UNP D5SUT9
B	0	HIS	-	expression tag	UNP D5SUT9
C	-19	MET	-	expression tag	UNP D5SUT9
C	-18	GLY	-	expression tag	UNP D5SUT9
C	-17	SER	-	expression tag	UNP D5SUT9
C	-16	SER	-	expression tag	UNP D5SUT9
C	-15	HIS	-	expression tag	UNP D5SUT9
C	-14	HIS	-	expression tag	UNP D5SUT9
C	-13	HIS	-	expression tag	UNP D5SUT9
C	-12	HIS	-	expression tag	UNP D5SUT9
C	-11	HIS	-	expression tag	UNP D5SUT9
C	-10	HIS	-	expression tag	UNP D5SUT9
C	-9	SER	-	expression tag	UNP D5SUT9
C	-8	SER	-	expression tag	UNP D5SUT9
C	-7	GLY	-	expression tag	UNP D5SUT9
C	-6	LEU	-	expression tag	UNP D5SUT9
C	-5	VAL	-	expression tag	UNP D5SUT9
C	-4	PRO	-	expression tag	UNP D5SUT9
C	-3	ARG	-	expression tag	UNP D5SUT9
C	-2	GLY	-	expression tag	UNP D5SUT9
C	-1	SER	-	expression tag	UNP D5SUT9
C	0	HIS	-	expression tag	UNP D5SUT9

- Molecule 2 is CYSTEINE (CCD ID: CYS) (formula: $C_3H_7NO_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
2	B	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
2	B	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

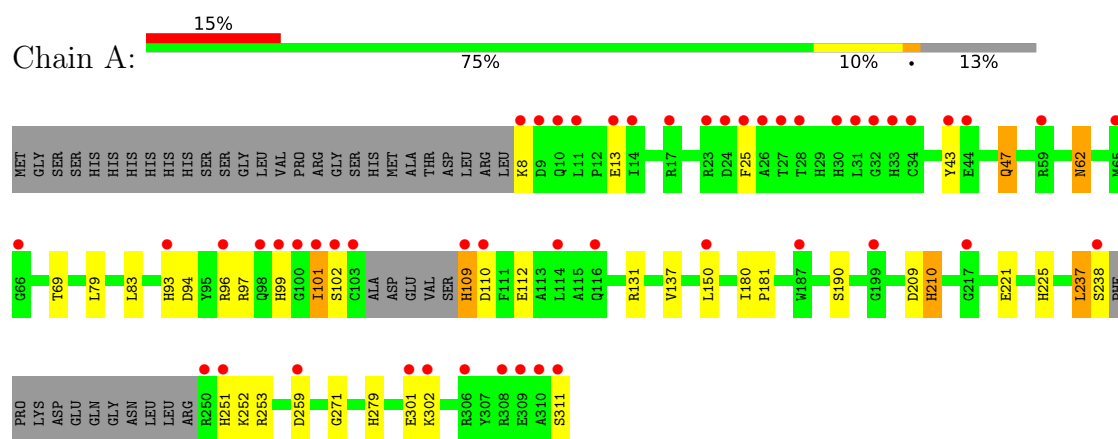
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total	O	0	0
			25	25		
3	B	23	Total	O	0	0
			23	23		
3	C	28	Total	O	0	0
			28	28		

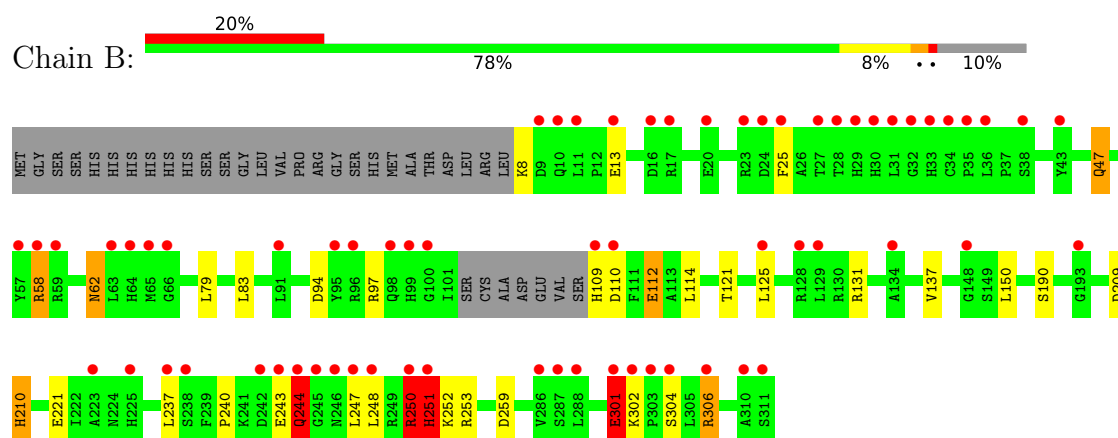
3 Residue-property plots [i](#)

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.

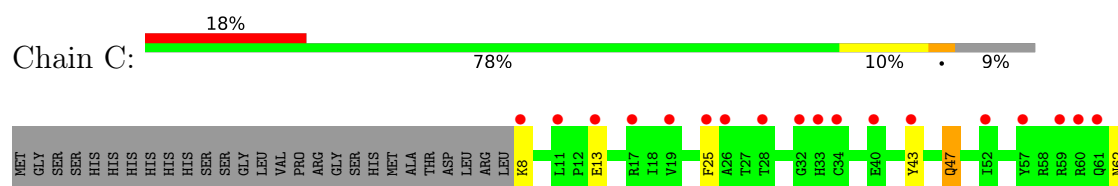
• Molecule 1: Serine O-acetyltransferase

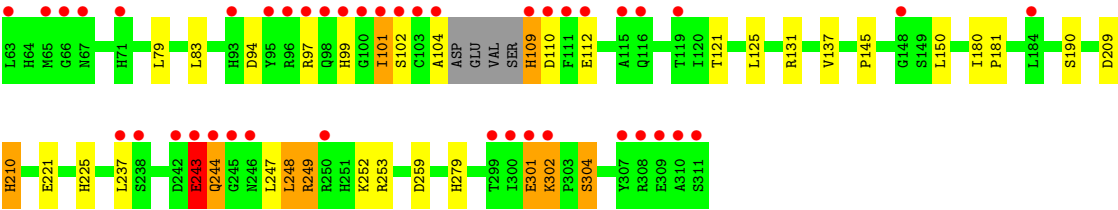


• Molecule 1: Serine O-acetyltransferase



• Molecule 1: Serine O-acetyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	127.75Å 88.80Å 101.40Å 90.00° 113.22° 90.00°	Depositor
Resolution (Å)	46.59 – 2.45 46.59 – 2.45	Depositor EDS
% Data completeness (in resolution range)	93.8 (46.59-2.45) 93.8 (46.59-2.45)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.239 , 0.284 0.239 , 0.284	Depositor DCC
R_{free} test set	1735 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.798	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7042	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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

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	0.67	2/2323 (0.1%)	1.08	3/3162 (0.1%)
1	B	0.65	0/2384	1.11	5/3247 (0.2%)
1	C	0.69	2/2410 (0.1%)	1.12	1/3282 (0.0%)
All	All	0.67	4/7117 (0.1%)	1.10	9/9691 (0.1%)

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	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	279	HIS	CE1-NE2	7.29	1.39	1.32
1	A	279	HIS	CE1-NE2	5.72	1.38	1.32
1	C	225	HIS	CE1-NE2	5.31	1.37	1.32
1	A	225	HIS	CE1-NE2	5.00	1.37	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	THR	CA-CB-OG1	-6.51	99.83	109.60
1	B	244	GLN	CA-C-N	6.49	126.15	119.92
1	B	244	GLN	C-N-CA	6.49	126.15	119.92
1	B	58	ARG	CG-CD-NE	-6.01	98.78	112.00
1	B	301	GLU	CB-CG-CD	5.89	122.61	112.60
1	C	301	GLU	CB-CG-CD	5.86	122.57	112.60
1	B	306	ARG	CB-CG-CD	5.22	123.31	111.30
1	A	96	ARG	CB-CG-CD	5.10	123.03	111.30
1	A	301	GLU	CB-CG-CD	5.01	121.11	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	247	LEU	Peptide
1	B	251	HIS	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	2267	0	2229	25	0
1	B	2327	0	2279	33	0
1	C	2351	0	2293	29	0
2	A	7	0	4	1	0
2	B	14	0	8	1	0
3	A	25	0	0	3	0
3	B	23	0	0	0	0
3	C	28	0	0	2	0
All	All	7042	0	6813	79	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (79) 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:250:ARG:HD2	1:B:251:HIS:H	1.05	1.05
1:C:244:GLN:HB2	1:C:247:LEU:CB	1.94	0.98
1:B:248:LEU:HD23	1:B:250:ARG:NH1	1.89	0.86
1:B:248:LEU:HD23	1:B:250:ARG:HH12	1.40	0.86
1:B:250:ARG:HD2	1:B:251:HIS:N	1.90	0.84
1:A:221:GLU:OE2	1:A:252:LYS:HE3	1.81	0.81
1:B:250:ARG:CD	1:B:251:HIS:H	1.93	0.80
1:B:301:GLU:OE1	1:C:304:SER:HB2	1.86	0.74
1:C:221:GLU:OE2	1:C:252:LYS:HE2	1.88	0.73
1:C:243:GLU:O	1:C:243:GLU:HG3	1.88	0.72
1:A:109:HIS:CB	1:A:112:GLU:HB3	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:GLU:O	1:C:243:GLU:CG	2.40	0.69
1:B:250:ARG:HH21	1:B:251:HIS:N	1.90	0.69
1:B:221:GLU:OE2	1:B:252:LYS:HE2	1.93	0.69
1:B:243:GLU:O	1:B:244:GLN:HB2	1.94	0.67
1:C:109:HIS:CB	1:C:112:GLU:HB3	2.24	0.67
1:C:131:ARG:HD3	3:C:412:HOH:O	1.95	0.67
1:B:109:HIS:CB	1:B:112:GLU:HB2	2.26	0.66
1:A:93:HIS:HD2	3:A:523:HOH:O	1.80	0.64
1:B:250:ARG:NH2	1:B:251:HIS:O	2.31	0.64
1:A:109:HIS:HB3	1:A:112:GLU:HB3	1.79	0.63
1:B:47:GLN:NE2	1:B:58:ARG:HH22	1.97	0.62
1:A:25:PHE:CZ	1:B:131:ARG:HG3	2.35	0.61
1:C:109:HIS:HB2	1:C:112:GLU:HB3	1.83	0.60
1:B:248:LEU:HD13	1:C:145:PRO:HG3	1.85	0.58
1:A:8:LYS:N	3:A:501:HOH:O	2.37	0.58
1:B:240:PRO:HD2	1:B:248:LEU:HD21	1.88	0.56
1:C:244:GLN:CB	1:C:247:LEU:CB	2.77	0.55
1:B:243:GLU:O	1:B:244:GLN:CB	2.55	0.55
1:A:109:HIS:HB3	1:A:112:GLU:CB	2.36	0.55
1:B:248:LEU:C	1:B:250:ARG:H	2.15	0.54
1:C:131:ARG:NH1	3:C:401:HOH:O	2.40	0.54
1:A:93:HIS:CD2	3:A:523:HOH:O	2.56	0.54
1:A:253:ARG:HD2	2:B:402:CYS:OXT	2.08	0.53
1:B:25:PHE:CZ	1:C:131:ARG:HG3	2.44	0.52
1:C:137:VAL:HG12	1:C:150:LEU:HD22	1.91	0.52
1:A:237:LEU:HD23	1:A:238:SER:H	1.74	0.52
1:C:209:ASP:O	1:C:210:HIS:HB2	2.10	0.51
1:B:221:GLU:OE2	1:B:252:LYS:CE	2.59	0.50
1:B:137:VAL:HG12	1:B:150:LEU:HD22	1.93	0.49
1:A:237:LEU:HD12	1:A:271:GLY:HA3	1.94	0.49
1:A:62:ASN:OD1	1:A:62:ASN:N	2.46	0.49
1:A:209:ASP:O	1:A:210:HIS:HB2	2.12	0.49
1:C:94:ASP:OD1	1:C:97:ARG:NH2	2.45	0.48
1:A:131:ARG:HG3	1:C:25:PHE:CZ	2.48	0.48
1:B:62:ASN:OD1	1:B:62:ASN:N	2.47	0.48
1:B:94:ASP:OD1	1:B:97:ARG:NH2	2.45	0.48
1:A:43[B]:TYR:CE1	1:A:47:GLN:OE1	2.66	0.48
1:A:137:VAL:HG12	1:A:150:LEU:HD22	1.96	0.47
1:A:94:ASP:OD1	1:A:97:ARG:NH2	2.47	0.46
1:B:248:LEU:HD22	1:B:253:ARG:HD3	1.97	0.46
1:B:209:ASP:O	1:B:210:HIS:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:HIS:N	1:A:109:HIS:CD2	2.84	0.45
1:B:58:ARG:HE	1:B:58:ARG:HB3	1.45	0.45
1:B:240:PRO:HD2	1:B:248:LEU:CG	2.48	0.44
1:B:248:LEU:HD13	1:C:145:PRO:CG	2.46	0.43
1:A:109:HIS:HB2	1:A:112:GLU:HB3	1.97	0.43
1:C:102:SER:C	1:C:104:ALA:H	2.25	0.43
1:C:248:LEU:O	1:C:249:ARG:HB2	2.17	0.43
1:A:79:LEU:O	1:A:83:LEU:HB2	2.19	0.43
1:A:99:HIS:C	1:A:101:ILE:H	2.27	0.43
1:C:79:LEU:O	1:C:83:LEU:HB2	2.20	0.42
2:A:401:CYS:OXT	1:C:253:ARG:HD2	2.19	0.42
1:B:248:LEU:HB2	1:C:145:PRO:HB3	2.01	0.42
1:B:121:THR:O	1:B:125:LEU:HG	2.20	0.42
1:B:240:PRO:HD2	1:B:248:LEU:CD2	2.49	0.42
1:C:180:ILE:N	1:C:181:PRO:CD	2.83	0.42
1:C:221:GLU:OE2	1:C:252:LYS:CE	2.62	0.41
1:C:99:HIS:C	1:C:101:ILE:H	2.28	0.41
1:C:302:LYS:HE2	1:C:302:LYS:HB3	1.93	0.41
1:B:79:LEU:O	1:B:83:LEU:HB2	2.19	0.41
1:A:180:ILE:N	1:A:181:PRO:CD	2.84	0.40
1:A:302:LYS:H	1:B:306:ARG:HH22	1.69	0.40
1:C:121:THR:O	1:C:125:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	283/331 (86%)	272 (96%)	8 (3%)	3 (1%)	11	12
1	B	294/331 (89%)	277 (94%)	13 (4%)	4 (1%)	9	8
1	C	297/331 (90%)	277 (93%)	14 (5%)	6 (2%)	6	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	874/993 (88%)	826 (94%)	35 (4%)	13 (2%)	8	7

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	244	GLN
1	B	250	ARG
1	C	243	GLU
1	A	110	ASP
1	C	110	ASP
1	C	248	LEU
1	C	249	ARG
1	A	210	HIS
1	B	210	HIS
1	C	210	HIS
1	A	101	ILE
1	B	110	ASP
1	C	101	ILE

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	245/282 (87%)	235 (96%)	10 (4%)	27	40
1	B	248/282 (88%)	234 (94%)	14 (6%)	19	27
1	C	251/282 (89%)	238 (95%)	13 (5%)	21	30
All	All	744/846 (88%)	707 (95%)	37 (5%)	22	32

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	47	GLN
1	A	62	ASN

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Mol	Chain	Res	Type
1	A	102	SER
1	A	109	HIS
1	A	190	SER
1	A	237	LEU
1	A	251	HIS
1	A	259	ASP
1	A	311	SER
1	B	8	LYS
1	B	13	GLU
1	B	47	GLN
1	B	62	ASN
1	B	112	GLU
1	B	114	LEU
1	B	190	SER
1	B	237	LEU
1	B	250	ARG
1	B	251	HIS
1	B	259	ASP
1	B	301	GLU
1	B	302	LYS
1	B	304	SER
1	C	8	LYS
1	C	13	GLU
1	C	47	GLN
1	C	62	ASN
1	C	109	HIS
1	C	190	SER
1	C	237	LEU
1	C	243	GLU
1	C	244	GLN
1	C	259	ASP
1	C	301	GLU
1	C	302	LYS
1	C	304	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	50	GLN
1	A	61	GLN
1	A	71	HIS

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Mol	Chain	Res	Type
1	A	93	HIS
1	A	109	HIS
1	A	225	HIS
1	B	47	GLN
1	B	50	GLN
1	B	71	HIS
1	B	225	HIS
1	C	47	GLN
1	C	50	GLN
1	C	61	GLN
1	C	71	HIS
1	C	93	HIS
1	C	98	GLN
1	C	225	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

3 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	CYS	A	401	-	5,6,6	1.31	1 (20%)	3,7,7	1.78	1 (33%)
2	CYS	B	402	-	5,6,6	1.36	1 (20%)	3,7,7	2.28	1 (33%)
2	CYS	B	401	-	5,6,6	0.58	0	3,7,7	1.62	1 (33%)

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	CYS	A	401	-	-	0/6/6/6	-
2	CYS	B	402	-	-	0/6/6/6	-
2	CYS	B	401	-	-	0/6/6/6	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	CYS	OXT-C	-2.58	1.22	1.30
2	A	401	CYS	O-C	2.20	1.28	1.22

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	CYS	OXT-C-O	-3.81	115.44	124.08
2	A	401	CYS	OXT-C-O	-3.02	117.23	124.08
2	B	401	CYS	OXT-C-O	-2.66	118.04	124.08

There are no chirality outliers.

There are no torsion outliers.

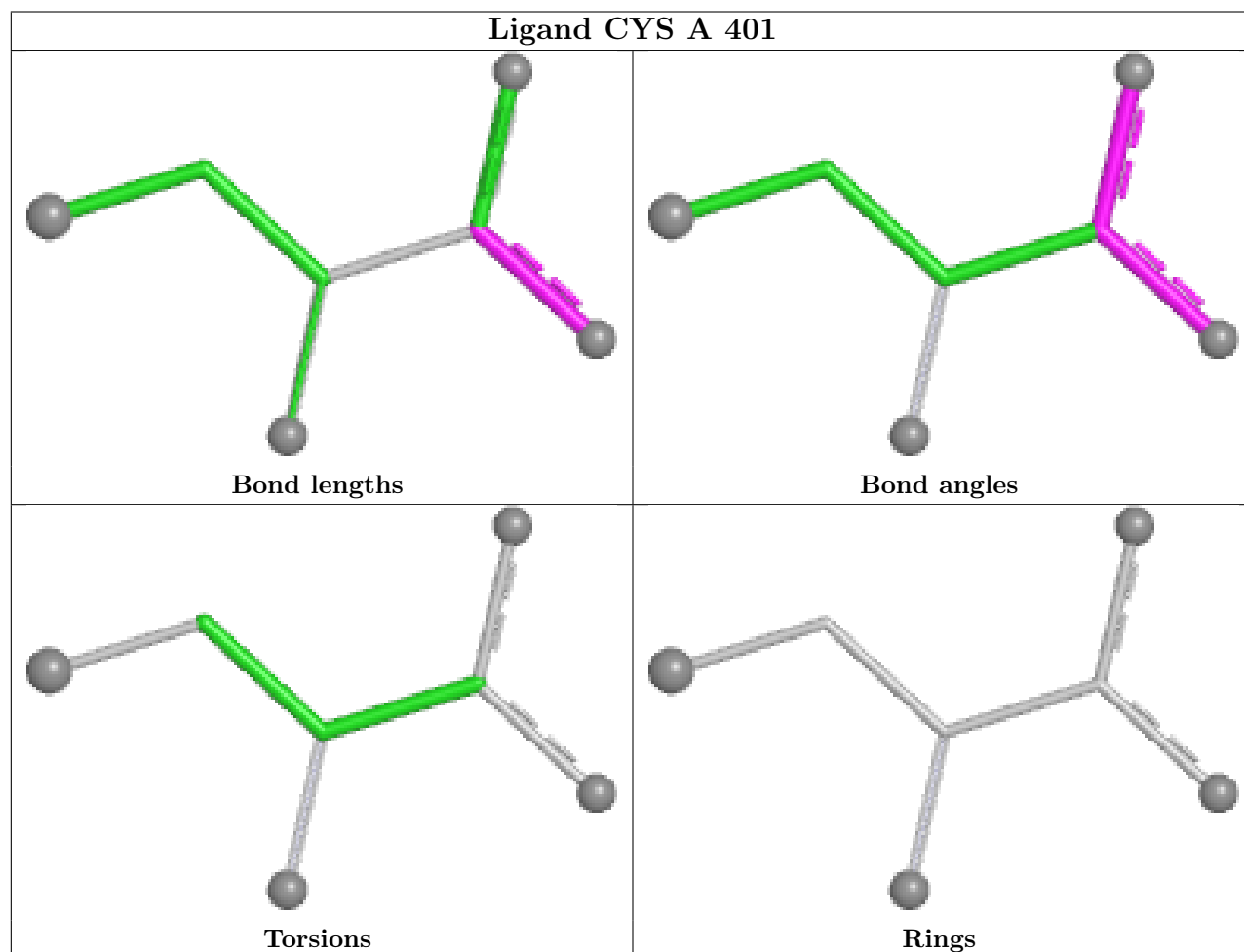
There are no ring outliers.

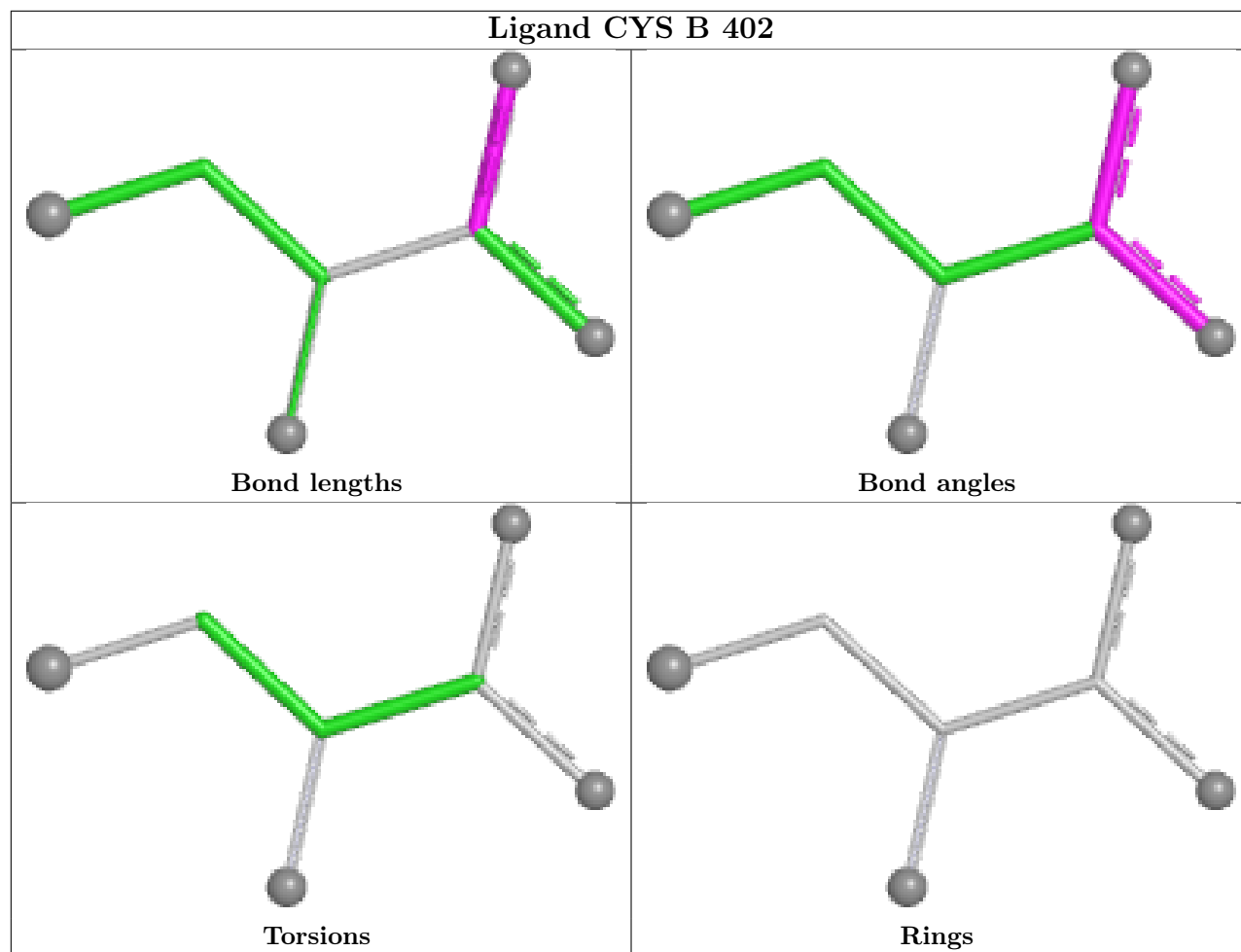
2 monomers are involved in 2 short contacts:

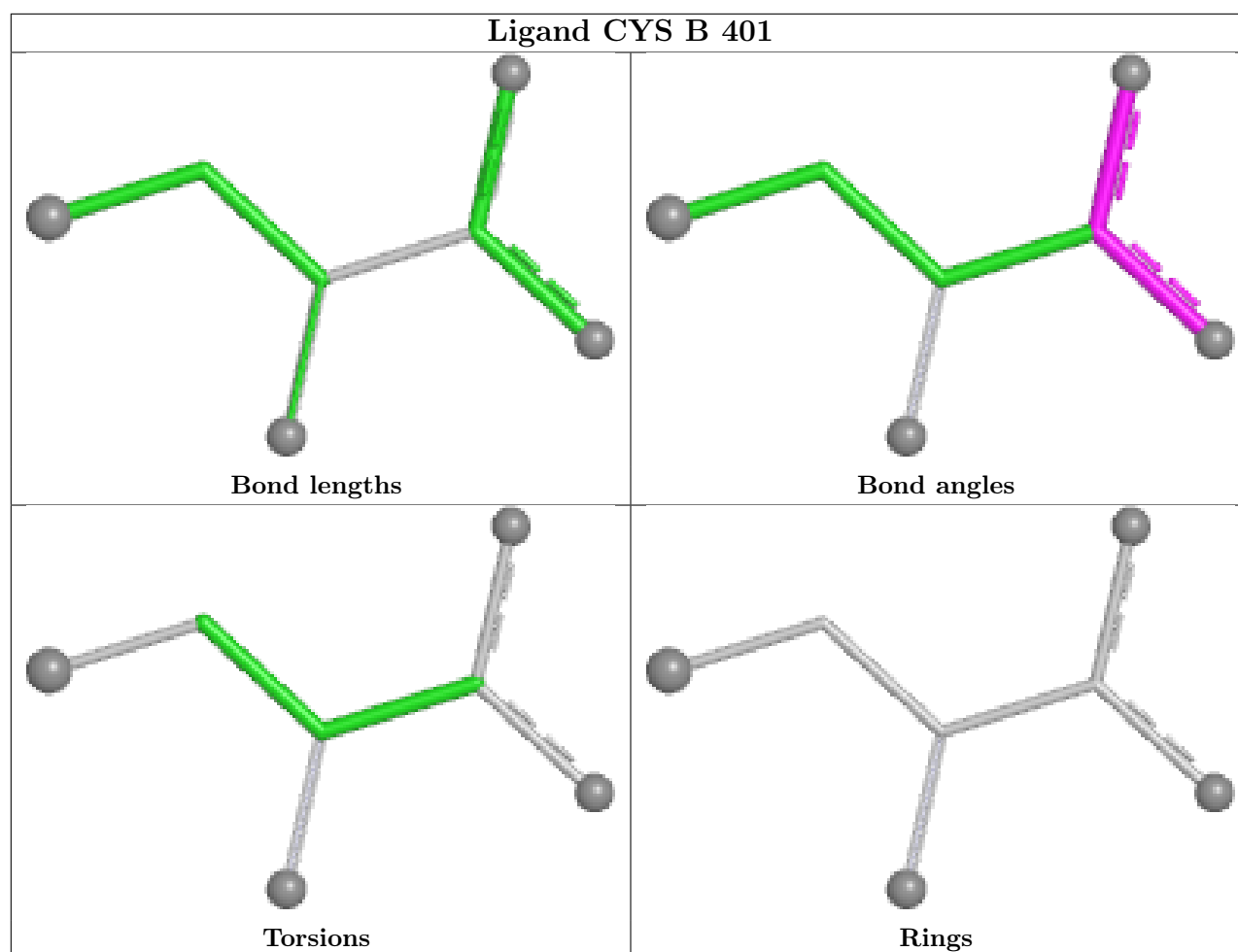
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	CYS	1	0
2	B	402	CYS	1	0

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	288/331 (87%)	1.10	50 (17%) 4 3	13, 26, 69, 120	1 (0%)
1	B	297/331 (89%)	1.40	66 (22%) 2 2	14, 33, 75, 95	1 (0%)
1	C	300/331 (90%)	1.26	60 (20%) 3 2	12, 29, 77, 167	1 (0%)
All	All	885/993 (89%)	1.25	176 (19%) 3 2	12, 30, 74, 167	3 (0%)

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	238	SER	7.2
1	C	245	GLY	7.0
1	C	109	HIS	7.0
1	C	246	ASN	6.9
1	B	251	HIS	6.1
1	A	103	CYS	6.1
1	B	28	THR	6.0
1	B	25	PHE	5.8
1	A	101	ILE	5.8
1	C	104	ALA	5.8
1	A	311	SER	5.5
1	B	243	GLU	5.4
1	B	310	ALA	5.2
1	A	109	HIS	5.2
1	C	244	GLN	5.2
1	C	310	ALA	5.0
1	A	34	CYS	5.0
1	A	310	ALA	4.9
1	B	109	HIS	4.9
1	B	311	SER	4.8
1	C	311	SER	4.7
1	B	246	ASN	4.6
1	C	110	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	17	ARG	4.6
1	B	27	THR	4.6
1	B	237	LEU	4.5
1	B	244	GLN	4.4
1	A	96	ARG	4.2
1	B	304	SER	4.1
1	A	59	ARG	4.1
1	B	33	HIS	4.1
1	A	13	GLU	4.0
1	C	96	ARG	3.9
1	A	65	MET	3.9
1	A	102	SER	3.9
1	C	65	MET	3.9
1	B	250	ARG	3.9
1	B	13	GLU	3.9
1	C	103	CYS	3.8
1	A	27	THR	3.8
1	A	301	GLU	3.7
1	A	24	ASP	3.7
1	A	251	HIS	3.7
1	C	99	HIS	3.7
1	B	248	LEU	3.7
1	C	308	ARG	3.7
1	C	102	SER	3.7
1	A	100	GLY	3.7
1	B	34	CYS	3.7
1	C	237	LEU	3.7
1	B	303	PRO	3.7
1	B	30	HIS	3.6
1	A	26	ALA	3.6
1	A	114	LEU	3.6
1	B	100	GLY	3.6
1	C	98	GLN	3.5
1	C	307	TYR	3.5
1	B	31	LEU	3.5
1	B	32	GLY	3.5
1	A	33	HIS	3.4
1	C	95	TYR	3.4
1	B	23	ARG	3.4
1	B	238	SER	3.3
1	B	59	ARG	3.3
1	A	250	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	97	ARG	3.2
1	A	23	ARG	3.1
1	A	25	PHE	3.1
1	B	95	TYR	3.1
1	C	61	GLN	3.1
1	C	59	ARG	3.1
1	C	100	GLY	3.1
1	C	250	ARG	3.1
1	C	101	ILE	3.1
1	A	306	ARG	3.0
1	C	17	ARG	3.0
1	C	60	ARG	3.0
1	C	309	GLU	2.9
1	C	8	LYS	2.9
1	B	223	ALA	2.9
1	B	301	GLU	2.9
1	C	66	GLY	2.9
1	B	306	ARG	2.9
1	B	63	LEU	2.9
1	C	43[A]	TYR	2.9
1	B	286	VAL	2.8
1	A	11	LEU	2.8
1	B	66	GLY	2.8
1	B	58	ARG	2.8
1	B	287	SER	2.8
1	C	238	SER	2.8
1	A	308	ARG	2.8
1	B	302	LYS	2.8
1	C	301	GLU	2.8
1	C	300	ILE	2.7
1	C	112	GLU	2.7
1	C	299	THR	2.7
1	B	24	ASP	2.7
1	B	110	ASP	2.7
1	A	43[A]	TYR	2.6
1	B	9	ASP	2.6
1	B	64	HIS	2.6
1	C	302	LYS	2.6
1	B	148	GLY	2.6
1	A	302	LYS	2.6
1	C	67	ASN	2.6
1	B	98	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	110	ASP	2.5
1	B	99	HIS	2.5
1	C	243	GLU	2.5
1	C	184	LEU	2.5
1	C	71	HIS	2.5
1	C	34	CYS	2.5
1	C	19	VAL	2.5
1	C	26	ALA	2.5
1	C	63	LEU	2.5
1	C	111	PHE	2.5
1	A	30	HIS	2.5
1	A	9	ASP	2.4
1	B	247	LEU	2.4
1	C	25	PHE	2.4
1	B	128	ARG	2.4
1	B	134	ALA	2.4
1	C	32	GLY	2.4
1	C	242	ASP	2.4
1	A	93	HIS	2.4
1	A	99	HIS	2.4
1	B	43[A]	TYR	2.4
1	B	96	ARG	2.4
1	C	93	HIS	2.4
1	C	28	THR	2.3
1	B	17	ARG	2.3
1	A	150	LEU	2.3
1	B	242	ASP	2.3
1	A	28	THR	2.3
1	C	148	GLY	2.3
1	B	11	LEU	2.3
1	B	245	GLY	2.3
1	A	14	ILE	2.3
1	A	8	LYS	2.3
1	A	31	LEU	2.3
1	C	13	GLU	2.2
1	C	119	THR	2.2
1	A	199	GLY	2.2
1	A	44	GLU	2.2
1	A	309	GLU	2.2
1	C	57	TYR	2.2
1	C	52	ILE	2.2
1	B	38	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	33	HIS	2.1
1	A	66	GLY	2.1
1	C	11	LEU	2.1
1	A	98	GLN	2.1
1	A	116	GLN	2.1
1	A	217	GLY	2.1
1	B	36	LEU	2.1
1	B	20	GLU	2.1
1	C	115	ALA	2.1
1	B	125	LEU	2.1
1	C	40	GLU	2.1
1	B	16	ASP	2.1
1	B	129	LEU	2.1
1	B	288	LEU	2.1
1	A	32	GLY	2.1
1	B	29	HIS	2.1
1	B	10	GLN	2.0
1	C	116	GLN	2.0
1	A	187	TRP	2.0
1	B	193	GLY	2.0
1	B	225	HIS	2.0
1	A	10	GLN	2.0
1	B	91	LEU	2.0
1	A	259	ASP	2.0
1	B	35	PRO	2.0
1	B	65	MET	2.0
1	B	57	TYR	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,

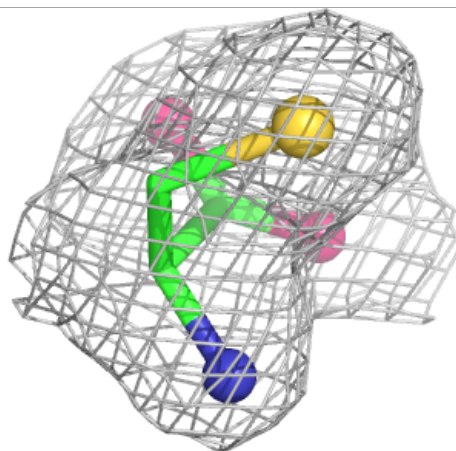
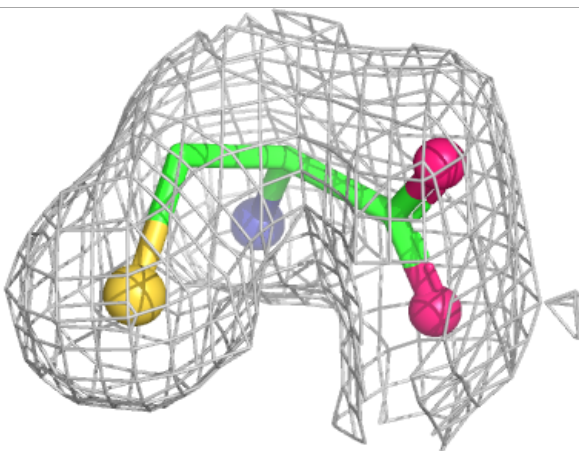
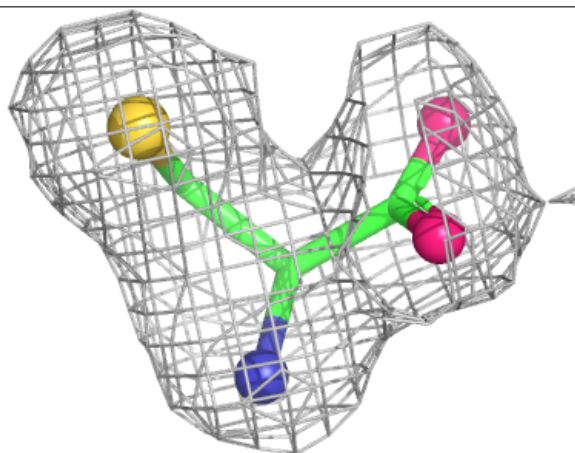
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CYS	B	401	7/7	0.89	0.12	18,20,21,22	0
2	CYS	B	402	7/7	0.92	0.10	18,19,20,24	0
2	CYS	A	401	7/7	0.94	0.10	14,19,22,24	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.

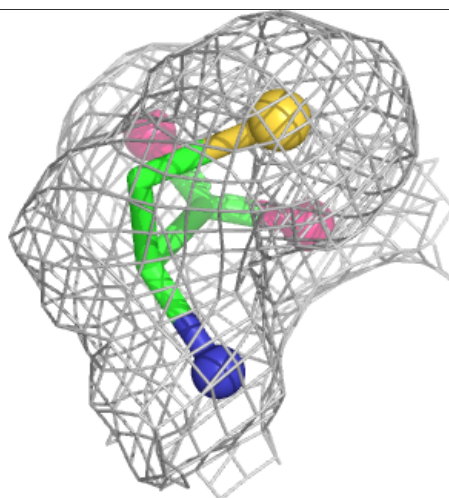
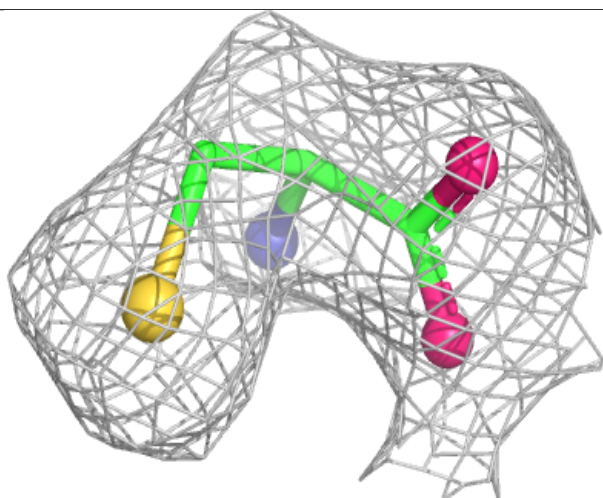
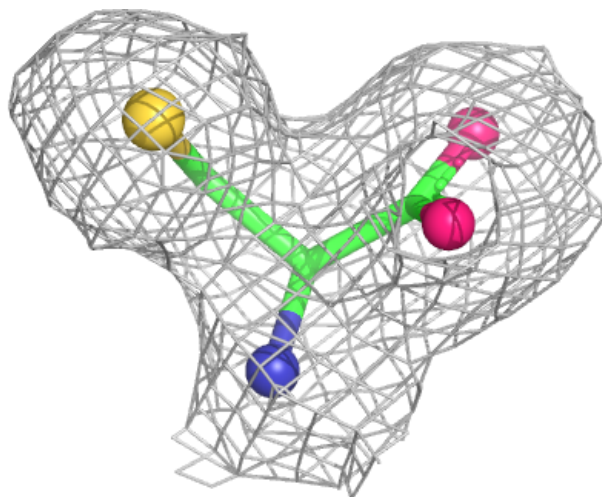
Electron density around CYS B 401:

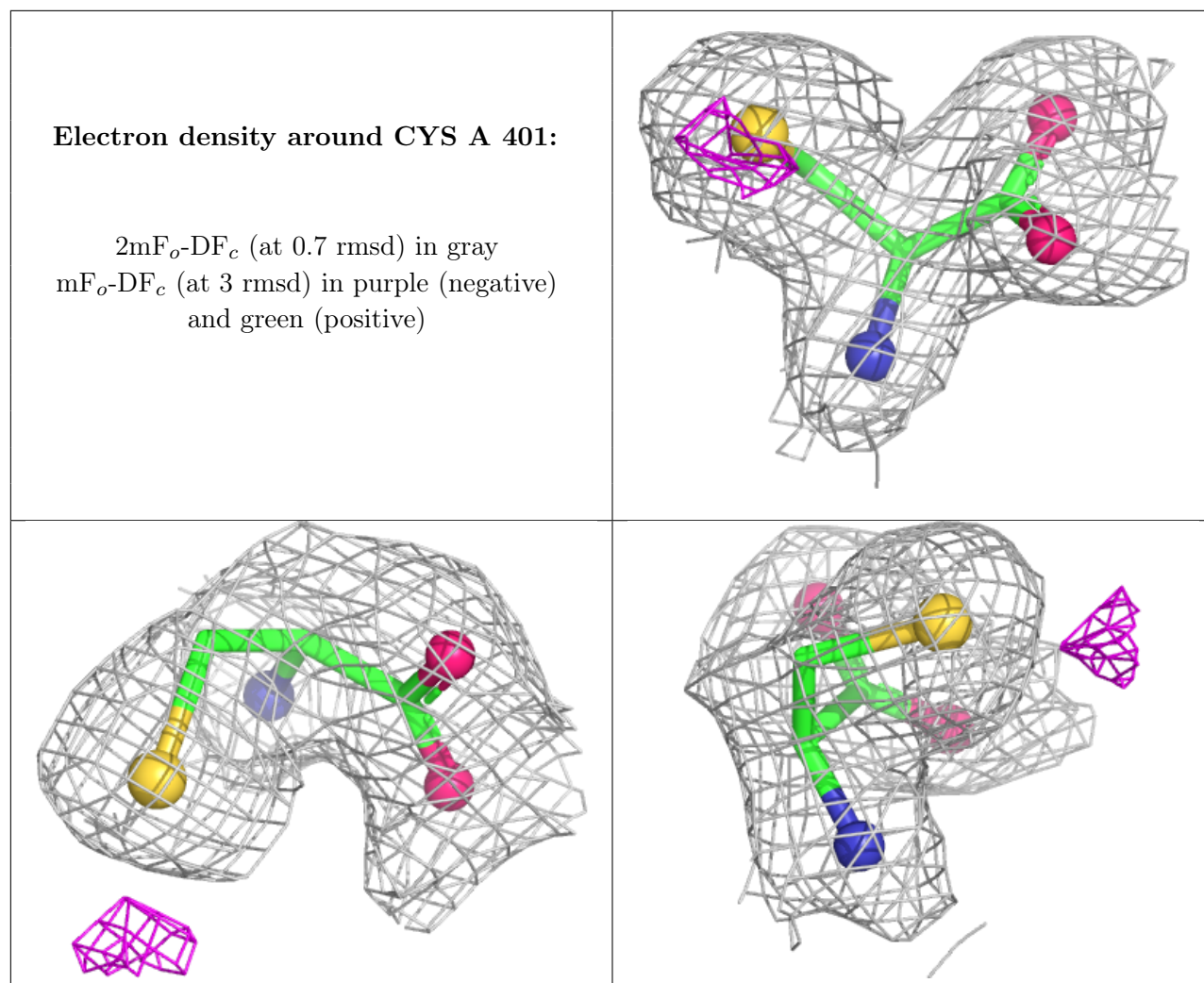
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CYS B 402:

$2mF_o-DF_c$ (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.