



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:07 AM UTC

PDB ID : 3P9K / pdb_00003p9k
Title : Crystal structure of perennial ryegrass LpOMT1 complexed with S-adenosyl-L-homocysteine and coniferaldehyde
Authors : Louie, G.V.; Noel, J.P.; Bowman, M.E.
Deposited on : 2010-10-17
Resolution : 2.25 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

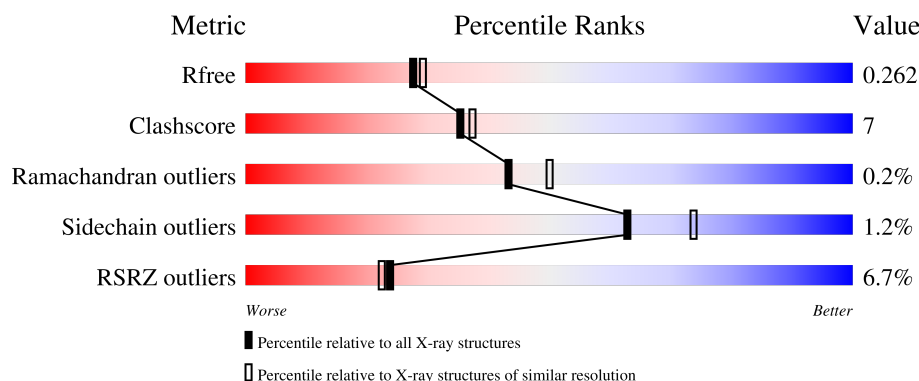
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	364	6% 79% 19% .
1	B	364	9% 77% 19% ..
1	C	364	6% 81% 16% ..
1	D	364	5% 79% 17% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11230 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 Caffeic acid O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2704	1726	453	506	19			
1	B	356	Total	C	N	O	S	0	0	0
			2692	1719	451	503	19			
1	C	357	Total	C	N	O	S	0	0	0
			2698	1723	453	504	18			
1	D	351	Total	C	N	O	S	0	0	0
			2666	1704	447	497	18			

There are 16 discrepancies between the modelled and reference sequences:

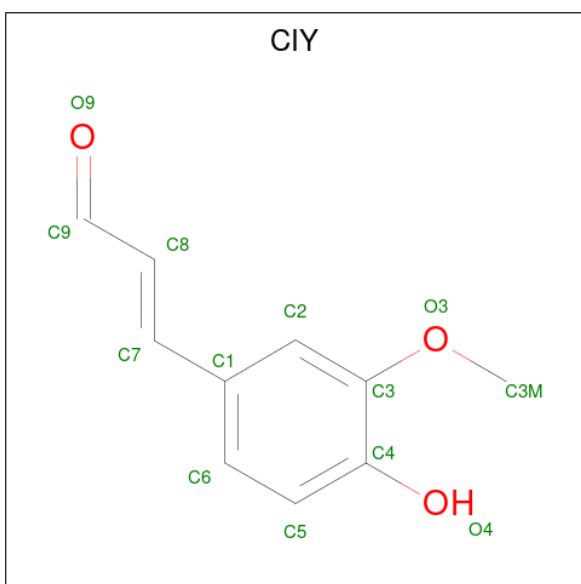
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q9ZTU2
A	-2	SER	-	expression tag	UNP Q9ZTU2
A	-1	HIS	-	expression tag	UNP Q9ZTU2
A	0	GLY	-	expression tag	UNP Q9ZTU2
B	-3	GLY	-	expression tag	UNP Q9ZTU2
B	-2	SER	-	expression tag	UNP Q9ZTU2
B	-1	HIS	-	expression tag	UNP Q9ZTU2
B	0	GLY	-	expression tag	UNP Q9ZTU2
C	-3	GLY	-	expression tag	UNP Q9ZTU2
C	-2	SER	-	expression tag	UNP Q9ZTU2
C	-1	HIS	-	expression tag	UNP Q9ZTU2
C	0	GLY	-	expression tag	UNP Q9ZTU2
D	-3	GLY	-	expression tag	UNP Q9ZTU2
D	-2	SER	-	expression tag	UNP Q9ZTU2
D	-1	HIS	-	expression tag	UNP Q9ZTU2
D	0	GLY	-	expression tag	UNP Q9ZTU2

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is (2E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enal (CCD ID: CIY) (formula: $C_{10}H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	10	3		
3	B	1	Total	C	O	0	0
			13	10	3		
3	C	1	Total	C	O	0	0
			13	10	3		
3	D	1	Total	C	O	0	0
			13	10	3		

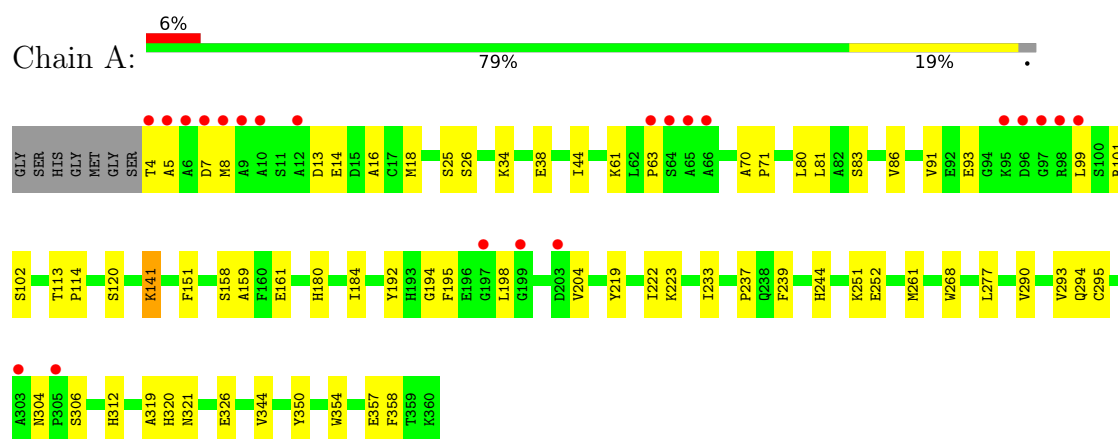
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	76	Total	O	0	0
			76	76		
4	B	59	Total	O	0	0
			59	59		
4	C	100	Total	O	0	0
			100	100		
4	D	79	Total	O	0	0
			79	79		

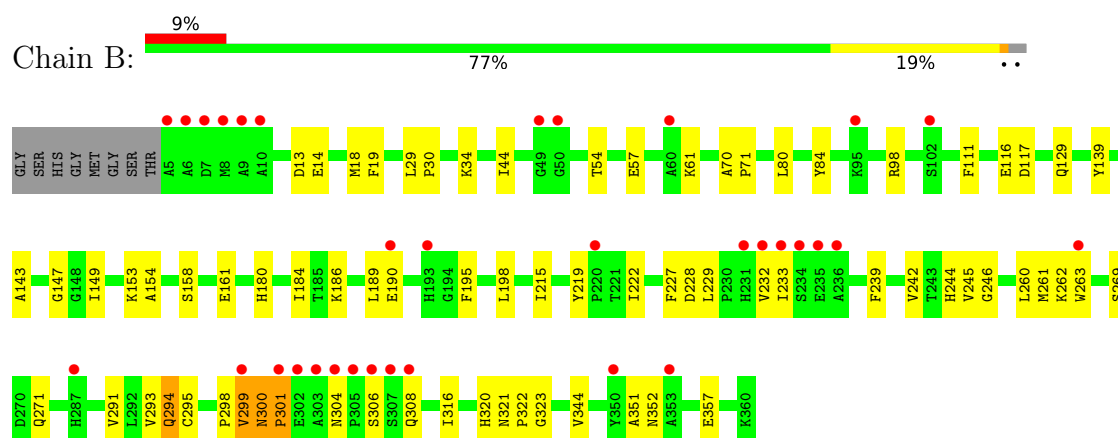
3 Residue-property plots [i](#)

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.

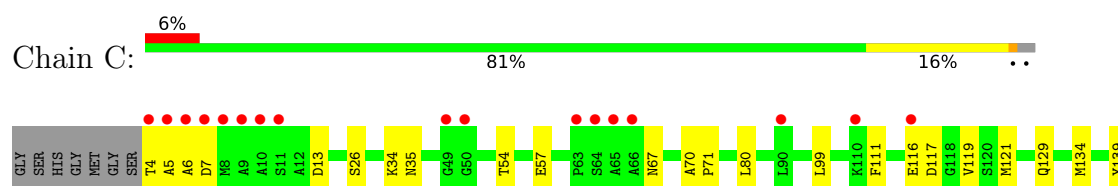
• Molecule 1: Caffeic acid O-methyltransferase

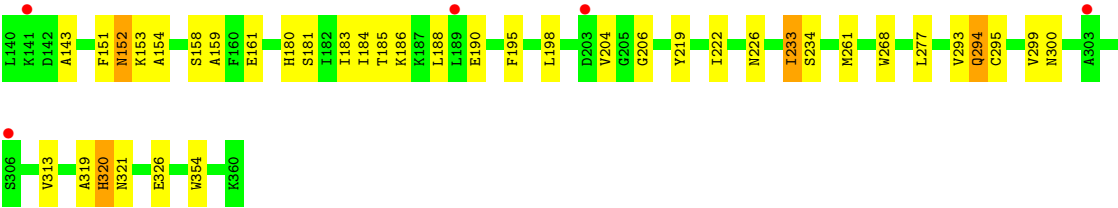


• Molecule 1: Caffeic acid O-methyltransferase

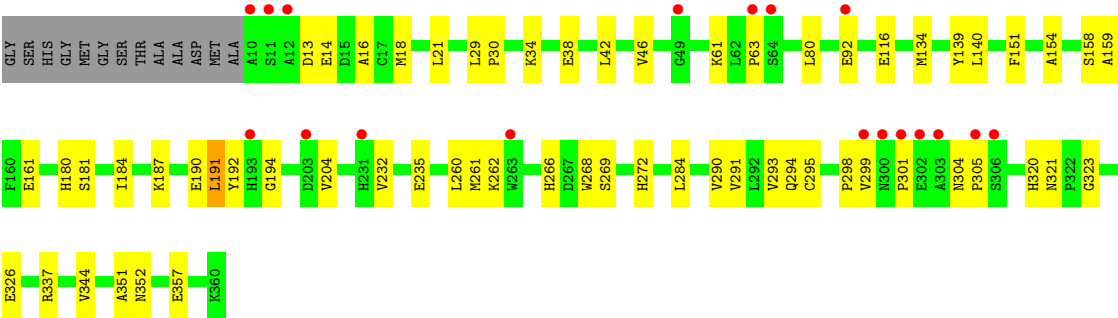
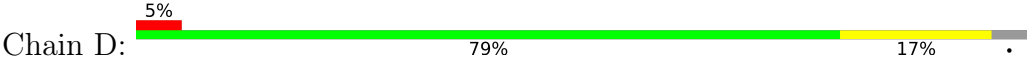


• Molecule 1: Caffeic acid O-methyltransferase





● Molecule 1: Caffeic acid O-methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.38Å 85.06Å 98.59Å 90.00° 111.75° 90.00°	Depositor
Resolution (Å)	48.69 – 2.25 48.69 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.69-2.25) 99.5 (48.69-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.232 , 0.262 0.232 , 0.262	Depositor DCC
R_{free} test set	4808 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.914	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11230	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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 47.93 % 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 9.2468e-05. 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: SAH, CIY

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	0.41	0/2767	0.89	10/3759 (0.3%)
1	B	0.40	0/2755	0.88	8/3742 (0.2%)
1	C	0.41	0/2761	0.91	7/3752 (0.2%)
1	D	0.43	0/2729	0.89	6/3707 (0.2%)
All	All	0.41	0/11012	0.89	31/14960 (0.2%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	ASN	N-CA-C	8.39	121.39	110.40
1	C	321	ASN	N-CA-C	8.12	121.03	110.40
1	D	321	ASN	N-CA-C	7.62	120.38	110.40
1	B	321	ASN	N-CA-C	6.71	119.19	110.40
1	C	268	TRP	N-CA-C	6.41	119.98	109.85
1	B	147	GLY	N-CA-C	-6.36	103.40	112.81
1	C	67	ASN	CA-C-N	6.35	126.04	119.56
1	C	67	ASN	C-N-CA	6.35	126.04	119.56
1	D	321	ASN	CA-C-N	6.26	127.67	119.84
1	D	321	ASN	C-N-CA	6.26	127.67	119.84
1	A	321	ASN	CA-C-N	6.15	127.53	119.84
1	A	321	ASN	C-N-CA	6.15	127.53	119.84
1	A	102	SER	N-CA-C	-5.88	100.21	109.50
1	C	320	HIS	N-CA-C	5.85	121.30	114.04
1	A	320	HIS	N-CA-C	5.70	120.89	113.88
1	C	295	CYS	N-CA-C	-5.65	102.15	110.52
1	D	295	CYS	N-CA-C	-5.64	102.17	110.52
1	A	295	CYS	N-CA-C	-5.55	102.30	110.52
1	B	232	VAL	N-CA-C	-5.50	107.44	111.90
1	B	321	ASN	CA-C-N	5.47	126.68	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	321	ASN	C-N-CA	5.47	126.68	119.84
1	A	268	TRP	N-CA-C	5.46	117.98	109.52
1	C	319	ALA	N-CA-C	5.35	117.19	111.36
1	A	63	PRO	N-CA-C	-5.31	105.31	112.48
1	A	326	GLU	N-CA-C	-5.31	103.38	110.55
1	B	19	PHE	N-CA-C	-5.27	105.62	111.36
1	D	320	HIS	N-CA-C	5.26	120.56	114.04
1	D	326	GLU	N-CA-C	-5.19	103.54	110.55
1	A	319	ALA	N-CA-C	5.18	116.93	111.28
1	B	320	HIS	N-CA-C	5.11	120.89	114.31
1	B	295	CYS	N-CA-C	-5.01	103.78	110.55

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	2704	0	2677	45	0
1	B	2692	0	2659	54	0
1	C	2698	0	2668	39	0
1	D	2666	0	2642	40	0
2	A	26	0	19	0	0
2	B	26	0	19	1	0
2	C	26	0	19	1	0
2	D	26	0	19	0	0
3	A	13	0	9	0	0
3	B	13	0	9	3	0
3	C	13	0	10	0	0
3	D	13	0	9	0	0
4	A	76	0	0	1	0
4	B	59	0	0	3	0
4	C	100	0	0	1	0
4	D	79	0	0	1	0
All	All	11230	0	10759	161	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 (161) 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:D:299:VAL:O	1:D:301:PRO:HD3	1.84	0.75
1:C:4:THR:HG22	1:C:6:ALA:H	1.53	0.72
1:A:80:LEU:C	1:A:80:LEU:HD13	2.15	0.72
1:A:18:MET:HE2	1:B:352:ASN:ND2	2.04	0.71
1:D:190:GLU:C	1:D:191:LEU:HD23	2.15	0.71
1:A:91:VAL:HG22	1:A:101:ARG:HG2	1.73	0.70
1:C:99:LEU:HD11	1:D:299:VAL:HG13	1.72	0.70
1:B:180:HIS:CE1	1:B:184:ILE:HG13	2.28	0.69
1:A:233:ILE:HG23	1:A:244:HIS:HB3	1.77	0.67
1:A:83:SER:HB2	1:B:308:GLN:HG2	1.77	0.66
1:B:299:VAL:O	1:B:300:ASN:HB2	1.96	0.65
1:D:14:GLU:O	1:D:18:MET:HG3	1.96	0.65
1:D:116:GLU:H	1:D:116:GLU:CD	2.05	0.65
1:C:158:SER:OG	1:C:161:GLU:HG3	1.98	0.64
1:C:80:LEU:C	1:C:80:LEU:HD13	2.23	0.63
1:D:304:ASN:HB2	1:D:305:PRO:HD2	1.79	0.63
1:D:294:GLN:NE2	4:D:1113:HOH:O	2.31	0.63
1:A:14:GLU:O	1:A:18:MET:HG3	1.98	0.62
1:A:158:SER:OG	1:A:161:GLU:HG3	2.00	0.62
1:C:186:LYS:O	1:C:190:GLU:HG3	1.99	0.62
1:C:134:MET:HE2	1:D:134:MET:HE2	1.82	0.62
1:C:152:ASN:H	1:C:152:ASN:HD22	1.48	0.61
1:B:263:TRP:O	3:B:602:CIY:H3M	2.01	0.61
1:C:119:VAL:HG23	1:C:183:ILE:HD11	1.81	0.61
1:A:91:VAL:HG11	1:A:99:LEU:HD13	1.82	0.61
1:D:139:TYR:CD2	1:D:154:ALA:HB2	2.36	0.60
1:D:180:HIS:CE1	1:D:184:ILE:HG13	2.37	0.59
1:C:180:HIS:CE1	1:C:184:ILE:HG13	2.38	0.59
1:D:299:VAL:C	1:D:301:PRO:HD3	2.29	0.57
1:B:139:TYR:CD2	1:B:154:ALA:HB2	2.39	0.57
1:A:16:ALA:HB3	1:B:111:PHE:HE2	1.68	0.57
1:C:4:THR:HB	1:C:7:ASP:CB	2.34	0.57
1:B:233:ILE:HG23	1:B:244:HIS:HB3	1.87	0.56
1:A:180:HIS:CE1	1:A:184:ILE:HG13	2.40	0.56
1:D:204:VAL:HB	1:D:261:MET:HG2	1.87	0.56
1:A:219:TYR:HB3	1:A:222:ILE:HD13	1.87	0.56
1:B:34:LYS:HD2	1:B:129:GLN:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ALA:HB3	1:C:71:PRO:HD3	1.88	0.56
1:B:260:LEU:HD12	1:B:291:VAL:O	2.06	0.56
1:A:4:THR:HA	1:A:7:ASP:HB2	1.88	0.56
1:C:143:ALA:HA	1:C:153:LYS:HE3	1.88	0.56
1:B:344:VAL:HA	1:B:357:GLU:O	2.07	0.55
1:C:152:ASN:HD22	1:C:152:ASN:N	2.04	0.55
1:A:70:ALA:HB3	1:A:71:PRO:HD3	1.89	0.55
1:B:271:GLN:HG3	4:B:1237:HOH:O	2.06	0.55
1:B:298:PRO:HG3	1:B:301:PRO:HB3	1.87	0.55
1:C:54:THR:OG1	1:C:57:GLU:HG3	2.06	0.55
1:D:192:TYR:CZ	1:D:194:GLY:HA3	2.42	0.54
1:A:237:PRO:HG2	1:A:239:PHE:CZ	2.43	0.53
1:B:262:LYS:HG3	1:B:293:VAL:HB	1.91	0.53
1:A:4:THR:O	1:A:8:MET:N	2.41	0.52
1:A:204:VAL:HB	1:A:261:MET:HG2	1.92	0.52
1:B:116:GLU:HG2	1:B:117:ASP:N	2.25	0.52
1:D:191:LEU:HD23	1:D:191:LEU:N	2.25	0.52
1:A:304:ASN:OD1	1:A:306:SER:HB3	2.10	0.51
1:B:304:ASN:C	1:B:306:SER:H	2.18	0.51
1:B:98:ARG:HD3	1:B:98:ARG:C	2.36	0.51
1:B:298:PRO:C	1:B:300:ASN:H	2.18	0.51
1:C:204:VAL:HB	1:C:261:MET:HG2	1.92	0.51
1:B:54:THR:OG1	1:B:57:GLU:HG3	2.10	0.51
1:D:139:TYR:CE2	1:D:154:ALA:HB2	2.45	0.50
1:B:186:LYS:O	1:B:190:GLU:HG3	2.12	0.50
1:A:195:PHE:HA	1:A:198:LEU:HD12	1.94	0.49
1:B:189:LEU:HD21	1:B:215:ILE:HG12	1.93	0.49
1:D:29:LEU:HB3	1:D:30:PRO:CD	2.42	0.49
1:C:134:MET:CE	1:D:134:MET:HE2	2.43	0.49
1:B:158:SER:OG	1:B:161:GLU:HG3	2.12	0.49
1:B:219:TYR:HB2	1:B:222:ILE:HD12	1.94	0.49
1:D:266:HIS:HB3	1:D:294:GLN:HE22	1.78	0.49
1:D:351:ALA:O	1:D:352:ASN:HB2	2.12	0.49
1:D:42:LEU:O	1:D:46:VAL:HG23	2.12	0.49
1:D:269:SER:HB3	1:D:323:GLY:HA3	1.94	0.49
1:B:98:ARG:HH11	1:B:98:ARG:HG3	1.78	0.49
1:B:294:GLN:NE2	4:B:1040:HOH:O	2.45	0.49
1:C:151:PHE:CE2	1:C:159:ALA:HA	2.48	0.49
1:D:80:LEU:C	1:D:80:LEU:HD13	2.38	0.49
1:C:4:THR:HG22	1:C:5:ALA:N	2.28	0.49
1:A:251:LYS:O	1:A:252:GLU:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:GLU:HG3	1:C:117:ASP:N	2.29	0.48
1:B:80:LEU:C	1:B:80:LEU:HD13	2.39	0.48
1:B:239:PHE:HB2	1:B:242:VAL:HB	1.95	0.48
1:D:262:LYS:HG3	1:D:293:VAL:HB	1.96	0.48
1:D:337:ARG:HH11	1:D:337:ARG:HG3	1.79	0.47
1:A:16:ALA:HB3	1:B:111:PHE:CE2	2.49	0.47
1:C:195:PHE:O	1:C:198:LEU:HB2	2.15	0.47
1:D:158:SER:OG	1:D:161:GLU:HG3	2.14	0.47
1:A:26:SER:OG	1:B:30:PRO:HB3	2.14	0.47
1:A:223:LYS:HD2	1:A:223:LYS:N	2.29	0.47
1:A:141:LYS:NZ	1:A:141:LYS:HB3	2.29	0.47
1:A:192:TYR:CZ	1:A:194:GLY:HA3	2.50	0.47
1:C:116:GLU:HG3	1:C:117:ASP:H	1.80	0.47
1:C:121:MET:HE3	1:D:21:LEU:HD21	1.96	0.47
1:A:113:THR:O	1:A:120:SER:HB3	2.16	0.46
1:B:298:PRO:CG	1:B:301:PRO:HB3	2.45	0.46
1:A:222:ILE:C	1:A:223:LYS:HD2	2.41	0.46
1:A:34:LYS:O	1:A:38:GLU:HG3	2.15	0.46
1:A:80:LEU:C	1:A:80:LEU:CD1	2.87	0.46
1:B:70:ALA:HB3	1:B:71:PRO:HD3	1.98	0.46
1:B:198:LEU:HB3	1:B:222:ILE:HG12	1.98	0.46
1:D:232:VAL:O	1:D:235:GLU:HG2	2.16	0.46
1:B:263:TRP:HB3	3:B:602:CIY:C3M	2.46	0.46
1:C:111:PHE:HE2	1:D:16:ALA:HB3	1.81	0.46
1:D:268:TRP:HB3	1:D:272:HIS:HB2	1.98	0.45
1:C:219:TYR:HB2	1:C:222:ILE:HD12	1.98	0.45
1:B:299:VAL:O	1:B:300:ASN:CB	2.63	0.45
1:D:298:PRO:HG2	1:D:301:PRO:HG3	1.98	0.45
1:C:233:ILE:HG13	1:C:234:SER:N	2.32	0.45
1:A:4:THR:HB	1:A:8:MET:HG3	1.99	0.45
1:B:261:MET:HA	4:B:1143:HOH:O	2.17	0.45
1:A:151:PHE:CE2	1:A:159:ALA:HA	2.51	0.44
1:B:269:SER:HB3	1:B:323:GLY:HA3	1.99	0.44
1:B:29:LEU:HB3	1:B:30:PRO:CD	2.47	0.44
1:D:260:LEU:HD12	1:D:291:VAL:O	2.17	0.44
1:B:149:ILE:HD11	1:B:322:PRO:HA	1.99	0.44
1:B:44:ILE:HD13	1:B:61:LYS:HB2	1.98	0.44
1:C:294:GLN:NE2	4:C:1074:HOH:O	2.51	0.44
1:A:290:VAL:HB	1:A:358:PHE:HB2	2.00	0.43
1:B:195:PHE:O	1:B:198:LEU:HB2	2.18	0.43
1:C:34:LYS:HD2	1:C:129:GLN:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:GLU:O	1:B:18:MET:HG3	2.18	0.43
1:C:35:ASN:CG	1:D:140:LEU:HB3	2.44	0.43
1:D:187:LYS:O	1:D:191:LEU:HG	2.19	0.43
1:A:18:MET:HE3	1:B:351:ALA:HA	2.01	0.43
1:A:350:TYR:CE1	1:B:14:GLU:HB2	2.53	0.43
1:B:263:TRP:HD1	1:B:294:GLN:NE2	2.15	0.43
2:B:402:SAH:SD	3:B:602:CIY:H3MB	2.58	0.43
1:B:143:ALA:HA	1:B:153:LYS:HE3	2.00	0.43
1:B:228:ASP:O	1:B:246:GLY:HA2	2.18	0.43
1:C:139:TYR:CD2	1:C:154:ALA:HB2	2.54	0.43
1:D:151:PHE:CE2	1:D:159:ALA:HA	2.53	0.43
1:D:284:LEU:HD11	1:D:290:VAL:HG23	2.00	0.43
1:C:293:VAL:HA	1:C:354:TRP:O	2.19	0.42
1:A:4:THR:O	1:A:7:ASP:N	2.52	0.42
1:A:114:PRO:HG3	4:A:1106:HOH:O	2.18	0.42
1:A:277:LEU:HD23	1:A:277:LEU:HA	1.86	0.42
1:A:293:VAL:HA	1:A:354:TRP:O	2.20	0.42
1:A:344:VAL:HA	1:A:357:GLU:O	2.20	0.42
1:C:206:GLY:HA3	1:C:226:ASN:OD1	2.20	0.42
1:B:227:PHE:HA	1:B:245:VAL:O	2.19	0.42
1:D:181:SER:HA	1:D:262:LYS:HE3	2.02	0.42
1:A:4:THR:O	1:A:5:ALA:C	2.61	0.42
1:C:195:PHE:HA	1:C:198:LEU:HD12	2.00	0.42
1:C:26:SER:OG	1:D:30:PRO:HB3	2.19	0.41
1:A:312:HIS:CE1	1:B:84:TYR:HH	2.38	0.41
1:D:61:LYS:O	1:D:63:PRO:HD3	2.21	0.41
1:A:44:ILE:HG23	1:A:61:LYS:HD2	2.02	0.41
1:A:18:MET:CE	1:B:352:ASN:ND2	2.80	0.41
1:D:344:VAL:HA	1:D:357:GLU:O	2.21	0.41
1:D:34:LYS:O	1:D:38:GLU:HG3	2.20	0.41
1:A:18:MET:SD	1:B:306:SER:HB2	2.61	0.41
1:A:25:SER:HB2	1:B:316:ILE:HD11	2.03	0.41
1:B:228:ASP:OD1	1:B:229:LEU:N	2.45	0.40
1:B:304:ASN:C	1:B:306:SER:N	2.80	0.40
1:C:181:SER:OG	2:C:403:SAH:O	2.35	0.40
1:C:185:THR:O	1:C:188:LEU:HB3	2.21	0.40
1:C:277:LEU:HD23	1:C:277:LEU:HA	1.90	0.40
1:C:299:VAL:O	1:C:300:ASN:C	2.63	0.40
1:C:313:VAL:HG12	1:C:326:GLU:OE2	2.21	0.40
1:B:139:TYR:CE2	1:B:154:ALA:HB2	2.56	0.40
1:A:81:LEU:HB3	1:A:86:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:PHE:HB2	1:C:320:HIS:HA	2.03	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	355/364 (98%)	348 (98%)	7 (2%)	0	100	100
1	B	354/364 (97%)	341 (96%)	10 (3%)	3 (1%)	16	14
1	C	355/364 (98%)	346 (98%)	9 (2%)	0	100	100
1	D	349/364 (96%)	337 (97%)	12 (3%)	0	100	100
All	All	1413/1456 (97%)	1372 (97%)	38 (3%)	3 (0%)	43	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	300	ASN
1	B	301	PRO
1	B	299	VAL

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	284/288 (99%)	280 (99%)	4 (1%)	59	70
1	B	281/288 (98%)	279 (99%)	2 (1%)	76	82
1	C	282/288 (98%)	278 (99%)	4 (1%)	59	70
1	D	281/288 (98%)	278 (99%)	3 (1%)	65	75
All	All	1128/1152 (98%)	1115 (99%)	13 (1%)	63	74

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	A	93	GLU
1	A	141	LYS
1	A	294	GLN
1	B	13	ASP
1	B	294	GLN
1	C	13	ASP
1	C	152	ASN
1	C	233	ILE
1	C	294	GLN
1	D	13	ASP
1	D	92	GLU
1	D	191	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	85	ASN
1	A	193	HIS
1	A	218	HIS
1	A	294	GLN
1	A	300	ASN
1	A	308	GLN
1	B	85	ASN
1	B	294	GLN
1	B	333	GLN
1	B	352	ASN
1	C	22	GLN
1	C	152	ASN
1	C	218	HIS

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Mol	Chain	Res	Type
1	C	294	GLN
1	C	300	ASN
1	C	333	GLN
1	D	22	GLN
1	D	85	ASN
1	D	180	HIS
1	D	271	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	SAH	A	401	-	27,28,28	0.86	1 (3%)	36,40,40	1.96	8 (22%)
3	CIY	B	602	-	13,13,13	2.38	4 (30%)	16,16,16	1.79	3 (18%)
3	CIY	A	601	-	13,13,13	2.40	4 (30%)	16,16,16	2.02	3 (18%)
2	SAH	B	402	-	27,28,28	0.87	0	36,40,40	1.99	8 (22%)
3	CIY	D	604	-	13,13,13	2.14	4 (30%)	16,16,16	1.72	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SAH	D	404	-	27,28,28	0.79	0	36,40,40	1.99	7 (19%)
3	CIY	C	603	-	13,13,13	2.32	4 (30%)	16,16,16	1.77	5 (31%)
2	SAH	C	403	-	27,28,28	0.90	1 (3%)	36,40,40	1.98	8 (22%)

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	SAH	A	401	-	-	2/15/31/31	0/3/3/3
3	CIY	B	602	-	-	2/6/6/6	0/1/1/1
3	CIY	A	601	-	-	2/6/6/6	0/1/1/1
2	SAH	B	402	-	-	1/15/31/31	0/3/3/3
3	CIY	D	604	-	-	2/6/6/6	0/1/1/1
2	SAH	D	404	-	-	1/15/31/31	0/3/3/3
3	CIY	C	603	-	-	2/6/6/6	0/1/1/1
2	SAH	C	403	-	-	3/15/31/31	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	CIY	C4-C3	6.25	1.51	1.40
3	B	602	CIY	C4-C3	5.88	1.50	1.40
3	D	604	CIY	C4-C3	5.78	1.50	1.40
3	C	603	CIY	C4-C3	5.68	1.50	1.40
3	A	601	CIY	C6-C5	3.81	1.45	1.38
3	C	603	CIY	C6-C5	3.70	1.44	1.38
3	B	602	CIY	C6-C5	3.45	1.44	1.38
3	B	602	CIY	C5-C4	3.16	1.45	1.39
3	D	604	CIY	C6-C5	2.98	1.43	1.38
3	C	603	CIY	C6-C1	2.94	1.45	1.39
3	C	603	CIY	C5-C4	2.94	1.44	1.39
3	A	601	CIY	C6-C1	2.84	1.45	1.39
3	B	602	CIY	C6-C1	2.84	1.45	1.39
3	A	601	CIY	C5-C4	2.75	1.44	1.39
3	D	604	CIY	C5-C4	2.63	1.44	1.39
2	A	401	SAH	C5-C4	2.40	1.43	1.39
3	D	604	CIY	C6-C1	2.24	1.44	1.39
2	C	403	SAH	C5-C4	2.14	1.42	1.39

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	SAH	C5-C4-N3	-5.15	119.62	126.72
2	D	404	SAH	C5-C4-N3	-5.03	119.79	126.72
2	B	402	SAH	N3-C2-N1	-5.03	120.97	128.58
2	D	404	SAH	N3-C2-N1	-4.93	121.12	128.58
2	C	403	SAH	C5-C4-N3	-4.92	119.94	126.72
2	A	401	SAH	N3-C2-N1	-4.80	121.32	128.58
2	B	402	SAH	C5-C4-N3	-4.74	120.19	126.72
2	C	403	SAH	N3-C2-N1	-4.74	121.41	128.58
2	A	401	SAH	N3-C4-N9	4.47	134.76	127.17
2	D	404	SAH	N3-C4-N9	4.39	134.63	127.17
2	B	402	SAH	N3-C4-N9	4.35	134.56	127.17
2	C	403	SAH	N3-C4-N9	4.29	134.46	127.17
3	A	601	CIY	C3M-O3-C3	-4.26	111.26	117.51
3	D	604	CIY	C3M-O3-C3	-4.23	111.31	117.51
2	D	404	SAH	C2-N3-C4	3.93	121.43	111.83
3	A	601	CIY	O3-C3-C4	3.84	120.31	114.55
2	A	401	SAH	C2-N3-C4	3.84	121.21	111.83
2	C	403	SAH	C2-N3-C4	3.79	121.08	111.83
2	B	402	SAH	C2-N3-C4	3.78	121.06	111.83
2	D	404	SAH	C5-N7-C8	3.71	109.29	103.45
3	B	602	CIY	C3M-O3-C3	-3.71	112.07	117.51
2	C	403	SAH	C5-N7-C8	3.68	109.23	103.45
2	B	402	SAH	C5-N7-C8	3.65	109.19	103.45
3	C	603	CIY	O3-C3-C4	3.56	119.89	114.55
2	A	401	SAH	C5-N7-C8	3.50	108.95	103.45
3	B	602	CIY	O3-C3-C4	3.29	119.48	114.55
3	D	604	CIY	O3-C3-C4	3.07	119.16	114.55
3	C	603	CIY	C3M-O3-C3	-2.89	113.28	117.51
3	A	601	CIY	O3-C3-C2	-2.87	119.13	124.08
2	C	403	SAH	C4-C5-N7	-2.82	107.36	110.58
2	B	402	SAH	N9-C8-N7	-2.77	110.00	113.94
2	C	403	SAH	N9-C8-N7	-2.73	110.06	113.94
2	D	404	SAH	C4-C5-N7	-2.70	107.49	110.58
2	D	404	SAH	N9-C8-N7	-2.65	110.18	113.94
2	C	403	SAH	O4'-C1'-N9	2.63	113.14	108.09
3	C	603	CIY	O3-C3-C2	-2.62	119.57	124.08
2	A	401	SAH	C4-C5-N7	-2.56	107.65	110.58
2	B	402	SAH	C4-C5-N7	-2.56	107.66	110.58
3	B	602	CIY	C1-C7-C8	-2.53	122.73	127.11
2	A	401	SAH	N9-C8-N7	-2.38	110.56	113.94
2	A	401	SAH	O4'-C1'-N9	2.15	112.21	108.09
2	B	402	SAH	C4-N9-C8	2.07	107.91	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	603	CIY	C1-C7-C8	-2.06	123.54	127.11
3	C	603	CIY	O9-C9-C8	-2.05	119.06	125.61

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	CIY	C4-C3-O3-C3M
3	D	604	CIY	C2-C3-O3-C3M
3	B	602	CIY	C2-C3-O3-C3M
3	C	603	CIY	C2-C3-O3-C3M
3	A	601	CIY	C2-C3-O3-C3M
3	D	604	CIY	C4-C3-O3-C3M
3	C	603	CIY	C4-C3-O3-C3M
3	A	601	CIY	C4-C3-O3-C3M
2	C	403	SAH	C-CA-CB-CG
2	C	403	SAH	CB-CG-SD-C5'
2	C	403	SAH	OXT-C-CA-N
2	A	401	SAH	OXT-C-CA-N
2	B	402	SAH	OXT-C-CA-N
2	D	404	SAH	OXT-C-CA-N
2	A	401	SAH	O-C-CA-N

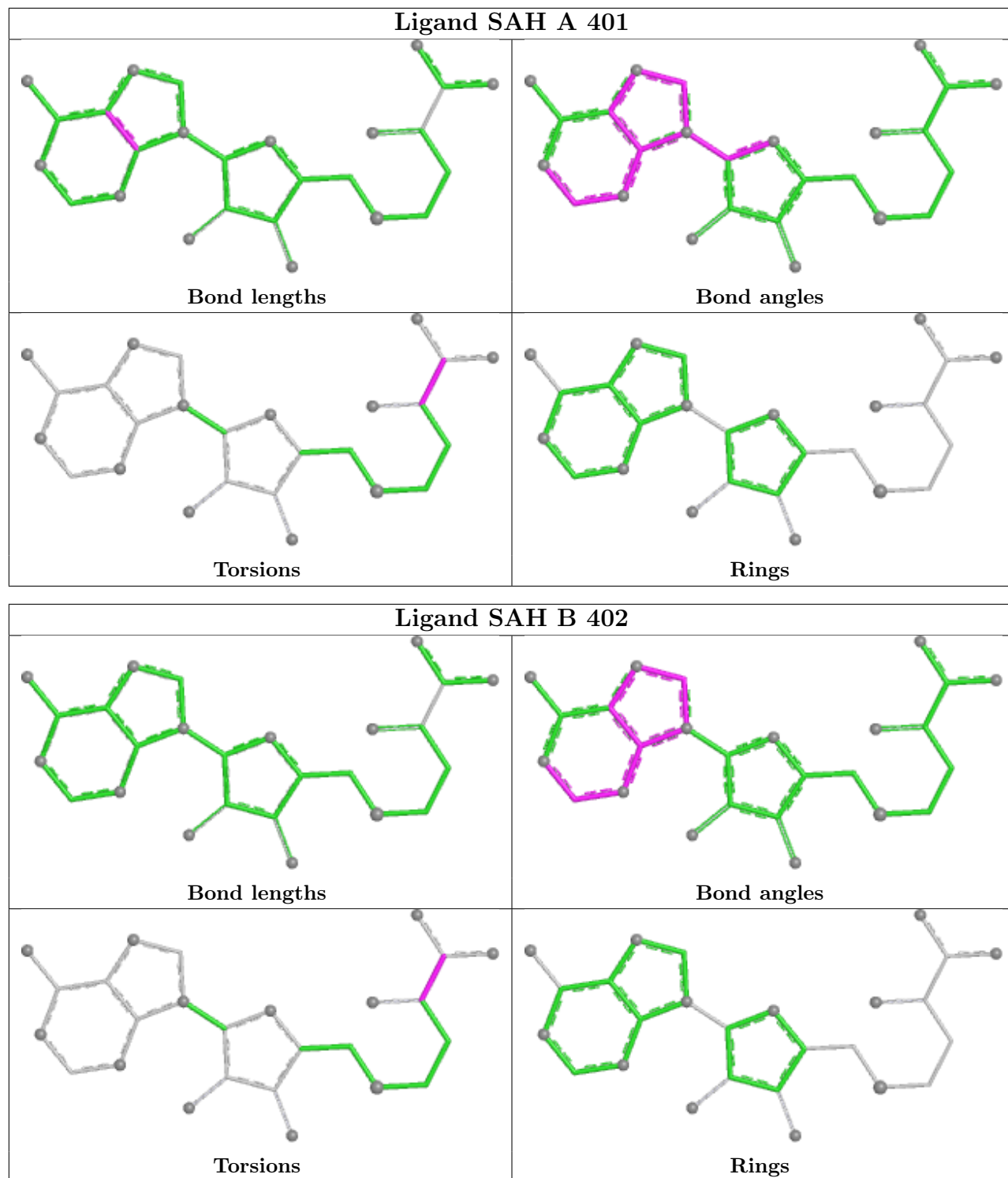
There are no ring outliers.

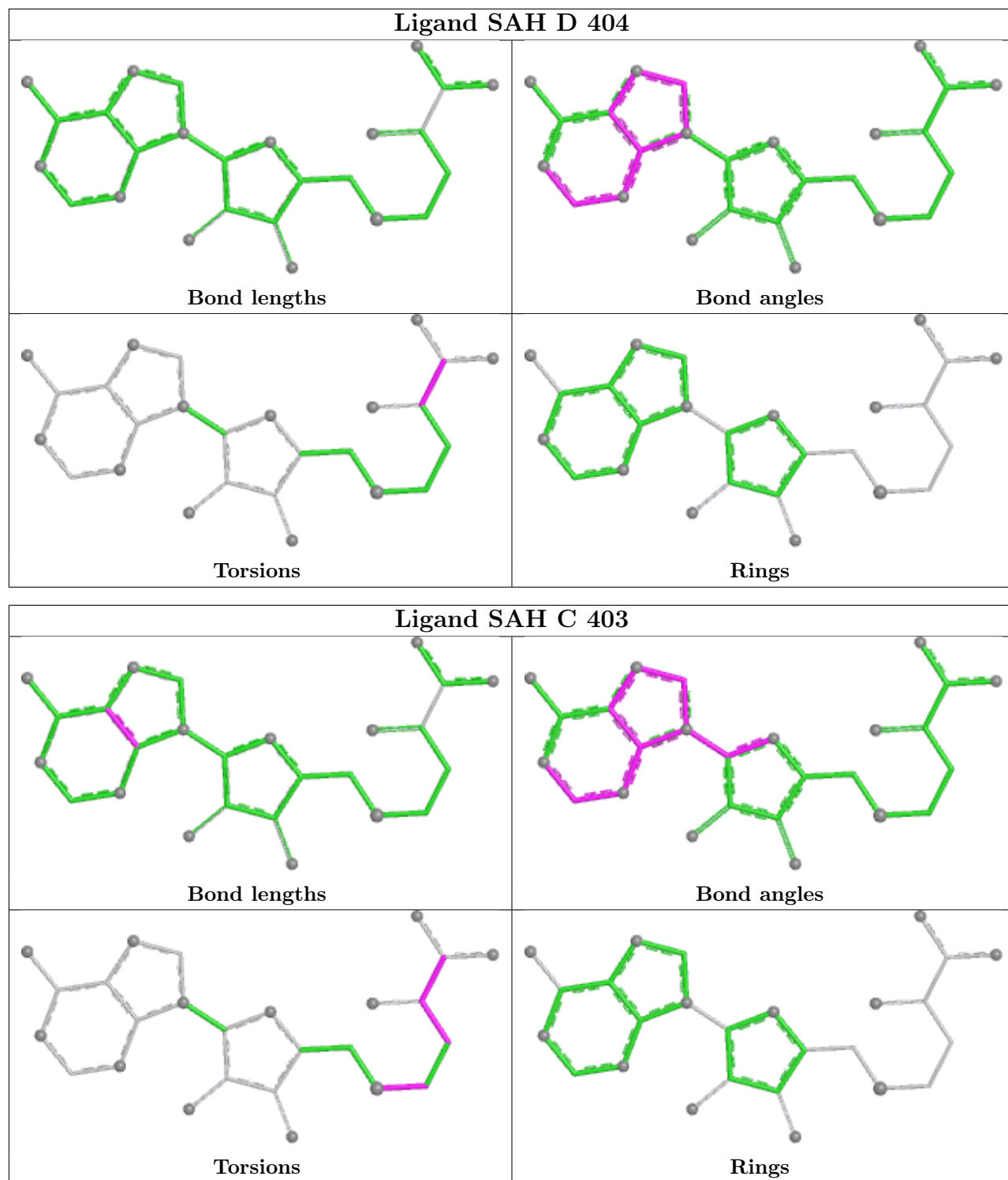
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	CIY	3	0
2	B	402	SAH	1	0
2	C	403	SAH	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 ⓘ

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	357/364 (98%)	0.48	22 (6%) 26 24	19, 32, 59, 82	0
1	B	356/364 (97%)	0.76	33 (9%) 14 13	21, 36, 63, 105	0
1	C	357/364 (98%)	0.46	22 (6%) 26 24	16, 29, 58, 81	0
1	D	351/364 (96%)	0.41	18 (5%) 33 32	12, 31, 53, 91	0
All	All	1421/1456 (97%)	0.53	95 (6%) 24 22	12, 32, 59, 105	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	10	ALA	6.1
1	B	5	ALA	5.7
1	B	304	ASN	5.7
1	C	64	SER	5.5
1	B	306	SER	5.5
1	B	303	ALA	5.4
1	B	305	PRO	5.2
1	C	66	ALA	5.1
1	C	4	THR	4.7
1	C	6	ALA	4.6
1	A	4	THR	4.6
1	A	65	ALA	4.6
1	C	65	ALA	4.4
1	B	299	VAL	4.2
1	D	301	PRO	4.1
1	B	301	PRO	4.0
1	A	64	SER	3.8
1	C	63	PRO	3.8
1	D	305	PRO	3.8
1	B	9	ALA	3.8
1	C	5	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	12	ALA	3.7
1	C	9	ALA	3.6
1	B	6	ALA	3.6
1	B	8	MET	3.4
1	A	66	ALA	3.4
1	A	8	MET	3.4
1	B	307	SER	3.4
1	D	299	VAL	3.3
1	D	63	PRO	3.3
1	D	302	GLU	3.3
1	B	302	GLU	3.1
1	B	10	ALA	3.1
1	A	7	ASP	3.1
1	A	10	ALA	3.1
1	C	203	ASP	3.1
1	A	6	ALA	3.1
1	A	9	ALA	3.0
1	B	50	GLY	3.0
1	A	203	ASP	3.0
1	B	231	HIS	2.9
1	B	236	ALA	2.9
1	C	303	ALA	2.8
1	C	7	ASP	2.8
1	A	5	ALA	2.8
1	A	98	ARG	2.8
1	D	203	ASP	2.7
1	A	95	LYS	2.7
1	D	263	TRP	2.7
1	B	234	SER	2.7
1	C	116	GLU	2.7
1	B	263	TRP	2.7
1	D	303	ALA	2.6
1	B	233	ILE	2.6
1	A	303	ALA	2.6
1	D	306	SER	2.6
1	B	235	GLU	2.5
1	A	63	PRO	2.5
1	C	50	GLY	2.5
1	C	189	LEU	2.5
1	C	8	MET	2.5
1	A	97	GLY	2.4
1	C	11	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	193	HIS	2.4
1	B	232	VAL	2.4
1	B	353	ALA	2.3
1	C	10	ALA	2.3
1	B	7	ASP	2.3
1	B	102	SER	2.3
1	C	90	LEU	2.2
1	A	199	GLY	2.2
1	C	141	LYS	2.2
1	A	99	LEU	2.2
1	C	110	LYS	2.2
1	C	306	SER	2.2
1	B	350	TYR	2.2
1	B	220	PRO	2.2
1	B	308	GLN	2.2
1	D	193	HIS	2.2
1	D	11	SER	2.2
1	C	49	GLY	2.1
1	D	64	SER	2.1
1	A	305	PRO	2.1
1	B	95	LYS	2.1
1	B	190	GLU	2.1
1	B	49	GLY	2.1
1	A	12	ALA	2.1
1	B	60	ALA	2.1
1	D	92	GLU	2.1
1	A	96	ASP	2.0
1	A	197	GLY	2.0
1	D	49	GLY	2.0
1	B	287	HIS	2.0
1	D	231	HIS	2.0
1	D	300	ASN	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](#)

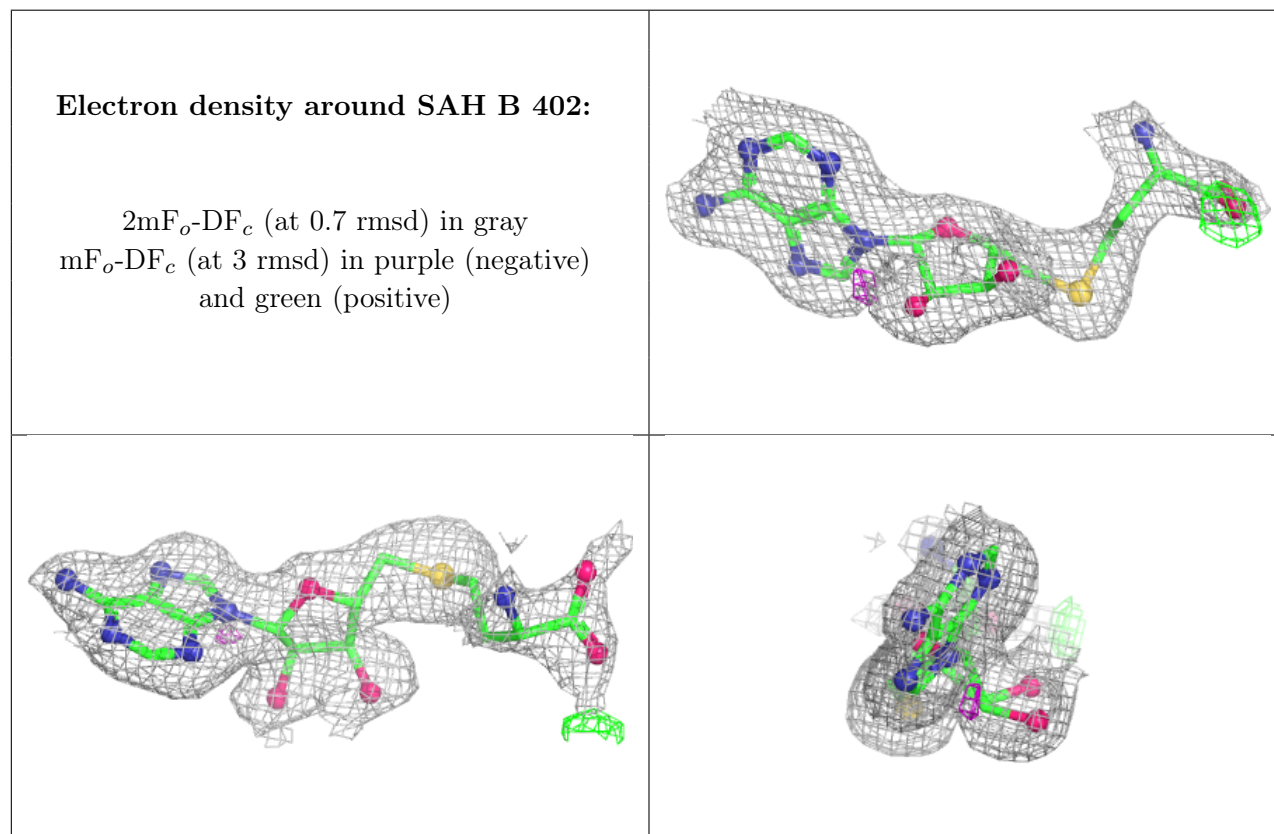
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

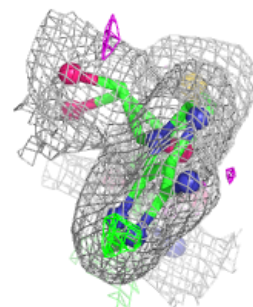
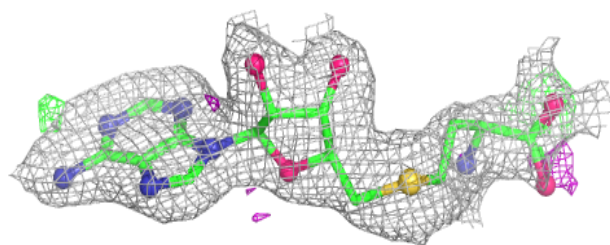
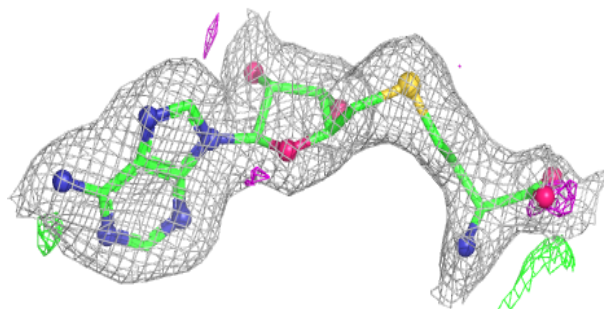
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CIY	B	602	13/13	0.76	0.19	44,53,59,59	0
3	CIY	D	604	13/13	0.78	0.18	35,38,50,53	0
3	CIY	A	601	13/13	0.82	0.14	33,37,40,42	0
3	CIY	C	603	13/13	0.83	0.14	31,36,43,43	0
2	SAH	B	402	26/26	0.92	0.10	24,29,49,51	0
2	SAH	C	403	26/26	0.94	0.09	14,20,41,46	0
2	SAH	A	401	26/26	0.95	0.08	19,23,38,42	0
2	SAH	D	404	26/26	0.95	0.08	12,22,45,49	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.

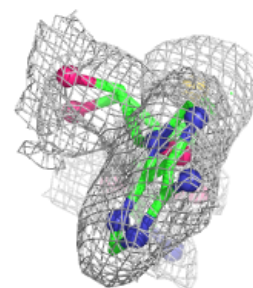
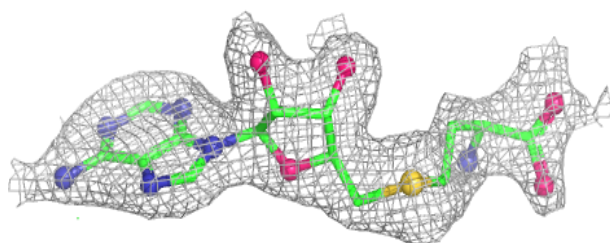
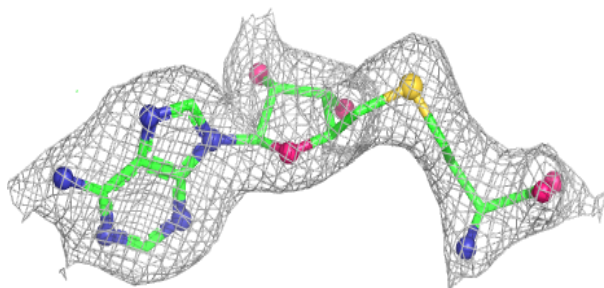


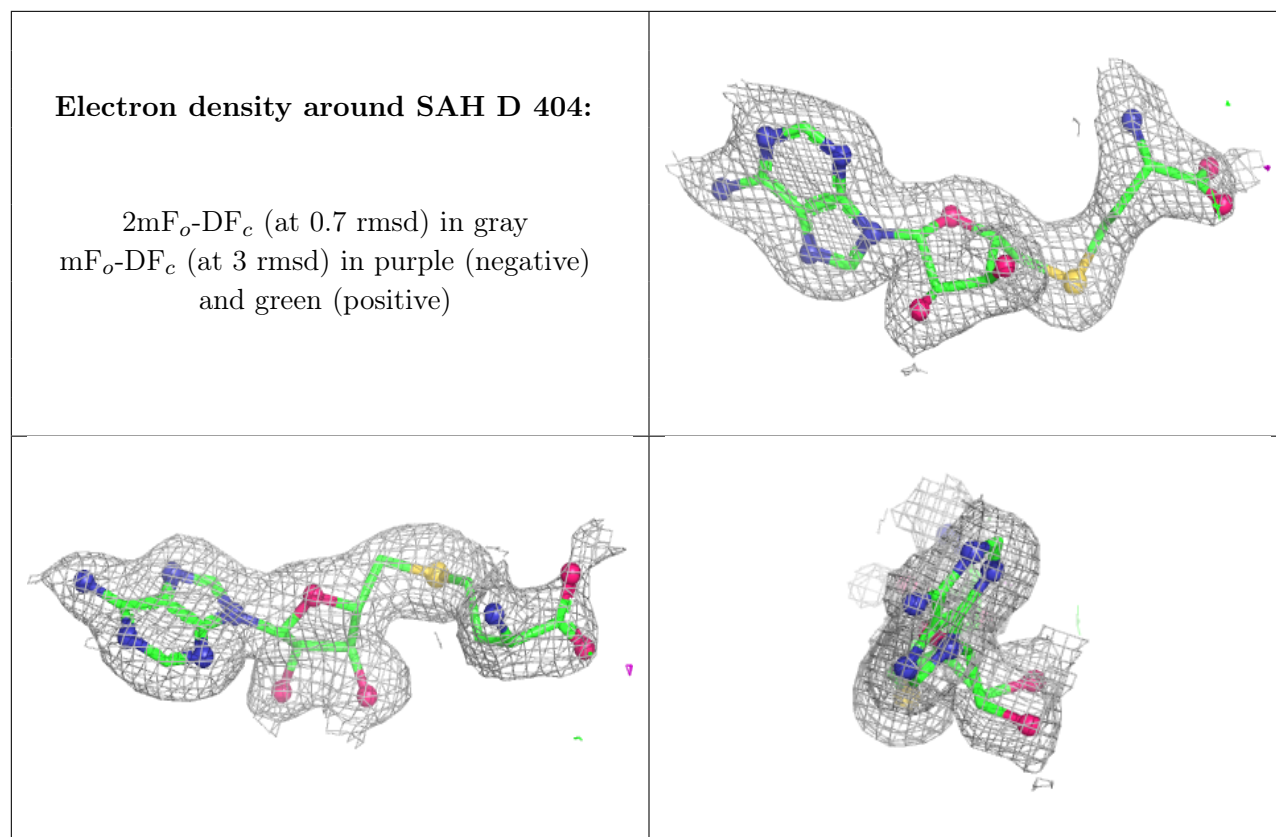
Electron density around SAH C 403:

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

**Electron density around SAH A 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 [i](#)

There are no such residues in this entry.