



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:30 AM UTC

PDB ID : 3REO / pdb_00003reo
Title : Monolignol O-methyltransferase (MOMT)
Authors : Bhuiya, M.W.; Liu, C.J.
Deposited on : 2011-04-04
Resolution : 1.90 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

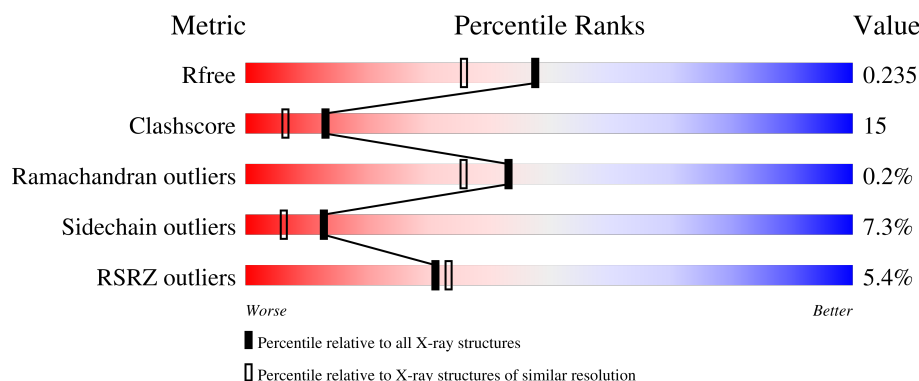
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	368	4% 72% 21% • 5%
1	B	368	3% 69% 23% • •
1	C	368	8% 68% 25% • • •
1	D	368	6% 68% 25% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EUG	C	369	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11187 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.

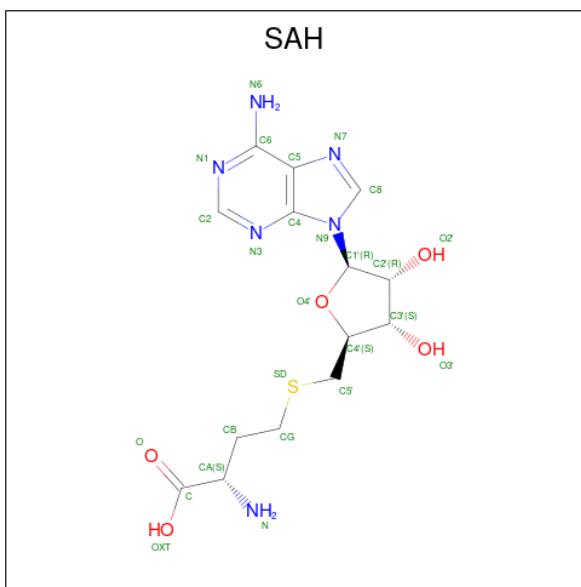
- Molecule 1 is a protein called (Iso)eugenol O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	0	0
			2688	1741	432	497	18			
1	B	352	Total	C	N	O	S	0	0	0
			2694	1744	433	499	18			
1	C	358	Total	C	N	O	S	0	0	0
			2747	1779	442	508	18			
1	D	356	Total	C	N	O	S	0	0	0
			2731	1769	440	504	18			

There are 12 discrepancies between the modelled and reference sequences:

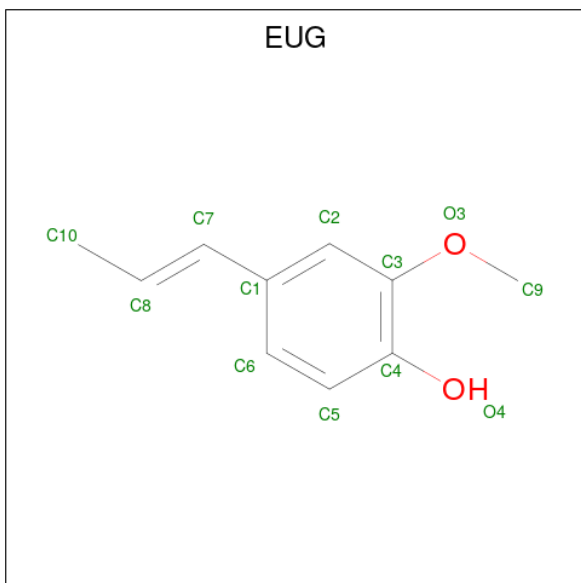
Chain	Residue	Modelled	Actual	Comment	Reference
A	133	LEU	THR	engineered mutation	UNP O04385
A	165	ILE	GLU	engineered mutation	UNP O04385
A	175	ILE	PHE	engineered mutation	UNP O04385
B	133	LEU	THR	engineered mutation	UNP O04385
B	165	ILE	GLU	engineered mutation	UNP O04385
B	175	ILE	PHE	engineered mutation	UNP O04385
C	133	LEU	THR	engineered mutation	UNP O04385
C	165	ILE	GLU	engineered mutation	UNP O04385
C	175	ILE	PHE	engineered mutation	UNP O04385
D	133	LEU	THR	engineered mutation	UNP O04385
D	165	ILE	GLU	engineered mutation	UNP O04385
D	175	ILE	PHE	engineered mutation	UNP O04385

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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 2-methoxy-4-[(1E)-prop-1-en-1-yl]phenol (CCD ID: EUG) (formula: $C_{10}H_{12}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			12	10	2		
3	C	1	Total	C	O	0	0
			12	10	2		
3	D	1	Total	C	O	0	0
			12	10	2		

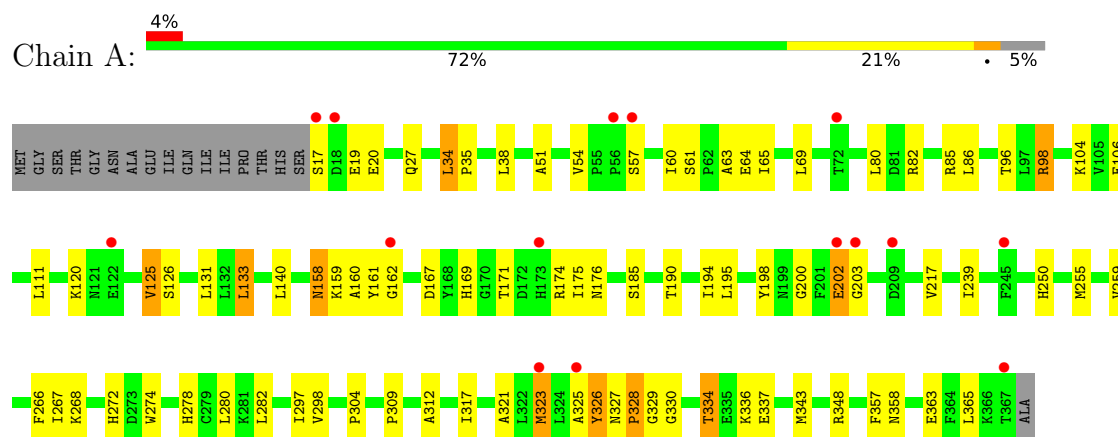
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	46	Total	O	0	0
			46	46		
4	B	69	Total	O	0	0
			69	69		
4	C	39	Total	O	0	0
			39	39		
4	D	33	Total	O	0	0
			33	33		

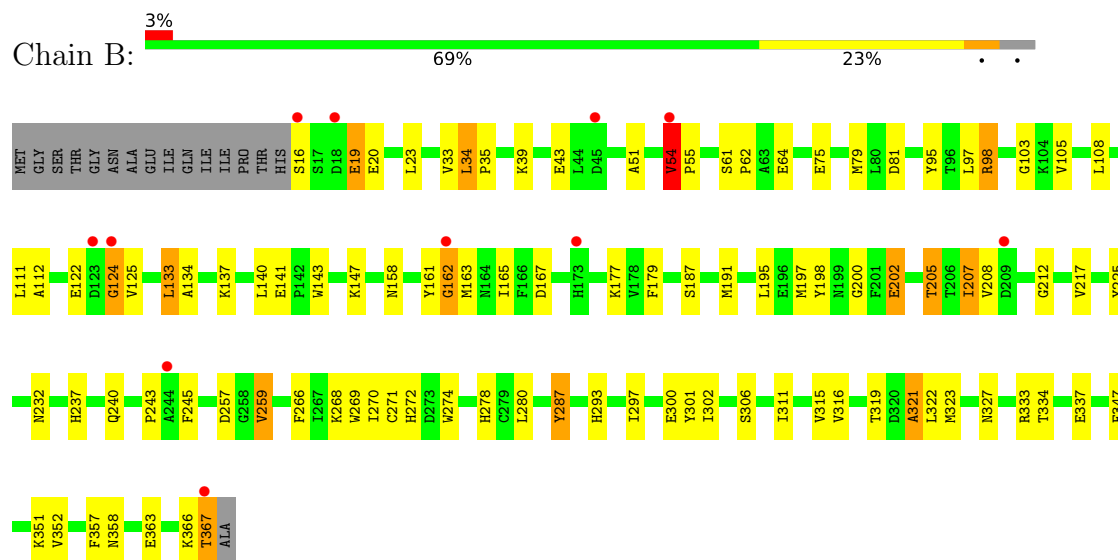
3 Residue-property plots [i](#)

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: (Iso)eugenol O-methyltransferase

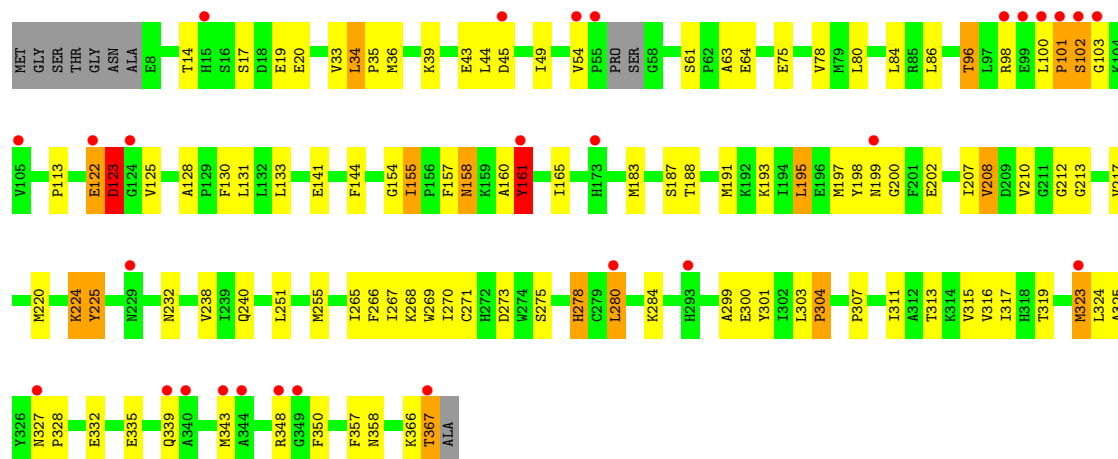


- Molecule 1: (Iso)eugenol O-methyltransferase

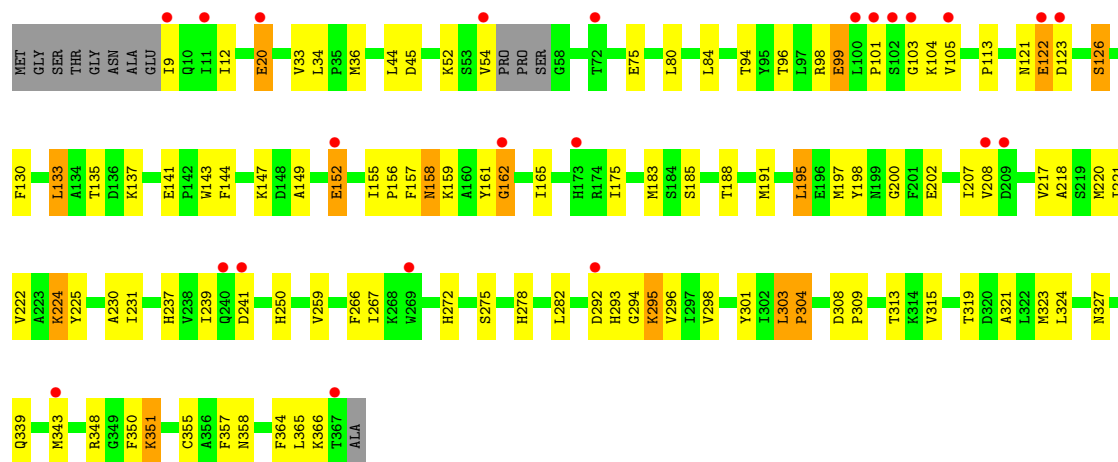


- Molecule 1: (Iso)eugenol O-methyltransferase





• Molecule 1: (Iso)eugenol 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	66.24Å 150.75Å 68.30Å 90.00° 92.67° 90.00°	Depositor
Resolution (Å)	44.37 – 1.90 44.37 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (44.37-1.90) 97.0 (44.37-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5, CNS 1.1	Depositor
R, R_{free}	0.188 , 0.232 0.196 , 0.235	Depositor DCC
R_{free} test set	5092 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.006 for l,k,-h 0.035 for h,-k,-l 0.025 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11187	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EUG, SAH

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.37	10/2753 (0.4%)	1.24	10/3741 (0.3%)
1	B	1.34	7/2759 (0.3%)	1.24	9/3749 (0.2%)
1	C	1.26	4/2812 (0.1%)	1.21	13/3820 (0.3%)
1	D	1.29	3/2795 (0.1%)	1.23	6/3796 (0.2%)
All	All	1.32	24/11119 (0.2%)	1.23	38/15106 (0.3%)

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	A	0	2
1	B	0	2
1	D	0	1
All	All	0	5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	54	VAL	CA-CB	6.65	1.62	1.54
1	A	326	TYR	CA-C	-6.64	1.43	1.52
1	A	328	PRO	CA-C	-6.12	1.47	1.53
1	C	267	ILE	CA-CB	6.07	1.62	1.54
1	D	155	ILE	N-CA	6.05	1.50	1.45
1	B	316	VAL	N-CA	5.92	1.53	1.46
1	C	325	ALA	C-O	-5.89	1.16	1.24
1	B	297	ILE	CA-CB	-5.83	1.47	1.53
1	D	221	ILE	CA-CB	-5.74	1.47	1.54
1	A	202	GLU	CA-C	5.55	1.59	1.52
1	B	95	TYR	C-O	5.51	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	ARG	C-O	-5.39	1.18	1.24
1	A	304	PRO	CA-C	5.38	1.57	1.52
1	C	63	ALA	CA-CB	5.37	1.61	1.53
1	A	159	LYS	C-O	-5.37	1.17	1.24
1	B	352	VAL	CA-CB	-5.28	1.47	1.53
1	C	49	ILE	CA-CB	5.26	1.60	1.54
1	A	63	ALA	CA-CB	5.24	1.61	1.53
1	B	321	ALA	CA-CB	5.24	1.61	1.53
1	A	312	ALA	CA-C	5.23	1.59	1.52
1	B	257	ASP	N-CA	5.21	1.53	1.46
1	D	161	TYR	C-O	-5.01	1.16	1.23
1	A	297	ILE	CA-CB	-5.01	1.48	1.54
1	A	160	ALA	C-O	-5.00	1.18	1.24

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	161	TYR	N-CA-C	9.91	126.58	113.30
1	C	324	LEU	N-CA-C	-9.56	100.47	113.18
1	D	122	GLU	N-CA-C	-9.48	97.92	110.24
1	A	203	GLY	N-CA-C	-9.04	102.84	115.32
1	B	270	ILE	N-CA-C	-8.39	104.34	111.56
1	A	328	PRO	N-CA-C	-8.18	101.43	112.48
1	D	162	GLY	N-CA-C	7.54	122.97	114.67
1	A	202	GLU	N-CA-C	6.95	120.31	110.23
1	C	304	PRO	CA-C-N	6.79	127.06	119.32
1	C	304	PRO	C-N-CA	6.79	127.06	119.32
1	B	259	VAL	N-CA-CB	-6.64	101.92	111.21
1	C	270	ILE	N-CA-C	-6.56	105.92	111.56
1	A	203	GLY	CA-C-N	-6.28	112.79	122.09
1	A	203	GLY	C-N-CA	-6.28	112.79	122.09
1	B	287	TYR	N-CA-C	-6.13	104.51	111.07
1	D	303	LEU	CA-C-N	6.10	126.67	120.38
1	D	303	LEU	C-N-CA	6.10	126.67	120.38
1	C	128	ALA	CA-C-N	-5.81	113.69	119.56
1	C	128	ALA	C-N-CA	-5.81	113.69	119.56
1	B	205	THR	N-CA-CB	5.74	118.85	110.47
1	A	202	GLU	CA-C-N	5.64	132.26	122.05
1	A	202	GLU	C-N-CA	5.64	132.26	122.05
1	B	367	THR	CB-CA-C	-5.62	96.74	109.10
1	A	125	VAL	CB-CA-C	-5.54	102.29	110.82
1	A	202	GLU	CA-C-O	-5.43	115.21	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	ALA	N-CA-C	-5.27	103.99	110.31
1	B	103	GLY	N-CA-C	-5.26	108.42	114.69
1	C	102	SER	N-CA-C	5.26	118.51	112.57
1	C	278	HIS	N-CA-C	-5.18	105.71	111.36
1	C	225	TYR	CA-C-N	-5.12	114.55	119.87
1	C	225	TYR	C-N-CA	-5.12	114.55	119.87
1	B	19	GLU	N-CA-C	-5.10	105.61	111.07
1	B	124	GLY	N-CA-C	5.09	125.25	113.18
1	D	304	PRO	CA-C-N	5.08	126.19	119.84
1	D	304	PRO	C-N-CA	5.08	126.19	119.84
1	C	125	VAL	N-CA-C	5.07	115.04	108.35
1	A	174	ARG	N-CA-C	-5.03	105.71	111.14
1	C	123	ASP	CB-CA-C	-5.00	100.46	110.42

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	GLY	Peptide
1	A	57	SER	Peptide
1	B	162	GLY	Peptide
1	B	98	ARG	Sidechain
1	D	162	GLY	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	2688	0	2706	66	0
1	B	2694	0	2711	83	0
1	C	2747	0	2766	112	0
1	D	2731	0	2753	98	0
2	A	26	0	19	4	0
2	B	26	0	19	1	0
2	C	26	0	19	6	0
2	D	26	0	19	0	0
3	B	12	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	12	0	11	8	0
3	D	12	0	11	5	0
4	A	46	0	0	1	0
4	B	69	0	0	1	0
4	C	39	0	0	5	0
4	D	33	0	0	6	0
All	All	11187	0	11046	328	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 15.

All (328) 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:98:ARG:NH1	1:B:108:LEU:HD21	1.57	1.20
1:B:98:ARG:HH11	1:B:108:LEU:HD21	1.07	1.18
1:C:122:GLU:O	1:C:123:ASP:HB2	1.45	1.16
1:A:255:MET:HE3	2:A:370:SAH:C2	1.86	1.05
1:A:133:LEU:C	1:A:133:LEU:HD23	1.82	1.03
1:A:140:LEU:HD12	1:C:144:PHE:HZ	1.24	1.02
1:A:343:MET:HE2	1:D:9:ILE:HG13	1.38	1.02
1:C:273:ASP:OD1	3:C:369:EUG:H93	1.58	1.02
1:D:191:MET:HE2	1:D:217:VAL:HG13	1.42	1.00
1:D:323:MET:HE3	1:D:323:MET:HA	1.43	1.00
1:B:323:MET:HA	1:B:323:MET:HE3	1.43	0.98
1:D:323:MET:HE1	1:D:327:ASN:OD1	1.61	0.98
1:C:80:LEU:O	1:C:84:LEU:HD13	1.64	0.96
1:C:273:ASP:OD1	3:C:369:EUG:C9	2.14	0.94
1:A:365:LEU:HD12	1:D:12:ILE:HD11	1.49	0.91
1:B:133:LEU:HD23	1:B:133:LEU:C	1.96	0.91
1:B:191:MET:HG3	1:B:217:VAL:HG22	1.51	0.90
1:B:311:ILE:HD12	1:D:20:GLU:OE2	1.71	0.89
1:A:365:LEU:CD1	1:D:12:ILE:HD11	2.04	0.88
1:C:255:MET:HE3	2:C:370:SAH:C2	2.04	0.86
1:B:323:MET:HE1	1:B:327:ASN:CG	2.01	0.86
1:B:315:VAL:O	1:B:319:THR:HG23	1.76	0.86
1:C:161:TYR:N	1:C:161:TYR:CD2	2.42	0.83
1:C:122:GLU:O	1:C:123:ASP:CB	2.24	0.83
1:A:140:LEU:HD12	1:C:144:PHE:CZ	2.15	0.81
1:B:98:ARG:HH11	1:B:108:LEU:CD2	1.90	0.81
1:A:323:MET:HE3	1:A:323:MET:HA	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ALA:CB	1:C:161:TYR:CE2	2.63	0.80
1:C:315:VAL:O	1:C:319:THR:HG23	1.80	0.80
1:C:323:MET:HE1	1:C:327:ASN:OD1	1.82	0.80
1:B:202:GLU:HG3	1:B:225:TYR:HE2	1.46	0.80
1:D:224:LYS:HD3	1:D:225:TYR:CE1	2.17	0.80
1:D:323:MET:CE	1:D:327:ASN:OD1	2.29	0.79
1:C:323:MET:HE3	1:C:323:MET:HA	1.65	0.79
1:A:343:MET:HE2	1:D:9:ILE:CG1	2.13	0.79
1:C:160:ALA:HB3	1:C:161:TYR:CE2	2.18	0.78
1:C:255:MET:HE3	2:C:370:SAH:N3	1.98	0.78
1:B:163:MET:HE2	1:B:167:ASP:C	2.07	0.78
1:C:160:ALA:HB3	1:C:161:TYR:CD2	2.20	0.77
1:B:202:GLU:HG3	1:B:225:TYR:CE2	2.19	0.77
1:A:133:LEU:C	1:A:133:LEU:CD2	2.56	0.77
1:B:323:MET:HE1	1:B:327:ASN:ND2	2.00	0.76
1:C:301:TYR:HE1	1:C:319:THR:HG21	1.48	0.76
1:C:304:PRO:HD3	1:C:316:VAL:HG11	1.66	0.76
1:D:133:LEU:C	1:D:133:LEU:HD23	2.11	0.76
1:A:140:LEU:CD1	1:C:144:PHE:HZ	1.98	0.75
1:C:100:LEU:O	1:C:102:SER:N	2.20	0.75
1:A:309:PRO:HD2	1:B:306:SER:OG	1.87	0.74
2:C:370:SAH:HB1	4:C:399:HOH:O	1.86	0.74
1:B:133:LEU:HD23	1:B:133:LEU:O	1.87	0.74
1:C:273:ASP:OD2	3:C:369:EUG:H92	1.88	0.74
1:C:323:MET:HE1	1:C:327:ASN:CG	2.12	0.74
1:D:323:MET:HE1	1:D:327:ASN:CG	2.12	0.74
1:C:366:LYS:O	1:C:367:THR:HG22	1.88	0.74
1:D:301:TYR:HE1	1:D:319:THR:HG21	1.53	0.74
1:D:122:GLU:O	1:D:123:ASP:HB2	1.87	0.73
1:C:154:GLY:C	1:C:155:ILE:HD12	2.13	0.73
1:B:293:HIS:ND1	1:B:367:THR:HG22	2.03	0.73
2:C:370:SAH:CB	4:C:399:HOH:O	2.37	0.73
1:B:301:TYR:HE1	1:B:319:THR:HG21	1.54	0.72
1:C:273:ASP:CG	3:C:369:EUG:C9	2.63	0.72
1:A:133:LEU:HD23	1:A:133:LEU:O	1.88	0.72
1:A:61:SER:OG	1:A:64:GLU:HG3	1.90	0.71
1:A:255:MET:HE3	2:A:370:SAH:N3	2.06	0.71
1:C:44:LEU:O	1:C:45:ASP:OD1	2.08	0.71
1:D:272:HIS:HE1	3:D:369:EUG:H12	1.54	0.71
1:B:133:LEU:C	1:B:133:LEU:CD2	2.63	0.71
1:C:100:LEU:C	1:C:102:SER:N	2.45	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ALA:HB1	1:C:161:TYR:CE2	2.26	0.71
1:D:191:MET:HE3	1:D:195:LEU:HD21	1.73	0.70
1:B:140:LEU:HD12	1:D:144:PHE:HZ	1.56	0.70
1:B:79:MET:HE3	1:D:324:LEU:HD11	1.74	0.70
1:B:137:LYS:HE2	1:D:141:GLU:OE1	1.92	0.70
1:B:323:MET:CE	1:B:327:ASN:ND2	2.54	0.70
1:B:39:LYS:HE2	1:B:43:GLU:OE1	1.91	0.70
1:C:273:ASP:CG	3:C:369:EUG:H92	2.17	0.69
1:D:208:VAL:HG22	1:D:231:ILE:HB	1.73	0.69
1:B:163:MET:HE2	1:B:167:ASP:HB3	1.72	0.69
1:D:315:VAL:O	1:D:319:THR:HG23	1.93	0.69
1:B:367:THR:O	1:B:367:THR:OG1	2.05	0.69
1:B:323:MET:CE	1:B:327:ASN:CG	2.65	0.69
1:A:365:LEU:CD1	1:D:12:ILE:CD1	2.72	0.68
1:C:160:ALA:CB	1:C:161:TYR:CD2	2.77	0.68
1:A:158:ASN:N	1:A:158:ASN:HD22	1.92	0.68
1:C:78:VAL:HG13	4:C:406:HOH:O	1.93	0.67
1:B:163:MET:CE	1:B:167:ASP:HB3	2.25	0.67
1:C:100:LEU:C	1:C:102:SER:H	2.02	0.66
1:A:158:ASN:HD22	1:A:158:ASN:H	1.43	0.66
1:A:82:ARG:NH2	1:C:323:MET:O	2.29	0.66
1:A:327:ASN:HB3	1:A:328:PRO:CD	2.26	0.66
1:D:301:TYR:CE1	1:D:319:THR:HG21	2.30	0.65
1:A:365:LEU:HD11	1:D:12:ILE:CD1	2.26	0.65
1:C:188:THR:HA	1:C:220:MET:HE1	1.79	0.64
1:D:191:MET:HE3	1:D:195:LEU:CD2	2.27	0.64
1:D:323:MET:CE	1:D:327:ASN:CG	2.71	0.64
3:D:369:EUG:H2	4:D:399:HOH:O	1.97	0.64
1:C:323:MET:CE	1:C:327:ASN:CG	2.70	0.64
1:D:272:HIS:HE1	3:D:369:EUG:C10	2.11	0.64
1:A:327:ASN:HB3	1:A:328:PRO:HD2	1.80	0.64
1:C:199:ASN:O	1:C:202:GLU:HG2	1.98	0.63
1:B:207:ILE:HD13	1:B:208:VAL:N	2.14	0.62
1:B:33:VAL:HG23	1:D:143:TRP:CH2	2.34	0.62
1:C:161:TYR:N	1:C:161:TYR:HD2	1.91	0.62
1:C:224:LYS:HD2	1:C:225:TYR:CE1	2.34	0.62
1:C:323:MET:CE	1:C:327:ASN:OD1	2.47	0.62
1:D:323:MET:CE	1:D:327:ASN:HB2	2.30	0.62
1:D:20:GLU:OE1	1:D:20:GLU:O	2.18	0.62
1:D:191:MET:HE2	1:D:217:VAL:CG1	2.25	0.61
1:B:287:TYR:CE1	1:B:366:LYS:HG2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:ASP:OD2	3:C:369:EUG:C9	2.48	0.61
1:C:304:PRO:CD	1:C:316:VAL:HG11	2.30	0.61
1:B:23:LEU:HD21	1:D:358:ASN:HB2	1.82	0.61
1:C:131:LEU:C	1:C:131:LEU:HD23	2.26	0.61
1:B:301:TYR:C	1:B:302:ILE:HD12	2.27	0.60
1:B:301:TYR:O	1:B:302:ILE:HD12	2.02	0.60
1:D:351:LYS:HB3	4:D:397:HOH:O	2.00	0.59
1:A:27:GLN:OE1	1:C:311:ILE:HD12	2.01	0.59
1:C:161:TYR:HD2	1:C:161:TYR:H	1.49	0.59
1:B:323:MET:CE	1:B:327:ASN:HB2	2.31	0.59
1:C:271:CYS:HB2	1:C:300:GLU:OE2	2.03	0.59
1:C:366:LYS:C	1:C:367:THR:CG2	2.76	0.59
1:D:294:GLY:O	1:D:366:LYS:HG2	2.03	0.59
1:B:323:MET:HE3	1:B:323:MET:CA	2.21	0.58
1:A:327:ASN:CB	1:A:328:PRO:CD	2.80	0.58
1:C:275:SER:OG	1:C:278:HIS:HD2	1.87	0.58
1:A:325:ALA:O	1:A:326:TYR:HD1	1.85	0.58
1:B:198:TYR:CZ	1:B:200:GLY:HA3	2.37	0.58
1:D:121:ASN:OD1	1:D:122:GLU:O	2.20	0.58
1:C:141:GLU:HB2	1:C:161:TYR:OH	2.04	0.58
1:C:323:MET:CE	1:C:327:ASN:HB2	2.33	0.58
1:D:122:GLU:O	1:D:123:ASP:CB	2.52	0.58
1:B:141:GLU:OE1	1:D:137:LYS:NZ	2.35	0.57
1:C:313:THR:O	1:C:316:VAL:HG12	2.05	0.57
1:B:133:LEU:HD12	1:B:179:PHE:HA	1.86	0.56
1:C:100:LEU:O	1:C:101:PRO:C	2.47	0.56
1:A:327:ASN:O	1:A:329:GLY:N	2.35	0.56
1:B:163:MET:HE2	1:B:167:ASP:CB	2.36	0.56
1:C:339:GLN:HG2	1:C:350:PHE:CE2	2.40	0.56
1:D:191:MET:HG3	1:D:217:VAL:HG22	1.87	0.56
1:B:191:MET:CG	1:B:217:VAL:HG22	2.32	0.55
1:B:51:ALA:HA	1:B:111:LEU:HD11	1.88	0.55
1:D:158:ASN:N	1:D:158:ASN:HD22	2.04	0.55
1:A:336:LYS:HG2	4:A:411:HOH:O	2.07	0.55
1:A:17:SER:HA	1:A:20:GLU:OE2	2.07	0.55
1:C:335:GLU:O	1:C:339:GLN:HG3	2.07	0.55
1:D:357:PHE:O	1:D:358:ASN:CB	2.55	0.55
1:A:34:LEU:HB3	1:A:35:PRO:CD	2.37	0.55
1:C:198:TYR:CZ	1:C:200:GLY:HA3	2.42	0.55
1:D:323:MET:CE	1:D:327:ASN:CB	2.85	0.55
1:C:273:ASP:OD1	3:C:369:EUG:H92	2.01	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:LEU:CD1	4:D:397:HOH:O	2.56	0.54
1:D:224:LYS:HD3	1:D:225:TYR:CZ	2.42	0.54
1:B:347:PHE:CE2	1:B:366:LYS:HG3	2.42	0.54
1:D:191:MET:CE	1:D:195:LEU:HD21	2.38	0.54
1:B:165:ILE:HD13	3:B:369:EUG:H93	1.90	0.54
1:C:366:LYS:O	1:C:367:THR:CG2	2.55	0.54
1:A:325:ALA:O	1:A:326:TYR:CD1	2.60	0.54
1:B:62:PRO:HG2	1:B:81:ASP:HB2	1.89	0.54
1:C:208:VAL:HG22	1:C:265:ILE:HG12	1.89	0.53
1:C:339:GLN:HG2	1:C:350:PHE:CD2	2.43	0.53
1:D:158:ASN:HD22	1:D:158:ASN:H	1.56	0.53
1:D:188:THR:HA	1:D:220:MET:HE1	1.90	0.53
1:D:133:LEU:C	1:D:133:LEU:CD2	2.82	0.53
1:B:134:ALA:HA	3:B:369:EUG:H12	1.91	0.53
1:D:237:HIS:HD2	4:D:385:HOH:O	1.90	0.53
1:C:34:LEU:HB3	1:C:35:PRO:CD	2.39	0.53
1:B:323:MET:CE	1:B:327:ASN:CB	2.87	0.53
1:B:140:LEU:HD12	1:D:144:PHE:CZ	2.39	0.53
1:D:308:ASP:HB2	1:D:309:PRO:HD2	1.90	0.53
1:D:339:GLN:HG2	1:D:343:MET:HE2	1.90	0.52
1:B:311:ILE:CD1	1:D:20:GLU:OE2	2.52	0.52
1:D:237:HIS:CD2	4:D:385:HOH:O	2.63	0.52
1:B:143:TRP:CH2	1:D:33:VAL:HG13	2.45	0.52
1:D:197:MET:HE1	1:D:355:CYS:O	2.10	0.51
1:C:299:ALA:O	1:C:300:GLU:HG2	2.10	0.51
1:D:272:HIS:CE1	3:D:369:EUG:H12	2.41	0.51
1:C:17:SER:O	1:C:20:GLU:HG2	2.11	0.51
1:C:130:PHE:HE2	1:C:183:MET:HE1	1.75	0.51
1:A:51:ALA:HA	1:A:111:LEU:HD11	1.92	0.51
1:A:126:SER:O	1:A:185:SER:HB3	2.11	0.50
1:D:152:GLU:O	1:D:152:GLU:HG3	2.11	0.50
1:B:357:PHE:O	1:B:358:ASN:HB2	2.10	0.50
1:C:240:GLN:O	1:C:240:GLN:NE2	2.45	0.50
1:C:303:LEU:HD13	1:C:332:GLU:HB2	1.93	0.50
1:D:44:LEU:O	1:D:45:ASP:HB2	2.10	0.50
1:D:198:TYR:CZ	1:D:200:GLY:HA3	2.47	0.50
1:D:295:LYS:HB3	1:D:365:LEU:HD23	1.92	0.50
1:A:198:TYR:CZ	1:A:200:GLY:HA3	2.47	0.50
1:D:202:GLU:HG3	1:D:225:TYR:CE2	2.46	0.50
1:C:187:SER:HA	1:C:268:LYS:HE3	1.95	0.49
1:B:34:LEU:HB3	1:B:35:PRO:CD	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:MET:HA	1:D:323:MET:CE	2.29	0.49
1:B:187:SER:OG	2:B:370:SAH:O	2.27	0.48
1:B:271:CYS:HB2	1:B:300:GLU:OE2	2.13	0.48
1:C:187:SER:OG	2:C:370:SAH:O	2.31	0.48
1:D:323:MET:HE2	1:D:327:ASN:HB2	1.93	0.48
1:A:272:HIS:O	1:A:330:GLY:HA3	2.13	0.48
1:D:296:VAL:HB	1:D:364:PHE:HB2	1.96	0.48
1:D:293:HIS:CD2	1:D:293:HIS:H	2.32	0.48
1:A:357:PHE:O	1:A:358:ASN:HB2	2.14	0.48
1:C:39:LYS:O	1:C:43:GLU:HG3	2.13	0.48
1:C:323:MET:CE	1:C:327:ASN:CB	2.91	0.48
1:A:327:ASN:C	1:A:329:GLY:N	2.72	0.48
1:D:36:MET:HE1	1:D:135:THR:HG22	1.96	0.48
1:B:323:MET:HE3	1:B:327:ASN:ND2	2.28	0.48
1:D:365:LEU:HD11	4:D:397:HOH:O	2.14	0.48
1:D:157:PHE:CE2	1:D:165:ILE:HA	2.49	0.47
1:C:154:GLY:C	1:C:155:ILE:CD1	2.86	0.47
1:C:158:ASN:HD22	1:C:158:ASN:N	2.11	0.47
1:C:191:MET:CG	1:C:217:VAL:HG22	2.45	0.47
1:A:34:LEU:HB3	1:A:35:PRO:HD3	1.96	0.47
1:A:323:MET:CE	1:A:327:ASN:ND2	2.77	0.47
1:B:161:TYR:O	1:B:162:GLY:C	2.58	0.47
1:D:267:ILE:HD11	1:D:298:VAL:HG22	1.97	0.47
1:D:357:PHE:O	1:D:358:ASN:HB2	2.14	0.47
1:A:325:ALA:C	1:A:326:TYR:CD1	2.93	0.47
1:B:54:VAL:HG13	1:B:55:PRO:O	2.14	0.47
1:B:207:ILE:HD11	1:B:266:PHE:HB2	1.97	0.47
1:B:322:LEU:HD13	3:B:369:EUG:H81	1.96	0.47
1:C:323:MET:HE2	1:C:327:ASN:HB2	1.95	0.47
1:B:79:MET:CE	1:D:324:LEU:HD11	2.41	0.47
1:D:217:VAL:HG11	1:D:266:PHE:CE1	2.50	0.47
1:C:100:LEU:HD23	1:C:100:LEU:HA	1.73	0.47
3:C:369:EUG:H92	3:C:369:EUG:O4	2.15	0.47
1:C:217:VAL:HG11	1:C:266:PHE:CE1	2.50	0.47
1:A:60:ILE:HG21	1:A:65:ILE:HD11	1.95	0.46
1:B:287:TYR:CD1	1:B:366:LYS:HG2	2.51	0.46
1:C:61:SER:OG	1:C:64:GLU:HG3	2.14	0.46
1:C:357:PHE:O	1:C:358:ASN:CB	2.61	0.46
1:D:130:PHE:HE2	1:D:183:MET:HE1	1.81	0.46
1:A:169:HIS:O	1:A:176:ASN:HB2	2.15	0.46
1:D:303:LEU:HA	1:D:304:PRO:HD3	1.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:LYS:HZ3	1:B:269:TRP:CD1	2.34	0.46
1:C:154:GLY:O	1:C:155:ILE:HD12	2.16	0.46
1:C:188:THR:OG1	1:C:220:MET:HE1	2.16	0.46
1:C:212:GLY:HA3	1:C:232:ASN:ND2	2.31	0.46
1:C:269:TRP:HA	1:C:300:GLU:OE1	2.15	0.46
1:B:198:TYR:OH	1:B:363:GLU:OE2	2.32	0.46
2:C:370:SAH:HB2	4:C:399:HOH:O	2.11	0.45
1:A:321:ALA:HB3	1:C:33:VAL:HG11	1.97	0.45
1:A:190:THR:HG22	1:A:194:ILE:HD12	1.96	0.45
1:A:217:VAL:HG11	1:A:266:PHE:CE1	2.52	0.45
1:D:339:GLN:HG3	1:D:350:PHE:CG	2.50	0.45
1:C:33:VAL:HG12	1:C:86:LEU:HD21	1.99	0.45
1:D:99:GLU:OE2	1:D:103:GLY:HA2	2.17	0.45
1:B:147:LYS:HG3	1:D:44:LEU:CD2	2.47	0.45
1:A:140:LEU:CD1	1:C:144:PHE:CZ	2.89	0.45
1:B:319:THR:O	1:B:323:MET:HG2	2.17	0.45
1:B:333:ARG:HB3	1:B:337:GLU:HB2	1.98	0.45
1:A:38:LEU:HD23	1:A:131:LEU:HD11	1.98	0.45
1:A:158:ASN:N	1:A:158:ASN:ND2	2.64	0.45
1:B:347:PHE:CD2	1:B:366:LYS:HG3	2.53	0.44
1:D:218:ALA:O	1:D:222:VAL:HG22	2.17	0.44
1:A:365:LEU:HD11	1:D:12:ILE:HD12	1.98	0.44
1:C:191:MET:HG3	1:C:217:VAL:HG22	1.99	0.44
1:C:188:THR:HG23	1:C:220:MET:CE	2.48	0.44
1:C:208:VAL:HG23	1:C:210:VAL:HG23	1.98	0.44
1:A:323:MET:HA	1:A:323:MET:CE	2.39	0.44
1:C:39:LYS:HE2	1:C:43:GLU:OE1	2.17	0.44
1:C:213:GLY:HA3	4:C:399:HOH:O	2.15	0.44
1:A:98:ARG:HD2	1:A:106:GLU:OE2	2.18	0.44
1:B:147:LYS:HG3	1:D:44:LEU:HD21	2.00	0.44
1:B:243:PRO:HG2	1:B:245:PHE:CZ	2.52	0.44
1:B:323:MET:HA	1:B:323:MET:CE	2.29	0.43
1:C:100:LEU:O	1:C:103:GLY:N	2.51	0.43
1:C:155:ILE:CD1	1:C:155:ILE:N	2.81	0.43
1:B:16:SER:O	1:B:20:GLU:HG3	2.18	0.43
1:C:197:MET:HE3	1:C:197:MET:HB2	1.79	0.43
1:A:86:LEU:HA	1:C:317:ILE:HG21	2.00	0.43
2:A:370:SAH:HB2	2:A:370:SAH:H4'	1.99	0.43
1:D:239:ILE:HG23	1:D:250:HIS:HB3	2.01	0.43
1:C:323:MET:HE3	1:C:323:MET:CA	2.43	0.43
1:C:280:LEU:O	1:C:284:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:VAL:HG13	1:D:230:ALA:HB2	1.99	0.43
1:B:212:GLY:HA3	1:B:232:ASN:ND2	2.33	0.43
1:C:131:LEU:HD23	1:C:131:LEU:O	2.19	0.43
1:C:366:LYS:C	1:C:367:THR:HG23	2.43	0.43
1:A:267:ILE:HD11	1:A:298:VAL:HG22	2.00	0.43
1:D:149:ALA:HA	1:D:159:LYS:HE3	1.99	0.43
1:A:239:ILE:HG23	1:A:250:HIS:HB3	2.00	0.43
1:B:158:ASN:H	1:B:158:ASN:HD22	1.67	0.43
1:A:19:GLU:OE1	1:C:193:LYS:NZ	2.52	0.42
1:A:317:ILE:HG21	1:C:86:LEU:HA	2.01	0.42
1:A:334:THR:HG23	1:A:337:GLU:OE1	2.18	0.42
1:D:308:ASP:HB2	1:D:309:PRO:CD	2.49	0.42
1:D:323:MET:HE2	1:D:327:ASN:CB	2.49	0.42
1:D:272:HIS:CE1	3:D:369:EUG:C10	2.96	0.42
1:B:124:GLY:C	1:B:125:VAL:HG23	2.45	0.42
1:C:158:ASN:HD22	1:C:158:ASN:H	1.66	0.42
1:A:69:LEU:HD11	1:A:80:LEU:HD11	2.01	0.42
1:A:80:LEU:HA	1:A:80:LEU:HD23	1.83	0.42
1:A:274:TRP:HB3	1:A:278:HIS:HB2	2.02	0.42
1:C:157:PHE:CE2	1:C:165:ILE:HA	2.55	0.42
1:D:197:MET:HE3	1:D:197:MET:HB2	1.83	0.42
1:D:80:LEU:O	1:D:84:LEU:HD13	2.20	0.42
1:D:275:SER:OG	1:D:278:HIS:HD2	2.03	0.42
1:D:126:SER:O	1:D:185:SER:HB3	2.20	0.41
1:A:198:TYR:OH	1:A:363:GLU:OE2	2.32	0.41
1:B:274:TRP:HB3	1:B:278:HIS:HB2	2.01	0.41
1:C:34:LEU:HB3	1:C:35:PRO:HD3	2.02	0.41
1:D:224:LYS:CD	1:D:225:TYR:CE1	2.99	0.41
1:A:167:ASP:O	1:A:171:THR:HG23	2.20	0.41
1:C:96:THR:HG23	1:D:94:THR:HG22	2.02	0.41
1:C:301:TYR:CE1	1:C:319:THR:HG21	2.40	0.41
1:D:80:LEU:HD23	1:D:80:LEU:HA	1.91	0.41
1:D:323:MET:HE3	1:D:323:MET:CA	2.28	0.41
1:A:268:LYS:HG2	2:A:370:SAH:OXT	2.21	0.41
1:B:33:VAL:HG21	1:D:321:ALA:HB3	2.02	0.41
1:D:84:LEU:N	1:D:84:LEU:CD1	2.83	0.41
1:A:327:ASN:HA	1:A:328:PRO:HD3	1.67	0.41
1:A:85:ARG:HG3	1:C:307:PRO:HB3	2.03	0.41
1:B:237:HIS:HE1	4:B:374:HOH:O	2.04	0.41
1:B:272:HIS:CD2	1:B:272:HIS:C	2.98	0.41
1:B:321:ALA:HB3	1:D:33:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:VAL:HG11	1:B:266:PHE:CE1	2.56	0.41
1:B:351:LYS:HG3	1:C:14:THR:CG2	2.51	0.41
1:C:224:LYS:HD2	1:C:225:TYR:CZ	2.55	0.41
1:C:195:LEU:HD12	1:C:195:LEU:HA	1.84	0.41
1:B:61:SER:OG	1:B:64:GLU:HG3	2.21	0.40
1:B:212:GLY:HA3	1:B:232:ASN:HD21	1.86	0.40
1:C:100:LEU:HA	1:C:101:PRO:HD2	1.74	0.40
1:C:357:PHE:O	1:C:358:ASN:HB2	2.21	0.40
1:D:304:PRO:HG2	1:D:313:THR:HG23	2.03	0.40
1:A:86:LEU:HA	1:C:317:ILE:CG2	2.51	0.40
1:A:158:ASN:O	1:A:161:TYR:O	2.40	0.40
1:B:334:THR:OG1	1:B:337:GLU:HG3	2.21	0.40
1:C:213:GLY:HA2	1:C:238:VAL:HG11	2.02	0.40
1:C:327:ASN:HA	1:C:328:PRO:HD3	1.88	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	349/368 (95%)	345 (99%)	4 (1%)	0	100	100
1	B	350/368 (95%)	342 (98%)	8 (2%)	0	100	100
1	C	354/368 (96%)	348 (98%)	4 (1%)	2 (1%)	21	13
1	D	352/368 (96%)	346 (98%)	5 (1%)	1 (0%)	36	29
All	All	1405/1472 (95%)	1381 (98%)	21 (2%)	3 (0%)	43	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	101	PRO

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Mol	Chain	Res	Type
1	C	123	ASP
1	D	101	PRO

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	289/302 (96%)	272 (94%)	17 (6%)	18	10
1	B	290/302 (96%)	273 (94%)	17 (6%)	18	10
1	C	296/302 (98%)	273 (92%)	23 (8%)	11	5
1	D	294/302 (97%)	266 (90%)	28 (10%)	8	3
All	All	1169/1208 (97%)	1084 (93%)	85 (7%)	13	6

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	54	VAL
1	A	96	THR
1	A	104	LYS
1	A	120	LYS
1	A	125	VAL
1	A	133	LEU
1	A	158	ASN
1	A	175	ILE
1	A	195	LEU
1	A	202	GLU
1	A	259	VAL
1	A	280	LEU
1	A	282	LEU
1	A	323	MET
1	A	334	THR
1	A	348	ARG
1	B	19	GLU
1	B	34	LEU

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Mol	Chain	Res	Type
1	B	54	VAL
1	B	75	GLU
1	B	97	LEU
1	B	105	VAL
1	B	122	GLU
1	B	133	LEU
1	B	177	LYS
1	B	195	LEU
1	B	197	MET
1	B	202	GLU
1	B	205	THR
1	B	207	ILE
1	B	240	GLN
1	B	259	VAL
1	B	280	LEU
1	C	19	GLU
1	C	34	LEU
1	C	36	MET
1	C	54	VAL
1	C	75	GLU
1	C	96	THR
1	C	98	ARG
1	C	113	PRO
1	C	122	GLU
1	C	133	LEU
1	C	155	ILE
1	C	158	ASN
1	C	161	TYR
1	C	195	LEU
1	C	207	ILE
1	C	208	VAL
1	C	224	LYS
1	C	251	LEU
1	C	280	LEU
1	C	323	MET
1	C	343	MET
1	C	348	ARG
1	C	367	THR
1	D	20	GLU
1	D	34	LEU
1	D	52	LYS
1	D	54	VAL

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Mol	Chain	Res	Type
1	D	75	GLU
1	D	96	THR
1	D	98	ARG
1	D	99	GLU
1	D	104	LYS
1	D	105	VAL
1	D	113	PRO
1	D	126	SER
1	D	133	LEU
1	D	147	LYS
1	D	152	GLU
1	D	156	PRO
1	D	158	ASN
1	D	175	ILE
1	D	195	LEU
1	D	207	ILE
1	D	224	LYS
1	D	241	ASP
1	D	259	VAL
1	D	282	LEU
1	D	292	ASP
1	D	295	LYS
1	D	348	ARG
1	D	351	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	158	ASN
1	A	169	HIS
1	A	176	ASN
1	A	180	ASN
1	A	232	ASN
1	A	237	HIS
1	A	278	HIS
1	A	293	HIS
1	A	327	ASN
1	B	158	ASN
1	B	180	ASN
1	B	232	ASN
1	B	237	HIS

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Mol	Chain	Res	Type
1	B	327	ASN
1	C	158	ASN
1	C	169	HIS
1	C	176	ASN
1	C	180	ASN
1	C	232	ASN
1	C	237	HIS
1	C	278	HIS
1	C	293	HIS
1	D	158	ASN
1	D	169	HIS
1	D	176	ASN
1	D	180	ASN
1	D	186	ASN
1	D	199	ASN
1	D	232	ASN
1	D	237	HIS
1	D	278	HIS
1	D	293	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 ⓘ

7 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	C	370	-	27,28,28	1.68	4 (14%)	36,40,40	2.13	13 (36%)
2	SAH	B	370	-	27,28,28	1.43	3 (11%)	36,40,40	1.83	9 (25%)
3	EUG	D	369	-	12,12,12	1.58	1 (8%)	15,15,15	1.84	5 (33%)
2	SAH	A	370	-	27,28,28	1.45	5 (18%)	36,40,40	2.47	14 (38%)
3	EUG	C	369	-	12,12,12	1.70	1 (8%)	15,15,15	1.87	4 (26%)
3	EUG	B	369	-	12,12,12	1.97	2 (16%)	15,15,15	1.73	3 (20%)
2	SAH	D	370	-	27,28,28	1.24	4 (14%)	36,40,40	2.70	13 (36%)

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	C	370	-	-	0/15/31/31	0/3/3/3
2	SAH	B	370	-	-	0/15/31/31	0/3/3/3
3	EUG	D	369	-	-	2/5/5/5	0/1/1/1
2	SAH	A	370	-	-	6/15/31/31	0/3/3/3
3	EUG	C	369	-	-	3/5/5/5	0/1/1/1
3	EUG	B	369	-	-	4/5/5/5	0/1/1/1
2	SAH	D	370	-	-	4/15/31/31	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	369	EUG	C4-C3	5.91	1.50	1.40
2	C	370	SAH	C5-C4	5.86	1.49	1.39
3	C	369	EUG	C4-C3	5.50	1.50	1.40
3	D	369	EUG	C4-C3	5.24	1.49	1.40
2	B	370	SAH	C5-C4	4.44	1.47	1.39
2	A	370	SAH	C8-N7	3.88	1.39	1.31
2	A	370	SAH	C5-C4	3.46	1.45	1.39
2	D	370	SAH	C5-N7	-3.32	1.33	1.39
2	C	370	SAH	C4-N9	-3.04	1.31	1.37
2	B	370	SAH	C5-C6	2.96	1.49	1.41
3	B	369	EUG	O3-C9	2.79	1.50	1.42
2	A	370	SAH	C4-N9	-2.62	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	370	SAH	C5-N7	-2.54	1.34	1.39
2	D	370	SAH	C5-C6	2.53	1.48	1.41
2	C	370	SAH	C8-N7	2.49	1.36	1.31
2	A	370	SAH	O-C	2.48	1.29	1.22
2	C	370	SAH	C5-N7	-2.46	1.34	1.39
2	D	370	SAH	C8-N9	-2.26	1.33	1.37
2	D	370	SAH	C5-C4	2.20	1.43	1.39
2	A	370	SAH	C5-C6	2.19	1.47	1.41

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	370	SAH	C5-C4-N3	-7.28	116.70	126.72
2	A	370	SAH	N3-C2-N1	-6.93	118.09	128.58
2	D	370	SAH	N3-C4-N9	5.78	137.00	127.17
2	C	370	SAH	N3-C2-N1	-4.86	121.23	128.58
2	D	370	SAH	C2-N3-C4	4.83	123.63	111.83
2	A	370	SAH	C2-N3-C4	4.77	123.47	111.83
2	D	370	SAH	CB-CG-SD	-4.76	102.82	113.45
2	D	370	SAH	C5-N7-C8	4.76	110.93	103.45
2	C	370	SAH	N3-C4-N9	4.72	135.19	127.17
2	D	370	SAH	C4-C5-N7	-4.65	105.26	110.58
3	B	369	EUG	O3-C3-C4	4.62	121.47	114.55
2	C	370	SAH	C4-N9-C8	4.57	110.54	105.74
2	A	370	SAH	C5-C4-N3	-4.49	120.54	126.72
2	B	370	SAH	N3-C4-N9	4.15	134.23	127.17
2	A	370	SAH	N3-C4-N9	4.08	134.11	127.17
2	A	370	SAH	C4-N9-C8	4.05	110.00	105.74
2	A	370	SAH	C5'-SD-CG	4.05	114.28	102.26
3	C	369	EUG	C1-C7-C8	-3.92	113.37	127.43
2	B	370	SAH	N3-C2-N1	-3.78	122.86	128.58
2	B	370	SAH	N6-C6-N1	3.78	126.79	118.38
2	D	370	SAH	N3-C2-N1	-3.75	122.90	128.58
2	B	370	SAH	C5-C4-N3	-3.75	121.55	126.72
2	C	370	SAH	C5-C4-N3	-3.72	121.59	126.72
3	D	369	EUG	C9-O3-C3	3.72	122.97	117.51
3	D	369	EUG	O3-C3-C4	3.66	120.04	114.55
2	D	370	SAH	N9-C8-N7	-3.65	108.76	113.94
3	C	369	EUG	O3-C3-C4	3.57	119.90	114.55
2	C	370	SAH	C2-N1-C6	3.53	124.53	118.73
2	A	370	SAH	C2-N1-C6	3.38	124.28	118.73
2	B	370	SAH	C2-N1-C6	3.33	124.20	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	370	SAH	CB-CA-N	-3.32	101.47	110.12
2	D	370	SAH	C5'-SD-CG	3.27	111.97	102.26
2	C	370	SAH	N6-C6-N1	3.04	125.16	118.38
2	A	370	SAH	C6-C5-C4	-2.98	113.11	117.18
2	D	370	SAH	OXT-C-O	-2.97	117.33	124.08
2	A	370	SAH	C5-C6-N6	-2.91	116.07	123.29
2	C	370	SAH	C2-N3-C4	2.91	118.95	111.83
3	D	369	EUG	C1-C7-C8	-2.90	117.03	127.43
2	B	370	SAH	C2-N3-C4	2.87	118.83	111.83
2	D	370	SAH	C4-N9-C8	2.86	108.74	105.74
3	B	369	EUG	C1-C7-C8	-2.81	117.36	127.43
3	C	369	EUG	C9-O3-C3	2.78	121.59	117.51
2	B	370	SAH	O4'-C1'-C2'	-2.71	100.82	106.62
2	D	370	SAH	C6-C5-N7	2.70	137.30	132.09
2	C	370	SAH	OXT-C-O	-2.68	118.00	124.08
2	C	370	SAH	CB-CG-SD	-2.64	107.57	113.45
2	A	370	SAH	C6-C5-N7	2.50	136.92	132.09
2	B	370	SAH	CB-CA-N	2.48	116.58	110.12
2	C	370	SAH	C5-C4-N9	-2.45	103.14	105.81
3	B	369	EUG	O3-C3-C2	-2.43	119.90	124.08
2	C	370	SAH	C5-C6-N6	-2.40	117.35	123.29
2	A	370	SAH	N6-C6-N1	2.38	123.68	118.38
2	B	370	SAH	C5-C6-N6	-2.37	117.43	123.29
3	D	369	EUG	C2-C3-C4	-2.36	117.66	120.04
3	D	369	EUG	C6-C1-C2	2.27	121.58	118.72
2	A	370	SAH	N9-C8-N7	-2.24	110.76	113.94
2	A	370	SAH	CB-CA-C	2.19	116.26	110.45
3	C	369	EUG	C6-C1-C2	2.15	121.42	118.72
2	D	370	SAH	O4'-C1'-C2'	-2.07	102.19	106.62
2	C	370	SAH	N9-C8-N7	-2.06	111.02	113.94
2	C	370	SAH	CB-CA-N	2.03	115.40	110.12

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	370	SAH	N-CA-CB-CG
2	A	370	SAH	C-CA-CB-CG
2	D	370	SAH	C4'-C5'-SD-CG
3	C	369	EUG	C1-C7-C8-C10
3	C	369	EUG	C2-C3-O3-C9
3	C	369	EUG	C4-C3-O3-C9

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Mol	Chain	Res	Type	Atoms
3	D	369	EUG	C6-C1-C7-C8
3	D	369	EUG	C2-C1-C7-C8
3	B	369	EUG	C2-C1-C7-C8
2	A	370	SAH	CA-CB-CG-SD
3	B	369	EUG	C4-C3-O3-C9
3	B	369	EUG	C6-C1-C7-C8
3	B	369	EUG	C2-C3-O3-C9
2	D	370	SAH	C-CA-CB-CG
2	D	370	SAH	N-CA-CB-CG
2	A	370	SAH	CB-CG-SD-C5'
2	D	370	SAH	OXT-C-CA-N
2	A	370	SAH	OXT-C-CA-N
2	A	370	SAH	O-C-CA-N

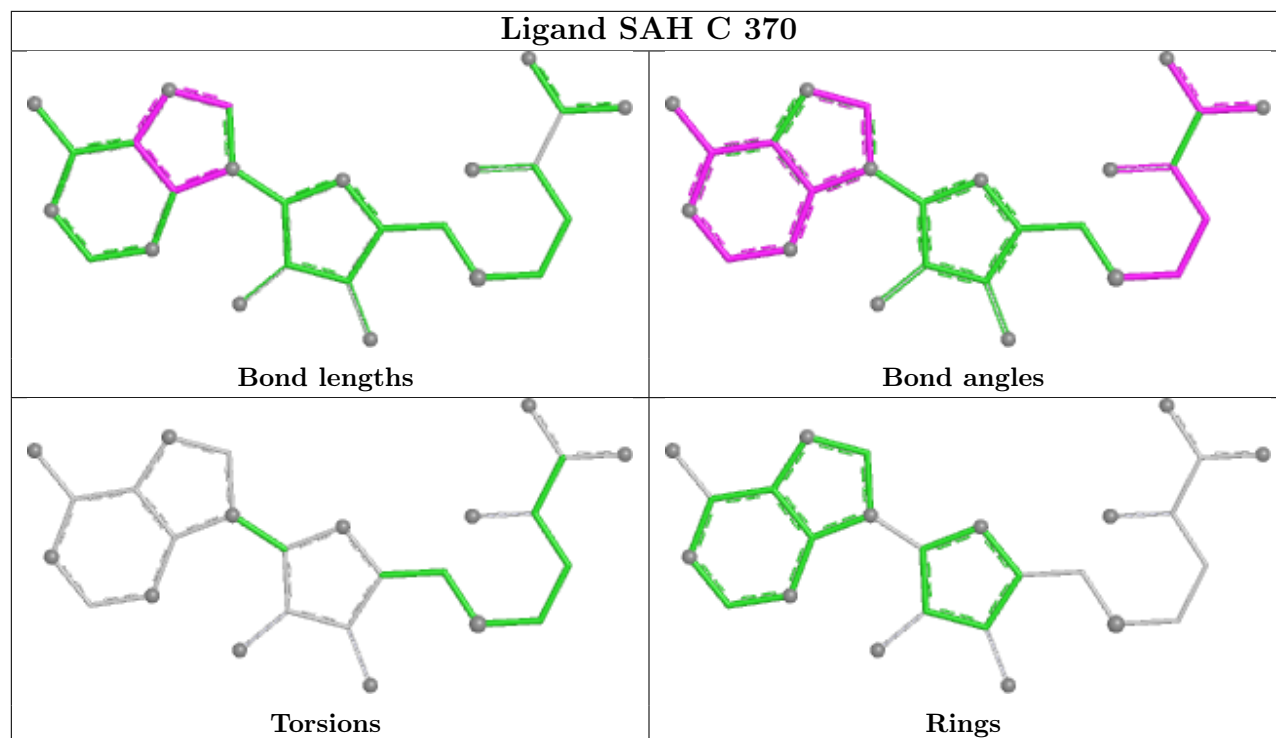
There are no ring outliers.

6 monomers are involved in 27 short contacts:

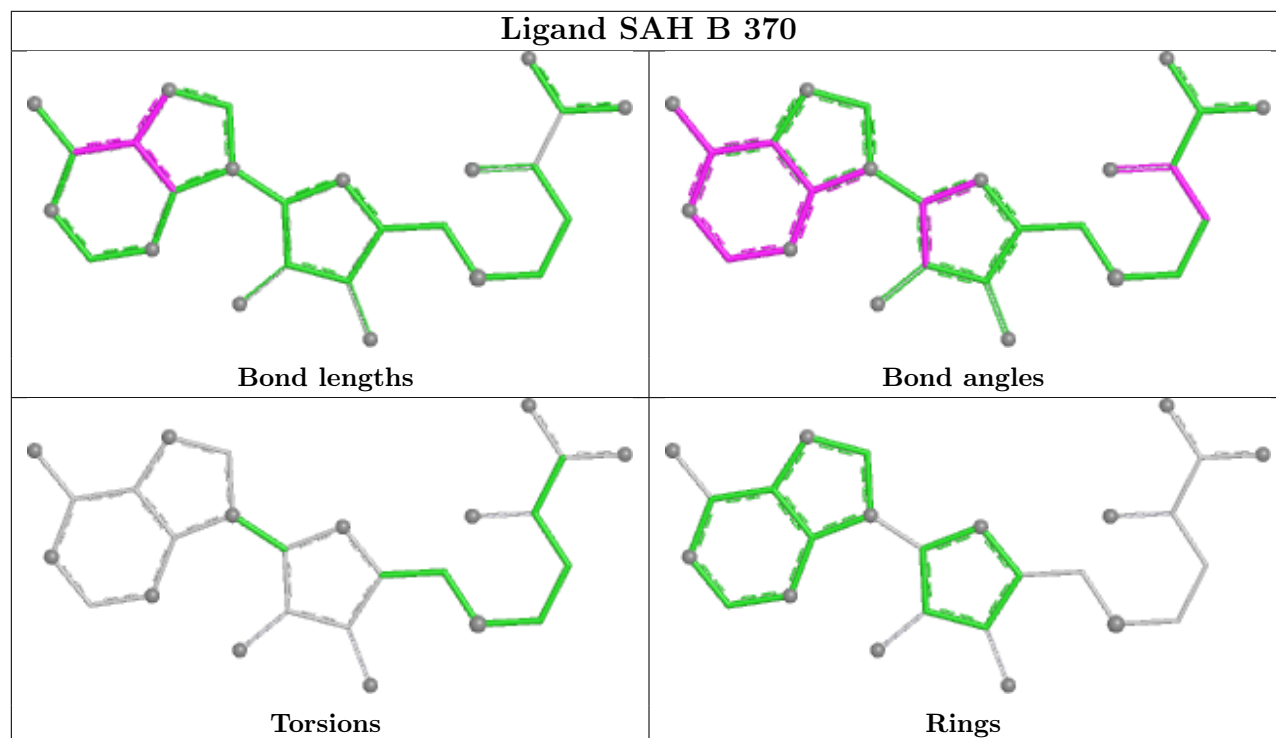
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	370	SAH	6	0
2	B	370	SAH	1	0
3	D	369	EUG	5	0
2	A	370	SAH	4	0
3	C	369	EUG	8	0
3	B	369	EUG	3	0

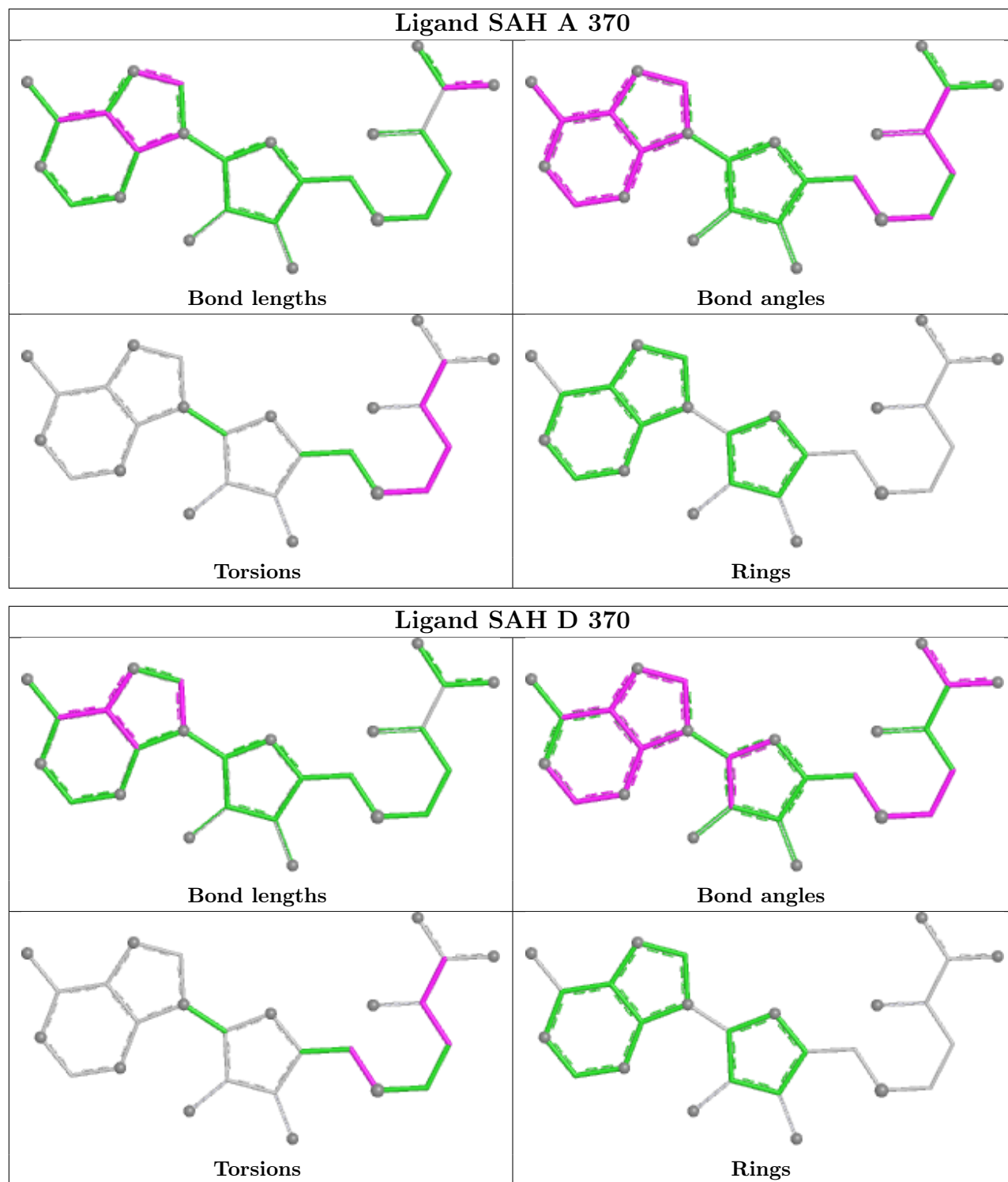
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand SAH C 370



Ligand SAH B 370





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	351/368 (95%)	0.27	15 (4%) 40 42	17, 29, 44, 55	0
1	B	352/368 (95%)	0.08	11 (3%) 51 55	16, 25, 38, 56	0
1	C	358/368 (97%)	0.54	28 (7%) 19 20	17, 31, 48, 62	0
1	D	356/368 (96%)	0.35	23 (6%) 25 26	17, 31, 46, 65	0
All	All	1417/1472 (96%)	0.31	77 (5%) 31 33	16, 29, 45, 65	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	GLY	6.3
1	C	161	TYR	5.5
1	D	241	ASP	5.4
1	C	54	VAL	5.3
1	A	56	PRO	4.5
1	C	102	SER	4.3
1	D	100	LEU	4.0
1	B	123	ASP	4.0
1	C	101	PRO	3.9
1	C	100	LEU	3.9
1	C	55	PRO	3.9
1	C	367	THR	3.8
1	A	325	ALA	3.8
1	C	122	GLU	3.6
1	C	124	GLY	3.5
1	C	280	LEU	3.3
1	C	344	ALA	3.3
1	C	343	MET	3.2
1	A	57	SER	3.2
1	D	9	ILE	3.2
1	A	367	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	173	HIS	3.1
1	C	99	GLU	3.0
1	C	105	VAL	3.0
1	A	72	THR	3.0
1	A	209	ASP	3.0
1	D	343	MET	2.9
1	C	327	ASN	2.9
1	C	103	GLY	2.9
1	B	209	ASP	2.9
1	D	123	ASP	2.9
1	C	323	MET	2.8
1	A	203	GLY	2.8
1	B	18	ASP	2.8
1	D	103	GLY	2.8
1	C	98	ARG	2.8
1	C	229	ASN	2.7
1	D	367	THR	2.7
1	D	240	GLN	2.7
1	A	245	PHE	2.6
1	D	101	PRO	2.6
1	B	16	SER	2.6
1	B	173	HIS	2.6
1	D	292	ASP	2.6
1	B	162	GLY	2.6
1	C	45	ASP	2.5
1	B	54	VAL	2.5
1	B	45	ASP	2.5
1	D	173	HIS	2.5
1	D	54	VAL	2.5
1	D	209	ASP	2.5
1	A	162	GLY	2.4
1	C	199	ASN	2.4
1	C	173	HIS	2.4
1	D	152	GLU	2.4
1	B	244	ALA	2.4
1	D	162	GLY	2.4
1	D	11	ILE	2.3
1	C	349	GLY	2.3
1	C	340	ALA	2.3
1	A	122	GLU	2.3
1	D	122	GLU	2.3
1	A	18	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	339	GLN	2.2
1	C	293	HIS	2.2
1	C	348	ARG	2.2
1	A	202	GLU	2.2
1	D	72	THR	2.2
1	D	102	SER	2.2
1	D	269	TRP	2.1
1	D	208	VAL	2.1
1	A	17	SER	2.1
1	A	323	MET	2.1
1	D	105	VAL	2.1
1	D	20	GLU	2.1
1	C	15	HIS	2.1
1	B	367	THR	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.

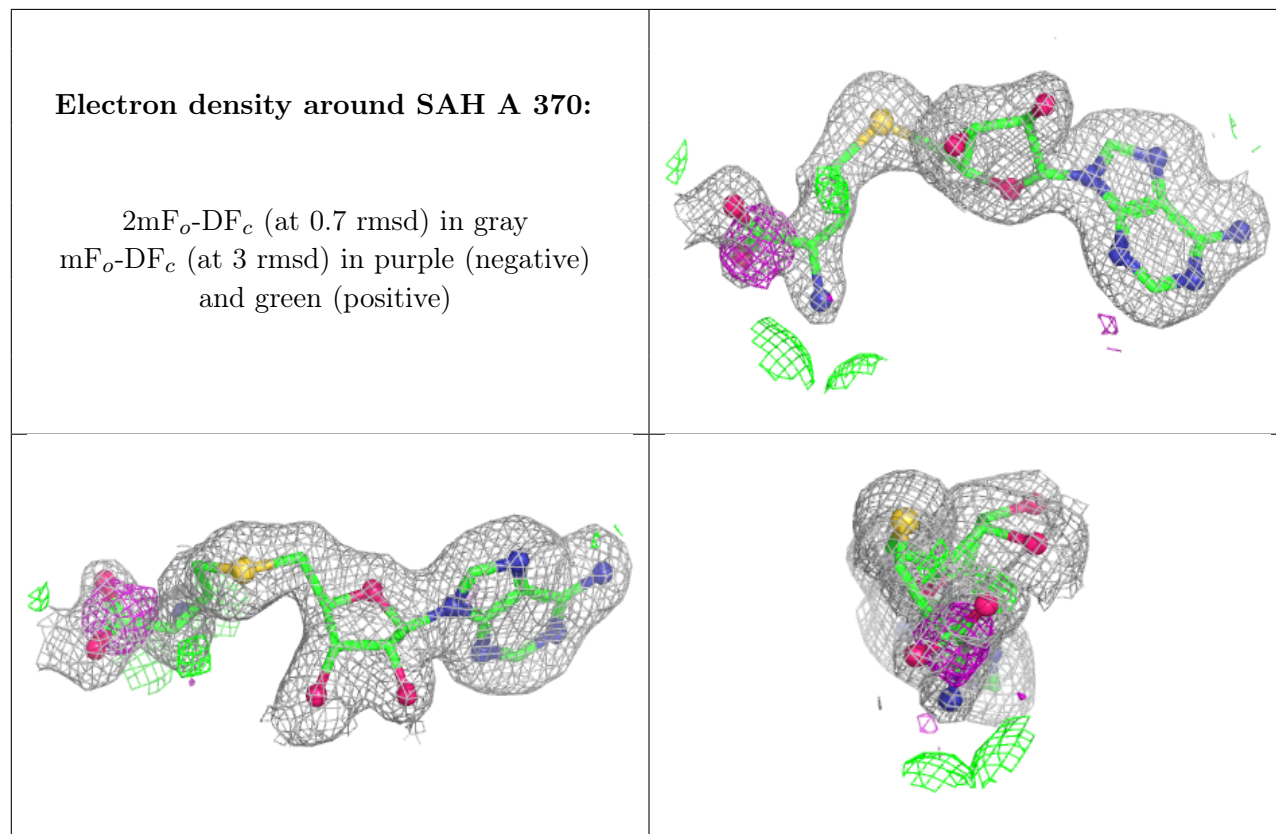
6.4 Ligands [i](#)

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
3	EUG	D	369	12/12	0.71	0.25	94,95,98,99	0
3	EUG	C	369	12/12	0.73	0.28	136,137,137,138	0
3	EUG	B	369	12/12	0.75	0.28	103,103,104,104	0
2	SAH	A	370	26/26	0.94	0.09	20,26,42,42	0
2	SAH	B	370	26/26	0.95	0.07	15,19,36,39	0
2	SAH	C	370	26/26	0.95	0.07	24,27,41,43	0
2	SAH	D	370	26/26	0.95	0.08	25,28,44,45	0

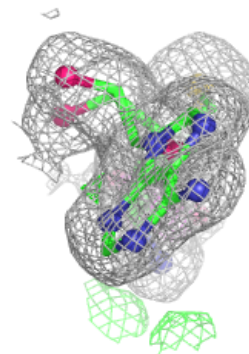
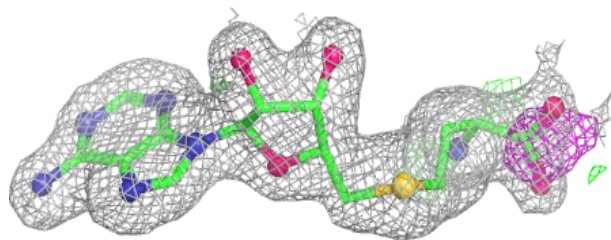
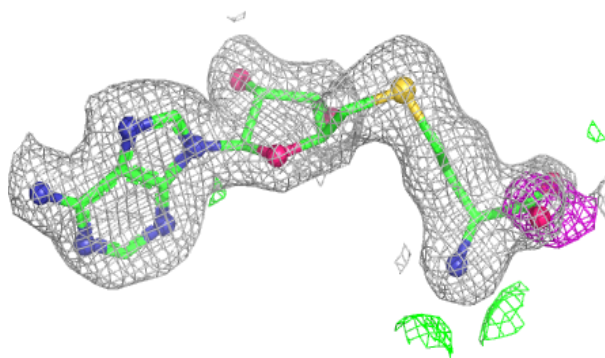
The following is a graphical depiction of the model fit to experimental electron density of all

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.

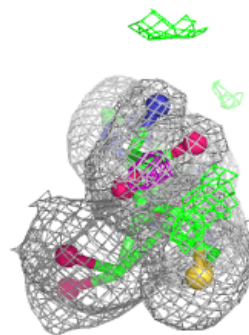
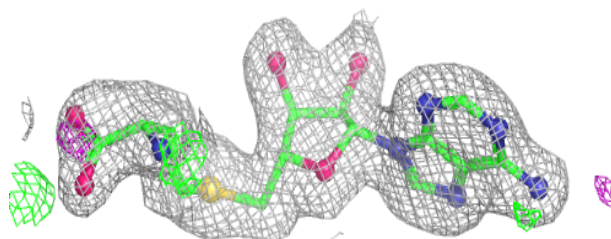
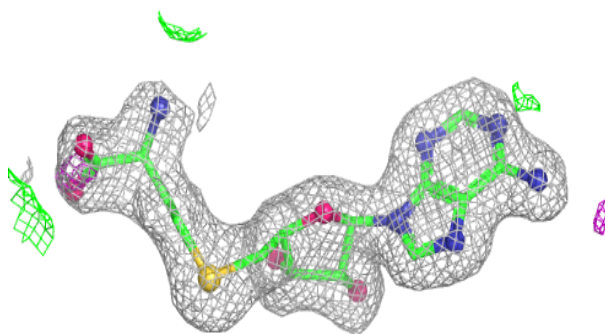


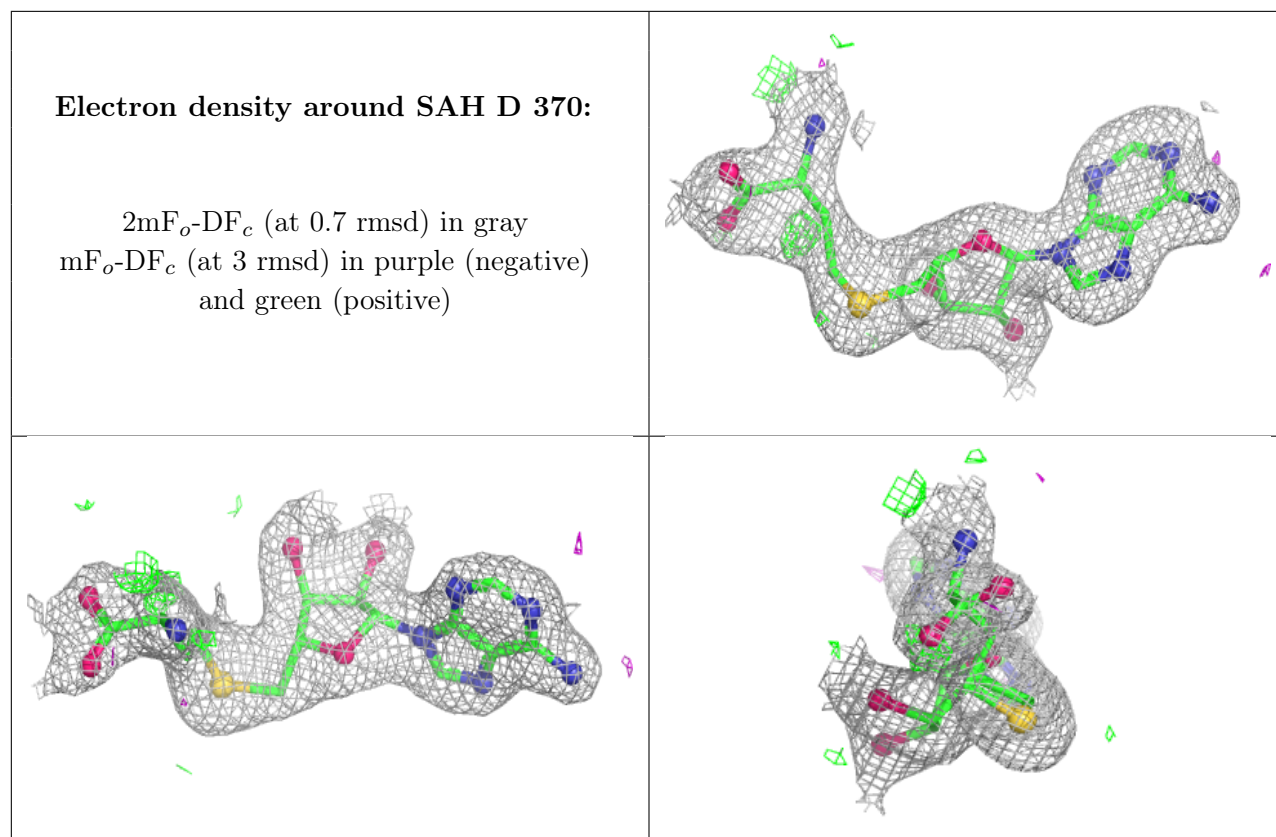
Electron density around SAH B 370:

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

**Electron density around SAH C 370:**

$2mF_o-DF_c$ (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.