



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:02 PM UTC

PDB ID : 3TKY / pdb_00003tky
Title : Monolignol o-methyltransferase (momt)
Authors : Bhuiya, M.W.; Liu, C.J.
Deposited on : 2011-08-29
Resolution : 2.47 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

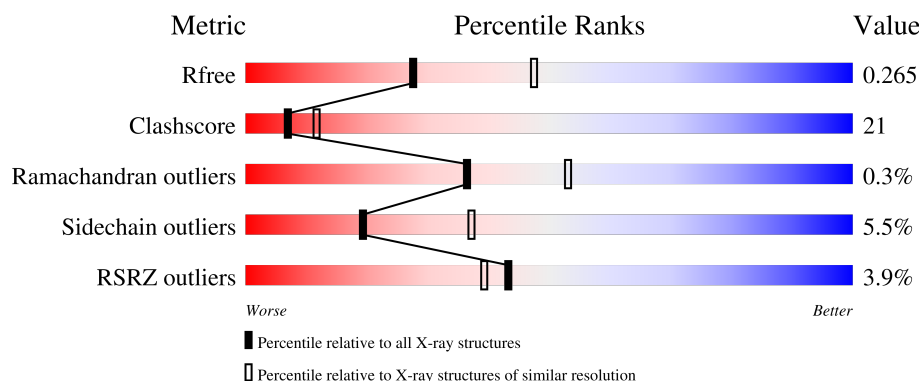
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	368	5% 64% 28% • •
1	B	368	4% 62% 28% 5% 5%
1	C	368	3% 67% 23% 5% •
1	D	368	3% 63% 27% • 5%

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
2	N7I	A	369	-	-	X	-
2	N7I	B	369	-	-	X	-
2	N7I	C	369	-	-	X	-
2	N7I	D	369	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11065 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.

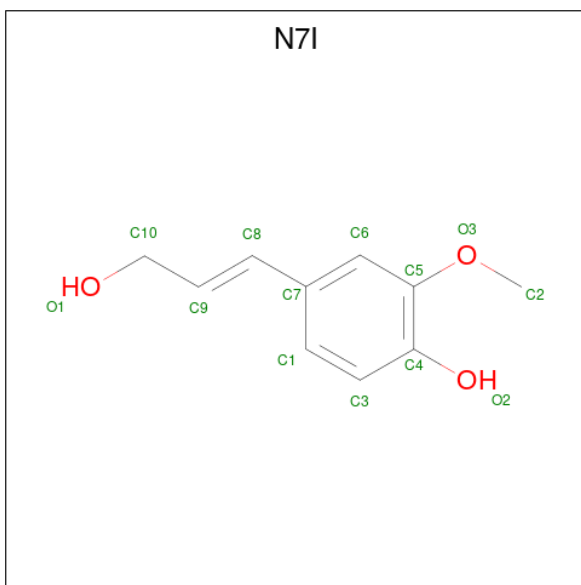
- Molecule 1 is a protein called (Iso)eugenol O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2694	1744	433	499	18			
1	B	349	Total	C	N	O	S	0	0	0
			2681	1737	432	494	18			
1	C	352	Total	C	N	O	S	0	0	0
			2694	1744	433	499	18			
1	D	348	Total	C	N	O	S	0	0	0
			2674	1732	431	493	18			

There are 12 discrepancies between the modelled and reference sequences:

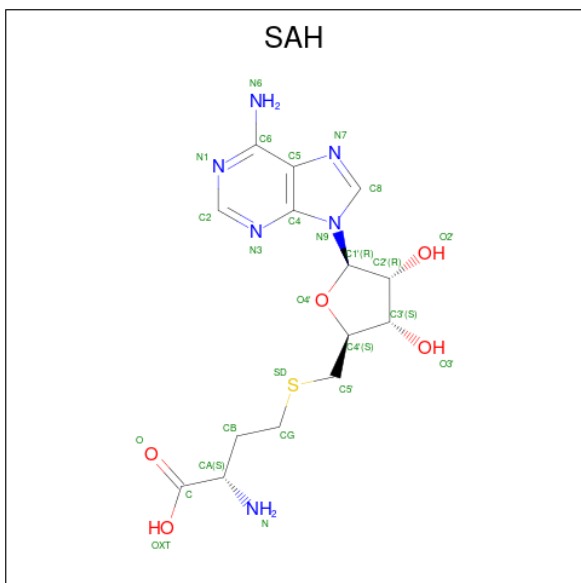
Chain	Residue	Modelled	Actual	Comment	Reference
A	133	LEU	THR	engineered mutation	UNP O04385
A	165	ILE	GLU	engineered mutation	UNP O04385
A	175	ILE	PHE	engineered mutation	UNP O04385
B	133	LEU	THR	engineered mutation	UNP O04385
B	165	ILE	GLU	engineered mutation	UNP O04385
B	175	ILE	PHE	engineered mutation	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 4-[(1E)-3-hydroxyprop-1-en-1-yl]-2-methoxyphenol (CCD ID: N7I) (formula: C₁₀H₁₂O₃).



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

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		
4	B	46	Total	O	0	0
			46	46		
4	C	50	Total	O	0	0
			50	50		
4	D	35	Total	O	0	0
			35	35		

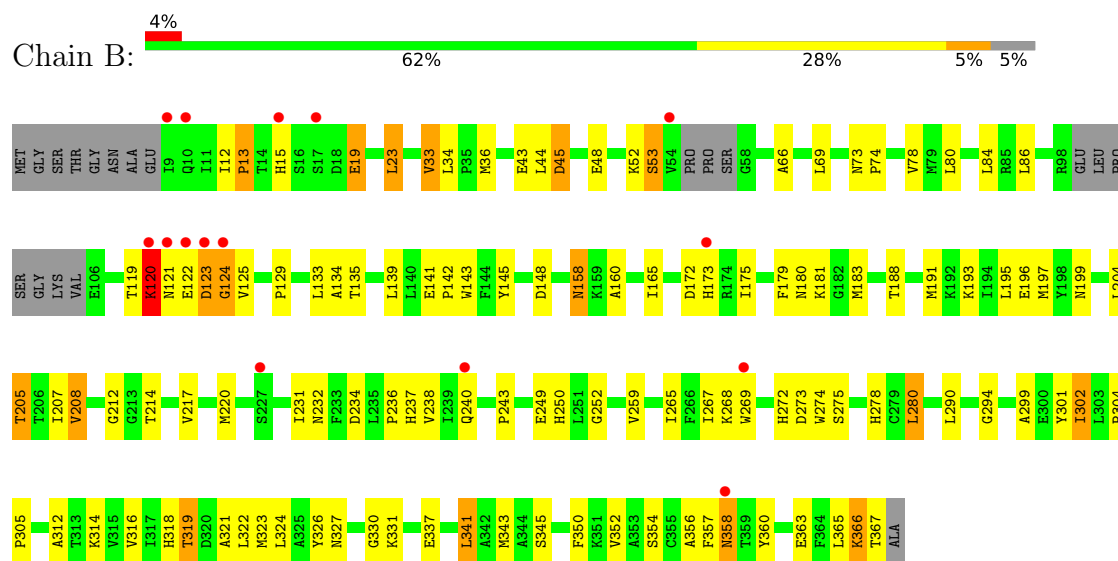
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

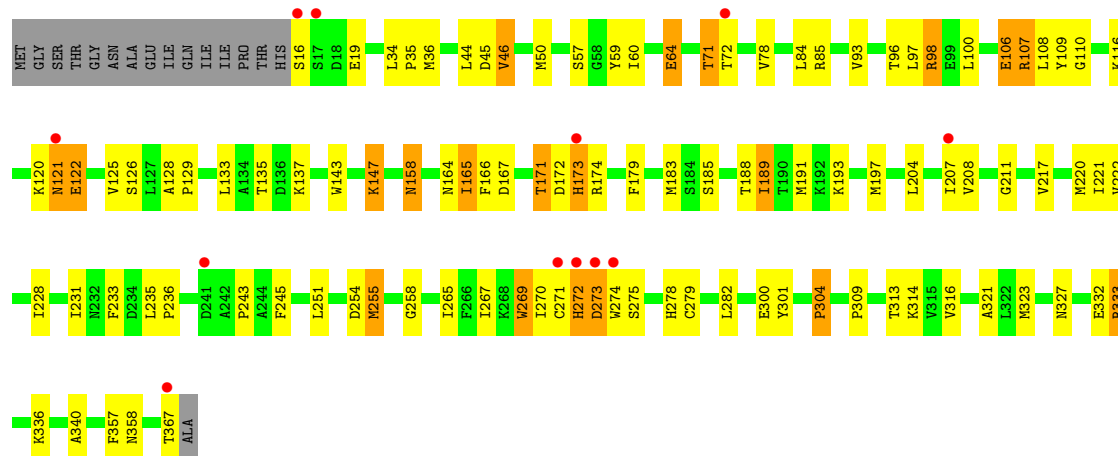
• Molecule 1: (Iso)eugenol O-methyltransferase



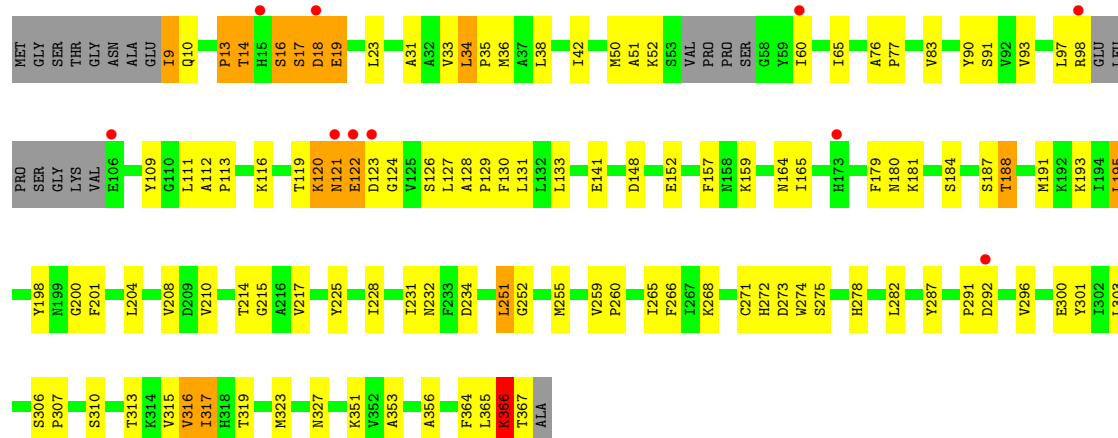
• Molecule 1: (Iso)eugenol O-methyltransferase



• 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	65.86Å 152.16Å 68.18Å 90.00° 94.92° 90.00°	Depositor
Resolution (Å)	50.00 – 2.47 50.00 – 2.47	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.47) 99.9 (50.00-2.47)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.67 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.5, CNS 1.1	Depositor
R, R_{free}	0.193 , 0.262 0.206 , 0.265	Depositor DCC
R_{free} test set	2447 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11065	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: N7I, 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	1.10	9/2759 (0.3%)	1.21	16/3749 (0.4%)
1	B	1.12	7/2743 (0.3%)	1.20	20/3724 (0.5%)
1	C	1.10	8/2759 (0.3%)	1.16	11/3749 (0.3%)
1	D	1.04	6/2736 (0.2%)	1.21	16/3714 (0.4%)
All	All	1.09	30/10997 (0.3%)	1.20	63/14936 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	MET	C-N	10.43	1.47	1.33
1	B	330	GLY	C-N	-8.08	1.23	1.33
1	B	78	VAL	CA-CB	7.45	1.63	1.54
1	A	359	THR	CA-CB	7.44	1.62	1.53
1	A	296	VAL	C-O	-7.21	1.16	1.24
1	C	174	ARG	C-O	-7.08	1.15	1.24
1	B	326	TYR	C-O	-6.65	1.15	1.24
1	B	352	VAL	C-O	-6.30	1.17	1.24
1	A	125	VAL	C-O	-6.16	1.17	1.24
1	A	358	ASN	CA-C	5.92	1.60	1.52
1	B	208	VAL	CA-CB	5.86	1.61	1.54
1	B	205	THR	CA-CB	5.81	1.62	1.53
1	D	17	SER	C-O	-5.74	1.17	1.24
1	C	106	GLU	N-CA	-5.62	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	10	GLN	C-O	-5.61	1.17	1.24
1	D	13	PRO	C-O	-5.60	1.17	1.23
1	D	16	SER	CA-C	5.56	1.59	1.52
1	C	340	ALA	CA-CB	5.56	1.62	1.53
1	C	258	GLY	N-CA	5.51	1.51	1.45
1	A	296	VAL	CA-CB	-5.44	1.47	1.54
1	C	107	ARG	C-O	-5.32	1.18	1.24
1	A	296	VAL	N-CA	-5.28	1.39	1.46
1	B	327	ASN	C-O	-5.22	1.18	1.24
1	C	172	ASP	C-O	-5.18	1.18	1.23
1	D	316	VAL	CA-CB	5.16	1.61	1.54
1	C	106	GLU	CA-C	-5.16	1.46	1.52
1	A	327	ASN	CA-C	-5.08	1.46	1.52
1	C	173	HIS	C-O	-5.05	1.18	1.24
1	D	18	ASP	C-N	-5.04	1.27	1.33
1	A	124	GLY	C-O	-5.01	1.17	1.24

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	ASP	N-CA-CB	-11.40	101.17	114.17
1	D	121	ASN	N-CA-C	10.57	122.56	111.14
1	B	330	GLY	O-C-N	-9.06	113.51	122.84
1	D	19	GLU	O-C-N	8.58	131.22	122.12
1	C	106	GLU	CA-C-O	8.48	130.22	120.80
1	A	329	GLY	CA-C-N	8.39	129.07	120.60
1	A	329	GLY	C-N-CA	8.39	129.07	120.60
1	A	126	SER	N-CA-C	8.12	120.72	109.18
1	D	16	SER	N-CA-C	8.04	120.12	111.36
1	A	329	GLY	N-CA-C	7.43	127.48	115.67
1	B	119	THR	O-C-N	7.38	132.27	123.27
1	C	106	GLU	CA-C-N	7.09	132.99	123.00
1	C	106	GLU	C-N-CA	7.09	132.99	123.00
1	C	165	ILE	CB-CA-C	-7.04	102.64	112.14
1	B	13	PRO	CB-CA-C	-6.97	100.06	111.56
1	B	318	HIS	N-CA-C	-6.47	104.14	111.07
1	A	123	ASP	N-CA-C	6.47	123.44	113.28
1	B	125	VAL	N-CA-C	6.39	117.06	108.11
1	B	120	LYS	N-CA-C	-6.34	97.29	110.80
1	D	34	LEU	CA-C-N	-6.30	112.51	119.19
1	D	34	LEU	C-N-CA	-6.30	112.51	119.19
1	A	295	LYS	N-CA-C	6.29	117.78	108.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	98	ARG	N-CA-C	6.22	118.57	107.80
1	B	23	LEU	CA-C-N	6.20	129.09	120.29
1	B	23	LEU	C-N-CA	6.20	129.09	120.29
1	D	23	LEU	CA-C-N	6.15	129.03	120.29
1	D	23	LEU	C-N-CA	6.15	129.03	120.29
1	D	16	SER	CA-C-N	5.92	128.49	120.44
1	D	16	SER	C-N-CA	5.92	128.49	120.44
1	A	329	GLY	CA-C-O	5.91	125.24	118.98
1	B	53	SER	N-CA-C	5.86	117.39	108.07
1	A	122	GLU	N-CA-C	-5.85	101.99	110.24
1	B	199	ASN	N-CA-C	5.78	120.45	113.17
1	C	121	ASN	CB-CA-C	-5.73	99.02	110.42
1	A	126	SER	N-CA-CB	-5.71	102.20	111.22
1	B	23	LEU	O-C-N	-5.69	115.57	122.22
1	B	331	LYS	O-C-N	-5.65	117.38	123.42
1	D	23	LEU	O-C-N	-5.64	115.62	122.22
1	D	366	LYS	CA-C-N	5.54	131.68	121.70
1	D	366	LYS	C-N-CA	5.54	131.68	121.70
1	B	330	GLY	CA-C-N	5.53	131.74	121.62
1	B	330	GLY	C-N-CA	5.53	131.74	121.62
1	C	147	LYS	N-CA-C	-5.43	105.27	111.14
1	B	205	THR	CB-CA-C	5.42	117.80	109.03
1	A	17	SER	CB-CA-C	5.40	116.13	109.16
1	A	47	LEU	N-CA-C	-5.39	106.01	113.18
1	B	354	SER	N-CA-C	5.38	115.39	108.34
1	A	125	VAL	N-CA-C	5.37	116.21	108.48
1	A	326	TYR	CA-C-N	5.34	134.82	121.80
1	A	326	TYR	C-N-CA	5.34	134.82	121.80
1	B	124	GLY	O-C-N	5.30	128.53	122.33
1	B	208	VAL	N-CA-C	5.27	115.55	108.17
1	C	71	THR	N-CA-C	5.27	119.46	112.72
1	D	251	LEU	N-CA-C	5.25	119.15	112.12
1	B	196	GLU	N-CA-C	-5.24	106.04	112.90
1	D	83	VAL	CB-CA-C	-5.21	105.26	112.24
1	D	19	GLU	CA-C-N	-5.20	112.90	120.29
1	D	19	GLU	C-N-CA	-5.20	112.90	120.29
1	C	304	PRO	CA-C-N	5.12	124.81	119.64
1	C	304	PRO	C-N-CA	5.12	124.81	119.64
1	C	120	LYS	N-CA-C	-5.09	102.67	110.30
1	B	319	THR	CB-CA-C	5.08	120.43	110.67
1	A	329	GLY	O-C-N	5.04	128.07	122.47

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	333	ARG	Sidechain

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	2694	0	2711	155	0
1	B	2681	0	2698	126	0
1	C	2694	0	2711	97	0
1	D	2674	0	2689	114	0
2	A	13	0	12	14	0
2	B	13	0	12	7	0
2	C	13	0	12	6	0
2	D	13	0	12	7	0
3	A	26	0	19	1	0
3	B	26	0	19	2	0
3	C	26	0	19	5	0
3	D	26	0	19	0	0
4	A	35	0	0	2	0
4	B	46	0	0	7	0
4	C	50	0	0	4	0
4	D	35	0	0	2	0
All	All	11065	0	10933	461	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 21.

All (461) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ASP:HA	1:A:323:MET:CE	1.47	1.44
1:B:273:ASP:HA	1:B:323:MET:CE	1.58	1.32
1:A:269:TRP:CD1	1:A:272:HIS:CE1	2.33	1.15
1:D:50:MET:HG2	1:D:60:ILE:HD11	1.16	1.14
1:A:30:SER:HB2	4:A:380:HOH:O	1.45	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LYS:CD	1:B:43:GLU:HB3	1.79	1.12
1:A:327:ASN:HA	2:A:369:N7I:H2	1.22	1.11
1:D:42:ILE:HD13	1:D:131:LEU:HD23	1.28	1.11
1:D:42:ILE:CD1	1:D:131:LEU:CD2	2.29	1.10
1:A:46:VAL:HG12	1:A:46:VAL:O	1.49	1.09
1:B:273:ASP:HA	1:B:323:MET:HE1	1.31	1.09
1:C:16:SER:OG	1:C:19:GLU:HB2	1.51	1.08
1:A:147:LYS:HD2	1:B:43:GLU:CB	1.86	1.06
1:A:273:ASP:HA	1:A:323:MET:HE1	1.14	1.06
1:D:42:ILE:CD1	1:D:131:LEU:HD23	1.87	1.05
1:B:319:THR:HG21	4:B:375:HOH:O	1.56	1.04
1:D:50:MET:HG2	1:D:60:ILE:CD1	1.88	1.04
1:A:269:TRP:CG	1:A:272:HIS:CE1	2.46	1.02
1:A:269:TRP:HA	1:A:272:HIS:CE1	1.95	1.01
1:D:184:SER:O	1:D:188:THR:HG23	1.60	1.01
1:A:208:VAL:HG22	1:A:231:ILE:HB	1.42	1.00
1:D:272:HIS:CD2	1:D:323:MET:SD	2.53	1.00
1:A:122:GLU:O	1:A:123:ASP:HB2	1.57	1.00
1:A:273:ASP:CA	1:A:323:MET:CE	2.40	0.98
1:C:183:MET:HE1	1:C:269:TRP:HE3	1.27	0.98
1:C:207:ILE:CD1	1:C:221:ILE:HG21	1.93	0.98
1:C:367:THR:HG23	1:C:367:THR:O	1.60	0.98
1:A:147:LYS:HD2	1:B:43:GLU:HB3	1.01	0.98
1:A:269:TRP:CA	1:A:272:HIS:HE1	1.76	0.98
1:B:366:LYS:HA	4:B:389:HOH:O	1.63	0.97
1:B:52:LYS:O	1:B:53:SER:OG	1.84	0.96
1:A:272:HIS:O	1:A:323:MET:HE2	1.64	0.96
1:C:207:ILE:HD13	1:C:221:ILE:HG21	1.47	0.95
1:B:272:HIS:O	1:B:323:MET:HE2	1.66	0.94
1:A:30:SER:O	1:A:33:VAL:HG23	1.66	0.94
1:A:272:HIS:C	1:A:323:MET:HE2	1.93	0.93
1:D:42:ILE:HD12	1:D:131:LEU:CD2	1.99	0.93
1:A:269:TRP:CB	1:A:272:HIS:HE1	1.81	0.92
1:D:273:ASP:HA	1:D:323:MET:HE2	1.50	0.92
1:B:208:VAL:HG23	1:B:231:ILE:HB	1.51	0.90
1:D:122:GLU:CD	1:D:122:GLU:N	2.28	0.90
1:A:46:VAL:O	1:A:46:VAL:CG1	2.20	0.90
1:A:193:LYS:HE3	1:B:15:HIS:CE1	2.06	0.89
1:A:269:TRP:CG	1:A:272:HIS:HE1	1.86	0.89
1:D:42:ILE:HD13	1:D:131:LEU:CD2	1.98	0.88
1:B:273:ASP:HA	1:B:323:MET:HE2	1.56	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:SER:OG	1:C:19:GLU:CB	2.22	0.88
1:B:366:LYS:CA	4:B:389:HOH:O	2.20	0.87
1:D:122:GLU:CD	1:D:122:GLU:H	1.80	0.87
1:A:133:LEU:HD13	1:A:179:PHE:HA	1.56	0.87
1:A:269:TRP:CA	1:A:272:HIS:CE1	2.57	0.87
1:A:273:ASP:CA	1:A:323:MET:HE1	2.01	0.87
1:B:188:THR:HA	1:B:220:MET:HE1	1.55	0.86
1:C:272:HIS:CE1	1:C:273:ASP:OD2	2.27	0.86
1:C:269:TRP:CE3	2:C:369:N7I:H3	2.11	0.86
1:A:273:ASP:HA	1:A:323:MET:HE2	1.55	0.86
1:C:188:THR:HA	1:C:220:MET:HE1	1.57	0.85
1:A:107:ARG:O	1:A:108:LEU:HD12	1.76	0.85
1:A:193:LYS:HE3	1:B:15:HIS:ND1	1.93	0.84
1:C:93:VAL:HG13	1:C:110:GLY:O	1.77	0.84
1:C:71:THR:O	1:C:72:THR:HG22	1.76	0.84
1:D:42:ILE:HD12	1:D:131:LEU:HD21	1.60	0.83
1:A:155:ILE:HG12	1:A:327:ASN:OD1	1.78	0.83
1:D:351:LYS:HE3	1:D:353:ALA:HB2	1.61	0.82
1:C:16:SER:HG	1:C:19:GLU:HB2	1.43	0.82
1:A:122:GLU:O	1:A:123:ASP:CB	2.27	0.82
1:A:133:LEU:CD1	1:A:179:PHE:HA	2.10	0.82
1:A:188:THR:HA	1:A:220:MET:HE1	1.62	0.81
1:C:272:HIS:HB3	1:C:300:GLU:OE1	1.80	0.81
1:A:323:MET:O	1:A:327:ASN:HB3	1.81	0.81
1:A:323:MET:CE	2:A:369:N7I:H2A	2.10	0.81
1:A:275:SER:OG	1:A:278:HIS:HD2	1.66	0.79
1:A:107:ARG:C	1:A:108:LEU:HD12	2.07	0.79
1:C:367:THR:O	1:C:367:THR:CG2	2.30	0.79
1:B:301:TYR:CG	1:B:316:VAL:HG22	2.19	0.78
1:B:337:GLU:O	1:B:341:LEU:HD23	1.83	0.78
1:B:273:ASP:CA	1:B:323:MET:CE	2.53	0.77
1:B:301:TYR:HD2	1:B:358:ASN:O	1.68	0.77
1:B:272:HIS:C	1:B:323:MET:HE2	2.09	0.76
1:D:191:MET:HG3	1:D:195:LEU:CD2	2.15	0.76
1:C:183:MET:HE1	1:C:269:TRP:CE3	2.17	0.75
1:B:139:LEU:HD21	2:B:369:N7I:H2B	1.68	0.75
1:D:148:ASP:O	1:D:152:GLU:HG2	1.88	0.74
1:A:343:MET:CG	1:D:9:ILE:HD12	2.18	0.74
1:B:191:MET:HG3	1:B:217:VAL:HG22	1.70	0.73
1:D:50:MET:CG	1:D:60:ILE:HD11	2.09	0.73
1:A:327:ASN:OD1	1:A:327:ASN:O	2.05	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:VAL:HG12	1:A:255:MET:HE2	1.70	0.72
1:D:133:LEU:HG	2:D:369:N7I:H3	1.72	0.72
1:A:220:MET:O	1:A:224:LYS:HG2	1.90	0.71
1:B:165:ILE:HD11	2:B:369:N7I:H2	1.71	0.71
1:A:255:MET:HE3	3:A:370:SAH:C2	2.20	0.71
1:A:73:ASN:O	1:A:75:GLU:N	2.24	0.71
1:B:366:LYS:C	4:B:389:HOH:O	2.33	0.71
1:D:275:SER:OG	1:D:278:HIS:HD2	1.73	0.70
1:A:45:ASP:OD1	1:A:48:GLU:HB2	1.91	0.70
1:A:172:ASP:HB3	1:A:175:ILE:HG22	1.72	0.70
1:A:323:MET:HE3	2:A:369:N7I:H2A	1.74	0.70
1:D:287:TYR:O	1:D:366:LYS:NZ	2.23	0.69
1:D:133:LEU:CG	2:D:369:N7I:H3	2.23	0.69
1:A:58:GLY:C	1:A:59:TYR:CD1	2.70	0.68
1:A:147:LYS:CE	1:B:43:GLU:HB3	2.23	0.68
1:B:273:ASP:OD2	1:B:323:MET:HE1	1.93	0.68
1:D:296:VAL:CG1	1:D:364:PHE:HB2	2.23	0.68
1:A:187:SER:OG	1:A:268:LYS:HE3	1.93	0.68
1:D:291:PRO:O	1:D:366:LYS:HE2	1.94	0.68
1:A:267:ILE:HG22	1:A:270:ILE:HG13	1.76	0.68
1:B:122:GLU:HG3	1:B:123:ASP:H	1.58	0.68
1:D:133:LEU:HD21	2:D:369:N7I:C3	2.23	0.68
1:C:84:LEU:HD13	1:C:109:TYR:CD1	2.29	0.67
1:D:315:VAL:O	1:D:319:THR:HG23	1.95	0.67
1:C:301:TYR:CG	1:C:316:VAL:HG22	2.28	0.67
1:B:122:GLU:HG3	1:B:123:ASP:N	2.10	0.67
1:B:366:LYS:O	1:B:367:THR:C	2.37	0.67
1:C:272:HIS:O	1:C:272:HIS:CG	2.46	0.67
1:A:272:HIS:O	1:A:323:MET:CE	2.42	0.67
1:B:301:TYR:CD2	1:B:358:ASN:O	2.48	0.67
1:D:193:LYS:HG2	1:D:356:ALA:HB1	1.77	0.67
1:B:193:LYS:O	1:B:197:MET:HG2	1.93	0.66
1:B:236:PRO:O	1:B:240:GLN:HG2	1.95	0.66
1:C:207:ILE:CD1	1:C:221:ILE:CG2	2.72	0.66
1:A:155:ILE:HG23	1:A:327:ASN:OD1	1.96	0.66
1:A:275:SER:OG	1:A:278:HIS:CD2	2.49	0.66
1:C:143:TRP:CH2	1:D:33:VAL:HG13	2.31	0.66
1:B:273:ASP:CA	1:B:323:MET:HE1	2.17	0.65
1:C:272:HIS:ND1	1:C:273:ASP:OD2	2.28	0.65
1:A:96:THR:HG22	1:A:97:LEU:N	2.10	0.65
1:B:172:ASP:HB3	1:B:175:ILE:HG22	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:PHE:CE2	1:D:19:GLU:HA	2.32	0.65
1:A:312:ALA:HA	1:B:23:LEU:HD13	1.79	0.65
1:B:208:VAL:CG2	1:B:231:ILE:HB	2.26	0.65
1:D:121:ASN:HB2	1:D:122:GLU:OE1	1.97	0.65
1:D:210:VAL:HG12	1:D:255:MET:HE2	1.79	0.65
1:B:129:PRO:HB3	1:B:181:LYS:HE3	1.77	0.64
1:D:296:VAL:HG12	1:D:364:PHE:HB2	1.77	0.64
1:B:158:ASN:H	1:B:158:ASN:HD22	1.45	0.64
1:A:327:ASN:CA	2:A:369:N7I:H2	2.14	0.64
1:D:122:GLU:N	1:D:122:GLU:OE1	2.29	0.64
1:B:208:VAL:HG13	1:B:265:ILE:HD12	1.79	0.64
1:D:255:MET:CG	1:D:282:LEU:HD13	2.28	0.64
1:C:98:ARG:N	1:C:106:GLU:O	2.26	0.64
1:A:343:MET:HG2	1:D:9:ILE:HD12	1.80	0.64
1:C:188:THR:HA	1:C:220:MET:CE	2.27	0.64
1:A:273:ASP:HA	1:A:323:MET:HE3	1.71	0.63
1:C:267:ILE:HD12	1:C:271:CYS:SG	2.38	0.63
1:A:80:LEU:O	1:A:84:LEU:HG	1.98	0.63
1:A:343:MET:HG3	1:D:9:ILE:HD12	1.79	0.62
1:C:357:PHE:HE2	1:D:19:GLU:HA	1.64	0.62
1:D:272:HIS:NE2	1:D:323:MET:SD	2.72	0.62
1:A:327:ASN:HB2	1:A:329:GLY:H	1.62	0.62
1:A:273:ASP:O	1:A:328:PRO:HD2	2.00	0.62
1:A:273:ASP:N	1:A:323:MET:HE2	2.14	0.62
2:A:369:N7I:O2	2:A:369:N7I:H2B	1.99	0.62
1:A:193:LYS:NZ	1:B:19:GLU:OE2	2.31	0.62
1:B:122:GLU:CG	1:B:123:ASP:H	2.13	0.62
1:B:274:TRP:HB3	1:B:278:HIS:HB2	1.82	0.62
1:C:282:LEU:C	1:C:282:LEU:HD23	2.25	0.61
1:D:60:ILE:HD12	1:D:65:ILE:HG12	1.81	0.61
1:D:121:ASN:CB	1:D:122:GLU:OE1	2.48	0.61
1:C:275:SER:OG	1:C:278:HIS:HD2	1.83	0.61
1:B:234:ASP:OD2	1:B:238:VAL:HG21	2.00	0.61
1:B:36:MET:HE1	1:B:135:THR:HB	1.83	0.61
1:C:158:ASN:HD22	1:C:158:ASN:H	1.48	0.61
1:D:208:VAL:HG23	1:D:231:ILE:CG2	2.31	0.61
1:D:255:MET:HB2	1:D:282:LEU:CD1	2.31	0.60
1:A:191:MET:O	1:A:195:LEU:HG	2.00	0.60
1:A:343:MET:HG2	1:D:9:ILE:HB	1.83	0.60
1:C:272:HIS:HB3	1:C:300:GLU:CD	2.26	0.60
1:C:179:PHE:CE1	2:C:369:N7I:H2A	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:VAL:HG13	1:D:265:ILE:HG12	1.84	0.60
1:D:60:ILE:HD12	1:D:65:ILE:CG1	2.30	0.60
1:C:273:ASP:HB3	1:C:327:ASN:OD1	2.02	0.60
1:D:184:SER:O	1:D:188:THR:CG2	2.44	0.60
1:A:301:TYR:CG	1:A:316:VAL:HG12	2.37	0.60
1:B:234:ASP:OD2	1:B:238:VAL:CG2	2.50	0.59
1:B:365:LEU:HB2	1:B:367:THR:HG22	1.83	0.59
1:D:210:VAL:CG1	1:D:255:MET:HE2	2.31	0.59
1:A:269:TRP:CB	1:A:272:HIS:CE1	2.72	0.59
1:D:208:VAL:HG23	1:D:231:ILE:HG22	1.85	0.59
1:B:122:GLU:HG3	1:B:123:ASP:CG	2.27	0.59
1:D:180:ASN:HB3	1:D:214:THR:CG2	2.32	0.59
1:B:134:ALA:HB2	2:B:369:N7I:H10	1.85	0.59
1:A:266:PHE:CE1	1:A:268:LYS:HB2	2.38	0.58
1:B:173:HIS:CE1	4:B:379:HOH:O	2.55	0.58
1:D:255:MET:HG3	1:D:282:LEU:HD13	1.85	0.58
1:B:268:LYS:O	1:B:269:TRP:HB2	2.03	0.58
1:C:207:ILE:HD13	1:C:221:ILE:CG2	2.27	0.58
1:B:208:VAL:HG23	1:B:231:ILE:CB	2.28	0.58
1:C:191:MET:HG3	1:C:217:VAL:HG22	1.85	0.58
1:C:85:ARG:HG3	1:D:307:PRO:HG3	1.85	0.58
1:D:272:HIS:HD2	1:D:323:MET:SD	2.23	0.58
1:A:59:TYR:CD1	1:A:59:TYR:N	2.70	0.58
1:A:56:PRO:O	1:A:57:SER:HB2	2.03	0.58
1:A:147:LYS:HE3	1:B:43:GLU:O	2.04	0.58
1:A:210:VAL:CG1	1:A:255:MET:HE2	2.34	0.58
1:C:179:PHE:CZ	2:C:369:N7I:H2A	2.39	0.58
1:A:304:PRO:HD3	1:A:316:VAL:HG21	1.84	0.58
1:C:301:TYR:CD1	1:C:316:VAL:HG22	2.39	0.57
1:D:76:ALA:HB3	1:D:77:PRO:HD3	1.86	0.57
1:C:204:LEU:HD13	1:C:207:ILE:HG22	1.86	0.57
1:B:208:VAL:CG1	1:B:265:ILE:HD12	2.34	0.57
1:C:272:HIS:HE1	2:C:369:N7I:C4	2.17	0.57
1:B:122:GLU:HG3	1:B:123:ASP:OD2	2.04	0.57
1:D:128:ALA:O	1:D:131:LEU:HB3	2.04	0.57
1:C:243:PRO:HG2	1:C:245:PHE:CZ	2.40	0.57
1:D:180:ASN:HB3	1:D:214:THR:HG21	1.87	0.57
1:D:198:TYR:CZ	1:D:200:GLY:HA3	2.40	0.57
1:A:155:ILE:HG21	1:A:327:ASN:O	2.05	0.56
1:A:73:ASN:C	1:A:75:GLU:N	2.62	0.56
1:A:59:TYR:HB3	1:A:109:TYR:C	2.30	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:TYR:CD1	1:A:316:VAL:HG12	2.41	0.56
1:A:321:ALA:HB3	1:B:33:VAL:HG21	1.87	0.56
1:A:326:TYR:HB2	2:A:369:N7I:H6	1.87	0.56
1:C:71:THR:O	1:C:72:THR:CG2	2.51	0.56
1:C:272:HIS:HD2	1:C:332:GLU:OE2	1.87	0.56
1:D:193:LYS:CG	1:D:356:ALA:HB1	2.35	0.56
1:B:183:MET:HE1	1:B:269:TRP:HZ3	1.70	0.56
1:A:155:ILE:CG2	1:A:327:ASN:OD1	2.54	0.56
1:C:173:HIS:HB3	4:C:416:HOH:O	2.06	0.56
1:B:145:TYR:CE2	1:B:160:ALA:HB2	2.40	0.56
1:C:183:MET:HE2	3:C:370:SAH:CG	2.35	0.55
1:D:128:ALA:HB3	1:D:129:PRO:HD3	1.87	0.55
1:A:28:LEU:CD2	1:B:34:LEU:HD21	2.36	0.55
1:A:273:ASP:CA	1:A:323:MET:HE2	2.22	0.55
1:C:34:LEU:HB3	1:C:35:PRO:CD	2.36	0.55
1:A:147:LYS:HE3	1:B:43:GLU:C	2.31	0.55
1:C:357:PHE:O	1:C:358:ASN:HB2	2.07	0.55
1:A:198:TYR:CZ	1:A:200:GLY:HA3	2.42	0.55
1:A:301:TYR:HE1	1:A:319:THR:HG21	1.72	0.55
1:B:183:MET:HE1	1:B:269:TRP:CZ3	2.42	0.55
1:C:122:GLU:O	1:C:125:VAL:HB	2.07	0.55
1:C:97:LEU:HD11	1:D:306:SER:HB3	1.89	0.54
1:C:272:HIS:HE1	2:C:369:N7I:O2	1.91	0.54
1:A:96:THR:CG2	1:A:97:LEU:N	2.70	0.54
1:B:145:TYR:CD2	1:B:160:ALA:HB2	2.43	0.54
1:B:66:ALA:HA	1:B:69:LEU:HD12	1.90	0.54
1:A:133:LEU:HD13	1:A:179:PHE:CA	2.34	0.53
1:B:280:LEU:HD13	1:B:341:LEU:HD13	1.89	0.53
1:C:164:ASN:CG	4:C:394:HOH:O	2.52	0.53
1:C:167:ASP:O	1:C:171:THR:HG23	2.09	0.53
1:D:51:ALA:HA	1:D:111:LEU:HD11	1.90	0.53
1:D:327:ASN:OD1	2:D:369:N7I:H2	2.08	0.53
1:A:301:TYR:HB3	1:A:316:VAL:HG12	1.90	0.53
1:A:34:LEU:HB3	1:A:35:PRO:CD	2.39	0.52
1:B:134:ALA:HB2	2:B:369:N7I:C10	2.39	0.52
1:D:217:VAL:HG23	4:D:399:HOH:O	2.08	0.52
1:B:214:THR:HG22	1:B:243:PRO:HD3	1.90	0.52
1:C:93:VAL:CG1	1:C:110:GLY:O	2.55	0.52
1:A:328:PRO:HD2	2:A:369:N7I:C2	2.39	0.52
1:C:314:LYS:HD2	1:D:90:TYR:CZ	2.45	0.52
1:A:315:VAL:O	1:A:319:THR:HG23	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:GLU:CG	1:B:123:ASP:N	2.71	0.52
1:D:90:TYR:O	1:D:91:SER:HB2	2.10	0.52
1:B:133:LEU:HD13	1:B:179:PHE:HA	1.92	0.52
1:B:273:ASP:CA	1:B:323:MET:HE2	2.29	0.52
1:C:275:SER:OG	1:C:278:HIS:CD2	2.62	0.52
1:B:33:VAL:HG13	1:B:86:LEU:HD21	1.92	0.52
1:B:301:TYR:CD1	1:B:316:VAL:HG22	2.45	0.52
1:C:183:MET:HE2	3:C:370:SAH:HG1	1.92	0.52
1:D:191:MET:HG3	1:D:195:LEU:HD21	1.91	0.52
1:C:78:VAL:HG23	4:C:380:HOH:O	2.09	0.52
1:C:125:VAL:HG12	1:C:189:ILE:HD11	1.91	0.51
1:B:173:HIS:HE1	4:B:379:HOH:O	1.93	0.51
1:A:73:ASN:C	1:A:75:GLU:H	2.18	0.51
1:B:120:LYS:HG2	1:B:124:GLY:C	2.36	0.51
1:B:299:ALA:HA	1:B:360:TYR:O	2.10	0.51
1:A:309:PRO:O	1:A:314:LYS:HE3	2.11	0.51
1:C:158:ASN:HD22	1:C:158:ASN:N	2.08	0.51
1:A:153:GLY:HA2	1:B:73:ASN:ND2	2.26	0.51
1:A:312:ALA:CA	1:B:23:LEU:HD13	2.41	0.51
1:A:274:TRP:HB3	1:A:278:HIS:HB2	1.93	0.51
1:C:193:LYS:HG2	1:C:197:MET:HE2	1.93	0.51
1:C:36:MET:HE1	1:C:135:THR:HB	1.92	0.50
1:C:304:PRO:HG2	1:C:313:THR:HG23	1.93	0.50
1:D:120:LYS:HG2	1:D:124:GLY:C	2.36	0.50
1:B:366:LYS:O	1:B:367:THR:O	2.29	0.50
1:C:166:PHE:CE2	3:C:370:SAH:H2'	2.46	0.50
1:D:187:SER:HB3	1:D:268:LYS:CE	2.42	0.50
1:D:217:VAL:HG11	1:D:266:PHE:CE2	2.47	0.50
1:B:265:ILE:HG12	1:B:290:LEU:HD21	1.93	0.50
1:B:274:TRP:HH2	3:B:370:SAH:N7	2.10	0.50
1:C:147:LYS:HB3	4:C:391:HOH:O	2.11	0.50
1:A:73:ASN:O	1:A:74:PRO:C	2.54	0.50
1:A:261:LYS:HE3	1:A:289:ALA:HA	1.92	0.49
1:A:121:ASN:OD1	1:A:122:GLU:O	2.30	0.49
1:C:269:TRP:CZ3	2:C:369:N7I:H3	2.47	0.49
1:B:19:GLU:O	1:B:23:LEU:HG	2.13	0.49
1:D:133:LEU:CD2	2:D:369:N7I:C3	2.89	0.49
1:C:133:LEU:HD22	1:C:179:PHE:HA	1.94	0.49
1:D:18:ASP:OD2	1:D:19:GLU:N	2.46	0.49
1:D:217:VAL:HG11	1:D:266:PHE:HE2	1.78	0.49
1:A:208:VAL:CG2	1:A:231:ILE:HB	2.29	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:ALA:CB	1:D:33:VAL:HG11	2.43	0.49
1:D:208:VAL:HG21	1:D:260:PRO:HB2	1.95	0.49
1:D:351:LYS:HE3	1:D:353:ALA:CB	2.37	0.49
1:A:254:ASP:OD2	1:A:254:ASP:C	2.55	0.48
1:A:158:ASN:N	1:A:158:ASN:HD22	2.10	0.48
1:D:187:SER:HB3	1:D:268:LYS:HE2	1.94	0.48
1:C:34:LEU:HB3	1:C:35:PRO:HD2	1.95	0.48
1:D:274:TRP:HB3	1:D:278:HIS:HB2	1.95	0.48
1:B:204:LEU:HD13	1:B:207:ILE:HD13	1.96	0.48
1:C:272:HIS:CB	1:C:300:GLU:OE1	2.57	0.48
1:B:343:MET:C	1:B:345:SER:H	2.21	0.48
1:A:58:GLY:C	1:A:59:TYR:HD1	2.20	0.48
1:D:34:LEU:HB3	1:D:35:PRO:HD3	1.96	0.48
1:B:321:ALA:O	1:B:324:LEU:HB3	2.13	0.48
1:C:35:PRO:HG3	1:D:31:ALA:HB3	1.95	0.48
1:A:45:ASP:CG	1:A:45:ASP:O	2.57	0.48
1:B:145:TYR:O	1:B:148:ASP:HB2	2.14	0.48
1:C:50:MET:HE1	1:C:93:VAL:CG1	2.44	0.48
1:A:323:MET:O	1:A:327:ASN:CB	2.58	0.47
1:B:275:SER:OG	1:B:278:HIS:HD2	1.98	0.47
2:D:369:N7I:H6	2:D:369:N7I:H9	1.40	0.47
1:A:55:PRO:O	1:A:58:GLY:N	2.47	0.47
1:A:102:SER:OG	1:A:104:LYS:HG3	2.14	0.47
1:B:268:LYS:O	3:B:370:SAH:OXT	2.32	0.47
1:A:90:TYR:CZ	1:B:314:LYS:HD3	2.48	0.47
1:A:191:MET:HG3	1:A:217:VAL:HG13	1.96	0.47
1:A:355:CYS:HA	1:A:359:THR:O	2.15	0.47
1:C:50:MET:HE1	1:C:93:VAL:HG13	1.95	0.47
1:C:269:TRP:O	1:C:273:ASP:OD1	2.32	0.47
1:D:234:ASP:O	1:D:252:GLY:HA2	2.15	0.47
1:D:313:THR:O	1:D:317:ILE:HG13	2.15	0.47
1:A:197:MET:HE1	1:A:355:CYS:O	2.14	0.47
1:A:273:ASP:O	1:A:328:PRO:HG2	2.15	0.47
1:B:234:ASP:O	1:B:252:GLY:HA2	2.15	0.47
1:C:274:TRP:HB3	1:C:278:HIS:HB2	1.97	0.47
1:C:282:LEU:HD23	1:C:282:LEU:O	2.14	0.47
1:C:255:MET:HB2	3:C:370:SAH:N1	2.31	0.46
1:A:158:ASN:O	1:A:161:TYR:O	2.33	0.46
1:A:328:PRO:HD2	2:A:369:N7I:H2	1.97	0.46
1:B:158:ASN:HD22	1:B:158:ASN:N	2.13	0.46
1:D:13:PRO:C	1:D:14:THR:CG2	2.87	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ASP:OD1	1:A:323:MET:HE1	2.15	0.46
1:B:48:GLU:OE2	1:B:120:LYS:N	2.27	0.46
1:C:60:ILE:HD11	1:C:64:GLU:HB3	1.98	0.46
1:D:112:ALA:HB1	1:D:113:PRO:HD2	1.97	0.46
1:C:128:ALA:HB3	1:C:129:PRO:HD3	1.97	0.46
1:D:273:ASP:OD1	1:D:323:MET:HE1	2.15	0.46
1:A:187:SER:OG	1:A:268:LYS:CE	2.63	0.46
1:A:319:THR:O	1:A:323:MET:HG2	2.15	0.46
1:B:212:GLY:HA3	1:B:232:ASN:ND2	2.31	0.46
1:B:312:ALA:HB1	1:B:358:ASN:OD1	2.16	0.46
1:C:59:TYR:CZ	1:C:96:THR:HG23	2.51	0.46
1:D:119:THR:O	1:D:126:SER:HB3	2.15	0.46
1:A:275:SER:HA	1:A:329:GLY:O	2.16	0.46
1:B:52:LYS:C	1:B:53:SER:OG	2.50	0.46
1:B:212:GLY:HA3	1:B:232:ASN:HD21	1.80	0.46
1:D:34:LEU:HB3	1:D:35:PRO:CD	2.46	0.46
1:C:44:LEU:O	1:C:45:ASP:CB	2.63	0.46
1:B:44:LEU:O	1:B:45:ASP:HB2	2.15	0.45
1:C:191:MET:HE2	1:C:217:VAL:HG13	1.98	0.45
1:D:296:VAL:HG13	1:D:364:PHE:HB2	1.95	0.45
1:A:30:SER:OG	1:B:322:LEU:HD11	2.16	0.45
1:B:237:HIS:CE1	1:B:238:VAL:HG13	2.51	0.45
1:A:33:VAL:HG13	1:B:143:TRP:CH2	2.52	0.45
1:A:157:PHE:C	1:A:157:PHE:CD2	2.95	0.45
1:A:193:LYS:CE	1:B:15:HIS:ND1	2.72	0.45
1:A:54:VAL:HG13	1:A:55:PRO:O	2.16	0.45
1:C:255:MET:HE3	1:C:282:LEU:HD12	1.99	0.45
1:B:183:MET:CE	1:B:269:TRP:HZ3	2.30	0.45
1:D:225:TYR:O	1:D:228:ILE:HG22	2.15	0.45
1:C:46:VAL:O	1:C:50:MET:HG3	2.15	0.45
1:D:42:ILE:CD1	1:D:131:LEU:HD22	2.38	0.45
1:A:301:TYR:HB3	1:A:316:VAL:CG1	2.47	0.45
1:B:121:ASN:HD22	1:B:121:ASN:HA	1.49	0.45
1:A:133:LEU:HD11	1:A:179:PHE:HA	1.95	0.44
1:D:201:PHE:HA	1:D:204:LEU:HD12	1.98	0.44
1:C:309:PRO:HA	1:C:314:LYS:HE3	2.00	0.44
1:D:130:PHE:CZ	2:D:369:N7I:H8	2.52	0.44
1:B:80:LEU:O	1:B:84:LEU:HG	2.17	0.44
1:B:134:ALA:CB	2:B:369:N7I:H10	2.48	0.44
1:C:272:HIS:O	1:C:323:MET:SD	2.75	0.44
1:A:59:TYR:HB3	1:A:109:TYR:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ALA:HB2	1:B:23:LEU:CD1	2.47	0.44
1:C:208:VAL:HG23	1:C:231:ILE:HB	1.98	0.44
1:D:273:ASP:HA	1:D:323:MET:CE	2.34	0.44
1:B:356:ALA:O	1:B:357:PHE:C	2.61	0.44
1:C:116:LYS:O	1:C:121:ASN:ND2	2.44	0.44
1:A:53:SER:O	1:A:54:VAL:CB	2.64	0.43
1:A:323:MET:SD	2:A:369:N7I:H2A	2.58	0.43
1:A:326:TYR:HD2	2:A:369:N7I:H6	1.81	0.43
1:B:350:PHE:HA	1:B:363:GLU:O	2.17	0.43
1:B:302:ILE:HG13	1:B:360:TYR:CD1	2.53	0.43
1:A:46:VAL:O	1:A:47:LEU:HD23	2.19	0.43
1:D:367:THR:HG21	4:D:401:HOH:O	2.17	0.43
1:A:155:ILE:HD13	1:A:327:ASN:O	2.18	0.43
1:D:215:GLY:HA2	1:D:232:ASN:ND2	2.33	0.43
1:A:269:TRP:CD1	1:A:272:HIS:NE2	2.80	0.43
1:A:343:MET:HG2	1:D:9:ILE:CB	2.47	0.43
1:B:319:THR:CG2	4:B:375:HOH:O	2.34	0.43
1:C:208:VAL:HG13	1:C:265:ILE:HG12	2.01	0.43
1:D:18:ASP:OD2	1:D:18:ASP:C	2.59	0.42
1:D:122:GLU:C	1:D:124:GLY:H	2.27	0.42
1:D:191:MET:O	1:D:195:LEU:HD23	2.18	0.42
1:D:292:ASP:O	1:D:366:LYS:HB3	2.20	0.42
1:A:323:MET:CE	2:A:369:N7I:C2	2.91	0.42
1:D:60:ILE:HG12	1:D:109:TYR:O	2.19	0.42
1:A:165:ILE:HD12	1:A:326:TYR:HB3	2.01	0.42
1:D:271:CYS:HB2	1:D:300:GLU:OE2	2.18	0.42
1:B:272:HIS:O	1:B:323:MET:CE	2.53	0.42
2:B:369:N7I:H9	2:B:369:N7I:H6	1.39	0.42
1:C:126:SER:O	1:C:185:SER:HB3	2.18	0.42
1:C:279:CYS:SG	1:C:333:ARG:NH1	2.92	0.42
1:A:256:PHE:HB3	1:A:281:LYS:HD3	2.01	0.42
1:A:51:ALA:HA	1:A:111:LEU:HD11	2.02	0.42
1:A:126:SER:O	1:A:185:SER:HB3	2.20	0.42
1:A:326:TYR:CD2	2:A:369:N7I:H6	2.54	0.42
1:B:301:TYR:HB3	1:B:316:VAL:CG2	2.49	0.42
1:D:38:LEU:HG	1:D:131:LEU:HD21	2.02	0.42
1:D:301:TYR:HE1	1:D:319:THR:HG21	1.83	0.42
1:B:273:ASP:HA	1:B:323:MET:HE3	1.81	0.42
1:C:321:ALA:HB3	1:D:33:VAL:HG11	2.02	0.42
1:D:97:LEU:C	1:D:98:ARG:HG2	2.44	0.42
1:B:12:ILE:HG22	1:B:13:PRO:N	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:ASP:OD1	1:C:254:ASP:C	2.63	0.42
1:A:139:LEU:C	1:A:142:PRO:HD2	2.45	0.41
1:B:294:GLY:O	1:B:366:LYS:HG3	2.20	0.41
1:B:273:ASP:N	1:B:323:MET:HE2	2.35	0.41
1:A:195:LEU:HD13	1:A:224:LYS:HG3	2.02	0.41
1:B:234:ASP:CG	1:B:238:VAL:CG2	2.93	0.41
1:A:53:SER:O	1:A:54:VAL:HB	2.21	0.41
1:A:102:SER:OG	1:A:104:LYS:HE3	2.20	0.41
1:C:270:ILE:C	1:C:272:HIS:H	2.29	0.41
1:D:116:LYS:O	1:D:121:ASN:OD1	2.38	0.41
1:D:152:GLU:HG3	1:D:159:LYS:HE3	2.02	0.41
1:D:191:MET:O	1:D:195:LEU:CD2	2.69	0.41
2:A:369:N7I:O2	2:A:369:N7I:C2	2.65	0.41
1:C:137:LYS:HE3	1:D:141:GLU:OE2	2.20	0.41
1:D:51:ALA:CA	1:D:111:LEU:HD11	2.50	0.41
1:D:157:PHE:CE1	1:D:165:ILE:HA	2.55	0.41
1:A:47:LEU:N	4:A:408:HOH:O	2.53	0.41
1:A:269:TRP:C	1:A:272:HIS:CE1	2.97	0.41
1:D:60:ILE:CD1	1:D:65:ILE:HD11	2.51	0.41
1:A:195:LEU:HD11	1:A:220:MET:HB3	2.03	0.41
1:B:134:ALA:CB	2:B:369:N7I:C10	2.99	0.41
1:B:180:ASN:HD21	1:B:238:VAL:HG12	1.85	0.41
1:B:191:MET:O	1:B:195:LEU:HG	2.20	0.41
1:B:191:MET:HE2	1:B:217:VAL:HG13	2.03	0.41
1:B:208:VAL:CG1	1:B:265:ILE:CD1	2.99	0.41
1:B:304:PRO:HA	1:B:305:PRO:HD3	1.88	0.41
1:D:36:MET:HE2	1:D:36:MET:N	2.36	0.41
1:C:85:ARG:HG2	1:D:317:ILE:HD13	2.03	0.41
1:C:235:LEU:HB3	1:C:236:PRO:HD2	2.02	0.41
1:D:133:LEU:HD13	1:D:179:PHE:HA	2.02	0.41
1:A:294:GLY:O	1:A:366:LYS:HG2	2.21	0.40
1:A:328:PRO:HD2	2:A:369:N7I:H2B	2.02	0.40
1:A:356:ALA:O	1:A:357:PHE:C	2.64	0.40
1:B:234:ASP:CG	1:B:238:VAL:HG21	2.45	0.40
1:B:232:ASN:HB3	1:B:250:HIS:ND1	2.37	0.40
1:B:343:MET:HE2	1:B:343:MET:HB3	2.01	0.40
1:A:354:SER:HB2	1:A:355:CYS:H	1.70	0.40
1:B:73:ASN:HA	1:B:74:PRO:HD2	1.90	0.40
1:C:233:PHE:HA	1:C:251:LEU:O	2.22	0.40
1:A:100:LEU:HD23	1:A:100:LEU:HA	1.84	0.40
1:A:301:TYR:CB	1:A:316:VAL:HG12	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ILE:HD13	1:B:249:GLU:HB3	2.03	0.40
1:A:39:LYS:HE2	1:A:43:GLU:OE1	2.22	0.40
1:A:255:MET:HB2	1:A:282:LEU:HD23	2.02	0.40
1:B:141:GLU:N	1:B:142:PRO:CD	2.85	0.40
1:C:211:GLY:O	3:C:370:SAH:OXT	2.40	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	350/368 (95%)	337 (96%)	10 (3%)	3 (1%)	14	25
1	B	343/368 (93%)	326 (95%)	17 (5%)	0	100	100
1	C	350/368 (95%)	340 (97%)	9 (3%)	1 (0%)	36	53
1	D	342/368 (93%)	333 (97%)	9 (3%)	0	100	100
All	All	1385/1472 (94%)	1336 (96%)	45 (3%)	4 (0%)	36	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	VAL
1	C	255	MET
1	A	328	PRO
1	A	46	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	290/302 (96%)	280 (97%)	10 (3%)	32	57
1	B	288/302 (95%)	274 (95%)	14 (5%)	22	42
1	C	290/302 (96%)	273 (94%)	17 (6%)	18	34
1	D	287/302 (95%)	265 (92%)	22 (8%)	12	23
All	All	1155/1208 (96%)	1092 (94%)	63 (6%)	19	37

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	54	VAL
1	A	59	TYR
1	A	91	SER
1	A	120	LYS
1	A	158	ASN
1	A	177	LYS
1	A	228	ILE
1	A	259	VAL
1	A	282	LEU
1	B	19	GLU
1	B	33	VAL
1	B	45	ASP
1	B	120	LYS
1	B	123	ASP
1	B	158	ASN
1	B	205	THR
1	B	259	VAL
1	B	267	ILE
1	B	280	LEU
1	B	302	ILE
1	B	341	LEU
1	B	358	ASN
1	B	366	LYS
1	C	46	VAL
1	C	57	SER
1	C	64	GLU
1	C	100	LEU
1	C	107	ARG
1	C	108	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	122	GLU
1	C	158	ASN
1	C	165	ILE
1	C	171	THR
1	C	189	ILE
1	C	222	VAL
1	C	228	ILE
1	C	269	TRP
1	C	272	HIS
1	C	273	ASP
1	C	336	LYS
1	D	9	ILE
1	D	14	THR
1	D	16	SER
1	D	17	SER
1	D	52	LYS
1	D	93	VAL
1	D	120	LYS
1	D	122	GLU
1	D	123	ASP
1	D	127	LEU
1	D	164	ASN
1	D	181	LYS
1	D	188	THR
1	D	195	LEU
1	D	251	LEU
1	D	259	VAL
1	D	303	LEU
1	D	310	SER
1	D	316	VAL
1	D	317	ILE
1	D	365	LEU
1	D	366	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	ASN
1	A	169	HIS
1	A	180	ASN
1	A	232	ASN
1	A	237	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	272	HIS
1	A	278	HIS
1	B	121	ASN
1	B	158	ASN
1	B	173	HIS
1	B	180	ASN
1	B	232	ASN
1	B	272	HIS
1	B	278	HIS
1	C	158	ASN
1	C	272	HIS
1	C	278	HIS
1	D	27	GLN
1	D	68	GLN
1	D	158	ASN
1	D	169	HIS
1	D	232	ASN
1	D	272	HIS
1	D	278	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](#)

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	$\# Z > 2$
3	SAH	C	370	-	27,28,28	1.63	5 (18%)	36,40,40	2.20	12 (33%)
2	N7I	B	369	-	13,13,13	0.63	0	16,16,16	2.62	4 (25%)
3	SAH	D	370	-	27,28,28	1.59	5 (18%)	36,40,40	2.10	9 (25%)
3	SAH	A	370	-	27,28,28	1.31	4 (14%)	36,40,40	2.14	12 (33%)
2	N7I	D	369	-	13,13,13	0.62	0	16,16,16	2.62	4 (25%)
2	N7I	C	369	-	13,13,13	0.59	0	16,16,16	1.87	4 (25%)
2	N7I	A	369	-	13,13,13	0.81	0	16,16,16	1.31	2 (12%)
3	SAH	B	370	-	27,28,28	1.41	5 (18%)	36,40,40	2.37	11 (30%)

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
3	SAH	C	370	-	-	2/15/31/31	0/3/3/3
2	N7I	B	369	-	-	2/6/6/6	0/1/1/1
3	SAH	D	370	-	-	3/15/31/31	0/3/3/3
3	SAH	A	370	-	-	6/15/31/31	0/3/3/3
2	N7I	D	369	-	-	2/6/6/6	0/1/1/1
2	N7I	C	369	-	-	1/6/6/6	0/1/1/1
2	N7I	A	369	-	-	4/6/6/6	0/1/1/1
3	SAH	B	370	-	-	3/15/31/31	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	370	SAH	C5-C4	5.18	1.48	1.39
3	D	370	SAH	C5-C4	4.94	1.47	1.39
3	A	370	SAH	C5-C4	4.13	1.46	1.39
3	B	370	SAH	C5-C4	3.55	1.45	1.39
3	B	370	SAH	C5-C6	3.24	1.50	1.41
3	C	370	SAH	C5-C6	3.18	1.49	1.41
3	D	370	SAH	C5-C6	2.74	1.48	1.41
3	D	370	SAH	OXT-C	-2.57	1.22	1.30
3	D	370	SAH	C5-N7	-2.45	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	370	SAH	C5-C6	2.44	1.47	1.41
3	C	370	SAH	C8-N7	2.41	1.36	1.31
3	C	370	SAH	OXT-C	-2.25	1.23	1.30
3	A	370	SAH	OXT-C	-2.24	1.23	1.30
3	B	370	SAH	C8-N7	2.23	1.36	1.31
3	B	370	SAH	C5-N7	-2.17	1.35	1.39
3	B	370	SAH	OXT-C	-2.16	1.23	1.30
3	A	370	SAH	C4-N9	-2.10	1.33	1.37
3	C	370	SAH	O-C	2.05	1.28	1.22
3	D	370	SAH	C4-N9	-2.01	1.33	1.37

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	370	SAH	C5-C4-N3	-6.64	117.58	126.72
3	D	370	SAH	C5-C4-N3	-6.56	117.68	126.72
2	D	369	N7I	O3-C5-C4	6.42	124.17	114.55
2	B	369	N7I	O3-C5-C4	6.39	124.14	114.55
3	C	370	SAH	C5-C4-N3	-6.25	118.11	126.72
2	B	369	N7I	C7-C8-C9	-5.50	113.52	126.99
2	D	369	N7I	C7-C8-C9	-5.47	113.59	126.99
3	B	370	SAH	N3-C4-N9	5.40	136.35	127.17
3	D	370	SAH	N3-C4-N9	5.40	136.34	127.17
3	A	370	SAH	N3-C2-N1	-4.96	121.07	128.58
3	C	370	SAH	N3-C4-N9	4.88	135.47	127.17
3	A	370	SAH	C5-C4-N3	-4.79	120.12	126.72
2	B	369	N7I	O3-C5-C6	-4.72	115.95	124.08
2	D	369	N7I	O3-C5-C6	-4.72	115.95	124.08
3	B	370	SAH	C2-N3-C4	4.71	123.33	111.83
3	A	370	SAH	N3-C4-N9	4.38	134.61	127.17
3	C	370	SAH	O4'-C1'-N9	4.24	116.24	108.09
3	C	370	SAH	C4-C5-N7	-4.01	106.00	110.58
3	B	370	SAH	N3-C2-N1	-3.98	122.55	128.58
3	D	370	SAH	C2-N3-C4	3.84	121.22	111.83
3	A	370	SAH	C2-N3-C4	3.82	121.17	111.83
2	C	369	N7I	C10-C9-C8	-3.79	115.89	124.56
2	C	369	N7I	O3-C5-C4	3.74	120.15	114.55
3	C	370	SAH	C2-N3-C4	3.69	120.84	111.83
2	C	369	N7I	C2-O3-C5	3.61	122.81	117.51
3	A	370	SAH	C4-N9-C8	3.46	109.37	105.74
3	D	370	SAH	C4-C5-N7	-3.20	106.92	110.58
3	B	370	SAH	OXT-C-O	-3.20	116.83	124.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	370	SAH	C2-N1-C6	3.18	123.95	118.73
3	A	370	SAH	OXT-C-O	-3.13	116.98	124.08
3	C	370	SAH	C4-N9-C8	3.07	108.97	105.74
3	B	370	SAH	C4-N9-C8	3.06	108.95	105.74
3	B	370	SAH	O3'-C3'-C4'	-3.04	102.34	111.08
3	B	370	SAH	C4-C5-N7	-3.04	107.11	110.58
3	D	370	SAH	N3-C2-N1	-3.04	123.99	128.58
3	A	370	SAH	CB-CA-C	-3.01	102.46	110.45
3	C	370	SAH	OXT-C-O	-2.93	117.43	124.08
3	D	370	SAH	OXT-C-O	-2.73	117.88	124.08
2	A	369	N7I	C10-C9-C8	-2.73	118.32	124.56
3	C	370	SAH	C5-N7-C8	2.70	107.70	103.45
3	B	370	SAH	O4'-C1'-N9	2.55	112.99	108.09
3	C	370	SAH	N3-C2-N1	-2.50	124.79	128.58
3	B	370	SAH	C5-N7-C8	2.46	107.31	103.45
3	B	370	SAH	N9-C8-N7	-2.40	110.53	113.94
3	D	370	SAH	C4-N9-C8	2.36	108.22	105.74
2	D	369	N7I	C6-C7-C8	-2.35	113.59	120.61
2	B	369	N7I	C6-C7-C8	-2.34	113.61	120.61
3	C	370	SAH	C6-C5-N7	2.28	136.50	132.09
3	A	370	SAH	O3'-C3'-C4'	-2.28	104.54	111.08
2	C	369	N7I	O3-C5-C6	-2.27	120.17	124.08
3	A	370	SAH	O4'-C1'-C2'	-2.26	101.78	106.62
3	D	370	SAH	CB-CA-C	-2.19	104.64	110.45
2	A	369	N7I	C2-O3-C5	2.16	120.68	117.51
3	C	370	SAH	N9-C8-N7	-2.13	110.91	113.94
3	D	370	SAH	C5-N7-C8	2.09	106.74	103.45
3	A	370	SAH	C4-C5-N7	-2.09	108.19	110.58
3	A	370	SAH	C6-C5-N7	2.09	136.12	132.09
3	C	370	SAH	CB-CA-C	-2.05	105.03	110.45

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	370	SAH	C-CA-CB-CG
3	B	370	SAH	N-CA-CB-CG
3	B	370	SAH	C-CA-CB-CG
3	C	370	SAH	N-CA-CB-CG
3	C	370	SAH	C-CA-CB-CG
3	D	370	SAH	N-CA-CB-CG
3	D	370	SAH	C-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	369	N7I	C6-C5-O3-C2
2	A	369	N7I	C4-C5-O3-C2
2	B	369	N7I	C4-C5-O3-C2
2	D	369	N7I	C4-C5-O3-C2
2	A	369	N7I	C1-C7-C8-C9
2	A	369	N7I	C6-C7-C8-C9
3	A	370	SAH	N-CA-CB-CG
2	B	369	N7I	C6-C5-O3-C2
2	D	369	N7I	C6-C5-O3-C2
3	B	370	SAH	CB-CG-SD-C5'
3	D	370	SAH	CB-CG-SD-C5'
3	A	370	SAH	OXT-C-CA-N
3	A	370	SAH	CB-CG-SD-C5'
3	A	370	SAH	CA-CB-CG-SD
2	C	369	N7I	C4-C5-O3-C2
3	A	370	SAH	O-C-CA-N

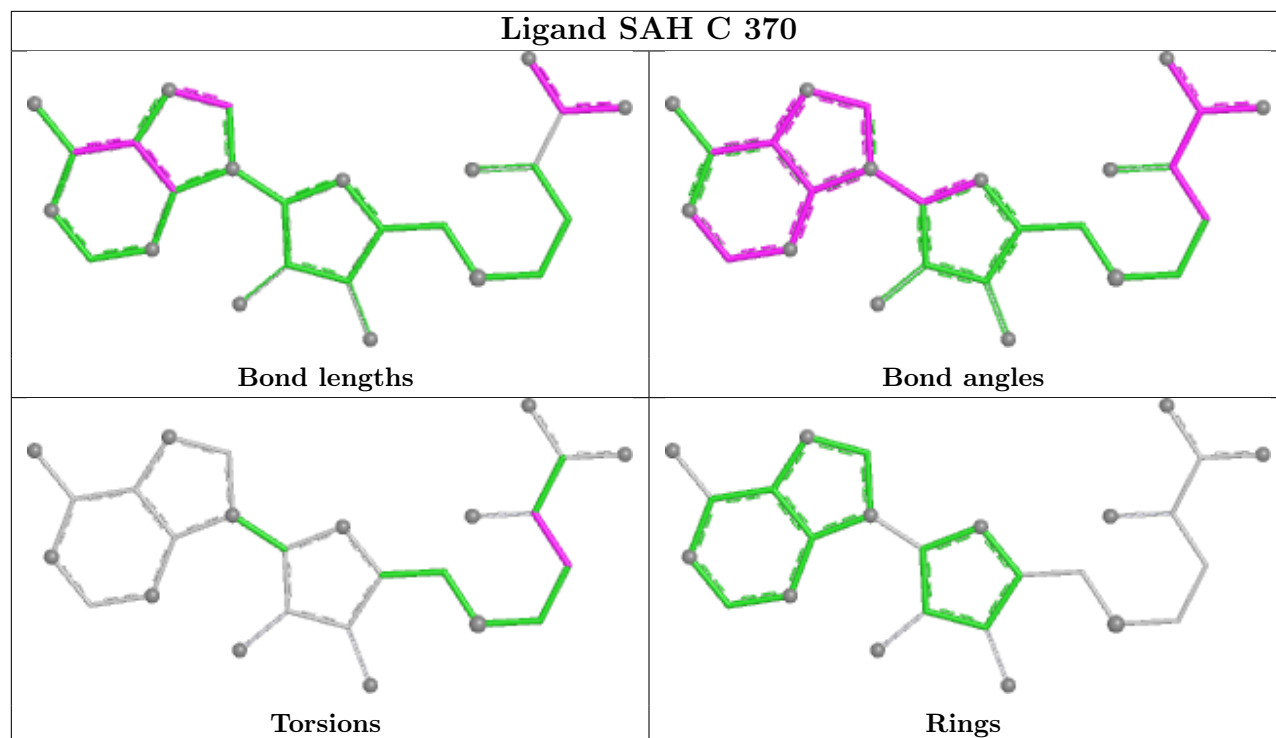
There are no ring outliers.

7 monomers are involved in 42 short contacts:

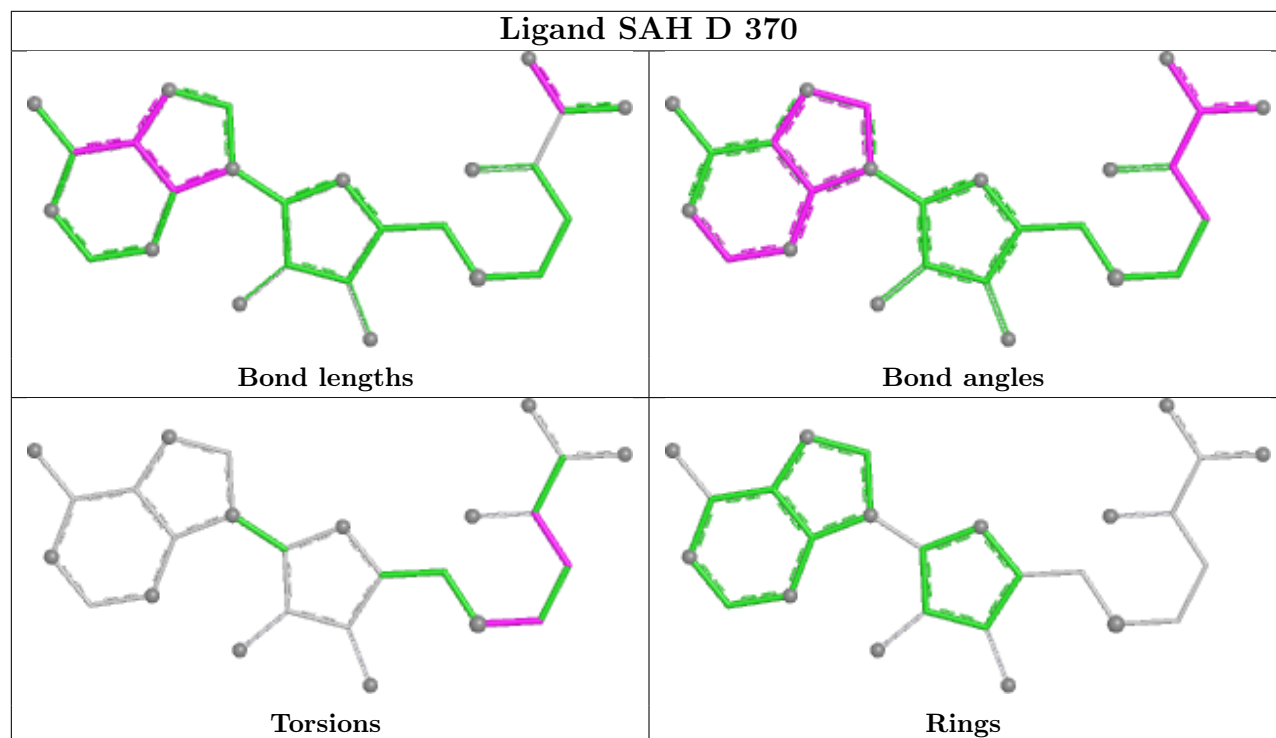
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	370	SAH	5	0
2	B	369	N7I	7	0
3	A	370	SAH	1	0
2	D	369	N7I	7	0
2	C	369	N7I	6	0
2	A	369	N7I	14	0
3	B	370	SAH	2	0

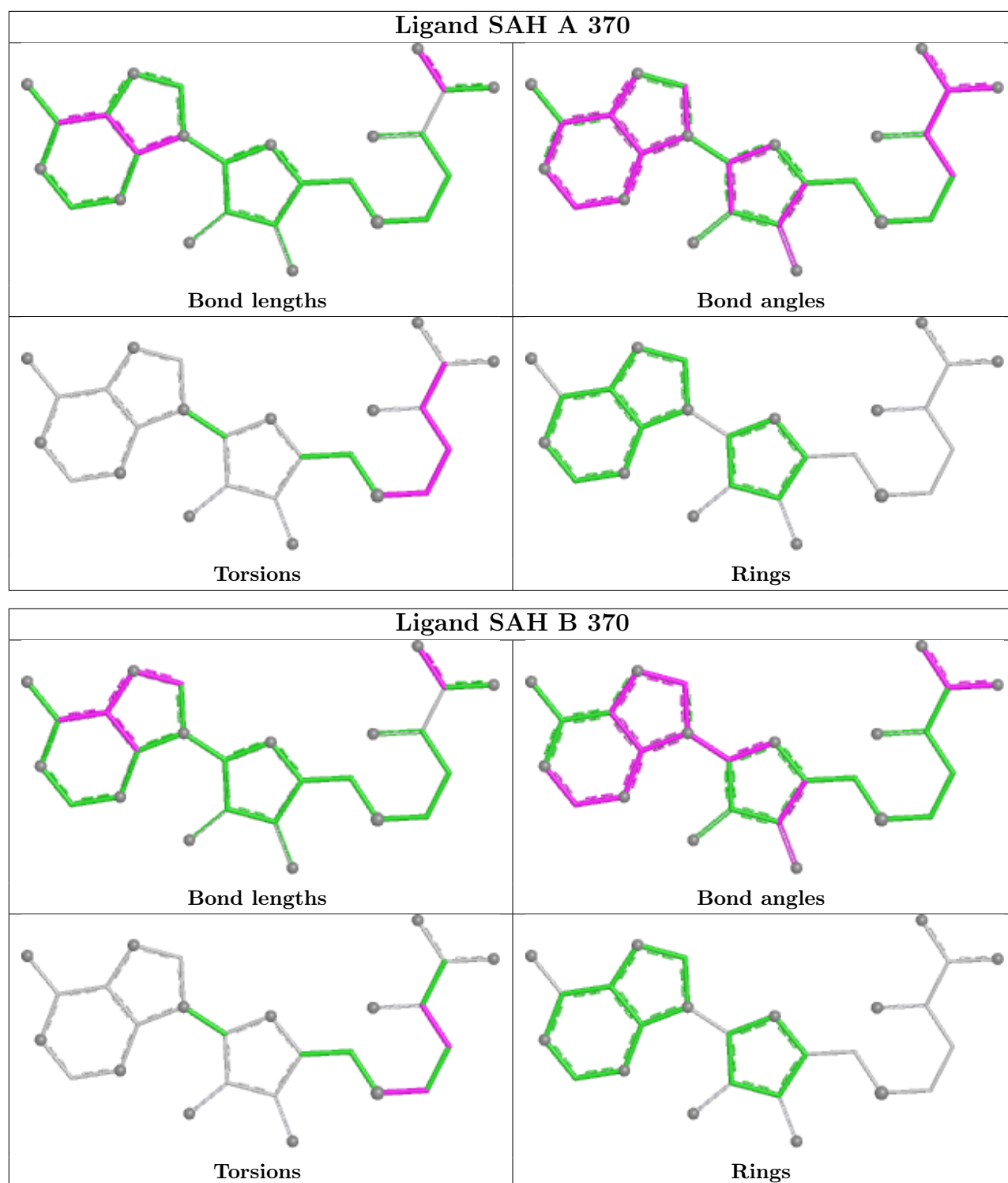
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 D 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	352/368 (95%)	0.07	18 (5%) 33 30	6, 21, 36, 58	0
1	B	349/368 (94%)	0.02	15 (4%) 40 36	6, 19, 36, 48	0
1	C	352/368 (95%)	-0.06	12 (3%) 48 44	9, 18, 34, 45	0
1	D	348/368 (94%)	-0.04	10 (2%) 53 50	7, 20, 34, 48	0
All	All	1401/1472 (95%)	-0.00	55 (3%) 43 39	6, 19, 35, 58	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	TYR	5.4
1	B	122	GLU	5.1
1	C	16	SER	5.0
1	B	121	ASN	4.6
1	A	72	THR	4.6
1	C	121	ASN	4.4
1	B	9	ILE	4.0
1	A	328	PRO	3.9
1	C	273	ASP	3.8
1	A	45	ASP	3.8
1	D	121	ASN	3.8
1	A	55	PRO	3.6
1	C	207	ILE	3.6
1	C	241	ASP	3.6
1	A	327	ASN	3.5
1	B	124	GLY	3.5
1	A	53	SER	3.4
1	A	224	LYS	3.4
1	D	98	ARG	3.4
1	B	10	GLN	3.3
1	D	106	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	271	CYS	3.2
1	A	329	GLY	3.2
1	D	292	ASP	3.1
1	D	122	GLU	3.0
1	C	72	THR	2.9
1	C	173	HIS	2.8
1	D	173	HIS	2.8
1	C	17	SER	2.7
1	C	272	HIS	2.7
1	D	60	ILE	2.7
1	A	17	SER	2.7
1	A	272	HIS	2.6
1	B	173	HIS	2.6
1	B	358	ASN	2.5
1	A	57	SER	2.5
1	B	54	VAL	2.4
1	B	17	SER	2.4
1	A	56	PRO	2.4
1	A	16	SER	2.4
1	B	123	ASP	2.4
1	D	18	ASP	2.4
1	B	227	SER	2.3
1	A	141	GLU	2.3
1	C	274	TRP	2.2
1	A	122	GLU	2.2
1	B	120	LYS	2.2
1	B	240	GLN	2.2
1	A	60	ILE	2.2
1	A	30	SER	2.2
1	B	269	TRP	2.2
1	C	367	THR	2.1
1	B	15	HIS	2.1
1	D	15	HIS	2.1
1	D	123	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

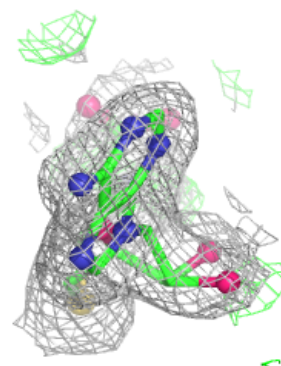
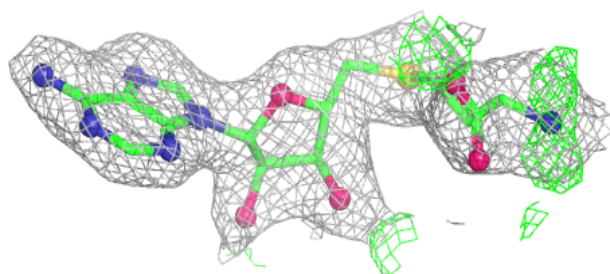
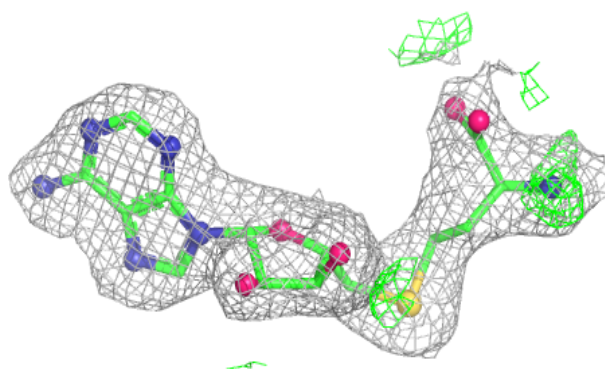
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	N7I	D	369	13/13	0.55	0.31	78,79,80,80	0
2	N7I	B	369	13/13	0.63	0.28	78,79,80,80	0
2	N7I	C	369	13/13	0.65	0.29	67,70,72,73	0
2	N7I	A	369	13/13	0.71	0.27	52,59,61,62	0
3	SAH	A	370	26/26	0.89	0.10	10,18,27,29	0
3	SAH	B	370	26/26	0.92	0.10	11,15,32,34	0
3	SAH	D	370	26/26	0.93	0.09	16,20,30,32	0
3	SAH	C	370	26/26	0.94	0.08	5,12,22,25	0

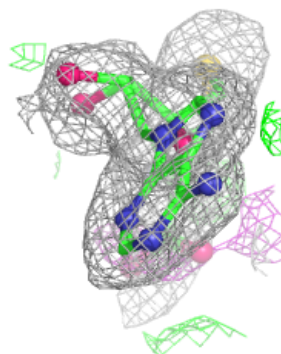
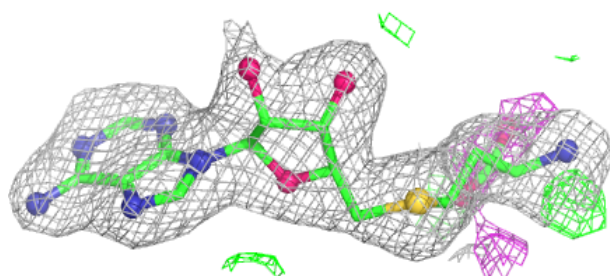
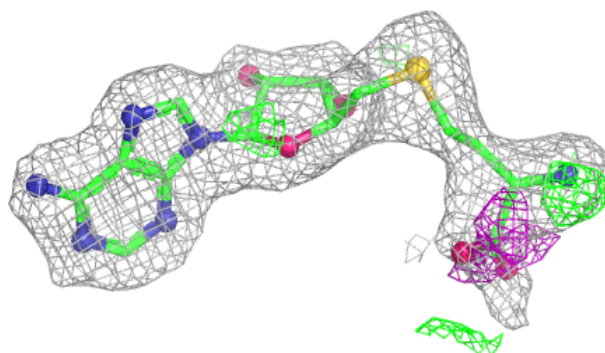
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SAH A 370:

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

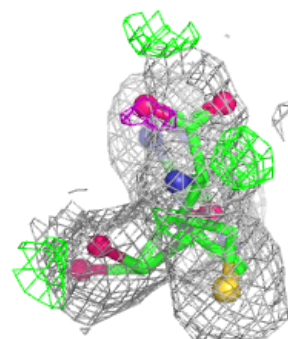
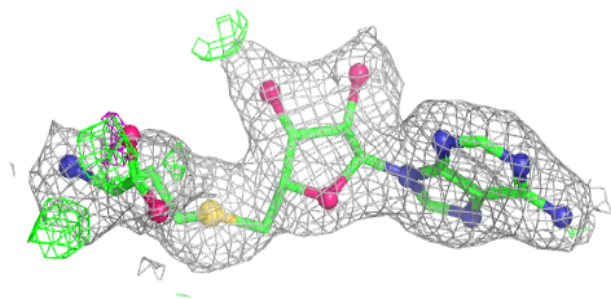
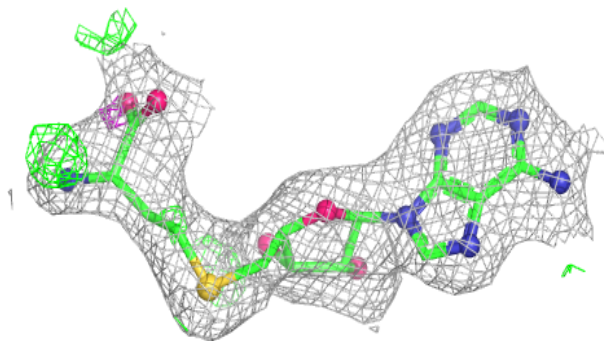
**Electron density around SAH B 370:**

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

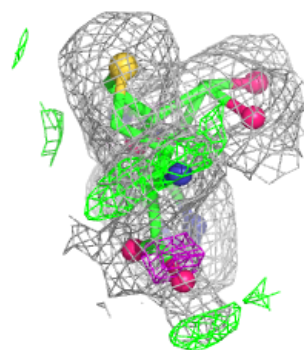
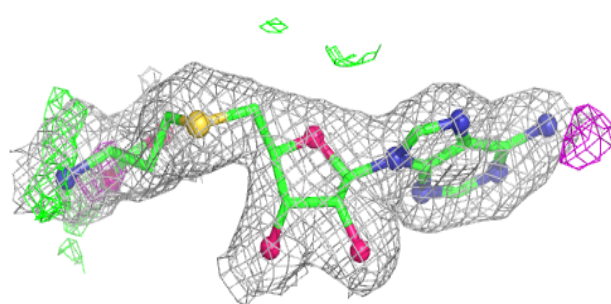
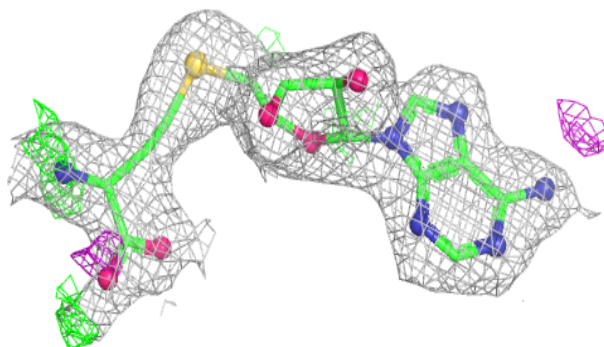


Electron density around SAH D 370:

$2mF_o-DF_c$ (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.