



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:15 PM UTC

PDB ID : 3I53 / pdb_00003i53
Title : Crystal structure of an O-methyltransferase (NcsB1) from neocarzinostatin biosynthesis in complex with S-adenosyl-L-homocysteine (SAH)
Authors : Cooke, H.A.; Bruner, S.D.
Deposited on : 2009-07-03
Resolution : 2.08 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)
Xtrriage (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

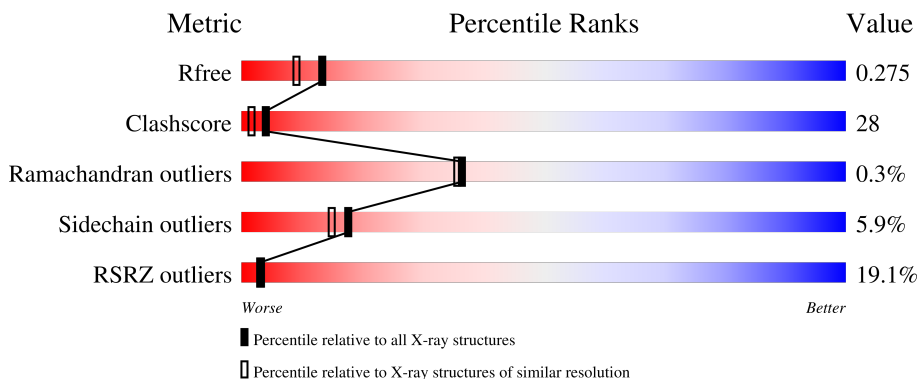
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	332	
1	B	332	



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 6 3 3	0	0

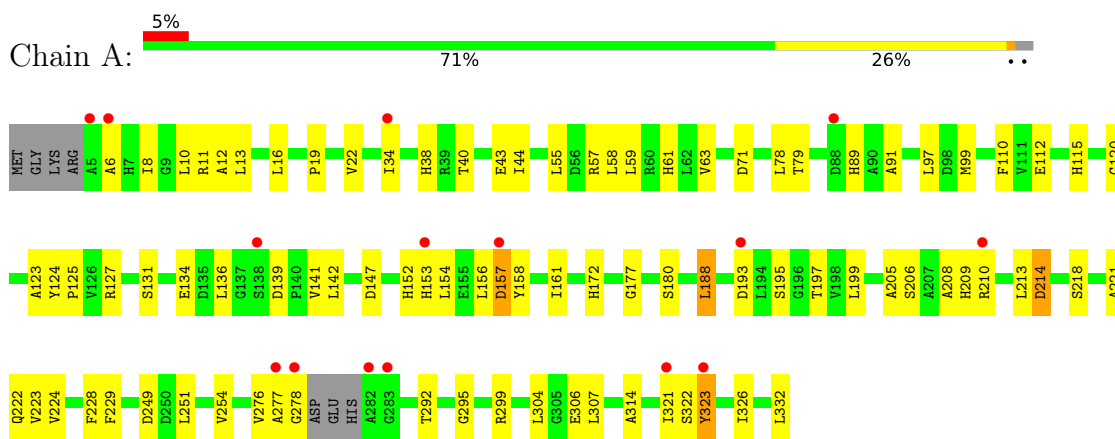
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	188	Total O 188 188	0	0
4	B	117	Total O 117 117	0	0

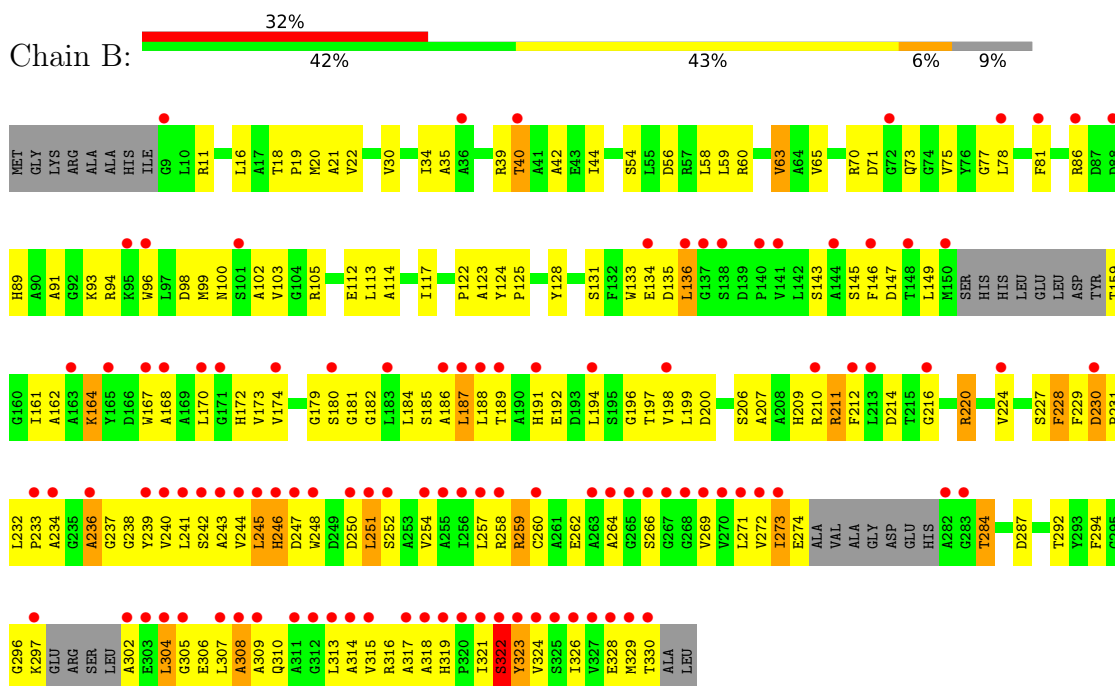
3 Residue-property plots [i](#)

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

- Molecule 1: O-methyltransferase



- Molecule 1: O-methyltransferase



4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	91.25Å 161.57Å 98.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.08 25.00 – 2.08	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.08) 93.7 (25.00-2.08)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.84 (at 2.08Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.272 0.242 , 0.275	Depositor DCC
R_{free} test set	2201 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.825	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.027 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4935	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/2424	0.90	7/3291 (0.2%)
1	B	0.40	0/2232	0.97	9/3029 (0.3%)
All	All	0.42	0/4656	0.94	16/6320 (0.3%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	284	THR	N-CA-C	-7.56	102.39	111.69
1	B	266	SER	CB-CA-C	-7.36	99.77	111.48
1	A	295	GLY	N-CA-C	-6.54	105.00	115.08
1	B	307	LEU	N-CA-C	-6.46	104.50	112.38
1	B	63	VAL	N-CA-C	-6.37	104.55	110.53
1	B	236	ALA	N-CA-C	6.33	119.66	110.42
1	B	236	ALA	CB-CA-C	-6.11	101.21	109.71
1	A	63	VAL	N-CA-C	-6.09	104.56	110.72
1	A	79	THR	N-CA-C	-5.87	102.08	110.59
1	A	177	GLY	N-CA-C	-5.82	103.92	114.46
1	B	128	TYR	N-CA-C	5.53	120.02	113.28
1	A	229	PHE	N-CA-C	-5.38	106.71	113.28
1	B	322	SER	CB-CA-C	-5.37	110.37	116.54
1	A	214	ASP	N-CA-C	5.30	116.75	111.07
1	B	308	ALA	N-CA-C	-5.10	105.42	111.69
1	A	323	TYR	N-CA-C	-5.08	106.59	112.89

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2379	0	2344	73	0
1	B	2193	0	2149	189	0
2	A	26	0	19	0	0
2	B	26	0	19	4	0
3	B	6	0	8	0	0
4	A	188	0	0	7	0
4	B	117	0	0	6	0
All	All	4935	0	4539	255	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 28.

All (255) 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:34:ILE:HD11	1:A:78:LEU:HG	1.30	1.13
1:B:164:LYS:HG2	1:B:321:ILE:HG22	1.24	1.13
1:B:164:LYS:HG2	1:B:321:ILE:CG2	1.87	1.05
1:B:316:ARG:HG3	1:B:330:THR:HG22	1.41	1.01
1:B:241:LEU:HD13	1:B:245:LEU:HD11	1.44	0.99
1:B:131:SER:OG	1:B:134:GLU:HG2	1.66	0.95
1:B:241:LEU:HD11	1:B:272:VAL:HG22	1.51	0.93
1:B:304:LEU:H	1:B:304:LEU:HD12	1.34	0.92
1:B:245:LEU:HD22	1:B:245:LEU:H	1.32	0.92
1:B:162:ALA:HA	1:B:167:TRP:HE1	1.38	0.89
1:A:11:ARG:HG2	1:A:11:ARG:HH11	1.38	0.88
1:B:257:LEU:HD13	1:B:308:ALA:HB1	1.57	0.86
1:B:322:SER:OG	1:B:323:TYR:N	1.99	0.86
1:A:161:ILE:HD11	1:A:326:ILE:HD11	1.59	0.85
1:B:254:VAL:HA	1:B:257:LEU:HD12	1.59	0.82
1:A:197:THR:HG22	1:A:222:GLN:HG2	1.64	0.80
1:A:34:ILE:HD11	1:A:78:LEU:CG	2.10	0.80
1:A:40:THR:HG23	1:A:43:GLU:H	1.46	0.80
1:B:245:LEU:HD22	1:B:245:LEU:N	1.96	0.80
1:B:246:HIS:HA	1:B:297:LYS:HE2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:GLY:H	1:B:211:ARG:NH2	1.79	0.79
1:B:309:ALA:HA	1:B:313:LEU:O	1.85	0.75
1:B:241:LEU:HD12	1:B:241:LEU:O	1.87	0.74
1:B:168:ALA:HA	1:B:194:LEU:HD21	1.70	0.74
1:B:309:ALA:HB2	1:B:315:VAL:HG23	1.69	0.74
1:A:34:ILE:HA	1:A:38:HIS:O	1.86	0.74
1:B:322:SER:OG	1:B:323:TYR:CD2	2.40	0.73
1:B:305:GLY:O	1:B:308:ALA:HB3	1.90	0.72
1:B:316:ARG:CG	1:B:330:THR:HG22	2.19	0.71
1:B:162:ALA:HA	1:B:167:TRP:NE1	2.06	0.70
1:B:174:VAL:HG23	1:B:236:ALA:HB2	1.74	0.70
1:B:241:LEU:CD1	1:B:245:LEU:HD11	2.20	0.70
1:B:245:LEU:H	1:B:245:LEU:CD2	2.02	0.69
1:B:304:LEU:HD12	1:B:304:LEU:N	2.08	0.69
1:B:321:ILE:HG12	1:B:324:VAL:O	1.93	0.69
1:B:11:ARG:HG3	1:B:11:ARG:HH11	1.57	0.69
1:B:39:ARG:NH1	1:B:77:GLY:HA2	2.09	0.68
1:B:273:ILE:HD12	1:B:273:ILE:N	2.09	0.68
1:B:182:GLY:HA3	4:B:575:HOH:O	1.93	0.68
1:B:96:TRP:HA	1:B:103:VAL:CG2	2.25	0.67
1:B:321:ILE:HG13	1:B:321:ILE:O	1.93	0.67
1:B:184:LEU:HD11	1:B:196:GLY:HA3	1.78	0.66
1:A:206:SER:O	1:A:210:ARG:HG3	1.96	0.65
1:A:147:ASP:HB2	4:A:773:HOH:O	1.97	0.64
1:B:96:TRP:CD1	1:B:149:LEU:HD11	2.32	0.64
1:B:321:ILE:CG1	1:B:324:VAL:O	2.46	0.64
1:B:60:ARG:HH21	1:B:70:ARG:NH2	1.95	0.64
1:B:185:SER:O	1:B:189:THR:HG23	1.98	0.64
1:B:123:ALA:HB3	1:B:292:THR:HG23	1.79	0.64
1:B:248:TRP:HB3	1:B:252:SER:HB2	1.80	0.63
1:B:248:TRP:HB3	1:B:252:SER:CB	2.27	0.63
1:A:172:HIS:NE2	1:A:197:THR:HG23	2.12	0.63
1:B:102:ALA:CB	1:B:146:PHE:HB2	2.28	0.63
1:B:304:LEU:H	1:B:304:LEU:CD1	2.10	0.63
1:B:234:ALA:HA	1:B:239:TYR:OH	1.99	0.62
1:B:245:LEU:HD23	1:B:274:GLU:OE2	1.98	0.62
1:A:154:LEU:O	1:A:158:TYR:HB2	1.99	0.62
1:A:314:ALA:HB2	1:A:332:LEU:HD13	1.81	0.62
1:B:230:ASP:HB2	1:B:231:PRO:HD2	1.82	0.62
1:A:61:HIS:ND1	1:B:284:THR:HG23	2.15	0.61
1:B:18:THR:O	1:B:22:VAL:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:LEU:HD13	1:B:143:SER:HA	1.83	0.61
1:B:329:MET:O	1:B:330:THR:HB	1.99	0.61
1:B:316:ARG:HG3	1:B:330:THR:CG2	2.24	0.61
1:B:246:HIS:HD2	1:B:247:ASP:H	1.46	0.61
1:A:6:ALA:HB3	4:A:776:HOH:O	2.00	0.61
1:B:172:HIS:CE1	1:B:197:THR:HG23	2.36	0.60
1:A:40:THR:HG22	1:A:43:GLU:CG	2.32	0.60
1:B:174:VAL:HG23	1:B:236:ALA:CB	2.32	0.60
1:A:136:LEU:HD22	1:A:142:LEU:HB3	1.83	0.60
1:B:315:VAL:O	1:B:316:ARG:HD3	2.03	0.59
1:A:34:ILE:CD1	1:A:78:LEU:HG	2.20	0.59
1:B:242:SER:O	1:B:244:VAL:HG23	2.03	0.59
1:B:164:LYS:HB2	1:B:164:LYS:NZ	2.18	0.59
1:B:39:ARG:HH12	1:B:77:GLY:HA2	1.67	0.59
1:A:40:THR:CG2	1:A:43:GLU:H	2.16	0.58
1:A:306:GLU:HB2	4:A:678:HOH:O	2.02	0.58
1:B:240:VAL:HG13	1:B:273:ILE:HD13	1.84	0.58
1:B:251:LEU:C	1:B:251:LEU:HD23	2.29	0.58
1:A:40:THR:HG22	1:A:43:GLU:CD	2.28	0.58
1:B:317:ALA:HB3	1:B:328:GLU:HG2	1.86	0.58
1:B:34:ILE:HG21	1:B:78:LEU:HD13	1.85	0.57
1:B:71:ASP:OD1	1:B:73:GLN:HB3	2.05	0.57
1:B:71:ASP:OD2	1:B:75:VAL:HB	2.05	0.57
1:B:241:LEU:HD12	1:B:272:VAL:HA	1.86	0.57
1:B:230:ASP:HB2	1:B:231:PRO:CD	2.35	0.56
1:B:269:VAL:HG12	1:B:330:THR:HB	1.86	0.56
1:B:161:ILE:HG13	1:B:326:ILE:HD11	1.88	0.56
1:B:164:LYS:CG	1:B:321:ILE:HG22	2.17	0.56
1:A:11:ARG:HG2	1:A:11:ARG:NH1	2.15	0.56
1:B:210:ARG:HG3	1:B:211:ARG:N	2.21	0.55
1:B:60:ARG:HH21	1:B:70:ARG:CZ	2.19	0.55
1:B:257:LEU:HD13	1:B:308:ALA:CB	2.33	0.55
1:B:309:ALA:HB1	1:B:314:ALA:HA	1.88	0.55
1:B:269:VAL:O	1:B:271:LEU:HD22	2.06	0.55
1:B:56:ASP:O	1:B:60:ARG:HG3	2.07	0.55
1:B:182:GLY:H	1:B:211:ARG:CZ	2.19	0.55
1:B:251:LEU:O	1:B:254:VAL:HG22	2.07	0.55
1:A:251:LEU:O	1:A:254:VAL:HG22	2.07	0.55
1:B:242:SER:O	2:B:401:SAH:HA	2.07	0.54
1:B:105:ARG:HH12	1:B:135:ASP:CG	2.15	0.54
1:B:172:HIS:NE2	1:B:197:THR:HG23	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ALA:HB1	1:B:93:LYS:HE3	1.91	0.53
1:A:205:ALA:HB1	1:A:223:VAL:CG1	2.39	0.53
1:B:16:LEU:C	1:B:19:PRO:HD2	2.34	0.53
1:B:162:ALA:C	1:B:164:LYS:H	2.16	0.53
1:A:99:MET:HE1	1:B:114:ALA:HB2	1.90	0.53
1:B:302:ALA:C	1:B:304:LEU:N	2.63	0.53
1:A:199:LEU:C	1:A:199:LEU:HD13	2.34	0.52
1:B:131:SER:HG	1:B:134:GLU:HG2	1.73	0.52
1:B:136:LEU:CD1	1:B:143:SER:HA	2.37	0.52
1:B:199:LEU:HD23	1:B:224:VAL:HG23	1.92	0.52
1:B:304:LEU:HD23	4:B:748:HOH:O	2.09	0.52
1:B:241:LEU:O	1:B:241:LEU:CD1	2.57	0.52
1:B:96:TRP:NE1	1:B:149:LEU:HD11	2.24	0.52
1:A:89:HIS:HD2	1:A:91:ALA:HB3	1.75	0.52
1:B:302:ALA:C	1:B:304:LEU:H	2.17	0.52
1:A:152:HIS:O	1:A:156:LEU:HG	2.10	0.52
1:B:122:PRO:HG3	1:B:294:PHE:O	2.10	0.52
1:B:322:SER:OG	1:B:323:TYR:CG	2.64	0.51
1:B:192:GLU:HA	1:B:220:ARG:NH2	2.26	0.51
1:B:21:ALA:HA	1:B:58:LEU:HD11	1.94	0.50
1:A:199:LEU:HD22	1:A:224:VAL:O	2.12	0.50
1:A:115:HIS:HD2	4:A:741:HOH:O	1.94	0.50
1:B:168:ALA:HA	1:B:194:LEU:CD2	2.40	0.50
1:A:89:HIS:CD2	1:A:91:ALA:H	2.29	0.49
1:A:205:ALA:HB1	1:A:223:VAL:HG11	1.94	0.49
1:B:162:ALA:HB2	1:B:187:LEU:HD12	1.94	0.49
1:A:10:LEU:HD23	1:B:93:LYS:CB	2.42	0.49
1:B:271:LEU:HD22	1:B:271:LEU:N	2.28	0.49
1:A:58:LEU:C	1:A:58:LEU:HD23	2.37	0.49
1:B:168:ALA:CA	1:B:194:LEU:HD21	2.41	0.49
1:B:145:SER:O	1:B:149:LEU:HB2	2.13	0.48
1:A:299:ARG:NE	1:A:307:LEU:HD11	2.28	0.48
1:A:8:ILE:HG22	1:A:12:ALA:HB3	1.94	0.48
1:A:16:LEU:C	1:A:19:PRO:HD2	2.37	0.48
1:A:222:GLN:HA	4:A:534:HOH:O	2.13	0.48
1:B:251:LEU:C	1:B:251:LEU:CD2	2.86	0.48
1:B:191:HIS:O	1:B:220:ARG:NH2	2.47	0.48
1:B:35:ALA:HB2	1:B:86:ARG:HE	1.78	0.48
1:B:30:VAL:HG11	1:B:59:LEU:HD21	1.96	0.47
1:A:34:ILE:HG22	1:A:44:ILE:HD11	1.96	0.47
1:B:96:TRP:HA	1:B:103:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:SAH:HB1	2:B:401:SAH:H4'	1.97	0.47
1:B:191:HIS:HB2	1:B:194:LEU:HD12	1.95	0.47
1:B:321:ILE:HG13	1:B:324:VAL:O	2.15	0.47
1:A:124:TYR:HB3	1:A:125:PRO:HD3	1.96	0.47
1:B:258:ARG:HG2	1:B:262:GLU:OE1	2.15	0.47
1:B:220:ARG:HD3	4:B:529:HOH:O	2.15	0.47
1:A:276:VAL:O	1:A:278:GLY:N	2.48	0.46
1:B:245:LEU:HG	1:B:272:VAL:HG13	1.96	0.46
1:B:102:ALA:HB1	1:B:146:PHE:HB2	1.97	0.46
1:A:13:LEU:HD21	1:B:65:VAL:CG1	2.44	0.46
1:B:59:LEU:O	1:B:63:VAL:HG23	2.15	0.46
1:B:214:ASP:C	1:B:216:GLY:H	2.22	0.46
1:B:164:LYS:HB2	1:B:164:LYS:HZ3	1.80	0.46
1:B:73:GLN:HA	4:B:602:HOH:O	2.15	0.46
1:A:89:HIS:CD2	1:A:91:ALA:HB3	2.50	0.46
1:A:157:ASP:C	1:A:158:TYR:HD1	2.24	0.46
1:A:276:VAL:C	1:A:278:GLY:N	2.73	0.46
1:A:323:TYR:N	1:A:323:TYR:CD2	2.84	0.46
1:B:11:ARG:HH11	1:B:11:ARG:CG	2.24	0.46
1:B:122:PRO:HG3	1:B:294:PHE:C	2.41	0.46
1:A:110:PHE:CD2	1:A:292:THR:HG21	2.51	0.45
1:B:244:VAL:O	1:B:248:TRP:HD1	1.99	0.45
1:B:167:TRP:HZ3	1:B:240:VAL:HG21	1.82	0.45
1:B:246:HIS:O	1:B:296:GLY:HA3	2.15	0.45
1:B:159:THR:C	1:B:161:ILE:N	2.74	0.45
1:B:199:LEU:HD13	1:B:199:LEU:C	2.41	0.45
1:B:246:HIS:HD2	1:B:247:ASP:N	2.14	0.45
1:B:241:LEU:CD1	1:B:272:VAL:HA	2.47	0.45
1:B:309:ALA:CB	1:B:314:ALA:HA	2.46	0.45
1:B:246:HIS:CD2	1:B:247:ASP:H	2.31	0.45
1:B:251:LEU:O	1:B:252:SER:C	2.58	0.45
1:B:181:GLY:HA3	1:B:211:ARG:NE	2.31	0.45
1:B:317:ALA:HB3	1:B:328:GLU:CG	2.47	0.45
1:B:260:CYS:O	1:B:264:ALA:N	2.50	0.44
1:B:159:THR:C	1:B:161:ILE:H	2.25	0.44
1:B:167:TRP:C	1:B:194:LEU:HD11	2.42	0.44
1:B:246:HIS:CA	1:B:297:LYS:HE2	2.41	0.44
1:B:297:LYS:HD2	4:B:748:HOH:O	2.16	0.44
1:B:167:TRP:CZ3	1:B:240:VAL:HG21	2.52	0.44
1:A:161:ILE:HD13	1:A:321:ILE:HD12	1.99	0.44
1:A:120:GLY:HA2	1:B:54:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:ILE:N	1:B:273:ILE:CD1	2.78	0.44
1:B:318:ALA:O	1:B:319:HIS:ND1	2.47	0.44
1:B:98:ASP:OD2	1:B:100:ASN:HB2	2.18	0.44
1:B:168:ALA:N	1:B:194:LEU:HD11	2.33	0.44
1:A:34:ILE:HD11	1:A:78:LEU:CD2	2.48	0.44
1:B:179:GLY:N	1:B:200:ASP:OD2	2.48	0.44
1:B:186:ALA:HA	1:B:189:THR:OG1	2.18	0.44
1:B:244:VAL:H	1:B:245:LEU:HD22	1.82	0.44
1:A:34:ILE:HG22	1:A:44:ILE:CD1	2.48	0.43
1:B:206:SER:O	1:B:209:HIS:HB3	2.18	0.43
1:A:161:ILE:CD1	1:A:326:ILE:HD11	2.40	0.43
1:A:71:ASP:OD2	1:A:71:ASP:C	2.61	0.43
1:A:136:LEU:CD2	1:A:142:LEU:HB3	2.48	0.43
1:B:232:LEU:HG	1:B:233:PRO:HD2	2.00	0.43
1:B:20:MET:HE1	1:B:99:MET:HE2	2.00	0.43
1:B:246:HIS:CB	1:B:297:LYS:HG2	2.49	0.43
1:B:184:LEU:HD23	1:B:198:VAL:HG23	2.01	0.43
1:B:188:LEU:HD22	1:B:194:LEU:O	2.18	0.43
1:A:172:HIS:CE1	1:A:197:THR:HG23	2.52	0.43
1:A:222:GLN:HB2	4:A:725:HOH:O	2.18	0.43
1:B:243:ALA:HB3	2:B:401:SAH:HG1	2.00	0.43
1:B:243:ALA:HB3	2:B:401:SAH:N	2.33	0.43
1:B:269:VAL:O	1:B:269:VAL:HG23	2.19	0.43
1:B:89:HIS:HD2	1:B:91:ALA:HB3	1.83	0.43
1:B:112:GLU:HB2	1:B:123:ALA:HB1	2.01	0.43
1:B:246:HIS:CD2	1:B:247:ASP:N	2.87	0.43
1:A:57:ARG:HD2	1:B:287:ASP:OD2	2.19	0.42
1:A:251:LEU:C	1:A:251:LEU:HD13	2.44	0.42
1:B:228:PHE:HE2	1:B:229:PHE:CE2	2.37	0.42
1:B:259:ARG:HG3	1:B:259:ARG:HH11	1.84	0.42
1:A:188:LEU:CD2	1:A:221:ALA:HB2	2.49	0.42
1:B:207:ALA:O	1:B:210:ARG:HG2	2.20	0.42
1:B:250:ASP:O	1:B:251:LEU:C	2.61	0.42
1:A:131:SER:OG	1:A:134:GLU:HG2	2.19	0.42
1:A:11:ARG:NH1	1:B:96:TRP:CD2	2.88	0.42
1:A:139:ASP:OD1	1:A:141:VAL:N	2.51	0.42
1:B:259:ARG:HG3	1:B:259:ARG:NH1	2.34	0.42
1:B:241:LEU:HD13	1:B:245:LEU:CD1	2.32	0.42
1:A:209:HIS:CE1	1:A:213:LEU:HD11	2.55	0.42
1:A:276:VAL:C	1:A:278:GLY:H	2.27	0.42
1:B:316:ARG:HE	1:B:330:THR:CG2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:LEU:O	1:B:117:ILE:HG12	2.20	0.41
1:B:133:TRP:HA	1:B:133:TRP:CE3	2.55	0.41
1:B:105:ARG:NH1	1:B:124:TYR:OH	2.54	0.41
1:B:187:LEU:HD12	1:B:187:LEU:HA	1.87	0.41
1:B:170:LEU:HD22	1:B:237:GLY:O	2.20	0.41
1:A:6:ALA:HB1	1:B:81:PHE:CE2	2.56	0.41
1:B:40:THR:HG22	1:B:42:ALA:N	2.35	0.41
1:B:180:SER:O	1:B:181:GLY:C	2.61	0.41
1:B:306:GLU:O	1:B:310:GLN:N	2.50	0.41
1:A:11:ARG:NH1	1:A:11:ARG:CG	2.79	0.41
1:A:172:HIS:HA	1:A:195:SER:O	2.21	0.41
1:B:71:ASP:OD1	1:B:71:ASP:C	2.63	0.41
1:B:173:VAL:HG23	1:B:238:GLY:O	2.21	0.41
1:A:249:ASP:OD1	1:A:251:LEU:HB3	2.20	0.41
1:B:71:ASP:C	1:B:73:GLN:H	2.29	0.41
1:B:124:TYR:HB3	1:B:125:PRO:HD3	2.03	0.41
1:B:227:SER:O	1:B:230:ASP:OD1	2.39	0.41
1:B:40:THR:O	1:B:44:ILE:HG13	2.21	0.41
1:B:184:LEU:HD23	1:B:212:PHE:CZ	2.56	0.41
1:A:180:SER:O	1:A:208:ALA:HA	2.21	0.40
1:A:323:TYR:H	1:A:323:TYR:HD2	1.68	0.40
1:B:89:HIS:CD2	1:B:91:ALA:HB3	2.57	0.40
1:B:273:ILE:HG22	1:B:274:GLU:N	2.36	0.40
1:A:55:LEU:O	1:A:59:LEU:HG	2.20	0.40
1:A:22:VAL:HG12	1:A:97:LEU:HD23	2.03	0.40
1:A:127:ARG:HG3	4:A:523:HOH:O	2.21	0.40
1:A:112:GLU:HB2	1:A:123:ALA:HB1	2.03	0.40
1:B:236:ALA:HA	4:B:676:HOH:O	2.21	0.40
1:B:302:ALA:O	1:B:304:LEU:N	2.53	0.40
1:B:89:HIS:CD2	1:B:91:ALA:H	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	321/332 (97%)	313 (98%)	6 (2%)	2 (1%)	21	17
1	B	295/332 (89%)	262 (89%)	33 (11%)	0	100	100
All	All	616/664 (93%)	575 (93%)	39 (6%)	2 (0%)	36	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	SER
1	A	277	ALA

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	231/237 (98%)	223 (96%)	8 (4%)	32	33
1	B	210/237 (89%)	192 (91%)	18 (9%)	10	6
All	All	441/474 (93%)	415 (94%)	26 (6%)	18	15

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	A	157	ASP
1	A	188	LEU
1	A	193	ASP
1	A	214	ASP
1	A	218	SER
1	A	228	PHE
1	A	304	LEU
1	B	40	THR
1	B	94	ARG
1	B	136	LEU

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Mol	Chain	Res	Type
1	B	147	ASP
1	B	164	LYS
1	B	187	LEU
1	B	211	ARG
1	B	220	ARG
1	B	228	PHE
1	B	230	ASP
1	B	245	LEU
1	B	246	HIS
1	B	251	LEU
1	B	259	ARG
1	B	273	ILE
1	B	304	LEU
1	B	322	SER
1	B	323	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	89	HIS
1	A	115	HIS
1	A	152	HIS
1	A	209	HIS
1	B	51	HIS
1	B	73	GLN
1	B	89	HIS
1	B	115	HIS
1	B	121	GLN
1	B	246	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	402	-	5,5,5	0.34	0	5,5,5	0.28	0
2	SAH	A	401	-	27,28,28	1.02	3 (11%)	36,40,40	1.92	9 (25%)
2	SAH	B	401	-	27,28,28	1.03	3 (11%)	36,40,40	1.92	10 (27%)

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	GOL	B	402	-	-	0/4/4/4	-
2	SAH	A	401	-	-	1/15/31/31	0/3/3/3
2	SAH	B	401	-	-	4/15/31/31	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	SAH	C5-N7	-3.13	1.33	1.39
2	A	401	SAH	C5-N7	-3.06	1.33	1.39
2	B	401	SAH	C8-N9	-2.29	1.33	1.37
2	A	401	SAH	C8-N9	-2.25	1.33	1.37
2	B	401	SAH	C4-N9	-2.11	1.33	1.37
2	A	401	SAH	C4-N9	-2.08	1.33	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	SAH	C5-C4-N3	-5.27	119.46	126.72
2	B	401	SAH	C5-C4-N3	-5.11	119.68	126.72
2	A	401	SAH	N3-C2-N1	-4.65	121.54	128.58
2	B	401	SAH	N3-C2-N1	-4.56	121.67	128.58
2	B	401	SAH	N3-C4-N9	3.67	133.41	127.17
2	A	401	SAH	C2-N3-C4	3.61	120.66	111.83
2	A	401	SAH	N3-C4-N9	3.53	133.18	127.17
2	B	401	SAH	C2-N3-C4	3.50	120.37	111.83
2	A	401	SAH	N9-C8-N7	-3.16	109.45	113.94
2	B	401	SAH	N9-C8-N7	-3.15	109.47	113.94
2	A	401	SAH	C4-C5-N7	-2.99	107.16	110.58
2	A	401	SAH	C5-N7-C8	2.94	108.07	103.45
2	B	401	SAH	C5-N7-C8	2.84	107.91	103.45
2	B	401	SAH	C4-C5-N7	-2.72	107.47	110.58
2	B	401	SAH	C4-N9-C8	2.38	108.24	105.74
2	B	401	SAH	C5'-C4'-C3'	-2.21	109.54	115.06
2	B	401	SAH	O4'-C1'-C2'	-2.15	102.01	106.62
2	A	401	SAH	C4-N9-C8	2.15	107.99	105.74
2	A	401	SAH	O4'-C1'-C2'	-2.13	102.06	106.62

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	SAH	O-C-CA-N
2	B	401	SAH	OXT-C-CA-N
2	B	401	SAH	O-C-CA-CB
2	B	401	SAH	OXT-C-CA-CB
2	A	401	SAH	C4'-C5'-SD-CG

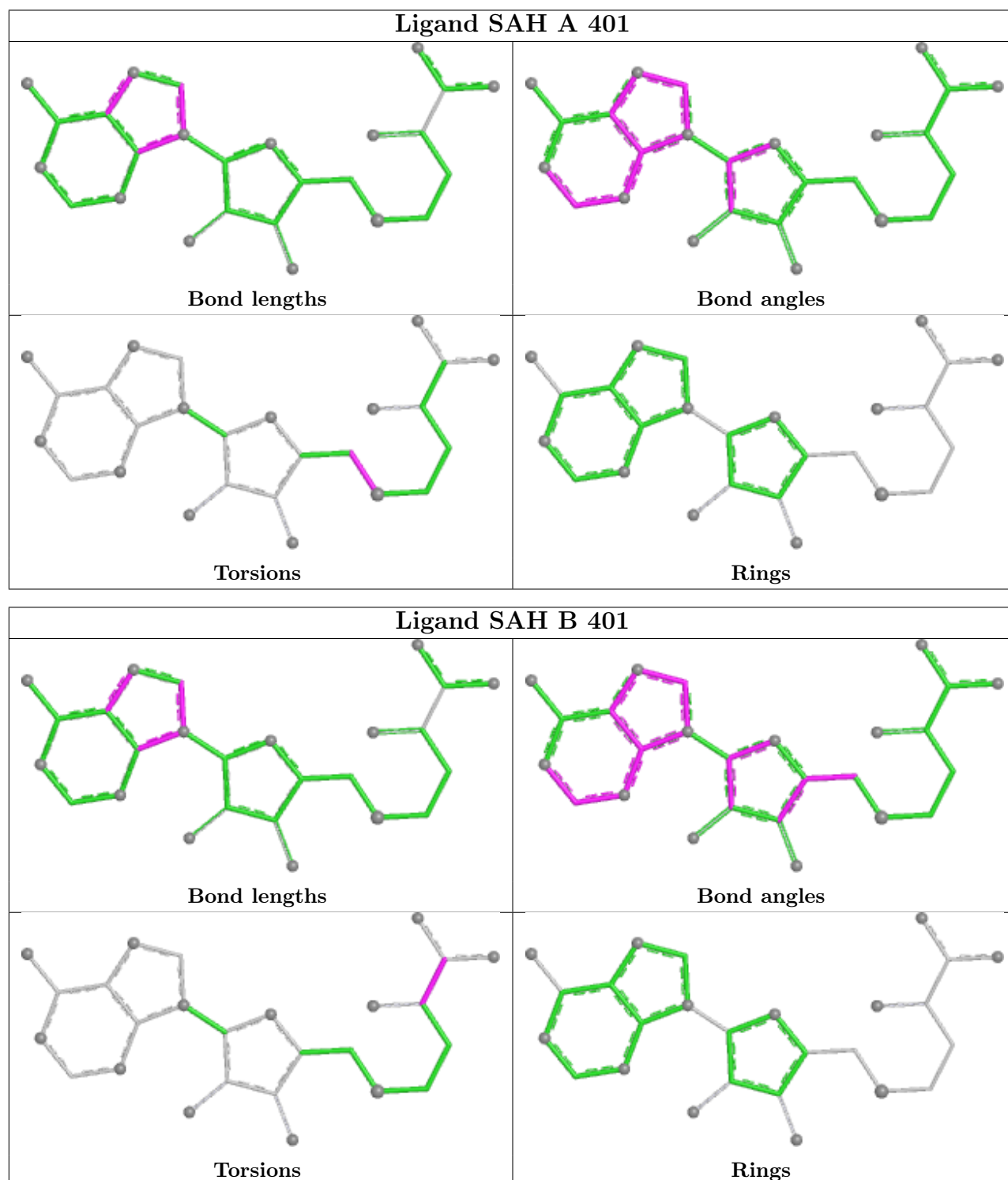
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	SAH	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	325/332 (97%)	0.39	15 (4%) 37 39	25, 37, 53, 72	0
1	B	303/332 (91%)	1.51	105 (34%) 1 1	27, 53, 83, 89	0
All	All	628/664 (94%)	0.93	120 (19%) 3 3	25, 42, 75, 89	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	313	LEU	6.8
1	B	251	LEU	5.5
1	B	304	LEU	5.5
1	B	266	SER	5.1
1	B	315	VAL	5.1
1	B	322	SER	4.9
1	B	321	ILE	4.8
1	B	9	GLY	4.7
1	B	183	LEU	4.7
1	B	234	ALA	4.6
1	A	210	ARG	4.5
1	B	194	LEU	4.4
1	B	323	TYR	4.4
1	B	318	ALA	4.3
1	B	317	ALA	4.2
1	B	163	ALA	4.2
1	B	268	GLY	4.1
1	B	324	VAL	4.1
1	B	330	THR	4.1
1	B	267	GLY	4.0
1	B	327	VAL	3.9
1	B	240	VAL	3.8
1	B	326	ILE	3.8
1	B	312	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	254	VAL	3.7
1	A	277	ALA	3.7
1	B	171	GLY	3.6
1	B	269	VAL	3.5
1	B	308	ALA	3.5
1	B	311	ALA	3.5
1	B	264	ALA	3.5
1	B	309	ALA	3.4
1	B	329	MET	3.4
1	B	303	GLU	3.4
1	B	265	GLY	3.3
1	B	282	ALA	3.3
1	B	188	LEU	3.2
1	B	212	PHE	3.2
1	B	302	ALA	3.2
1	B	148	THR	3.2
1	B	244	VAL	3.1
1	B	96	TRP	3.1
1	B	245	LEU	3.1
1	B	307	LEU	3.1
1	B	136	LEU	3.1
1	B	150	MET	3.1
1	B	305	GLY	3.0
1	B	319	HIS	3.0
1	A	5	ALA	3.0
1	B	243	ALA	3.0
1	B	216	GLY	3.0
1	A	278	GLY	2.9
1	B	252	SER	2.9
1	B	170	LEU	2.9
1	B	241	LEU	2.9
1	B	191	HIS	2.9
1	B	255	ALA	2.9
1	B	146	PHE	2.8
1	B	272	VAL	2.8
1	B	273	ILE	2.8
1	B	246	HIS	2.7
1	B	210	ARG	2.7
1	B	137	GLY	2.7
1	B	36	ALA	2.7
1	A	157	ASP	2.7
1	B	230	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	193	ASP	2.6
1	B	325	SER	2.6
1	B	40	THR	2.6
1	B	144	ALA	2.6
1	B	213	LEU	2.6
1	A	282	ALA	2.5
1	B	256	ILE	2.5
1	B	250	ASP	2.5
1	B	236	ALA	2.5
1	B	72	GLY	2.5
1	B	283	GLY	2.5
1	B	134	GLU	2.4
1	B	328	GLU	2.4
1	B	248	TRP	2.4
1	A	323	TYR	2.4
1	A	6	ALA	2.4
1	A	153	HIS	2.4
1	B	186	ALA	2.4
1	B	86	ARG	2.4
1	B	270	VAL	2.4
1	A	88	ASP	2.3
1	A	34	ILE	2.3
1	A	138	SER	2.3
1	B	101	SER	2.3
1	B	189	THR	2.3
1	B	242	SER	2.3
1	B	224	VAL	2.3
1	B	320	PRO	2.3
1	B	239	TYR	2.2
1	A	283	GLY	2.2
1	B	271	LEU	2.2
1	B	165	TYR	2.2
1	B	81	PHE	2.2
1	B	168	ALA	2.2
1	B	141	VAL	2.1
1	B	174	VAL	2.1
1	B	263	ALA	2.1
1	B	314	ALA	2.1
1	B	187	LEU	2.1
1	B	138	SER	2.1
1	B	95	LYS	2.1
1	B	233	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	167	TRP	2.1
1	B	198	VAL	2.1
1	B	260	CYS	2.1
1	B	88	ASP	2.1
1	B	140	PRO	2.1
1	A	321	ILE	2.1
1	B	257	LEU	2.0
1	B	247	ASP	2.0
1	B	180	SER	2.0
1	B	78	LEU	2.0
1	B	258	ARG	2.0
1	B	297	LYS	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](#)

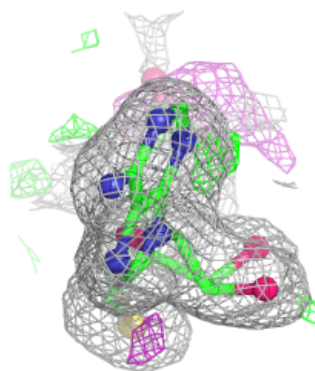
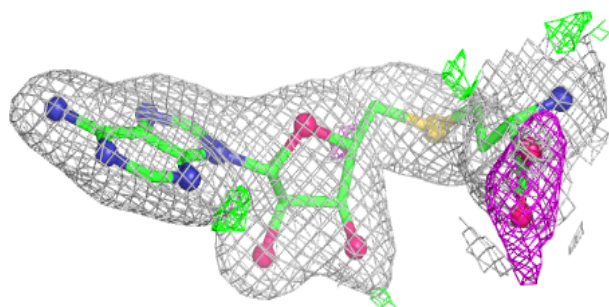
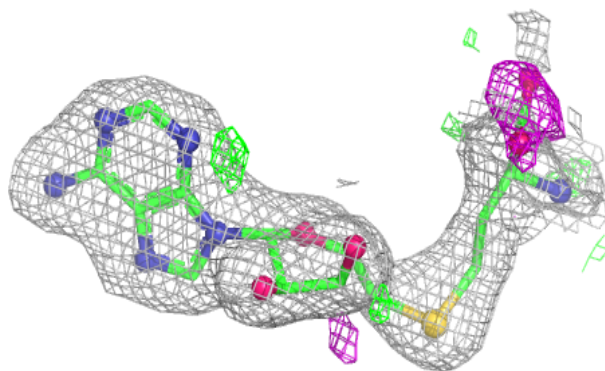
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GOL	B	402	6/6	0.61	0.16	69,72,73,73	0
2	SAH	B	401	26/26	0.88	0.12	34,37,59,61	0
2	SAH	A	401	26/26	0.94	0.08	22,28,34,38	0

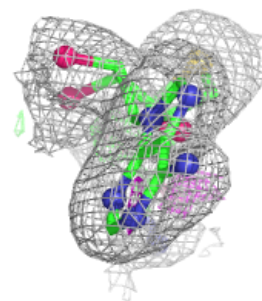
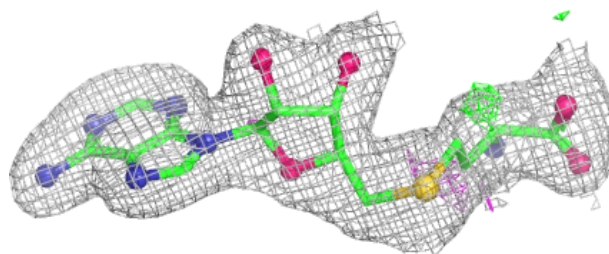
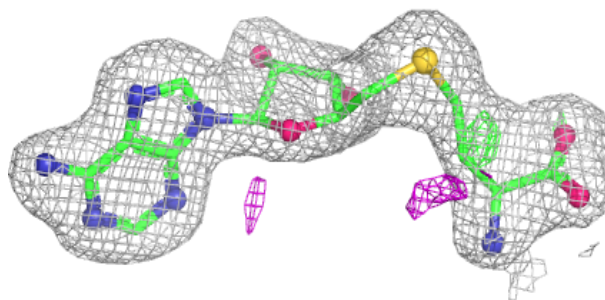
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH B 401:

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

**Electron density around SAH A 401:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.