



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 5, 2024 – 01:23 am GMT

PDB ID : 5ARF
Title : SMYD2 in complex with small molecule inhibitor compound-2
Authors : Hillig, R.C.; Badock, V.; Barak, N.; Stellfeld, T.; Eggert, E.; ter Laak, A.; Weiske, J.; Christ, C.D.; Koehr, S.; Stoeckigt, D.; Mowat, J.; Mueller, T.; Fernandez-Montalvan, A.E.; Hartung, I.V.; Stresemann, C.; Brumby, T.; Weinmann, H.
Deposited on : 2015-09-24
Resolution : 1.92 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

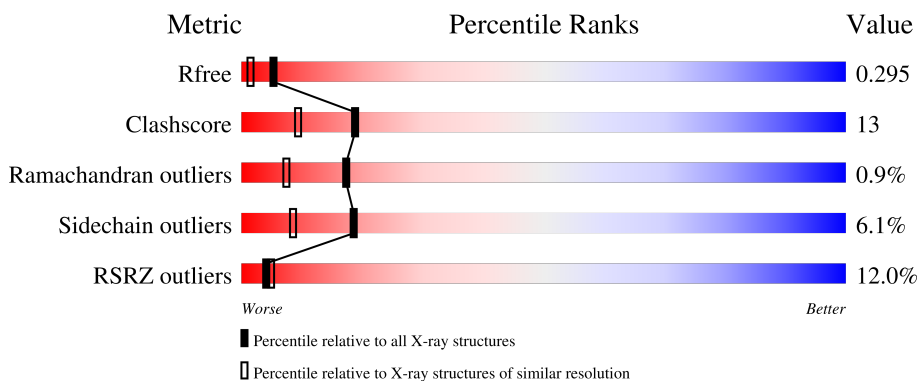
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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}	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	433	

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	SAM	A	1002	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3610 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.

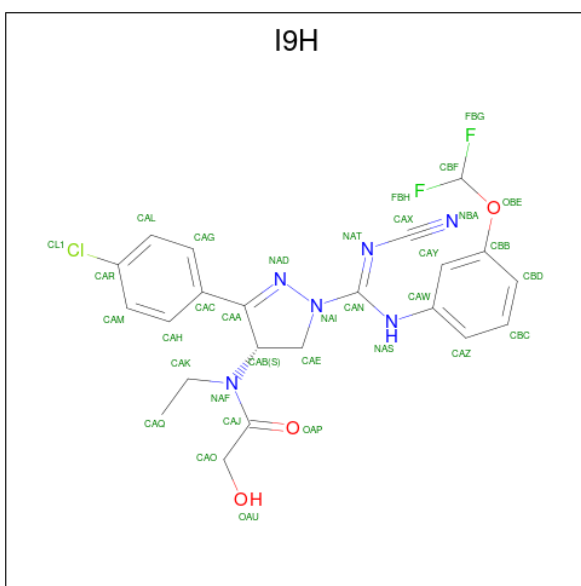
- Molecule 1 is a protein called N-LYSINE METHYLTRANSFERASE SMYD2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	425	3419	2171	584	634	30	0	0	0

There is a discrepancy between the modelled and reference sequences:

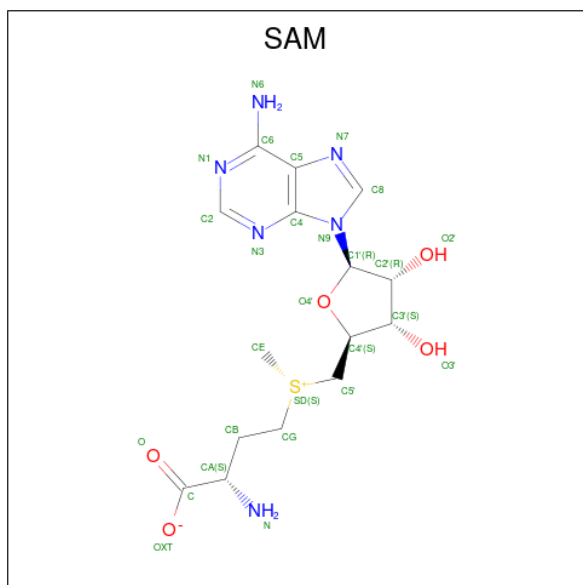
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q9NRG4

- Molecule 2 is N-[3-(4-CHLOROPHENYL)-1-{N'-CYANO-N-[3-(DIFLUOROMETHOXY)PHENYL]CARBAMIMIDOYL}-4,5-DIHYDRO-1H-PYRAZOL-4-YL]-N-ETHYL-2-HYDROXYACETAMIDE (three-letter code: I9H) (formula: C₂₂H₂₁ClF₂N₆O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	F	N			O
2	A	1	34	22	1	2	6	3	0	0

- Molecule 3 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C₁₅H₂₂N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Zn	0	0
			3	3		

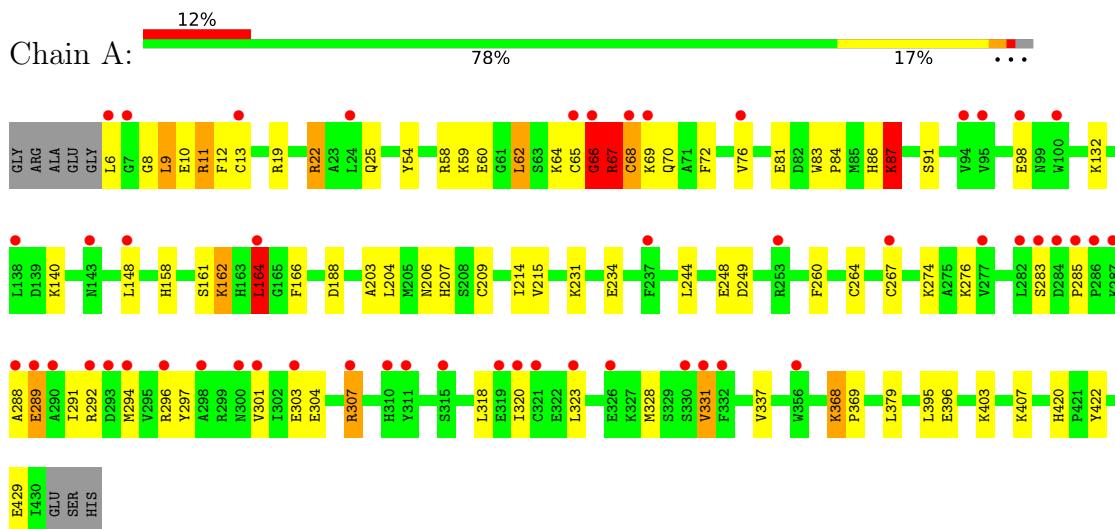
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	127	Total	O	0	0
			127	127		

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: N-LYSINE METHYLTRANSFERASE SMYD2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	130.49Å 51.76Å 69.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.59 – 1.92 47.59 – 1.92	Depositor EDS
% Data completeness (in resolution range)	97.9 (47.59-1.92) 98.0 (47.59-1.92)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 1.92Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.257 , 0.301 0.250 , 0.295	Depositor DCC
R_{free} test set	1808 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtrriage
Anisotropy	0.345	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3610	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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: SAM, I9H, ZN

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	0.83	3/3497 (0.1%)	0.92	7/4714 (0.1%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	267	CYS	CA-CB	7.83	1.71	1.53
1	A	267	CYS	CB-SG	7.73	1.95	1.82
1	A	267	CYS	CA-C	7.00	1.71	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	CYS	CB-CA-C	9.31	129.02	110.40
1	A	267	CYS	CA-CB-SG	7.94	128.28	114.00
1	A	164	LEU	CB-CG-CD1	-6.41	100.11	111.00
1	A	67	ARG	CA-CB-CG	5.50	125.51	113.40
1	A	164	LEU	CB-CG-CD2	5.17	119.79	111.00
1	A	87	LYS	CD-CE-NZ	5.16	123.56	111.70
1	A	188	ASP	CB-CG-OD1	5.11	122.90	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	66	GLY	Peptide

5.2 Too-close contacts [i](#)

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	3419	0	3368	87	1
2	A	34	0	0	1	0
3	A	27	0	22	13	0
4	A	3	0	0	1	0
5	A	127	0	0	19	0
All	All	3610	0	3390	89	1

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 13.

All (89) 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:164:LEU:HD11	1:A:166:PHE:CE1	1.98	0.99
1:A:206:ASN:HD22	3:A:1002:SAM:C8	1.79	0.95
1:A:206:ASN:HD21	3:A:1002:SAM:HN2	1.01	0.92
3:A:1002:SAM:O4'	3:A:1002:SAM:HA	1.73	0.88
1:A:19:ARG:O	3:A:1002:SAM:N	2.06	0.88
1:A:420:HIS:HD2	1:A:422:TYR:H	1.22	0.85
1:A:65:CYS:O	1:A:66:GLY:O	1.96	0.84
1:A:164:LEU:HD12	1:A:164:LEU:C	1.97	0.83
1:A:76:VAL:HA	5:A:2026:HOH:O	1.82	0.79
1:A:206:ASN:HD22	3:A:1002:SAM:H8	1.47	0.79
1:A:206:ASN:ND2	3:A:1002:SAM:C8	2.46	0.78
1:A:66:GLY:HA3	1:A:67:ARG:HG2	1.66	0.78
1:A:283:SER:HA	5:A:2093:HOH:O	1.88	0.72
1:A:68:CYS:SG	4:A:1005:ZN:ZN	1.79	0.70
1:A:203:ALA:O	3:A:1002:SAM:HE1	1.93	0.69
1:A:84:PRO:O	1:A:87:LYS:HE2	1.93	0.68
1:A:234:GLU:HG2	5:A:2077:HOH:O	1.95	0.67
1:A:368:LYS:HB2	1:A:369:PRO:HD3	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LYS:HA	1:A:231:LYS:HE2	1.77	0.64
1:A:209:CYS:HB2	1:A:264:CYS:SG	2.38	0.63
1:A:54:TYR:CZ	1:A:81:GLU:HB3	2.34	0.62
1:A:206:ASN:HB3	3:A:1002:SAM:N7	2.14	0.62
1:A:68:CYS:SG	1:A:86:HIS:NE2	2.72	0.61
1:A:368:LYS:NZ	1:A:368:LYS:HB3	2.15	0.61
1:A:162:LYS:CG	5:A:2045:HOH:O	2.48	0.61
1:A:234:GLU:CG	5:A:2077:HOH:O	2.49	0.59
1:A:162:LYS:CD	5:A:2045:HOH:O	2.52	0.58
1:A:396:GLU:HB3	5:A:2114:HOH:O	2.02	0.58
1:A:66:GLY:HA3	1:A:67:ARG:CG	2.34	0.56
1:A:59:LYS:HB2	1:A:62:LEU:HD13	1.88	0.56
1:A:303:GLU:HA	1:A:303:GLU:OE1	2.08	0.54
1:A:66:GLY:O	1:A:69:LYS:HG2	2.09	0.53
1:A:285:PRO:HB3	5:A:2092:HOH:O	2.07	0.53
1:A:214:ILE:HD11	1:A:379:LEU:HG	1.91	0.53
1:A:11:ARG:HB3	1:A:204:LEU:HD21	1.90	0.52
1:A:64:LYS:HE2	1:A:72:PHE:CZ	2.45	0.52
1:A:66:GLY:CA	1:A:67:ARG:HG2	2.36	0.51
1:A:161:SER:HB3	1:A:166:PHE:HE2	1.75	0.51
1:A:54:TYR:CE1	1:A:81:GLU:HB3	2.45	0.51
1:A:83:TRP:O	1:A:87:LYS:HG2	2.10	0.50
1:A:276:LYS:HD2	5:A:2088:HOH:O	2.11	0.50
1:A:158:HIS:ND1	5:A:2043:HOH:O	2.35	0.50
1:A:368:LYS:HB3	1:A:368:LYS:HZ3	1.76	0.50
1:A:294:MET:HG2	1:A:331:VAL:HG23	1.94	0.50
1:A:12:PHE:CE1	1:A:22:ARG:HB3	2.48	0.49
1:A:84:PRO:O	1:A:87:LYS:CE	2.60	0.49
1:A:206:ASN:ND2	3:A:1002:SAM:HN2	1.86	0.49
1:A:274:LYS:N	5:A:2090:HOH:O	2.46	0.49
1:A:66:GLY:HA3	1:A:67:ARG:CB	2.44	0.48
1:A:164:LEU:CD1	1:A:166:PHE:CE1	2.86	0.47
1:A:429:GLU:O	5:A:2125:HOH:O	2.20	0.47
1:A:65:CYS:SG	1:A:67:ARG:HG3	2.54	0.47
1:A:288:ALA:O	1:A:289:GLU:CB	2.63	0.47
1:A:244:LEU:HD21	1:A:337:VAL:HG13	1.96	0.46
2:A:1001:I9H:CAX	2:A:1001:I9H:CAW	2.93	0.46
1:A:207:HIS:HB3	1:A:260:PHE:HZ	1.80	0.46
1:A:292:ARG:NE	1:A:296:ARG:HH12	2.13	0.46
1:A:59:LYS:HB2	1:A:62:LEU:CD1	2.45	0.46
1:A:162:LYS:HD2	5:A:2045:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:VAL:CA	5:A:2026:HOH:O	2.53	0.45
1:A:368:LYS:HG3	5:A:2101:HOH:O	2.16	0.45
1:A:291:ILE:HG13	1:A:292:ARG:N	2.32	0.45
1:A:6:LEU:HA	1:A:9:LEU:HD12	1.98	0.44
1:A:76:VAL:N	5:A:2026:HOH:O	2.50	0.43
1:A:288:ALA:O	1:A:289:GLU:CG	2.67	0.43
1:A:231:LYS:HE2	1:A:231:LYS:CA	2.46	0.43
1:A:291:ILE:CG1	1:A:292:ARG:N	2.82	0.43
1:A:294:MET:HG2	1:A:331:VAL:CG2	2.49	0.43
1:A:294:MET:SD	1:A:328:MET:HA	2.58	0.43
1:A:8:GLY:C	1:A:9:LEU:HG	2.38	0.43
1:A:162:LYS:CB	5:A:2045:HOH:O	2.66	0.43
1:A:214:ILE:HD12	5:A:2069:HOH:O	2.19	0.42
1:A:132:LYS:HB3	1:A:132:LYS:HE3	1.83	0.42
1:A:70:GLN:HE21	1:A:70:GLN:HB2	1.70	0.42
1:A:83:TRP:CZ2	1:A:87:LYS:HB3	2.54	0.42
1:A:164:LEU:C	1:A:164:LEU:CD1	2.80	0.42
1:A:206:ASN:CB	3:A:1002:SAM:N7	2.79	0.42
1:A:206:ASN:HA	3:A:1002:SAM:H8	2.01	0.42
1:A:244:LEU:CD2	1:A:337:VAL:HG13	2.50	0.42
1:A:10:GLU:OE2	1:A:22:ARG:NE	2.51	0.41
1:A:297:TYR:O	1:A:301:VAL:HG23	2.20	0.41
1:A:303:GLU:O	1:A:307:ARG:CZ	2.69	0.41
1:A:203:ALA:O	3:A:1002:SAM:CE	2.63	0.41
1:A:206:ASN:HA	3:A:1002:SAM:C8	2.51	0.40
1:A:214:ILE:HG13	1:A:215:VAL:N	2.35	0.40
1:A:304:GLU:O	1:A:307:ARG:HG2	2.22	0.40
1:A:207:HIS:HB3	1:A:260:PHE:CZ	2.56	0.40
1:A:395:LEU:HD23	1:A:395:LEU:N	2.36	0.40
1:A:403:LYS:CE	5:A:2118:HOH:O	2.69	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLU:O	1:A:161:SER:O[2_555]	2.17	0.03

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	423/433 (98%)	404 (96%)	15 (4%)	4 (1%)	17 7

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	GLY
1	A	67	ARG
1	A	289	GLU
1	A	148	LEU

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	375/380 (99%)	352 (94%)	23 (6%)	18 8

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	11	ARG
1	A	13	CYS
1	A	22	ARG
1	A	25	GLN
1	A	58	ARG
1	A	62	LEU

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Mol	Chain	Res	Type
1	A	68	CYS
1	A	87	LYS
1	A	91	SER
1	A	98	GLU
1	A	140	LYS
1	A	162	LYS
1	A	164	LEU
1	A	248	GLU
1	A	249	ASP
1	A	307	ARG
1	A	318	LEU
1	A	320	ILE
1	A	323	LEU
1	A	331	VAL
1	A	368	LYS
1	A	407	LYS

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	70	GLN
1	A	79	GLN
1	A	150	GLN
1	A	169	ASN
1	A	182	ASN
1	A	206	ASN
1	A	251	ASN
1	A	397	HIS
1	A	416	HIS
1	A	420	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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	SAM	A	1002	-	24,29,29	1.91	6 (25%)	23,42,42	2.02	6 (26%)
2	I9H	A	1001	-	35,36,36	2.60	11 (31%)	37,49,49	1.62	9 (24%)

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	SAM	A	1002	-	-	6/12/33/33	0/3/3/3
2	I9H	A	1001	-	-	1/27/43/43	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	I9H	CAB-NAF	6.43	1.54	1.46
2	A	1001	I9H	CAC-CAA	-6.41	1.38	1.48
2	A	1001	I9H	NAI-NAD	-6.35	1.26	1.36
2	A	1001	I9H	CAO-CAJ	5.58	1.57	1.52
3	A	1002	SAM	O2'-C2'	4.97	1.54	1.43
2	A	1001	I9H	CAA-NAD	3.50	1.34	1.29
2	A	1001	I9H	CAE-CAB	-3.35	1.48	1.54
3	A	1002	SAM	O3'-C3'	3.33	1.50	1.43
3	A	1002	SAM	C5-C4	3.07	1.49	1.40
2	A	1001	I9H	CAW-NAS	-3.04	1.35	1.41
2	A	1001	I9H	CAX-NAT	2.74	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	SAM	O4'-C1'	2.69	1.44	1.41
2	A	1001	I9H	CAL-CAR	2.65	1.43	1.38
3	A	1002	SAM	C5'-C4'	2.53	1.60	1.53
3	A	1002	SAM	C8-N7	2.39	1.39	1.34
2	A	1001	I9H	OBE-CBF	2.33	1.49	1.36
2	A	1001	I9H	CAR-CL1	-2.02	1.70	1.74

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	SAM	CG-SD-C5'	5.03	116.22	103.40
3	A	1002	SAM	N3-C2-N1	-4.72	121.30	128.68
2	A	1001	I9H	CAC-CAA-NAD	4.21	127.21	120.59
2	A	1001	I9H	CAB-CAA-NAD	-3.33	107.61	115.20
3	A	1002	SAM	C2-N1-C6	3.31	124.41	118.75
2	A	1001	I9H	CAA-NAD-NAI	2.98	112.46	108.55
2	A	1001	I9H	CAM-CAR-CL1	2.86	123.82	119.35
2	A	1001	I9H	CAG-CAC-CAA	-2.61	117.66	120.75
2	A	1001	I9H	CAH-CAC-CAA	2.58	123.82	120.75
2	A	1001	I9H	CAL-CAR-CL1	-2.46	115.51	119.35
3	A	1002	SAM	O4'-C1'-C2'	-2.43	103.38	106.93
3	A	1002	SAM	O2'-C2'-C3'	2.16	118.82	111.82
3	A	1002	SAM	O4'-C4'-C5'	2.10	114.19	108.88
2	A	1001	I9H	CAG-CAL-CAR	-2.09	117.04	119.24
2	A	1001	I9H	CAL-CAG-CAC	2.01	123.11	120.78

There are no chirality outliers.

All (7) torsion outliers are listed below:

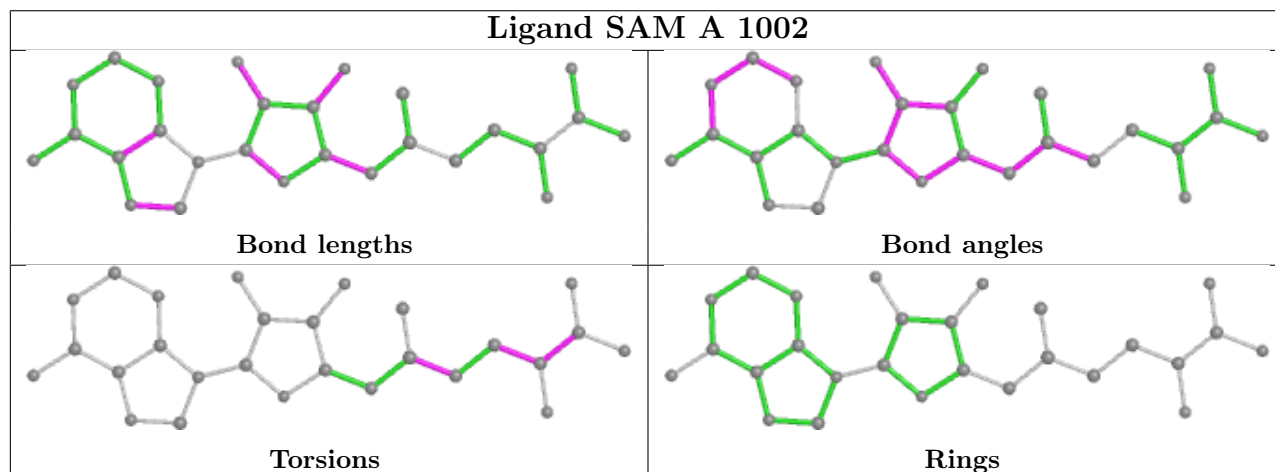
Mol	Chain	Res	Type	Atoms
3	A	1002	SAM	CB-CG-SD-CE
3	A	1002	SAM	CB-CG-SD-C5'
3	A	1002	SAM	OXT-C-CA-CB
3	A	1002	SAM	O-C-CA-CB
3	A	1002	SAM	C-CA-CB-CG
3	A	1002	SAM	N-CA-CB-CG
2	A	1001	I9H	CAE-CAB-NAF-CAK

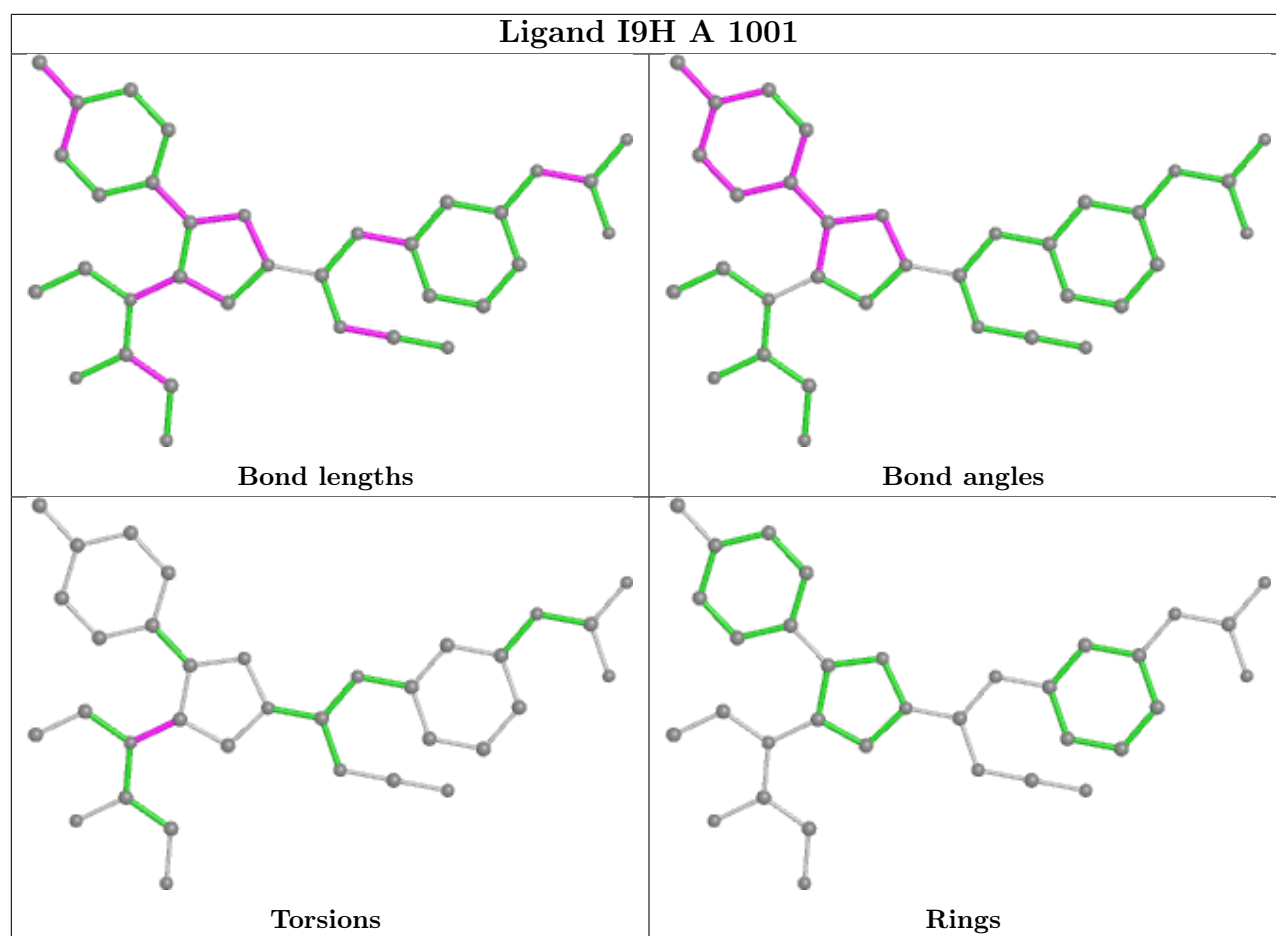
There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	SAM	13	0
2	A	1001	I9H	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	425/433 (98%)	0.76	51 (12%) 4 5	14, 48, 101, 175	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	298	ALA	5.7
1	A	332	PHE	5.5
1	A	323	LEU	5.4
1	A	284	ASP	4.8
1	A	66	GLY	4.7
1	A	283	SER	4.6
1	A	289	GLU	4.4
1	A	282	LEU	4.0
1	A	277	VAL	3.9
1	A	95	VAL	3.9
1	A	290	ALA	3.8
1	A	69	LYS	3.6
1	A	100	TRP	3.6
1	A	267	CYS	3.6
1	A	98	GLU	3.5
1	A	286	PRO	3.5
1	A	7	GLY	3.4
1	A	296	ARG	3.4
1	A	292	ARG	3.3
1	A	310	HIS	3.3
1	A	68	CYS	3.2
1	A	293	ASP	3.0
1	A	307	ARG	2.9
1	A	94	VAL	2.9
1	A	294	MET	2.9
1	A	285	PRO	2.8
1	A	287	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	311	TYR	2.8
1	A	237	PHE	2.7
1	A	331	VAL	2.6
1	A	330	SER	2.6
1	A	288	ALA	2.5
1	A	315	SER	2.4
1	A	65	CYS	2.4
1	A	148	LEU	2.3
1	A	24	LEU	2.3
1	A	303	GLU	2.3
1	A	300	ASN	2.3
1	A	321	CYS	2.3
1	A	164	LEU	2.3
1	A	319	GLU	2.3
1	A	326	GLU	2.2
1	A	76	VAL	2.2
1	A	301	VAL	2.2
1	A	356	TRP	2.2
1	A	6	LEU	2.2
1	A	138	LEU	2.2
1	A	13	CYS	2.2
1	A	320	ILE	2.1
1	A	143	ASN	2.1
1	A	253	ARG	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](#)

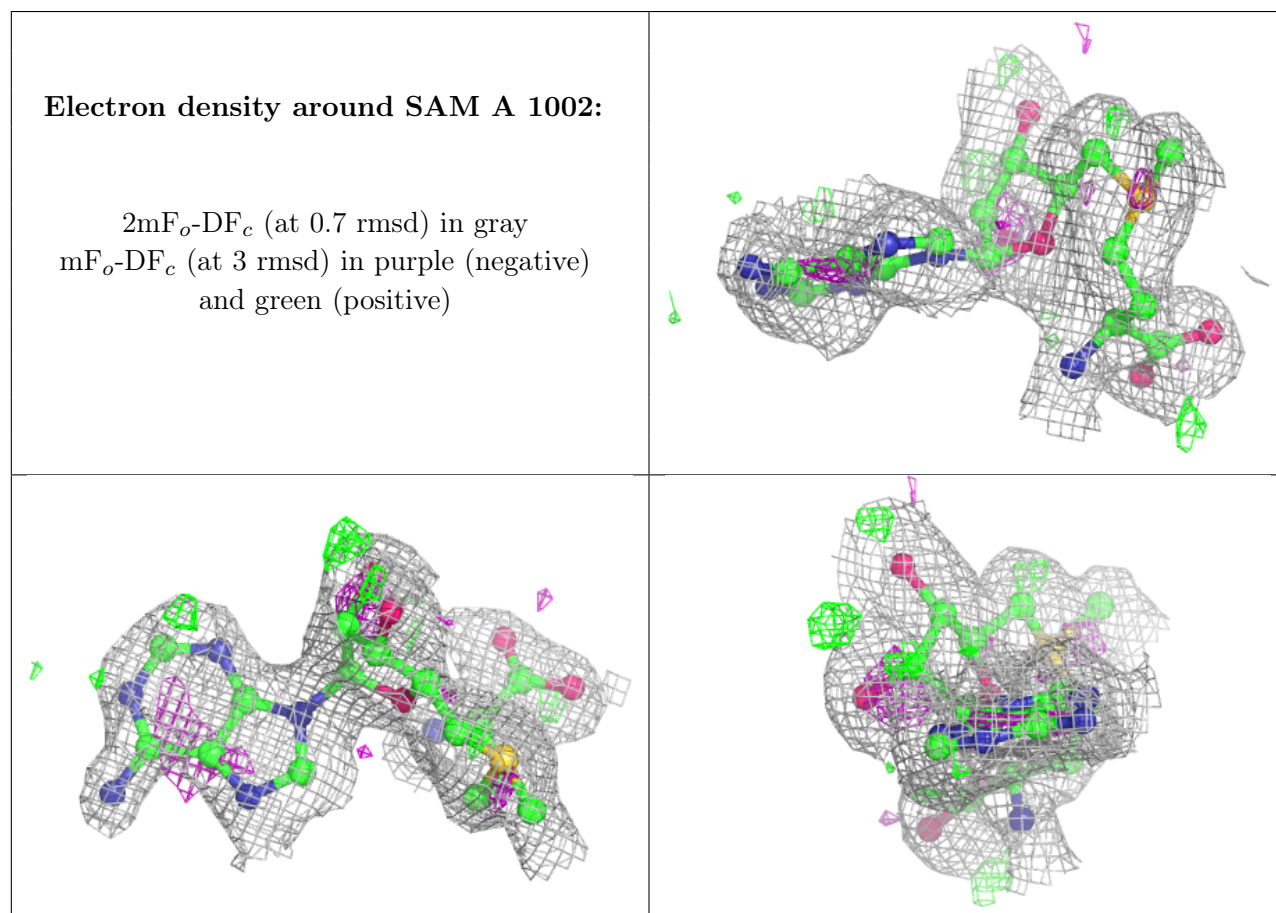
There are no monosaccharides in this entry.

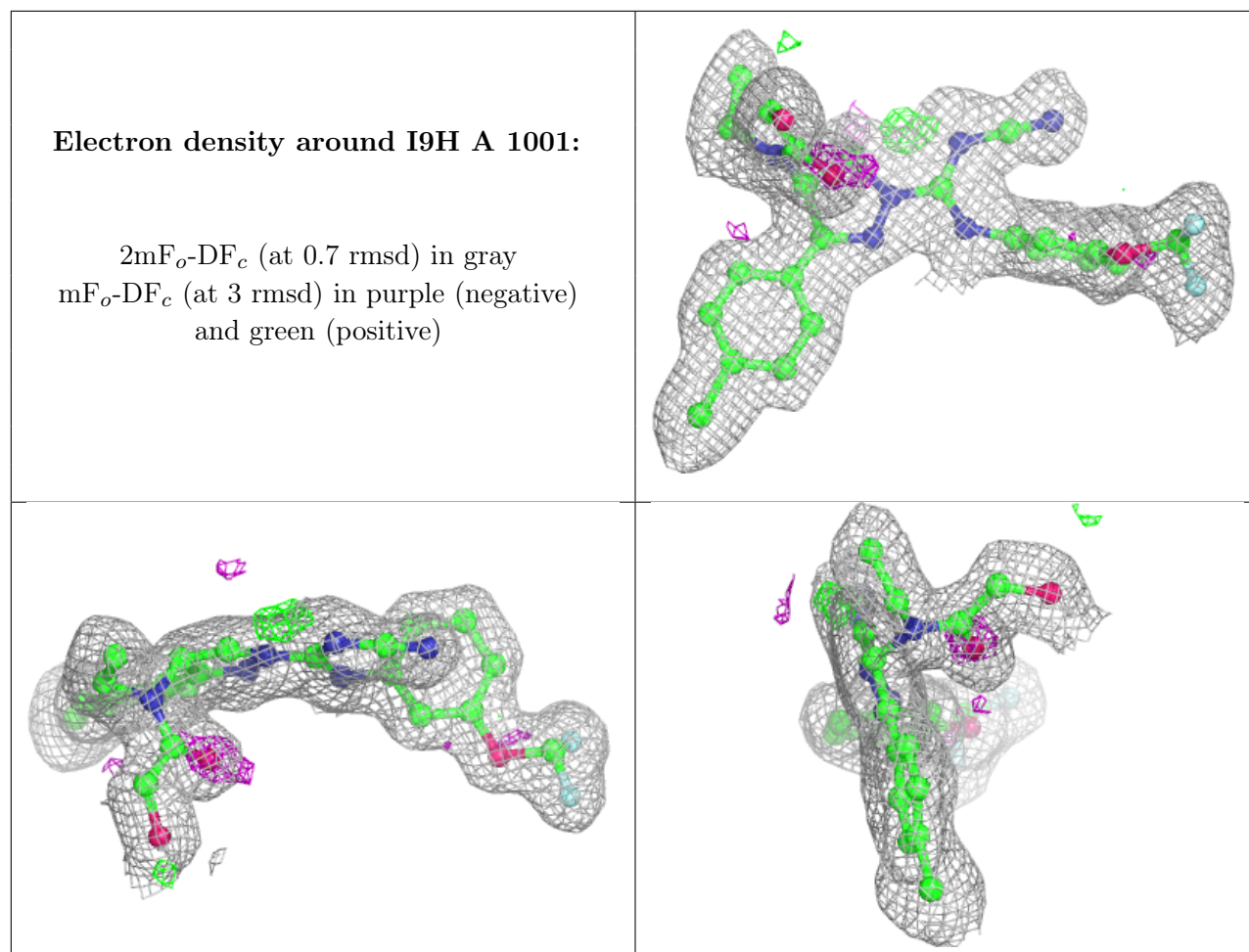
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
3	SAM	A	1002	27/27	0.87	0.18	13,29,38,53	0
4	ZN	A	1004	1/1	0.92	0.09	19,19,19,19	1
4	ZN	A	1003	1/1	0.93	0.09	35,35,35,35	1
2	I9H	A	1001	34/34	0.95	0.11	10,17,23,39	0
4	ZN	A	1005	1/1	0.98	0.04	16,16,16,16	1

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.