Full wwPDB X-ray Structure Validation Report (i)

Mar 10, 2024 – 08:02 AM EDT

PDB ID	:	4R29
Title	:	Crystal structure of bacterial cysteine methyltransferase effector NleE
Authors	:	Yao, Q.; Chen, J.; Hu, L.; Zhang, L.; Shao, F.
Deposited on	:	2014-08-11
Resolution	:	2.31 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 (i) 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 (i)) were used in the production of this report:

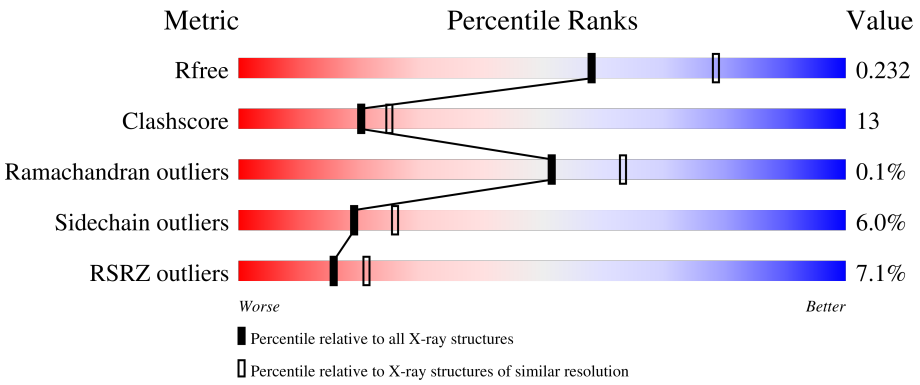
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 <=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	224	7%, 70%, 16%, •, 11%
1	B	224	5%, 70%, 18%, •, 9%
1	C	224	6%, 68%, 21%, •, 9%
1	D	224	8%, 66%, 20%, •, 11%

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	GOL	C	303	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7034 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.

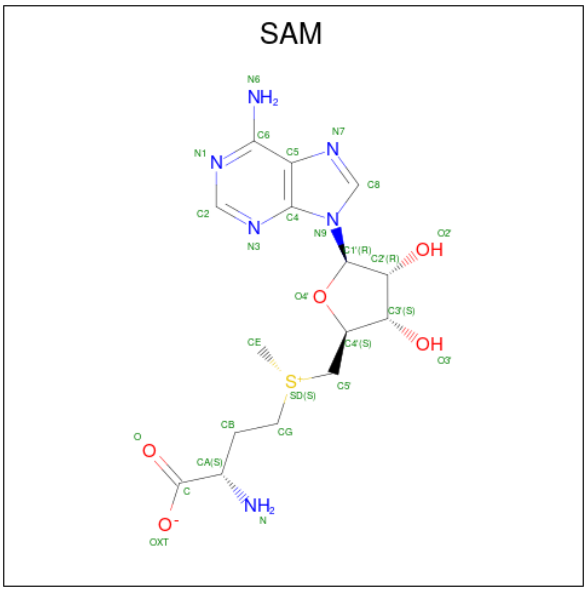
- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	199	1632	1046	267	307	12	0	0	0
1	B	203	1665	1066	273	314	12	0	0	0
1	C	203	1657	1060	274	311	12	0	0	0
1	D	199	1633	1047	269	305	12	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

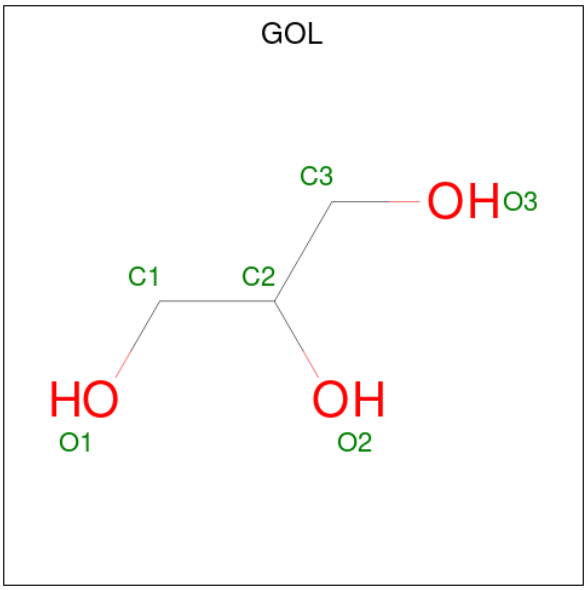
Chain	Residue	Modelled	Actual	Comment	Reference
A	181	ALA	GLU	engineered mutation	UNP Q7DBA6
B	181	ALA	GLU	engineered mutation	UNP Q7DBA6
C	181	ALA	GLU	engineered mutation	UNP Q7DBA6
D	181	ALA	GLU	engineered mutation	UNP Q7DBA6

- Molecule 2 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



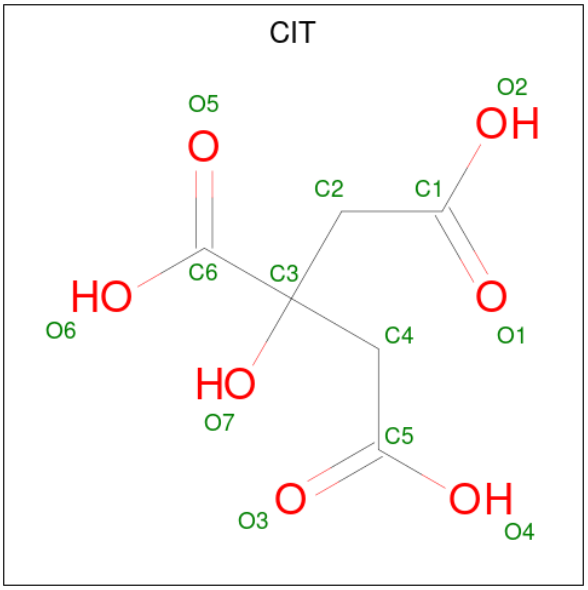
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	27	15	6	5	1	0	0
2	B	1	27	15	6	5	1	0	0
2	C	1	27	15	6	5	1	0	0
2	D	1	27	15	6	5	1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	B	1	13	6	7	0	0
			Total	C	O		
4	C	1	13	6	7	0	0

- Molecule 5 is water.

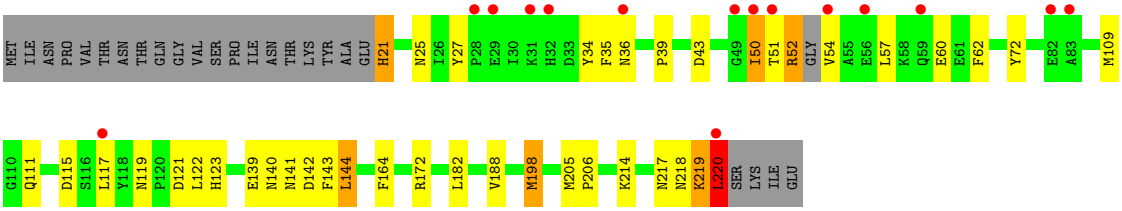
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	86	86	86	0	0
			Total	O		
5	B	87	87	87	0	0
			Total	O		
5	C	70	70	70	0	0
			Total	O		
5	D	52	52	52	0	0

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.

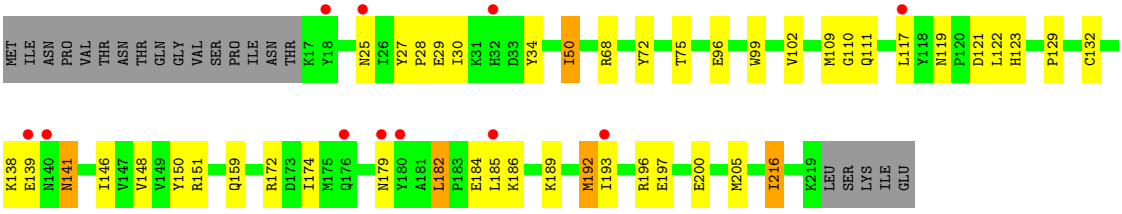
• Molecule 1: Uncharacterized protein

Chain A:



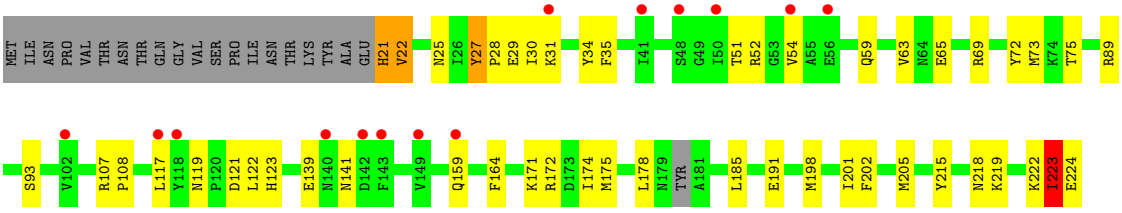
• Molecule 1: Uncharacterized protein

Chain B:



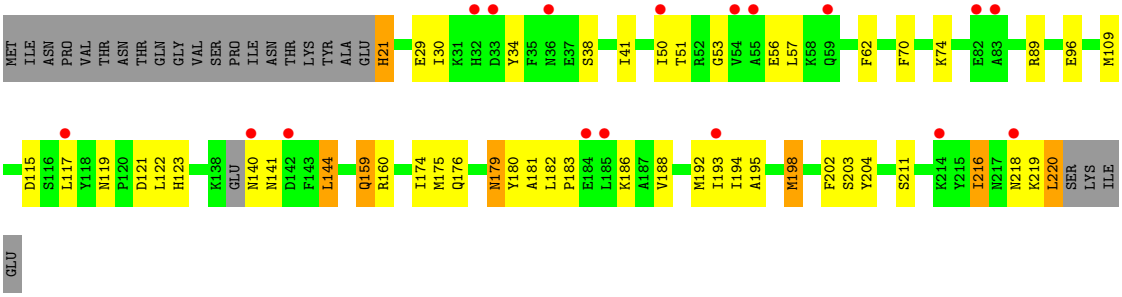
• Molecule 1: Uncharacterized protein

Chain C:



• Molecule 1: Uncharacterized protein

Chain D:


MET
ILE
ASN
PRO
VAL
THR
ASN
THR
GLN
GLY
VAL
SER
PRO
ILE
ASN
THR
LYS
TYR
ALA
GLU
H21
E29
I30
K31
H32
D33
Y34
F35
N36
E37
S38
I41
I50
T51
R52
G53
V54
A55
E56
L57
K58
Q59
F62
F70
K74
E82
A83
R89
E96
M109
D115
S116
L117
Y118
N119
P120
D121
L122
H123
K138
GLU
N140
N141
D142
F143
L144
Q159
R160
I174
M175
Q176
N179
Y180
A181
L182
P183
E184
L185
K186
A187
V188
M192
I193
I194
A195
M198
F202
S203
Y204
S211
K214
Y215
I216
N217
N218
K219
L220
SER
LYS
ILE
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	134.30Å 53.98Å 134.79Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	20.02 – 2.31 20.02 – 2.31	Depositor EDS
% Data completeness (in resolution range)	96.3 (20.02-2.31) 96.3 (20.02-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.83 (at 2.30Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.3_473)	Depositor
R, R_{free}	0.197 , 0.234 0.194 , 0.232	Depositor DCC
R_{free} test set	1943 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å^2)	28.3	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7034	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, CIT, 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	0.45	0/1669	0.58	1/2251 (0.0%)
1	B	0.42	0/1705	0.52	0/2302
1	C	0.40	0/1694	0.51	0/2283
1	D	0.39	0/1671	0.53	0/2254
All	All	0.41	0/6739	0.54	1/9090 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	220	LEU	CA-CB-CG	5.17	127.19	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1632	0	1607	45	0
1	B	1665	0	1628	44	0
1	C	1657	0	1637	43	0
1	D	1633	0	1610	42	0
2	A	27	0	22	1	0
2	B	27	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	27	0	22	4	0
2	D	27	0	22	2	0
3	A	6	0	8	1	0
3	C	6	0	8	4	0
3	D	6	0	8	0	0
4	B	13	0	5	0	0
4	C	13	0	5	0	0
5	A	86	0	0	1	0
5	B	87	0	0	3	0
5	C	70	0	0	3	0
5	D	52	0	0	3	0
All	All	7034	0	6604	167	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 13.

All (167) 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:51:THR:HG22	1:A:52:ARG:N	1.54	1.18
1:A:39:PRO:HD3	1:A:51:THR:O	1.45	1.17
1:A:51:THR:CG2	1:A:52:ARG:H	1.62	1.10
1:B:50:ILE:H	1:B:50:ILE:HD12	1.29	0.97
1:D:219:LYS:O	1:D:220:LEU:HB2	1.71	0.91
1:A:51:THR:HG22	1:A:52:ARG:H	0.76	0.89
1:A:220:LEU:HD23	1:A:220:LEU:O	1.75	0.86
1:B:119:ASN:HD22	1:B:122:LEU:H	1.23	0.83
1:C:164:PHE:HD1	1:C:198:MET:HE2	1.45	0.81
1:A:35:PHE:O	1:A:51:THR:CG2	2.30	0.80
1:C:119:ASN:HD22	1:C:122:LEU:H	1.27	0.79
1:B:192:MET:HE3	1:B:193:ILE:HD13	1.65	0.77
1:B:109:MET:CE	1:B:148:VAL:HG13	2.14	0.77
1:C:89:ARG:HG3	2:C:301:SAM:N1	2.00	0.76
1:B:192:MET:CE	1:D:192:MET:HE2	2.16	0.76
1:A:218:ASN:HB3	5:A:462:HOH:O	1.84	0.75
1:C:223:ILE:N	1:C:224:GLU:HA	2.04	0.73
1:B:119:ASN:HD21	1:B:121:ASP:HB2	1.53	0.72
1:D:179:ASN:HB2	1:D:186:LYS:HZ2	1.55	0.71
1:D:188:VAL:HG21	1:D:219:LYS:HE3	1.71	0.71
1:A:35:PHE:HA	1:A:52:ARG:HB3	1.71	0.71
1:C:29:GLU:H	1:C:29:GLU:CD	1.94	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PRO:CD	1:A:51:THR:O	2.34	0.70
1:A:188:VAL:HG21	1:A:219:LYS:HG2	1.73	0.70
1:D:119:ASN:HD21	1:D:121:ASP:HB2	1.57	0.70
1:A:51:THR:CG2	1:A:52:ARG:N	2.30	0.70
1:C:21:HIS:N	1:C:21:HIS:HD1	1.90	0.69
1:A:117:LEU:O	1:A:123:HIS:HE1	1.76	0.68
1:B:138:LYS:HD2	1:B:146:ILE:HD11	1.75	0.68
1:B:109:MET:HE2	1:B:148:VAL:HG13	1.74	0.68
1:B:192:MET:HE1	1:D:192:MET:HE2	1.76	0.68
1:C:164:PHE:CD1	1:C:198:MET:HE2	2.28	0.68
1:B:50:ILE:H	1:B:50:ILE:CD1	2.06	0.67
1:D:50:ILE:HG22	1:D:51:THR:HG23	1.76	0.67
1:A:54:VAL:O	1:A:54:VAL:HG23	1.95	0.67
1:A:119:ASN:HD21	1:A:121:ASP:HB2	1.61	0.66
1:B:68:ARG:HD3	5:B:484:HOH:O	1.95	0.66
1:D:174:ILE:HD13	1:D:193:ILE:HG13	1.79	0.65
1:A:143:PHE:CE1	1:A:144:LEU:HD13	2.32	0.65
1:B:109:MET:HE3	1:B:148:VAL:HG13	1.79	0.65
1:C:164:PHE:HD1	1:C:198:MET:CE	2.10	0.65
1:B:117:LEU:O	1:B:123:HIS:HE1	1.80	0.64
1:C:219:LYS:HE2	5:D:401:HOH:O	1.97	0.64
1:D:188:VAL:HG23	5:D:441:HOH:O	1.96	0.64
1:C:119:ASN:ND2	1:C:122:LEU:H	1.95	0.64
1:C:171:LYS:HE2	1:C:191:GLU:OE1	1.98	0.63
1:A:188:VAL:HG11	1:A:219:LYS:HB3	1.79	0.63
1:A:119:ASN:HD22	1:A:122:LEU:H	1.45	0.63
1:B:72:TYR:O	1:B:75:THR:HB	1.98	0.62
1:D:117:LEU:O	1:D:123:HIS:HE1	1.81	0.62
1:A:43:ASP:OD2	1:A:52:ARG:NH2	2.19	0.62
1:C:172:ARG:HD3	5:C:447:HOH:O	1.99	0.62
2:A:301:SAM:HN2	3:A:302:GOL:H2	1.65	0.61
1:B:192:MET:CE	1:B:193:ILE:HD13	2.30	0.61
1:A:35:PHE:O	1:A:51:THR:HG22	2.01	0.61
1:B:30:ILE:HD11	1:B:34:TYR:CG	2.35	0.61
1:C:117:LEU:O	1:C:123:HIS:HE1	1.84	0.60
1:D:119:ASN:HD22	1:D:122:LEU:H	1.49	0.60
1:C:119:ASN:HD21	1:C:121:ASP:HB2	1.66	0.60
1:B:50:ILE:HD12	1:B:50:ILE:N	2.10	0.60
1:B:174:ILE:HD12	1:B:193:ILE:HG13	1.83	0.60
1:B:119:ASN:ND2	1:B:122:LEU:H	1.99	0.60
1:B:28:PRO:HD2	1:B:29:GLU:OE1	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:ASP:HA	1:D:144:LEU:HD12	1.85	0.59
1:B:197:GLU:HG2	1:D:182:LEU:HD21	1.85	0.58
1:D:21:HIS:HE1	1:D:53:GLY:HA2	1.69	0.58
1:D:30:ILE:HD11	1:D:34:TYR:CD2	2.39	0.57
1:D:179:ASN:HB2	1:D:186:LYS:NZ	2.18	0.57
1:B:109:MET:HE1	1:B:111:GLN:HB2	1.86	0.57
1:C:164:PHE:CD1	1:C:198:MET:CE	2.87	0.56
1:D:194:ILE:HD12	1:D:195:ALA:N	2.21	0.56
1:A:139:GLU:O	1:A:140:ASN:CG	2.44	0.56
1:B:184:GLU:HG2	1:B:185:LEU:HD12	1.87	0.55
1:C:159:GLN:HG3	5:C:448:HOH:O	2.06	0.55
1:C:21:HIS:N	1:C:21:HIS:ND1	2.50	0.54
1:C:30:ILE:HD11	1:C:34:TYR:CG	2.42	0.54
1:B:182:LEU:HD22	5:B:476:HOH:O	2.08	0.54
1:A:111:GLN:HG3	1:A:164:PHE:CZ	2.43	0.54
1:D:159:GLN:HG3	1:D:160:ARG:N	2.23	0.53
1:D:30:ILE:HD11	1:D:34:TYR:CG	2.44	0.53
1:A:220:LEU:HD23	1:A:220:LEU:C	2.30	0.53
1:B:159:GLN:NE2	1:C:218:ASN:HD22	2.05	0.53
1:C:222:LYS:C	1:C:223:ILE:HG13	2.28	0.53
1:A:115:ASP:HA	1:A:144:LEU:HD12	1.91	0.52
1:A:217:ASN:O	1:A:220:LEU:HB3	2.09	0.52
1:D:204:TYR:OH	2:D:301:SAM:HB2	2.10	0.52
1:A:143:PHE:CD1	1:A:144:LEU:HD13	2.45	0.51
1:A:35:PHE:O	1:A:51:THR:HG21	2.10	0.51
1:A:72:TYR:CD1	1:B:129:PRO:CB	2.94	0.51
1:C:139:GLU:HB3	1:C:172:ARG:NH1	2.25	0.51
1:D:194:ILE:HD12	1:D:194:ILE:C	2.30	0.51
1:D:182:LEU:N	1:D:183:PRO:HD3	2.26	0.51
1:A:21:HIS:N	1:A:21:HIS:ND1	2.57	0.51
1:C:198:MET:CE	1:C:201:ILE:HD11	2.41	0.50
1:A:220:LEU:O	1:A:220:LEU:CD2	2.55	0.50
1:C:174:ILE:O	1:C:178:LEU:HG	2.12	0.50
1:D:96:GLU:HB2	5:D:411:HOH:O	2.12	0.49
1:B:123:HIS:HD2	5:B:419:HOH:O	1.95	0.49
1:C:35:PHE:HA	1:C:52:ARG:HB2	1.93	0.49
1:C:198:MET:HG3	1:C:202:PHE:CE2	2.48	0.49
1:D:198:MET:HB3	2:D:301:SAM:H1'	1.94	0.49
1:A:34:TYR:CE2	1:A:52:ARG:HD3	2.48	0.49
1:A:72:TYR:CD1	1:B:129:PRO:HB2	2.48	0.49
1:A:50:ILE:CG2	1:A:51:THR:N	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:LYS:HG3	1:B:139:GLU:N	2.29	0.48
1:D:202:PHE:O	1:D:203:SER:HB2	2.14	0.48
1:B:102:VAL:O	1:B:151:ARG:HD3	2.14	0.48
2:C:301:SAM:HN2	3:C:303:GOL:H11	1.79	0.48
1:A:141:ASN:OD1	1:A:144:LEU:HB2	2.14	0.48
1:A:72:TYR:HD1	1:B:129:PRO:CB	2.27	0.47
1:D:57:LEU:HD13	1:D:62:PHE:CE2	2.49	0.47
1:C:72:TYR:O	1:C:75:THR:HB	2.14	0.47
1:C:93:SER:C	3:C:303:GOL:H12	2.35	0.47
1:D:140:ASN:CG	1:D:141:ASN:H	2.17	0.47
1:D:70:PHE:CD2	1:D:74:LYS:HE2	2.49	0.47
1:B:109:MET:HE1	1:B:110:GLY:C	2.36	0.46
1:C:29:GLU:CD	1:C:29:GLU:N	2.66	0.46
2:C:301:SAM:HN2	3:C:303:GOL:H32	1.81	0.46
1:B:159:GLN:HE22	1:C:215:TYR:HA	1.81	0.46
1:B:179:ASN:OD1	1:B:186:LYS:NZ	2.49	0.46
1:A:21:HIS:N	1:A:21:HIS:HD1	2.14	0.45
1:C:223:ILE:HA	1:C:224:GLU:HG3	1.98	0.45
1:D:192:MET:CE	1:D:193:ILE:HD13	2.47	0.45
1:B:216:ILE:HD12	1:B:216:ILE:HA	1.83	0.45
1:C:198:MET:HE3	1:C:201:ILE:HD11	1.98	0.45
1:D:38:SER:HA	1:D:51:THR:HA	1.98	0.45
1:B:109:MET:HE2	1:B:110:GLY:O	2.16	0.45
1:B:192:MET:SD	1:D:192:MET:HE2	2.56	0.44
1:C:185:LEU:CD2	1:D:183:PRO:HG2	2.47	0.44
1:C:107:ARG:HB2	1:C:108:PRO:HD2	2.00	0.44
1:A:119:ASN:ND2	1:A:121:ASP:HB2	2.30	0.44
1:C:31:LYS:HB3	1:C:31:LYS:HE2	1.77	0.44
1:B:139:GLU:HA	1:B:139:GLU:OE1	2.17	0.44
1:A:144:LEU:HD12	1:A:144:LEU:HA	1.89	0.43
1:B:139:GLU:OE1	1:B:172:ARG:CZ	2.66	0.43
1:C:22:VAL:HG13	1:C:123:HIS:NE2	2.33	0.43
1:C:51:THR:OG1	1:C:54:VAL:HG22	2.19	0.43
1:C:159:GLN:CG	5:C:448:HOH:O	2.64	0.43
1:A:164:PHE:CD1	1:A:198:MET:HE1	2.53	0.43
1:D:56:GLU:O	1:D:56:GLU:HG2	2.18	0.43
1:D:180:TYR:CD1	1:D:180:TYR:C	2.92	0.43
1:D:194:ILE:C	1:D:194:ILE:CD1	2.86	0.43
1:A:54:VAL:O	1:A:54:VAL:CG2	2.66	0.43
1:A:60:GLU:HA	1:A:60:GLU:OE1	2.18	0.43
1:D:216:ILE:O	1:D:219:LYS:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:LYS:O	1:D:220:LEU:CB	2.54	0.42
1:A:57:LEU:HD13	1:A:62:PHE:CE2	2.55	0.42
1:B:96:GLU:HG3	1:B:99:TRP:CZ2	2.55	0.42
1:C:27:TYR:N	1:C:28:PRO:HD3	2.35	0.42
1:C:119:ASN:HD22	1:C:122:LEU:N	2.07	0.42
1:D:180:TYR:HD1	1:D:181:ALA:HB2	1.84	0.42
1:C:69:ARG:O	1:C:73:MET:HG3	2.19	0.41
1:A:205:MET:HA	1:A:206:PRO:HD3	1.92	0.41
1:A:36:ASN:O	1:A:51:THR:HG23	2.20	0.41
1:A:21:HIS:HE1	1:A:35:PHE:CE1	2.38	0.41
1:B:196:ARG:O	1:B:200:GLU:HG3	2.20	0.41
1:C:65:GLU:HA	1:C:65:GLU:OE1	2.20	0.41
1:D:29:GLU:OE1	1:D:29:GLU:N	2.52	0.41
1:B:138:LYS:HG2	1:B:141:ASN:HB2	2.02	0.41
1:D:140:ASN:CG	1:D:141:ASN:N	2.74	0.41
1:A:217:ASN:O	1:A:220:LEU:HD13	2.20	0.40
1:C:59:GLN:O	1:C:63:VAL:HB	2.21	0.40
1:B:132:CYS:HB2	1:B:150:TYR:CZ	2.56	0.40
1:C:185:LEU:HD23	1:D:183:PRO:HG2	2.03	0.40
1:B:189:LYS:O	1:B:192:MET:HG3	2.21	0.40
2:C:301:SAM:N	3:C:303:GOL:H11	2.36	0.40
1:D:192:MET:HE1	1:D:193:ILE:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	195/224 (87%)	186 (95%)	9 (5%)	0	100 100
1	B	201/224 (90%)	195 (97%)	6 (3%)	0	100 100
1	C	199/224 (89%)	190 (96%)	8 (4%)	1 (0%)	29 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	195/224 (87%)	186 (95%)	9 (5%)	0	100	100
All	All	790/896 (88%)	757 (96%)	32 (4%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	223	ILE

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	182/205 (89%)	168 (92%)	14 (8%)	13	16
1	B	184/205 (90%)	176 (96%)	8 (4%)	29	40
1	C	185/205 (90%)	177 (96%)	8 (4%)	29	40
1	D	182/205 (89%)	168 (92%)	14 (8%)	13	16
All	All	733/820 (89%)	689 (94%)	44 (6%)	19	26

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	25	ASN
1	A	27	TYR
1	A	50	ILE
1	A	52	ARG
1	A	109	MET
1	A	142	ASP
1	A	144	LEU
1	A	172	ARG
1	A	182	LEU
1	A	198	MET
1	A	214	LYS
1	A	219	LYS

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Mol	Chain	Res	Type
1	A	220	LEU
1	B	25	ASN
1	B	27	TYR
1	B	50	ILE
1	B	141	ASN
1	B	182	LEU
1	B	192	MET
1	B	205	MET
1	B	216	ILE
1	C	21	HIS
1	C	22	VAL
1	C	25	ASN
1	C	27	TYR
1	C	141	ASN
1	C	175	MET
1	C	205	MET
1	C	223	ILE
1	D	21	HIS
1	D	41	ILE
1	D	89	ARG
1	D	109	MET
1	D	144	LEU
1	D	159	GLN
1	D	175	MET
1	D	176	GLN
1	D	179	ASN
1	D	198	MET
1	D	211	SER
1	D	216	ILE
1	D	218	ASN
1	D	220	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	119	ASN
1	A	123	HIS
1	B	64	ASN
1	B	119	ASN
1	B	123	HIS
1	B	159	GLN

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Mol	Chain	Res	Type
1	C	32	HIS
1	C	64	ASN
1	C	119	ASN
1	C	123	HIS
1	D	21	HIS
1	D	64	ASN
1	D	119	ASN
1	D	123	HIS
1	D	176	GLN

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)

9 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	A	302	-	5,5,5	0.36	0	5,5,5	0.45	0
2	SAM	B	301	-	24,29,29	1.24	3 (12%)	23,42,42	1.54	3 (13%)
3	GOL	C	303	-	5,5,5	0.39	0	5,5,5	0.71	0
4	CIT	B	302	-	12,12,12	1.15	1 (8%)	17,17,17	1.37	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SAM	C	301	-	24,29,29	1.36	3 (12%)	23,42,42	1.49	2 (8%)
3	GOL	D	302	-	5,5,5	0.32	0	5,5,5	0.22	0
4	CIT	C	302	-	12,12,12	1.06	0	17,17,17	1.55	3 (17%)
2	SAM	D	301	-	24,29,29	1.33	2 (8%)	23,42,42	1.75	4 (17%)
2	SAM	A	301	-	24,29,29	1.20	2 (8%)	23,42,42	1.57	3 (13%)

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	A	302	-	-	2/4/4/4	-
2	SAM	B	301	-	-	0/12/33/33	0/3/3/3
3	GOL	C	303	-	-	0/4/4/4	-
4	CIT	B	302	-	-	6/16/16/16	-
2	SAM	C	301	-	-	3/12/33/33	0/3/3/3
3	GOL	D	302	-	-	0/4/4/4	-
4	CIT	C	302	-	-	5/16/16/16	-
2	SAM	D	301	-	-	7/12/33/33	0/3/3/3
2	SAM	A	301	-	-	1/12/33/33	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	SAM	C2-N3	4.52	1.39	1.32
2	D	301	SAM	C2-N3	4.21	1.38	1.32
2	A	301	SAM	C2-N3	3.98	1.38	1.32
2	B	301	SAM	C2-N3	3.89	1.38	1.32
2	D	301	SAM	C2-N1	2.82	1.39	1.33
2	A	301	SAM	C2-N1	2.67	1.38	1.33
2	B	301	SAM	C2-N1	2.50	1.38	1.33
2	C	301	SAM	C2-N1	2.48	1.38	1.33
2	B	301	SAM	OXT-C	-2.29	1.23	1.30
2	C	301	SAM	OXT-C	-2.22	1.23	1.30
4	B	302	CIT	C3-C6	-2.18	1.51	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	SAM	N3-C2-N1	-5.76	119.68	128.68
2	A	301	SAM	N3-C2-N1	-5.27	120.44	128.68
2	B	301	SAM	N3-C2-N1	-5.14	120.64	128.68
2	C	301	SAM	N3-C2-N1	-5.14	120.64	128.68
4	C	302	CIT	O6-C6-C3	3.99	119.98	113.05
4	B	302	CIT	O6-C6-C3	3.11	118.45	113.05
2	D	301	SAM	OXT-C-O	-3.09	117.08	124.09
2	A	301	SAM	C3'-C2'-C1'	2.76	105.14	100.98
4	B	302	CIT	O5-C6-C3	-2.65	118.51	122.25
2	D	301	SAM	C3'-C2'-C1'	2.56	104.83	100.98
4	C	302	CIT	O4-C5-C4	2.54	122.51	114.35
2	B	301	SAM	OXT-C-O	-2.50	118.40	124.09
2	B	301	SAM	C3'-C2'-C1'	2.49	104.73	100.98
4	C	302	CIT	O4-C5-O3	-2.19	117.84	123.30
2	D	301	SAM	OXT-C-CA	2.17	120.78	113.38
2	A	301	SAM	OXT-C-CA	2.14	120.69	113.38
2	C	301	SAM	OXT-C-CA	2.04	120.34	113.38

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	SAM	O-C-CA-N
2	D	301	SAM	O4'-C4'-C5'-SD
3	A	302	GOL	O1-C1-C2-C3
4	C	302	CIT	C1-C2-C3-O7
4	C	302	CIT	C1-C2-C3-C4
4	C	302	CIT	C1-C2-C3-C6
2	D	301	SAM	OXT-C-CA-N
3	A	302	GOL	O1-C1-C2-O2
4	B	302	CIT	C2-C3-C6-O6
2	A	301	SAM	O4'-C4'-C5'-SD
2	C	301	SAM	O4'-C4'-C5'-SD
2	C	301	SAM	C3'-C4'-C5'-SD
2	D	301	SAM	CA-CB-CG-SD
2	D	301	SAM	C3'-C4'-C5'-SD
4	B	302	CIT	C2-C3-C6-O5
4	C	302	CIT	C3-C4-C5-O4
4	B	302	CIT	C4-C3-C6-O5
4	C	302	CIT	C3-C4-C5-O3
2	D	301	SAM	O-C-CA-CB
4	B	302	CIT	C3-C4-C5-O3
4	B	302	CIT	C3-C4-C5-O4

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Mol	Chain	Res	Type	Atoms
4	B	302	CIT	C4-C3-C6-O6
2	D	301	SAM	OXT-C-CA-CB
2	C	301	SAM	CB-CG-SD-C5'

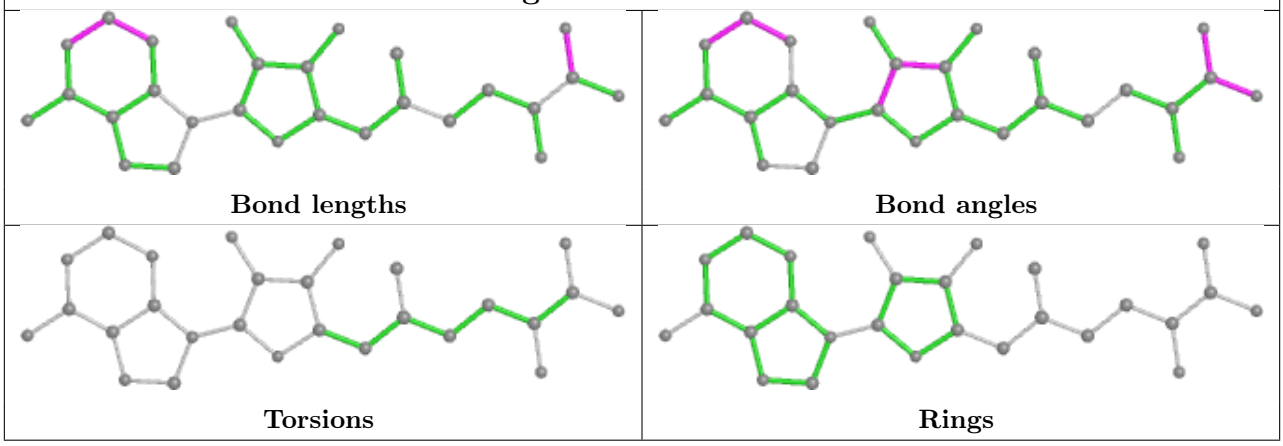
There are no ring outliers.

5 monomers are involved in 8 short contacts:

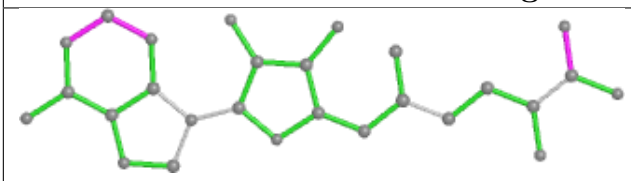
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	GOL	1	0
3	C	303	GOL	4	0
2	C	301	SAM	4	0
2	D	301	SAM	2	0
2	A	301	SAM	1	0

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 then 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.

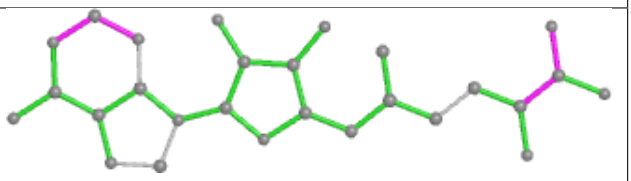
Ligand SAM B 301



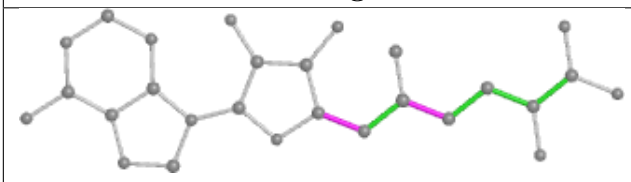
Ligand SAM C 301



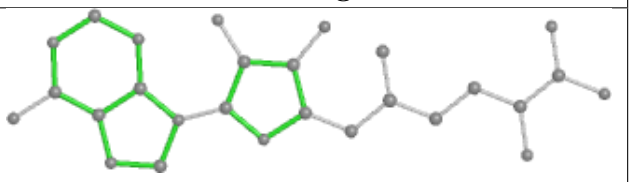
Bond lengths



Bond angles

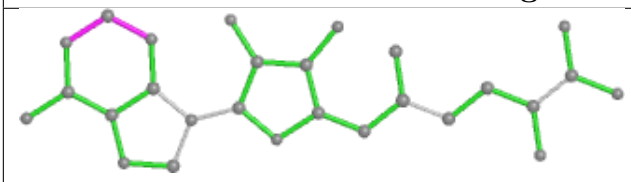


Torsions

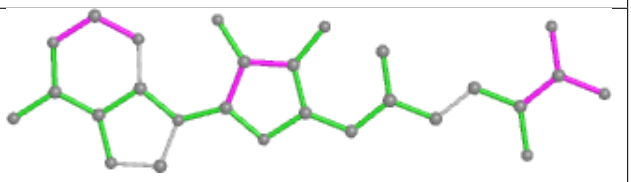


Rings

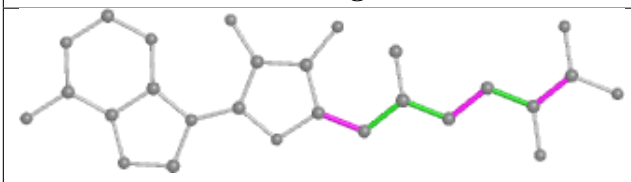
Ligand SAM D 301



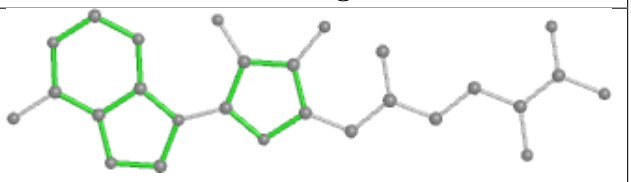
Bond lengths



Bond angles

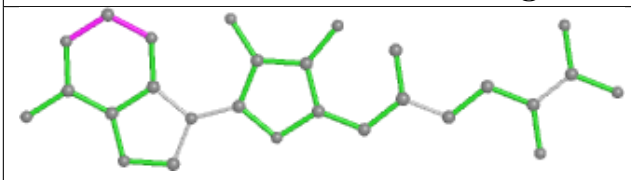


Torsions

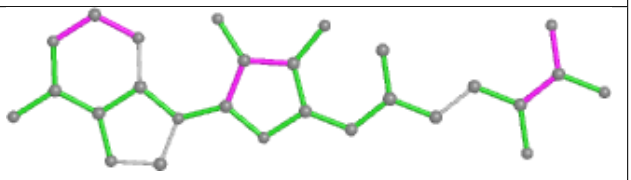


Rings

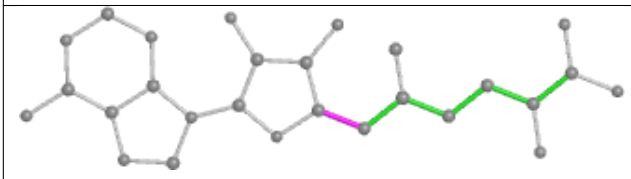
Ligand SAM A 301



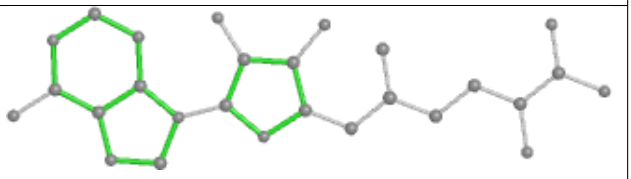
Bond lengths



Bond angles



Torsions



Rings

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	199/224 (88%)	0.15	15 (7%)	14	19	16, 27, 60, 65	0
1	B	203/224 (90%)	0.02	11 (5%)	25	32	16, 28, 55, 77	0
1	C	203/224 (90%)	0.21	14 (6%)	16	22	18, 30, 58, 72	0
1	D	199/224 (88%)	0.27	17 (8%)	10	15	19, 36, 60, 73	0
All	All	804/896 (89%)	0.16	57 (7%)	16	21	16, 30, 59, 77	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	180	TYR	6.6
1	B	140	ASN	6.3
1	A	54	VAL	4.8
1	A	50	ILE	4.6
1	C	41	ILE	4.5
1	B	18	TYR	4.4
1	C	143	PHE	4.3
1	C	50	ILE	4.3
1	D	82	GLU	4.2
1	A	83	ALA	4.1
1	B	32	HIS	3.5
1	A	59	GLN	3.4
1	D	184	GLU	3.3
1	C	117	LEU	3.2
1	D	140	ASN	3.1
1	C	140	ASN	3.0
1	A	220	LEU	3.0
1	B	176	GLN	3.0
1	D	218	ASN	2.9
1	D	32	HIS	2.9
1	B	117	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	51	THR	2.8
1	A	49	GLY	2.7
1	B	179	ASN	2.7
1	A	36	ASN	2.7
1	D	59	GLN	2.7
1	D	54	VAL	2.6
1	D	214	LYS	2.6
1	C	54	VAL	2.5
1	A	31	LYS	2.5
1	D	55	ALA	2.5
1	B	139	GLU	2.4
1	C	48	SER	2.4
1	B	185	LEU	2.4
1	B	25	ASN	2.4
1	A	28	PRO	2.3
1	C	159	GLN	2.3
1	D	50	ILE	2.3
1	D	83	ALA	2.3
1	C	149	VAL	2.3
1	A	82	GLU	2.3
1	D	185	LEU	2.3
1	A	117	LEU	2.2
1	D	193	ILE	2.2
1	D	36	ASN	2.2
1	D	142	ASP	2.2
1	C	56	GLU	2.2
1	A	32	HIS	2.2
1	C	118	TYR	2.1
1	C	102	VAL	2.1
1	A	29	GLU	2.1
1	A	56	GLU	2.1
1	D	117	LEU	2.1
1	C	31	LYS	2.1
1	B	193	ILE	2.0
1	D	33	ASP	2.0
1	C	142	ASP	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)

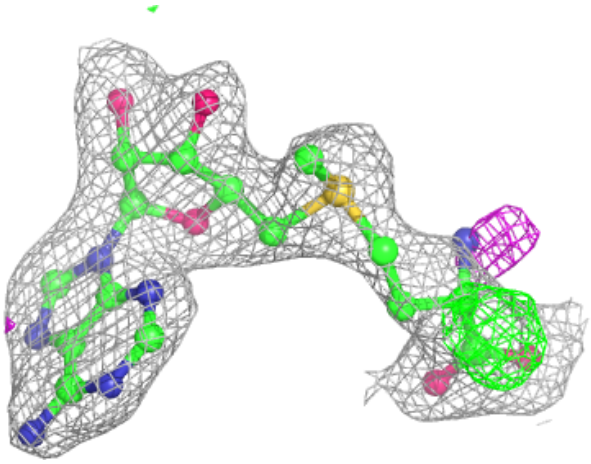
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

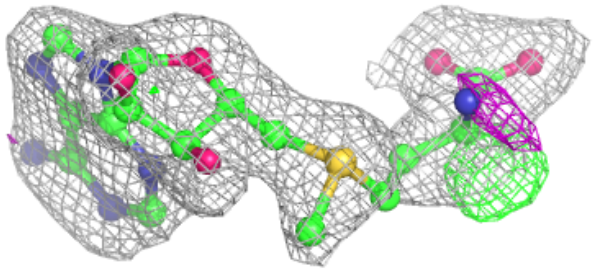
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	C	303	6/6	0.79	0.24	34,37,41,42	0
4	CIT	B	302	13/13	0.86	0.24	20,20,20,20	0
4	CIT	C	302	13/13	0.88	0.17	41,45,50,50	0
3	GOL	A	302	6/6	0.91	0.11	31,35,36,37	0
2	SAM	D	301	27/27	0.92	0.16	25,37,40,49	0
3	GOL	D	302	6/6	0.93	0.13	43,48,51,52	0
2	SAM	A	301	27/27	0.96	0.13	19,24,30,36	0
2	SAM	C	301	27/27	0.96	0.12	22,25,32,34	0
2	SAM	B	301	27/27	0.97	0.15	19,24,29,32	0

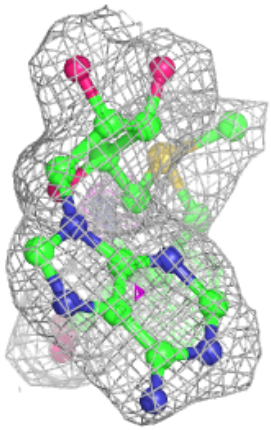
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAM D 301:

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

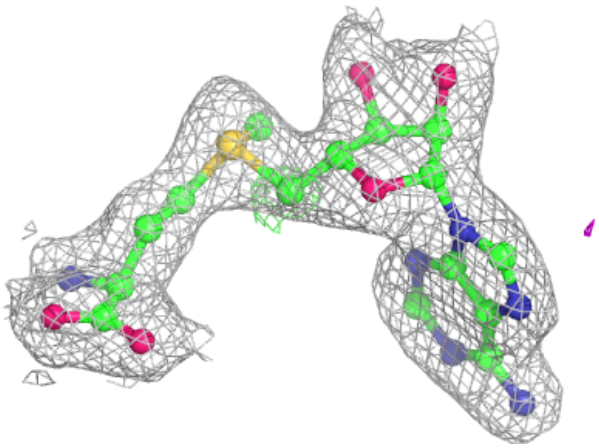


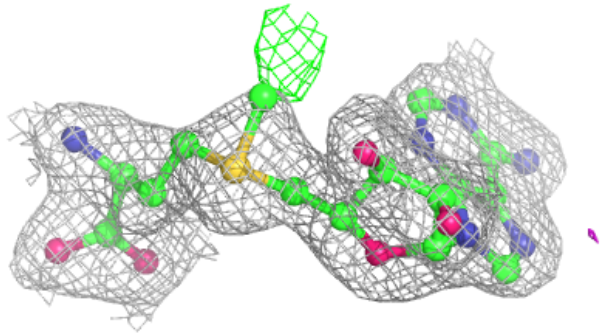


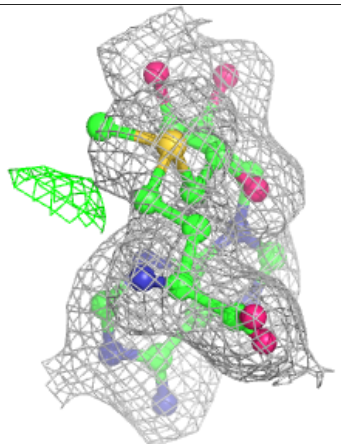


Electron density around SAM A 301:

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

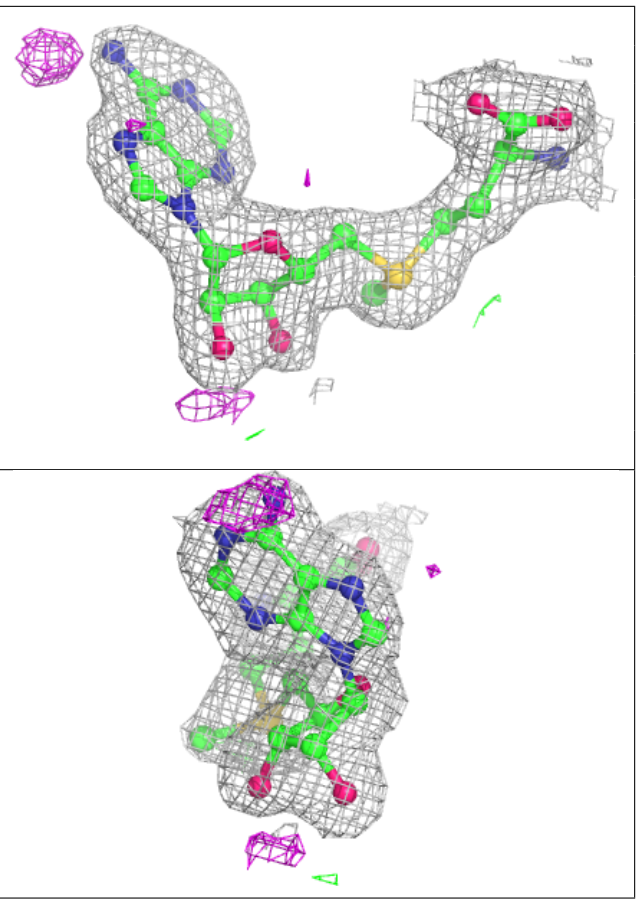


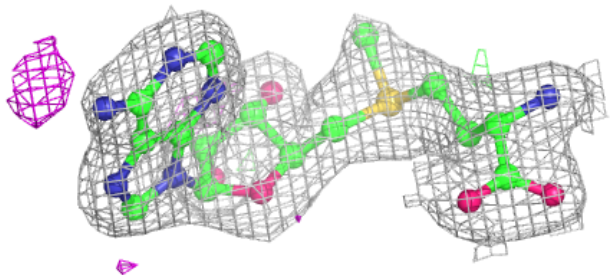




Electron density around SAM C 301:

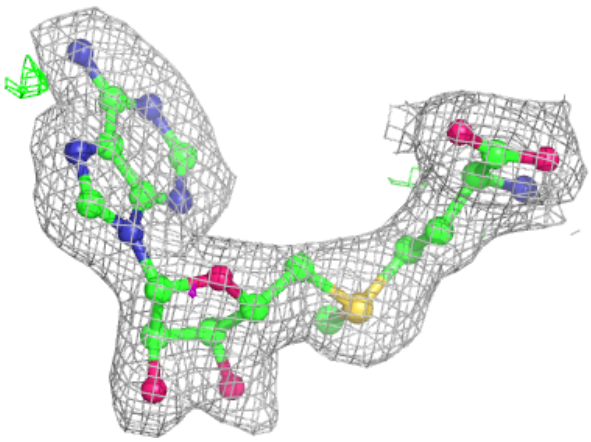
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

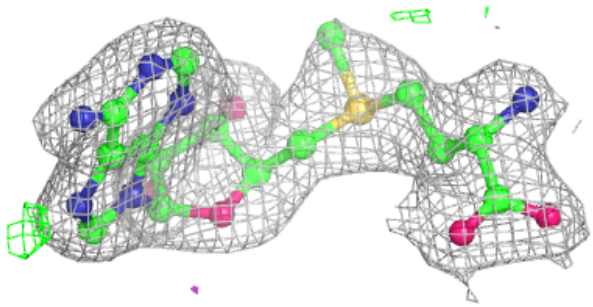


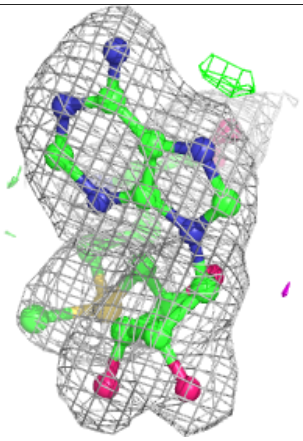


Electron density around SAM B 301:

$2mF_o$-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.