



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 05:24 AM EDT

PDB ID : 3IVA
Title : Structure of the B12-dependent Methionine Synthase (MetH) C-terminal half with AdoHcy bound
Authors : Pattridge, K.A.; Koutmos, M.; Smith, J.L.
Deposited on : 2009-08-31
Resolution : 2.70 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

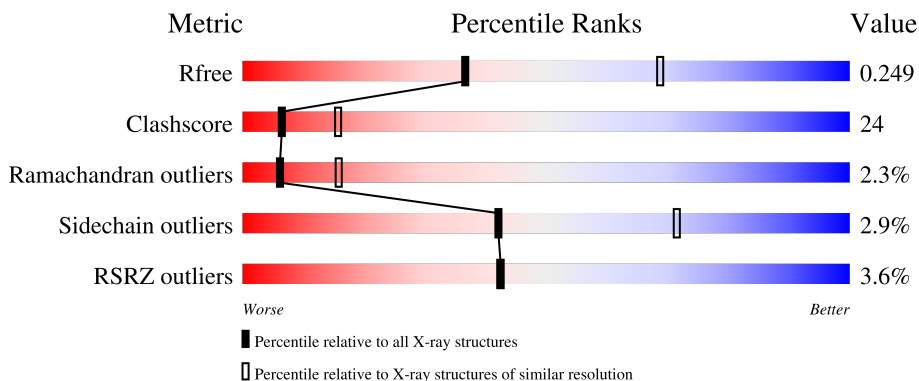
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	579	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	B12	A	1301	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NO3	A	1305	-	-	-	X

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 4722 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.

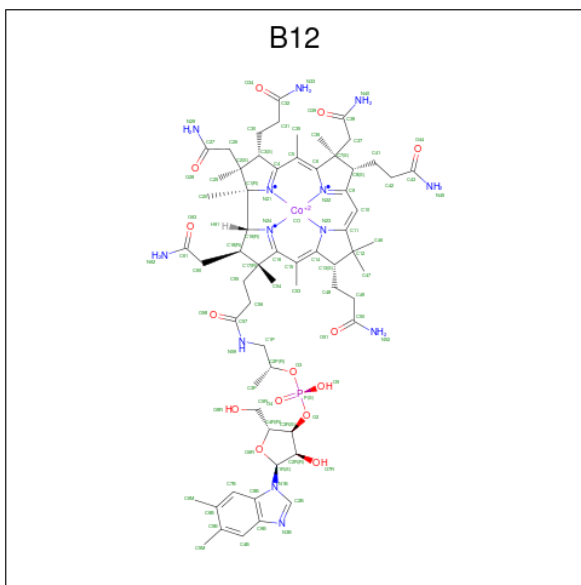
- Molecule 1 is a protein called Methionine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	576	4563	2886	788	870	19	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	690	CYS	ILE	engineered mutation	UNP P13009
A	743	CYS	GLY	engineered mutation	UNP P13009

- Molecule 2 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Co	N	O	P		
2	A	1	91	62	1	13	14	1	0	0

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

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	O		
4	A	1	4	1	3	0	0

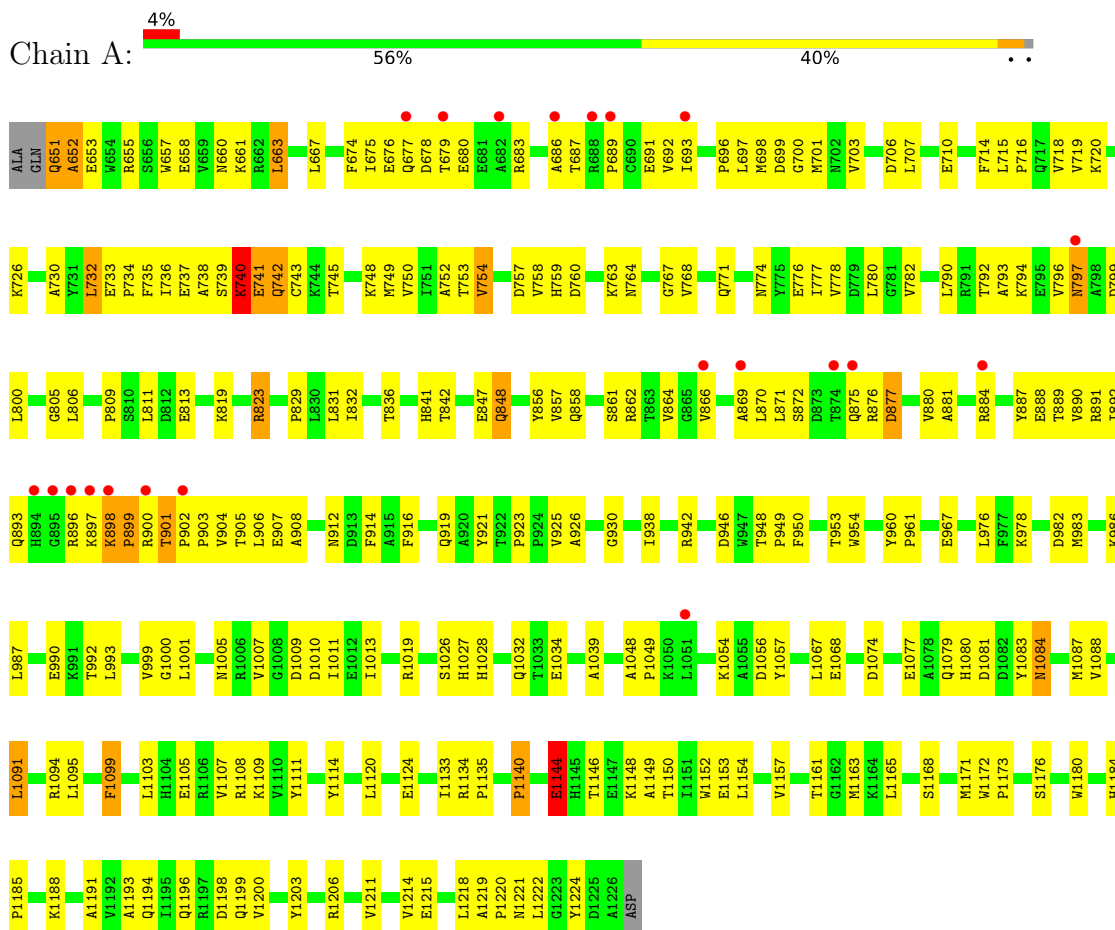
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	26	26	26	0	0

3 Residue-property plots

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

- Molecule 1: Methionine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.01Å 107.01Å 141.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.32 – 2.70 45.32 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.32-2.70) 100.0 (45.32-2.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.69Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.246 , 0.300 0.241 , 0.249	Depositor DCC
R_{free} test set	1119 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	66.2	Xtrriage
Anisotropy	0.174	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4722	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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: B12, SAH, NO3

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	0.32	0/4662	0.58	0/6325

There are no bond length outliers.

There are no bond angle outliers.

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	4563	0	4478	221	0
2	A	91	0	73	1	0
3	A	26	0	19	0	0
4	A	16	0	0	0	0
5	A	26	0	0	0	0
All	All	4722	0	4570	221	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 24.

All (221) 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:657:TRP:HB3	1:A:661:LYS:HE2	1.52	0.90
1:A:819:LYS:O	1:A:823:ARG:HG2	1.77	0.84
1:A:692:VAL:HG23	1:A:693:ILE:HD12	1.61	0.82
1:A:987:LEU:HD13	1:A:992:THR:HG23	1.61	0.81
1:A:1194:GLN:HA	1:A:1221:ASN:O	1.82	0.80
1:A:1120:LEU:HB3	1:A:1124:GLU:HB3	1.66	0.77
1:A:983:MET:HE3	1:A:1088:VAL:HA	1.67	0.76
1:A:938:ILE:O	1:A:942:ARG:HG3	1.86	0.76
1:A:1144:GLU:OE1	1:A:1146:THR:HB	1.86	0.75
1:A:660:ASN:HB3	1:A:696:PRO:HB3	1.67	0.74
1:A:750:VAL:HA	1:A:778:VAL:HG23	1.70	0.74
1:A:805:GLY:O	1:A:836:THR:HG22	1.88	0.73
1:A:983:MET:HE2	1:A:1091:LEU:HD23	1.70	0.72
1:A:799:ASP:C	1:A:800:LEU:HD12	2.09	0.72
1:A:1084:ASN:HA	1:A:1087:MET:HB3	1.73	0.70
1:A:753:THR:HB	1:A:782:VAL:HA	1.74	0.69
1:A:858:GLN:HB2	1:A:862:ARG:HD2	1.73	0.69
1:A:983:MET:CE	1:A:1088:VAL:HA	2.21	0.69
1:A:1219:ALA:HB3	1:A:1220:PRO:HD3	1.73	0.69
1:A:888:GLU:O	1:A:892:ILE:HG12	1.93	0.69
1:A:748:LYS:HE3	1:A:776:GLU:OE2	1.93	0.69
1:A:750:VAL:HG22	1:A:778:VAL:HG21	1.75	0.69
1:A:1211:VAL:O	1:A:1215:GLU:HG3	1.93	0.68
1:A:950:PHE:HZ	1:A:1087:MET:HE1	1.58	0.68
1:A:750:VAL:HA	1:A:778:VAL:CG2	2.23	0.67
1:A:730:ALA:O	1:A:733:GLU:HG2	1.94	0.67
1:A:950:PHE:CZ	1:A:1087:MET:HE1	2.30	0.67
1:A:754:VAL:HG13	1:A:813:GLU:HG2	1.75	0.67
1:A:1150:THR:O	1:A:1154:LEU:HD13	1.95	0.66
1:A:726:LYS:HG2	1:A:1080:HIS:HB3	1.77	0.65
1:A:758:VAL:HG11	1:A:1171:MET:O	1.96	0.65
1:A:983:MET:O	1:A:987:LEU:HD23	1.96	0.65
1:A:703:VAL:O	1:A:707:LEU:HB2	1.96	0.65
1:A:832:ILE:HD11	1:A:842:THR:OG1	1.97	0.64
1:A:1152:TRP:HA	1:A:1157:VAL:HG23	1.78	0.64
1:A:948:THR:HB	1:A:949:PRO:HD3	1.80	0.64
1:A:967:GLU:CD	1:A:967:GLU:H	2.02	0.63
1:A:683:ARG:HH21	1:A:735:PHE:HB3	1.64	0.63
1:A:658:GLU:HB3	1:A:661:LYS:HB2	1.79	0.62
1:A:692:VAL:HG21	1:A:732:LEU:CD1	2.29	0.62
1:A:754:VAL:HG13	1:A:813:GLU:CG	2.29	0.62
1:A:887:TYR:O	1:A:891:ARG:HB2	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:THR:O	1:A:893:GLN:HB2	2.01	0.61
1:A:900:ARG:HD3	1:A:901:THR:N	2.16	0.61
1:A:732:LEU:O	1:A:732:LEU:HD23	2.01	0.61
1:A:745:THR:HA	1:A:774:ASN:ND2	2.16	0.61
1:A:692:VAL:HG21	1:A:732:LEU:HD11	1.82	0.60
1:A:652:ALA:HB3	1:A:655:ARG:HG2	1.83	0.60
1:A:667:LEU:HB3	1:A:701:MET:HE2	1.84	0.59
1:A:1084:ASN:HA	1:A:1087:MET:CB	2.32	0.59
1:A:745:THR:HA	1:A:774:ASN:HD21	1.67	0.59
1:A:861:SER:O	1:A:864:VAL:HG12	2.02	0.59
1:A:862:ARG:O	1:A:866:VAL:HG23	2.02	0.59
1:A:950:PHE:HZ	1:A:1087:MET:CE	2.15	0.59
1:A:692:VAL:O	1:A:697:LEU:HB2	2.03	0.59
1:A:790:LEU:O	1:A:794:LYS:HG3	2.03	0.58
1:A:683:ARG:NH2	1:A:735:PHE:HB3	2.19	0.58
1:A:651:GLN:O	1:A:652:ALA:HB2	2.02	0.58
1:A:689:PRO:O	1:A:692:VAL:HG22	2.03	0.58
1:A:950:PHE:HE2	1:A:976:LEU:CD1	2.17	0.57
1:A:663:LEU:O	1:A:667:LEU:HG	2.04	0.57
1:A:706:ASP:O	1:A:710:GLU:HG3	2.05	0.57
1:A:800:LEU:HD11	1:A:871:LEU:HD13	1.86	0.57
1:A:674:PHE:O	1:A:678:ASP:HB2	2.05	0.57
1:A:901:THR:O	1:A:901:THR:HG23	2.05	0.56
1:A:950:PHE:CZ	1:A:1087:MET:CE	2.88	0.56
1:A:809:PRO:HB2	1:A:1168:SER:OG	2.05	0.56
1:A:829:PRO:HB3	1:A:870:LEU:HD21	1.87	0.56
1:A:1007:VAL:O	1:A:1007:VAL:HG23	2.05	0.56
1:A:693:ILE:CD1	1:A:732:LEU:HD22	2.35	0.56
1:A:1032:GLN:HE22	1:A:1196:GLN:HB2	1.71	0.56
1:A:1108:ARG:HG2	1:A:1114:TYR:CZ	2.42	0.55
1:A:1133:ILE:HG13	1:A:1135:PRO:HD3	1.88	0.55
1:A:752:ALA:HB2	1:A:780:LEU:HB2	1.89	0.55
1:A:987:LEU:HD12	1:A:993:LEU:HB2	1.88	0.55
1:A:905:THR:HG22	1:A:907:GLU:H	1.71	0.54
1:A:872:SER:O	1:A:876:ARG:HB2	2.07	0.54
1:A:1019:ARG:HH12	1:A:1056:ASP:H	1.54	0.54
1:A:750:VAL:HG22	1:A:778:VAL:CG2	2.37	0.54
1:A:869:ALA:HB1	1:A:875:GLN:HG2	1.90	0.54
1:A:1105:GLU:HG2	1:A:1109:LYS:HD3	1.90	0.54
1:A:1148:LYS:O	1:A:1152:TRP:HD1	1.90	0.54
1:A:904:VAL:HG12	1:A:908:ALA:HB3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:ILE:O	1:A:698:MET:HG2	2.09	0.53
1:A:732:LEU:O	1:A:736:ILE:HG13	2.09	0.53
1:A:733:GLU:N	1:A:734:PRO:CD	2.72	0.53
1:A:692:VAL:HG23	1:A:693:ILE:CD1	2.36	0.53
1:A:1196:GLN:O	1:A:1200:VAL:HG23	2.09	0.52
1:A:900:ARG:HD3	1:A:900:ARG:C	2.29	0.52
1:A:749:MET:O	1:A:778:VAL:HG22	2.10	0.52
1:A:1148:LYS:O	1:A:1152:TRP:CD1	2.62	0.52
1:A:680:GLU:O	1:A:683:ARG:HG2	2.10	0.52
1:A:749:MET:HE1	1:A:831:LEU:HD12	1.91	0.52
1:A:1218:LEU:O	1:A:1222:LEU:HD13	2.10	0.52
1:A:983:MET:HE2	1:A:1091:LEU:CD2	2.38	0.51
1:A:1011:ILE:HB	1:A:1026:SER:HB3	1.93	0.51
1:A:950:PHE:HE2	1:A:976:LEU:HD13	1.75	0.51
1:A:1010:ASP:OD2	1:A:1206:ARG:HD2	2.11	0.51
1:A:1010:ASP:OD1	1:A:1027:HIS:HA	2.10	0.51
1:A:686:ALA:HB1	1:A:691:GLU:HB2	1.93	0.51
1:A:1032:GLN:NE2	1:A:1196:GLN:HB2	2.26	0.51
1:A:880:VAL:HG23	1:A:881:ALA:N	2.26	0.51
1:A:652:ALA:O	1:A:653:GLU:HB3	2.11	0.50
1:A:715:LEU:HB3	1:A:716:PRO:HD3	1.93	0.50
1:A:1152:TRP:CE3	1:A:1157:VAL:HB	2.45	0.50
1:A:926:ALA:HB1	1:A:1001:LEU:HD13	1.92	0.50
1:A:904:VAL:CG1	1:A:908:ALA:HB3	2.42	0.50
1:A:759:HIS:CB	1:A:806:LEU:HD22	2.42	0.50
1:A:950:PHE:CE2	1:A:976:LEU:CD1	2.94	0.50
1:A:760:ASP:HB2	1:A:763:LYS:HE3	1.94	0.50
1:A:778:VAL:HG23	1:A:778:VAL:O	2.12	0.50
1:A:857:VAL:HG23	1:A:862:ARG:HG3	1.95	0.49
1:A:987:LEU:HD13	1:A:992:THR:CG2	2.36	0.49
1:A:737:GLU:HG3	1:A:738:ALA:N	2.28	0.49
1:A:750:VAL:HG21	1:A:793:ALA:HA	1.95	0.49
1:A:1013:ILE:CD1	1:A:1154:LEU:HD21	2.42	0.49
1:A:1163:MET:HE3	1:A:1176:SER:HB2	1.95	0.49
1:A:857:VAL:CG2	1:A:862:ARG:HG3	2.42	0.49
1:A:960:TYR:CD1	1:A:961:PRO:HA	2.48	0.48
1:A:1107:VAL:HA	1:A:1111:TYR:HB2	1.95	0.48
1:A:1152:TRP:HZ3	1:A:1163:MET:O	1.97	0.48
1:A:748:LYS:NZ	1:A:796:VAL:HB	2.29	0.47
1:A:906:LEU:HD22	1:A:1199:GLN:HA	1.95	0.47
1:A:978:LYS:HE3	1:A:982:ASP:OD1	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:950:PHE:CE2	1:A:976:LEU:HD11	2.49	0.47
1:A:912:ASN:O	1:A:1039:ALA:HB1	2.14	0.47
1:A:946:ASP:O	1:A:949:PRO:HD2	2.14	0.47
1:A:1149:ALA:O	1:A:1153:GLU:HG3	2.15	0.47
1:A:1152:TRP:CE2	1:A:1165:LEU:HD13	2.49	0.47
1:A:753:THR:HG22	1:A:757:ASP:HB3	1.97	0.47
1:A:776:GLU:C	1:A:777:ILE:HD12	2.35	0.47
1:A:780:LEU:HD11	1:A:792:THR:HG21	1.95	0.47
1:A:869:ALA:HB1	1:A:875:GLN:CG	2.45	0.47
1:A:896:ARG:HG3	1:A:897:LYS:HG3	1.96	0.47
1:A:767:GLY:O	1:A:771:GLN:HG3	2.15	0.47
1:A:1108:ARG:HG2	1:A:1114:TYR:OH	2.15	0.47
1:A:1140:PRO:HB3	1:A:1191:ALA:HB2	1.96	0.46
1:A:904:VAL:HG21	1:A:1034:GLU:HA	1.97	0.46
1:A:921:TYR:CE2	1:A:923:PRO:HG3	2.50	0.46
1:A:652:ALA:HB3	1:A:655:ARG:CG	2.45	0.46
1:A:676:GLU:HB2	1:A:677:GLN:NE2	2.31	0.46
1:A:792:THR:O	1:A:796:VAL:HG22	2.16	0.46
1:A:877:ASP:O	1:A:880:VAL:HG22	2.14	0.46
1:A:904:VAL:HG12	1:A:905:THR:N	2.31	0.46
1:A:1198:ASP:OD1	1:A:1199:GLN:N	2.48	0.46
1:A:1087:MET:HE2	1:A:1087:MET:HA	1.97	0.46
1:A:1144:GLU:CD	1:A:1146:THR:HB	2.34	0.46
1:A:950:PHE:HB2	1:A:1094:ARG:HD2	1.97	0.46
1:A:733:GLU:CG	1:A:734:PRO:HD3	2.46	0.46
1:A:737:GLU:C	1:A:739:SER:H	2.20	0.46
1:A:898:LYS:HA	1:A:899:PRO:HD3	1.83	0.46
1:A:1200:VAL:HG13	1:A:1214:VAL:HG23	1.97	0.46
1:A:657:TRP:HB3	1:A:661:LYS:CE	2.34	0.45
1:A:683:ARG:NH2	1:A:689:PRO:HG3	2.31	0.45
1:A:1005:ASN:OD1	1:A:1019:ARG:NH1	2.45	0.45
1:A:880:VAL:O	1:A:884:ARG:HG3	2.17	0.45
1:A:1013:ILE:HD13	1:A:1154:LEU:HD21	1.98	0.45
1:A:953:THR:HG23	2:A:1301:B12:H3P3	1.99	0.45
1:A:987:LEU:HA	1:A:992:THR:CG2	2.47	0.45
1:A:692:VAL:HG23	1:A:693:ILE:N	2.32	0.45
1:A:733:GLU:HG2	1:A:734:PRO:HD3	1.99	0.45
1:A:719:VAL:CG2	1:A:1083:TYR:HD1	2.31	0.44
1:A:1144:GLU:HG3	1:A:1203:TYR:OH	2.18	0.44
1:A:651:GLN:NE2	1:A:651:GLN:N	2.66	0.44
1:A:651:GLN:O	1:A:652:ALA:CB	2.66	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1099:PHE:HD1	1:A:1099:PHE:O	2.00	0.44
1:A:740:LYS:O	1:A:741:GLU:HB2	2.18	0.44
1:A:848:GLN:NE2	1:A:891:ARG:HD3	2.33	0.44
1:A:1194:GLN:HG3	1:A:1222:LEU:O	2.18	0.43
1:A:719:VAL:HG23	1:A:1083:TYR:HD1	1.83	0.43
1:A:742:GLN:HE21	1:A:742:GLN:N	2.16	0.43
1:A:847:GLU:OE2	1:A:891:ARG:NH2	2.51	0.43
1:A:1009:ASP:HB2	1:A:1206:ARG:HH12	1.83	0.43
1:A:799:ASP:O	1:A:800:LEU:HD12	2.18	0.43
1:A:888:GLU:C	1:A:890:VAL:H	2.21	0.43
1:A:986:LYS:O	1:A:990:GLU:HG3	2.18	0.43
1:A:1081:ASP:CG	1:A:1084:ASN:OD1	2.57	0.43
1:A:1163:MET:CE	1:A:1176:SER:HB2	2.48	0.43
1:A:1172:TRP:HA	1:A:1173:PRO:C	2.37	0.43
1:A:720:LYS:HE3	1:A:1083:TYR:CZ	2.53	0.43
1:A:1134:ARG:HA	1:A:1180:TRP:O	2.19	0.43
1:A:1140:PRO:HB3	1:A:1191:ALA:CB	2.48	0.42
1:A:1184:HIS:ND1	1:A:1185:PRO:HD2	2.34	0.42
1:A:1200:VAL:HG21	1:A:1224:TYR:OH	2.19	0.42
1:A:716:PRO:O	1:A:719:VAL:HG22	2.20	0.42
1:A:888:GLU:C	1:A:890:VAL:N	2.73	0.42
1:A:1103:LEU:O	1:A:1107:VAL:HG23	2.19	0.42
1:A:1194:GLN:NE2	1:A:1220:PRO:O	2.52	0.42
1:A:764:ASN:O	1:A:768:VAL:HG23	2.20	0.42
1:A:796:VAL:O	1:A:797:ASN:C	2.57	0.42
1:A:1193:ALA:O	1:A:1221:ASN:HB3	2.19	0.42
1:A:898:LYS:HE3	1:A:900:ARG:HH21	1.84	0.42
1:A:876:ARG:NH2	1:A:877:ASP:OD1	2.53	0.42
1:A:1091:LEU:HD12	1:A:1091:LEU:HA	1.82	0.42
1:A:1068:GLU:OE1	1:A:1068:GLU:N	2.51	0.42
1:A:733:GLU:O	1:A:737:GLU:HG2	2.20	0.42
1:A:999:VAL:HG22	1:A:1000:GLY:N	2.34	0.42
1:A:987:LEU:HD12	1:A:993:LEU:CB	2.50	0.41
1:A:754:VAL:CG1	1:A:813:GLU:HB3	2.49	0.41
1:A:1067:LEU:HD11	1:A:1161:THR:O	2.20	0.41
1:A:739:SER:C	1:A:740:LYS:HG2	2.40	0.41
1:A:930:GLY:O	1:A:1000:GLY:HA2	2.19	0.41
1:A:811:LEU:HD13	1:A:841:HIS:CD2	2.56	0.41
1:A:700:GLY:O	1:A:703:VAL:HB	2.21	0.41
1:A:716:PRO:HG3	1:A:954:TRP:HB3	2.03	0.41
1:A:856:TYR:CE2	1:A:858:GLN:NE2	2.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:ILE:O	1:A:679:THR:HG22	2.21	0.41
1:A:760:ASP:HB3	1:A:782:VAL:CG1	2.51	0.40
1:A:914:PHE:CE2	1:A:916:PHE:HB2	2.56	0.40
1:A:919:GLN:HA	1:A:1054:LYS:NZ	2.36	0.40
1:A:925:VAL:HA	1:A:1057:TYR:CE2	2.55	0.40
1:A:687:THR:N	1:A:691:GLU:OE1	2.49	0.40
1:A:1074:ASP:O	1:A:1077:GLU:HB3	2.21	0.40
1:A:699:ASP:O	1:A:703:VAL:HG23	2.20	0.40
1:A:714:PHE:O	1:A:718:VAL:HG23	2.21	0.40
1:A:693:ILE:HD11	1:A:732:LEU:HD22	2.03	0.40
1:A:900:ARG:O	1:A:901:THR:HB	2.21	0.40
1:A:919:GLN:HA	1:A:1054:LYS:HZ2	1.86	0.40
1:A:1152:TRP:CZ3	1:A:1163:MET:O	2.74	0.40
1:A:902:PRO:HA	1:A:903:PRO:HD3	1.87	0.40
1:A:1048:ALA:HA	1:A:1049:PRO:HD3	1.92	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	574/579 (99%)	523 (91%)	38 (7%)	13 (2%)	6 16

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	652	ALA
1	A	743	CYS
1	A	797	ASN
1	A	898	LYS
1	A	901	THR
1	A	754	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1144	GLU
1	A	740	LYS
1	A	848	GLN
1	A	899	PRO
1	A	1028	HIS
1	A	1079	GLN
1	A	741	GLU

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	482/484 (100%)	468 (97%)	14 (3%)	42 71

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	651	GLN
1	A	663	LEU
1	A	732	LEU
1	A	740	LYS
1	A	742	GLN
1	A	823	ARG
1	A	877	ASP
1	A	1084	ASN
1	A	1091	LEU
1	A	1095	LEU
1	A	1099	PHE
1	A	1140	PRO
1	A	1144	GLU
1	A	1188	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	651	GLN
1	A	742	GLN
1	A	848	GLN
1	A	912	ASN
1	A	1040	ASN

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](#)

6 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	$\# Z > 2$
4	NO3	A	1306	-	1,3,3	0.35	0	0,3,3	-	-
4	NO3	A	1304	-	1,3,3	0.34	0	0,3,3	-	-
4	NO3	A	1305	-	1,3,3	0.32	0	0,3,3	-	-
4	NO3	A	1303	-	1,3,3	0.29	0	0,3,3	-	-
3	SAH	A	1401	-	24,28,28	0.85	1 (4%)	25,40,40	1.37	2 (8%)
2	B12	A	1301	-	90,101,101	2.52	40 (44%)	137,166,166	2.50	47 (34%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAH	A	1401	-	-	0/11/31/31	0/3/3/3
2	B12	A	1301	-	2/2/36/38	15/52/223/223	0/3/11/11

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	B12	C7B-C8B	5.62	1.52	1.40
2	A	1301	B12	O6R-C1R	5.38	1.48	1.41
2	A	1301	B12	C7B-C6B	5.30	1.51	1.37
2	A	1301	B12	C3-C4	5.23	1.65	1.51
2	A	1301	B12	C8B-C9B	5.09	1.50	1.40
2	A	1301	B12	C6-C5	4.82	1.50	1.36
2	A	1301	B12	C1-C19	-4.82	1.44	1.55
2	A	1301	B12	C14-N23	4.67	1.41	1.35
2	A	1301	B12	C60-C18	4.54	1.64	1.54
2	A	1301	B12	C54-C17	4.03	1.61	1.54
2	A	1301	B12	C36-C7	4.02	1.61	1.54
2	A	1301	B12	C55-C56	3.99	1.62	1.53
2	A	1301	B12	C12-C11	3.99	1.59	1.52
2	A	1301	B12	C25-C2	3.91	1.62	1.54
2	A	1301	B12	C48-C13	3.59	1.62	1.54
2	A	1301	B12	C7-C6	3.25	1.62	1.54
2	A	1301	B12	C6B-C5B	3.15	1.48	1.40
2	A	1301	B12	C13-C14	3.13	1.58	1.52
2	A	1301	B12	C4B-C5B	3.05	1.45	1.37
2	A	1301	B12	C43-N45	-3.02	1.22	1.32
2	A	1301	B12	O6R-C4R	2.94	1.51	1.45
2	A	1301	B12	C61-N62	-2.93	1.23	1.32
2	A	1301	B12	C55-C17	2.80	1.61	1.54
2	A	1301	B12	C38-N40	-2.80	1.23	1.32
2	A	1301	B12	C32-N33	-2.78	1.23	1.32
2	A	1301	B12	C30-C31	-2.77	1.44	1.52
2	A	1301	B12	C1-C2	2.75	1.65	1.58
2	A	1301	B12	C17-C16	2.73	1.61	1.54
2	A	1301	B12	C27-N29	-2.72	1.23	1.32
2	A	1301	B12	O8R-C5R	-2.71	1.31	1.42
2	A	1301	B12	C53-C15	2.56	1.56	1.50
2	A	1301	B12	C37-C7	2.50	1.64	1.56
2	A	1301	B12	O3-C2P	-2.50	1.39	1.45
2	A	1301	B12	C50-N52	-2.49	1.24	1.32
3	A	1401	SAH	O4'-C1'	2.48	1.44	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	B12	O58-C57	2.45	1.28	1.23
2	A	1301	B12	C30-C3	2.27	1.59	1.54
2	A	1301	B12	C18-C19	2.18	1.58	1.53
2	A	1301	B12	C4B-C9B	2.09	1.45	1.41
2	A	1301	B12	C20-C1	2.08	1.57	1.53
2	A	1301	B12	C48-C49	2.08	1.59	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	B12	C30-C3-C4	8.92	130.39	109.63
2	A	1301	B12	C48-C13-C14	7.19	126.39	108.49
2	A	1301	B12	C3-C4-N21	-6.67	103.61	111.97
2	A	1301	B12	C1-C19-C18	6.42	132.42	121.88
2	A	1301	B12	C2-C3-C4	5.51	107.89	101.63
2	A	1301	B12	C1-C19-N24	5.31	112.22	106.24
2	A	1301	B12	C2-C26-C27	5.17	129.75	115.22
2	A	1301	B12	C17-C18-C19	4.99	109.99	102.36
2	A	1301	B12	C7-C6-C5	4.90	135.78	128.07
2	A	1301	B12	C48-C13-C12	4.59	129.47	116.63
2	A	1301	B12	C41-C8-C7	4.47	126.44	114.14
2	A	1301	B12	C49-C48-C13	4.40	127.44	114.73
3	A	1401	SAH	N3-C2-N1	-4.38	121.84	128.68
2	A	1301	B12	C3-C4-C5	4.08	130.69	123.81
2	A	1301	B12	O3-C2P-C1P	-3.97	98.99	106.92
2	A	1301	B12	C56-C55-C17	3.93	123.09	115.52
2	A	1301	B12	C17-C16-N24	-3.87	105.18	111.15
2	A	1301	B12	C2-C1-C19	3.84	124.66	118.60
2	A	1301	B12	O34-C32-C31	-3.83	109.83	121.07
2	A	1301	B12	O6R-C4R-C5R	3.82	117.47	109.21
2	A	1301	B12	C20-C1-N21	-3.76	104.10	110.27
2	A	1301	B12	C31-C30-C3	3.74	125.53	114.73
2	A	1301	B12	C41-C8-C9	-3.71	104.66	111.19
2	A	1301	B12	C31-C32-N33	3.65	127.89	116.51
2	A	1301	B12	C56-C57-N59	-3.64	110.30	116.42
2	A	1301	B12	O58-C57-N59	3.47	129.56	123.01
2	A	1301	B12	C7-C37-C38	3.44	124.60	114.25
2	A	1301	B12	C55-C17-C16	-3.44	109.86	116.65
2	A	1301	B12	C60-C18-C19	3.13	122.78	114.62
2	A	1301	B12	C9-C10-C11	3.11	130.45	125.97
2	A	1301	B12	C3R-C2R-C1R	2.96	106.45	99.89
2	A	1301	B12	C20-C1-C19	-2.90	106.56	109.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	B12	C17-C16-C15	2.71	130.53	126.26
3	A	1401	SAH	C2'-C3'-C4'	-2.68	97.43	102.64
2	A	1301	B12	C25-C2-C26	-2.68	104.30	109.71
2	A	1301	B12	C5M-C5B-C4B	-2.66	113.98	120.34
2	A	1301	B12	C13-C14-N23	-2.65	105.49	109.10
2	A	1301	B12	C18-C17-C16	2.50	103.70	100.67
2	A	1301	B12	O7R-C2R-C3R	2.50	118.26	111.17
2	A	1301	B12	C7-C6-N22	-2.40	103.54	107.94
2	A	1301	B12	C48-C49-C50	2.40	120.73	112.59
2	A	1301	B12	C30-C31-C32	-2.34	104.66	112.59
2	A	1301	B12	C13-C14-C15	2.24	127.76	124.32
2	A	1301	B12	C26-C2-C3	-2.23	103.47	107.41
2	A	1301	B12	C49-C50-N52	2.22	123.41	116.51
2	A	1301	B12	C47-C12-C46	-2.19	105.66	109.35
2	A	1301	B12	C16-C15-C14	-2.18	117.94	121.25
2	A	1301	B12	C25-C2-C3	2.12	118.39	112.96
2	A	1301	B12	C5-C6-N22	-2.09	120.68	123.88

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1301	B12	C13
2	A	1301	B12	C3

All (15) torsion outliers are listed below:

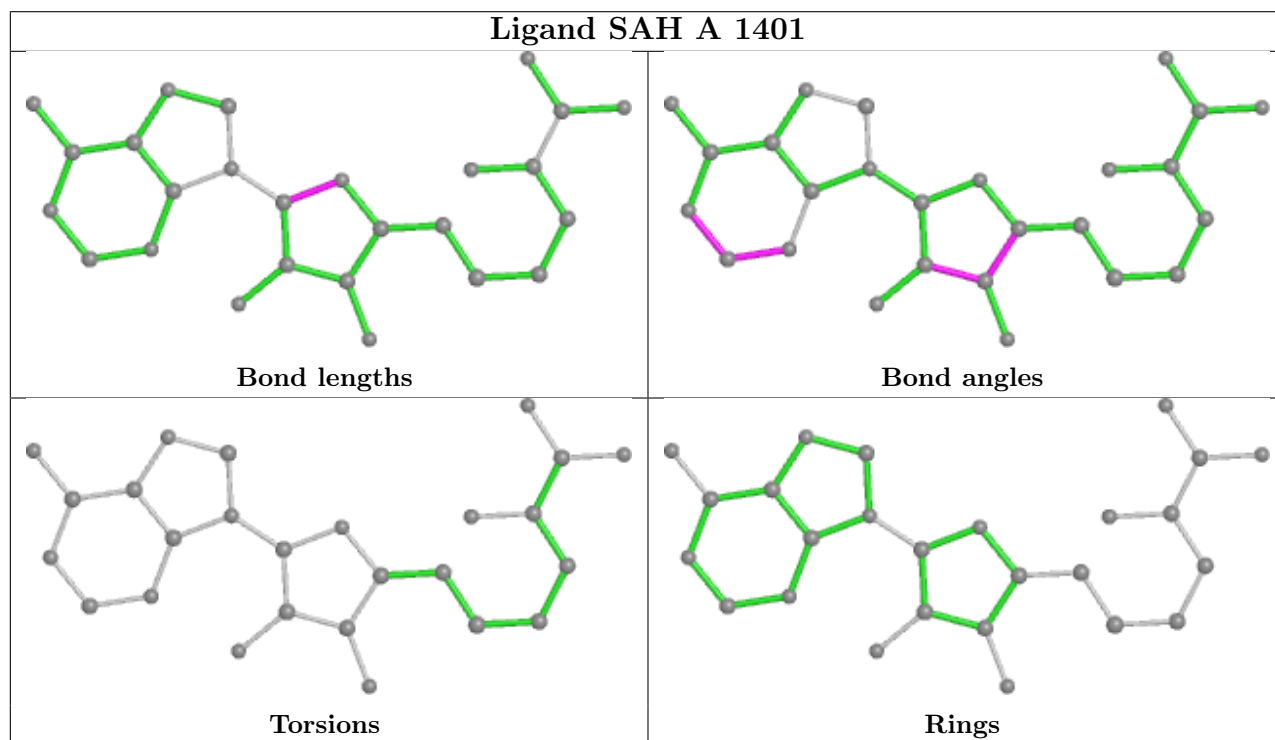
Mol	Chain	Res	Type	Atoms
2	A	1301	B12	C42-C41-C8-C7
2	A	1301	B12	C42-C41-C8-C9
2	A	1301	B12	C2P-O3-P-O4
2	A	1301	B12	C2P-O3-P-O5
2	A	1301	B12	C12-C13-C48-C49
2	A	1301	B12	C3-C30-C31-C32
2	A	1301	B12	C14-C13-C48-C49
2	A	1301	B12	C2P-O3-P-O2
2	A	1301	B12	C2-C3-C30-C31
2	A	1301	B12	C30-C31-C32-O34
2	A	1301	B12	C30-C31-C32-N33
2	A	1301	B12	N59-C1P-C2P-O3
2	A	1301	B12	C8-C41-C42-C43
2	A	1301	B12	C48-C49-C50-N52
2	A	1301	B12	C48-C49-C50-O51

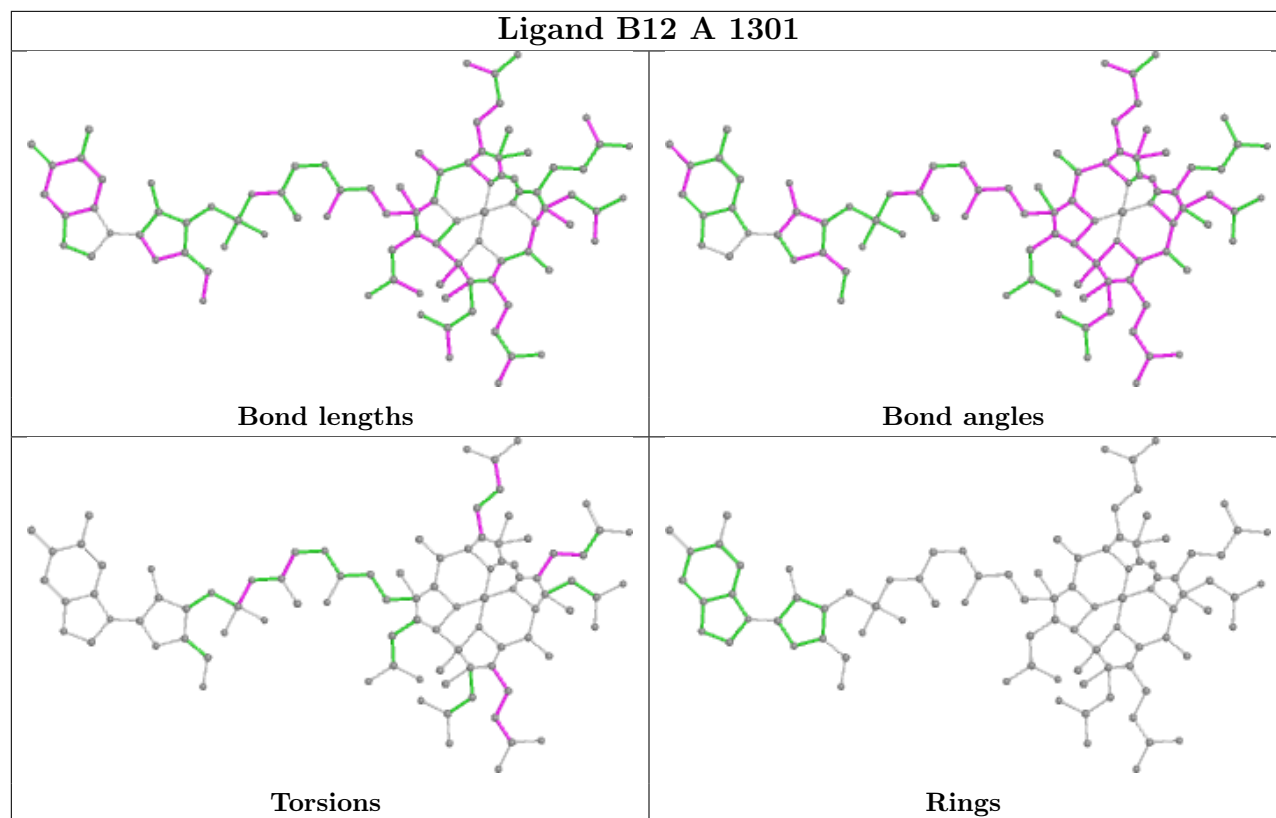
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	B12	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 [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	576/579 (99%)	0.24	21 (3%) 42 42	27, 69, 139, 181	2 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	898	LYS	11.0
1	A	897	LYS	6.4
1	A	895	GLY	6.4
1	A	896	ARG	6.0
1	A	875	GLN	5.0
1	A	874	THR	3.1
1	A	677	GLN	2.9
1	A	679	THR	2.9
1	A	900	ARG	2.8
1	A	902	PRO	2.8
1	A	869	ALA	2.5
1	A	1051	LEU	2.4
1	A	686	ALA	2.4
1	A	682	ALA	2.3
1	A	693	ILE	2.3
1	A	688	ARG	2.2
1	A	689	PRO	2.2
1	A	894	HIS	2.2
1	A	884	ARG	2.1
1	A	797	ASN	2.0
1	A	866	VAL	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](#)

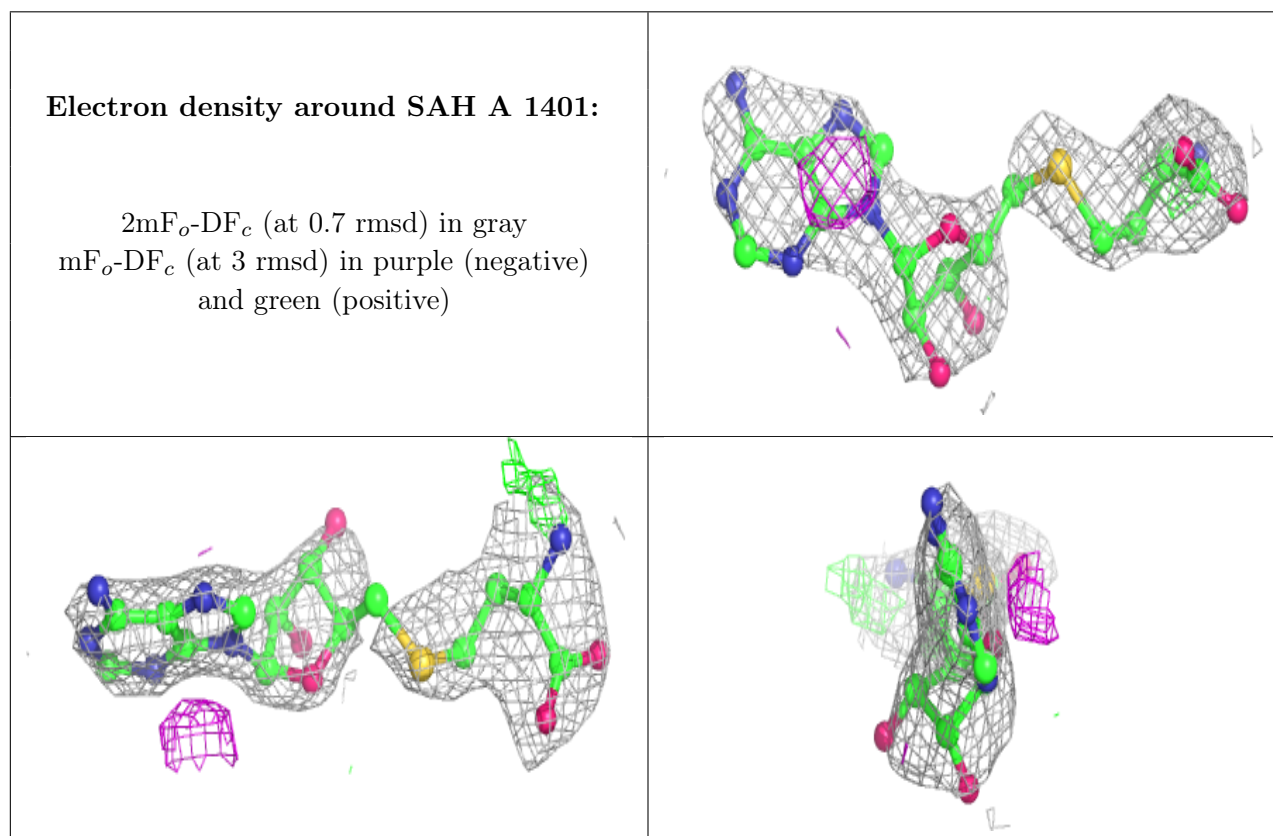
There are no monosaccharides in this entry.

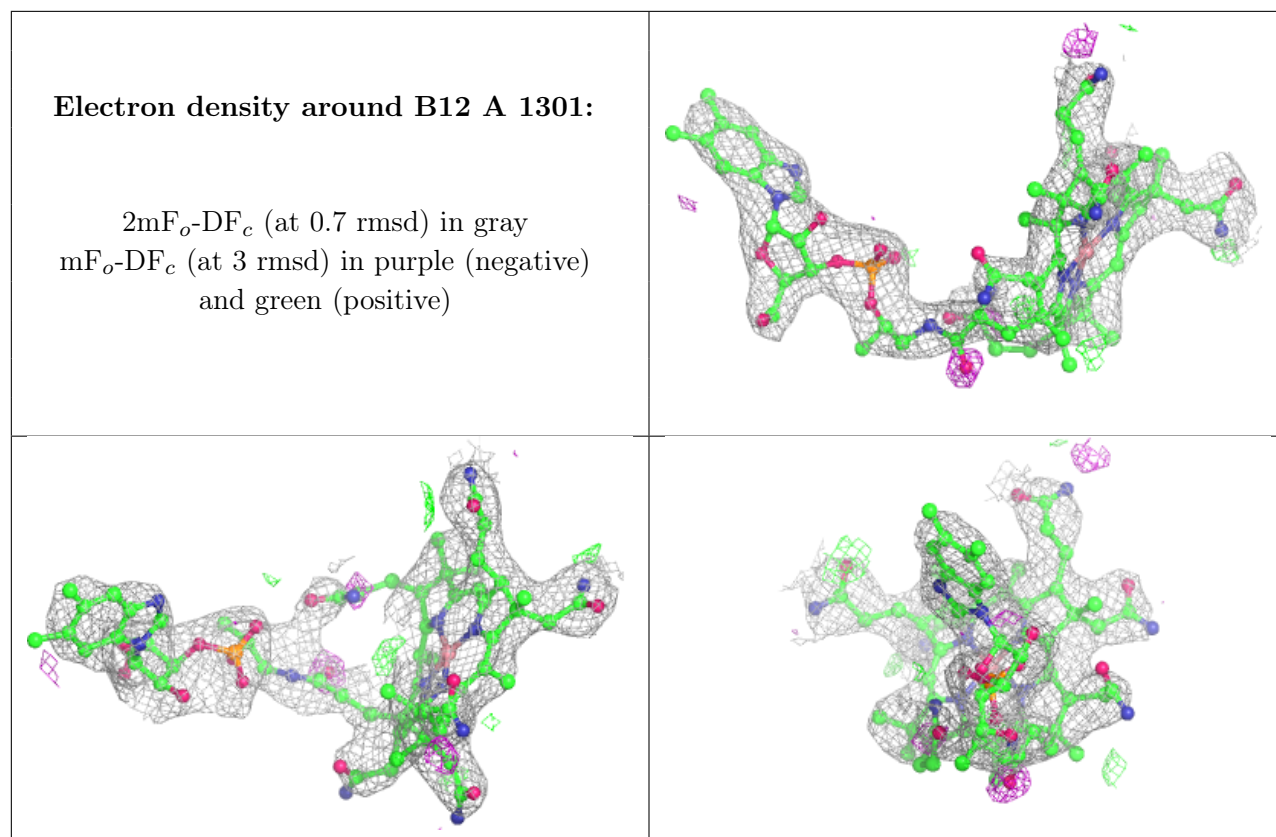
6.4 Ligands [i](#)

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
4	NO3	A	1306	4/4	0.61	0.20	146,147,147,147	0
4	NO3	A	1303	4/4	0.62	0.27	124,124,125,125	0
4	NO3	A	1305	4/4	0.65	0.52	121,122,122,123	0
3	SAH	A	1401	26/26	0.83	0.33	115,117,118,119	0
4	NO3	A	1304	4/4	0.89	0.22	120,120,120,120	0
2	B12	A	1301	91/91	0.94	0.21	59,81,89,95	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.