



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:48 PM UTC

PDB ID : 2JHP / pdb_00002jhp
Title : The structure of bluetongue virus VP4 reveals a multifunctional RNA- capping production-line
Authors : Sutton, G.; Grimes, J.M.; Stuart, D.I.; Roy, P.
Deposited on : 2007-02-23
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

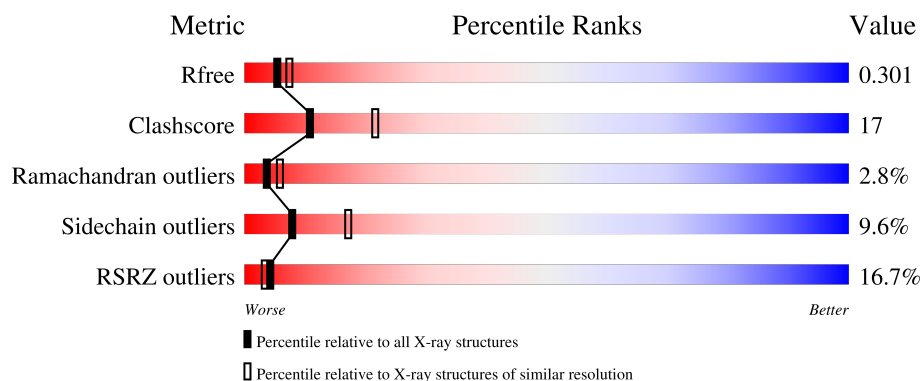
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	644	16% 68% 20% 5% 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5205 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 VP4 CORE PROTEIN.

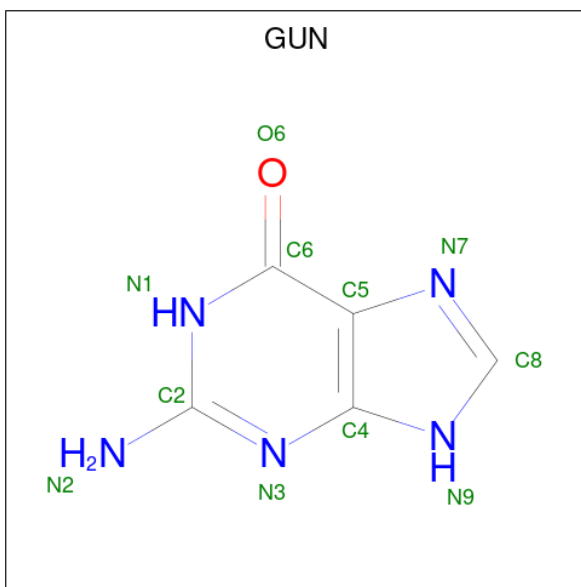
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	613	Total	C	N	O	S	0	0	0
			5040	3219	892	901	28			

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

- Molecule 3 is GUANINE (CCD ID: GUN) (formula: $C_5H_5N_5O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	5	5	1		
3	A	1	Total	C	N	O	0	0
			11	5	5	1		

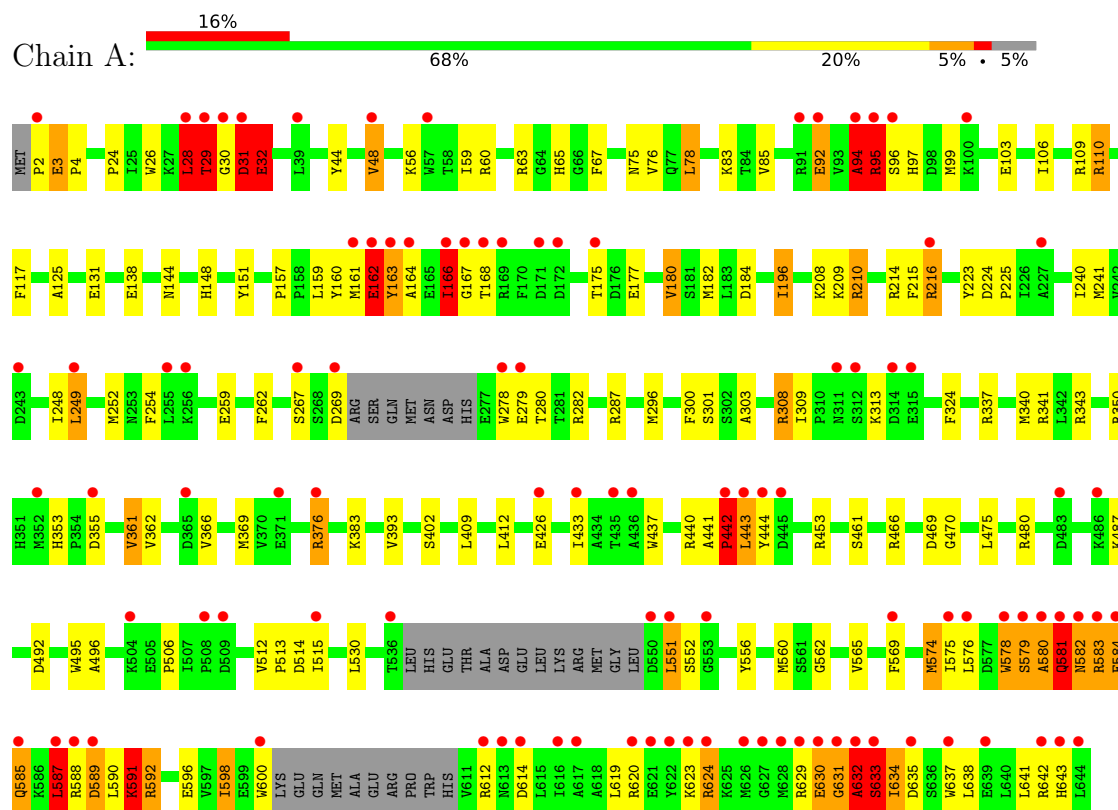
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	91	Total	O	0	0
			91	91		

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: VP4 CORE PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	76.24Å 76.24Å 421.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (20.00-2.50) 97.4 (20.00-2.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.31 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.226 , 0.289 0.238 , 0.301	Depositor DCC
R_{free} test set	1244 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 22.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	5205	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.60	0/5167	0.99	17/6981 (0.2%)

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	15

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	579	SER	N-CA-C	12.45	129.20	113.88
1	A	96	SER	N-CA-C	12.26	126.66	112.93
1	A	581	GLN	N-CA-C	10.29	132.71	110.80
1	A	580	ALA	N-CA-C	8.12	122.01	110.23
1	A	591	LYS	N-CA-C	7.70	123.34	111.56
1	A	162	GLU	N-CA-C	6.81	125.30	110.80
1	A	32	GLU	N-CA-C	6.11	123.80	110.80
1	A	162	GLU	CA-C-N	6.03	132.56	121.70
1	A	162	GLU	C-N-CA	6.03	132.56	121.70
1	A	591	LYS	CA-C-N	5.94	132.40	121.70
1	A	591	LYS	C-N-CA	5.94	132.40	121.70
1	A	94	ALA	N-CA-C	5.80	118.07	111.11
1	A	442	PRO	N-CA-C	5.76	124.34	112.47
1	A	632	ALA	N-CA-C	5.41	122.33	110.80
1	A	280	THR	N-CA-C	-5.39	105.51	111.71
1	A	442	PRO	CA-C-N	5.16	129.66	121.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	442	PRO	C-N-CA	5.16	129.66	121.72

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	28	LEU	Peptide
1	A	29	THR	Peptide
1	A	31	ASP	Peptide
1	A	442	PRO	Peptide
1	A	443	LEU	Peptide
1	A	578	TRP	Peptide
1	A	579	SER	Peptide
1	A	580	ALA	Peptide
1	A	587	LEU	Peptide
1	A	591	LYS	Peptide
1	A	631	GLY	Peptide
1	A	632	ALA	Peptide
1	A	633	SER	Peptide
1	A	94	ALA	Peptide
1	A	95	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5040	0	4985	168	0
2	A	52	0	38	3	0
3	A	22	0	10	5	0
4	A	91	0	0	9	0
All	All	5205	0	5033	168	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 17.

All (168) 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:28:LEU:HA	1:A:29:THR:CG2	1.66	1.23
1:A:28:LEU:C	1:A:29:THR:HG22	1.60	1.22
1:A:631:GLY:O	1:A:633:SER:HB2	1.40	1.18
1:A:28:LEU:CA	1:A:29:THR:HG22	1.77	1.13
1:A:29:THR:HG23	1:A:32:GLU:OE2	1.49	1.12
1:A:216:ARG:HH11	1:A:216:ARG:HG3	1.15	1.11
1:A:28:LEU:CA	1:A:29:THR:CG2	2.32	1.07
1:A:94:ALA:HB3	1:A:95:ARG:CB	1.84	1.07
1:A:28:LEU:HA	1:A:29:THR:HG23	1.33	1.06
1:A:225:PRO:HG2	1:A:241:MET:HE3	1.43	1.01
1:A:94:ALA:HB3	1:A:95:ARG:HB3	1.41	0.98
1:A:95:ARG:H	1:A:97:HIS:N	1.61	0.97
1:A:2:PRO:HD3	1:A:440:ARG:H	1.30	0.96
1:A:441:ALA:O	1:A:443:LEU:HB2	1.65	0.95
1:A:513:PRO:HB3	1:A:574:MET:HE3	1.50	0.93
1:A:95:ARG:N	1:A:97:HIS:H	1.66	0.93
1:A:631:GLY:HA3	1:A:634:ILE:HD12	1.50	0.93
1:A:210:ARG:HH11	1:A:210:ARG:HG3	1.36	0.91
1:A:630:GLU:HB3	1:A:631:GLY:HA2	1.53	0.90
1:A:631:GLY:O	1:A:633:SER:CB	2.22	0.88
1:A:634:ILE:HG22	1:A:635:ASP:H	1.35	0.88
1:A:2:PRO:HG3	1:A:453:ARG:HH22	1.40	0.85
1:A:2:PRO:HD2	1:A:453:ARG:HH12	1.40	0.84
1:A:94:ALA:HB3	1:A:95:ARG:HB2	1.57	0.84
1:A:589:ASP:HA	1:A:592:ARG:HG2	1.58	0.83
1:A:591:LYS:H	1:A:592:ARG:HB3	1.44	0.82
1:A:630:GLU:HB3	1:A:631:GLY:CA	2.09	0.82
1:A:633:SER:O	1:A:637:TRP:CD1	2.31	0.81
1:A:630:GLU:CB	1:A:631:GLY:HA2	2.07	0.81
1:A:495:TRP:HE1	3:A:1648:GUN:HN21	1.29	0.80
1:A:210:ARG:HH11	1:A:210:ARG:CG	1.94	0.80
1:A:95:ARG:H	1:A:97:HIS:H	0.84	0.80
1:A:28:LEU:C	1:A:29:THR:CG2	2.31	0.80
1:A:634:ILE:HG22	1:A:635:ASP:N	1.96	0.80
1:A:94:ALA:CB	1:A:95:ARG:HB2	2.13	0.78
1:A:94:ALA:CB	1:A:95:ARG:CB	2.62	0.78
1:A:2:PRO:HB3	1:A:440:ARG:HB2	1.66	0.77
1:A:3:GLU:H	1:A:4:PRO:CD	1.98	0.77
1:A:437:TRP:HZ2	1:A:443:LEU:HD13	1.49	0.76
1:A:216:ARG:HG3	1:A:216:ARG:NH1	1.94	0.76
1:A:512:VAL:HG22	1:A:513:PRO:HD2	1.68	0.76
1:A:383:LYS:HG2	3:A:1647:GUN:HN22	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:MET:CE	4:A:2042:HOH:O	2.36	0.74
1:A:629:ARG:O	1:A:630:GLU:HB2	1.87	0.73
1:A:28:LEU:CA	1:A:29:THR:HG23	2.09	0.73
1:A:591:LYS:N	1:A:592:ARG:HB3	2.03	0.73
1:A:177:GLU:HG3	1:A:180:VAL:HG13	1.72	0.71
1:A:633:SER:H	1:A:634:ILE:CB	2.04	0.70
1:A:2:PRO:HD3	1:A:440:ARG:N	2.05	0.70
1:A:28:LEU:HB3	1:A:32:GLU:CD	2.18	0.69
1:A:248:ILE:HB	1:A:296:MET:HE1	1.73	0.69
1:A:210:ARG:HG3	1:A:210:ARG:NH1	2.05	0.69
1:A:633:SER:H	1:A:634:ILE:HB	1.58	0.68
1:A:92:GLU:OE2	4:A:2003:HOH:O	2.12	0.67
1:A:633:SER:H	1:A:634:ILE:CA	2.08	0.66
1:A:631:GLY:C	1:A:633:SER:HB2	2.21	0.66
1:A:166:ILE:HA	1:A:167:GLY:O	1.96	0.66
1:A:341:ARG:HD2	1:A:350:ARG:O	1.97	0.65
1:A:75:ASN:HA	1:A:85:VAL:HG23	1.77	0.64
1:A:437:TRP:CZ2	1:A:443:LEU:HD13	2.30	0.64
1:A:512:VAL:CG2	1:A:513:PRO:HD2	2.29	0.63
1:A:633:SER:N	1:A:634:ILE:HB	2.14	0.62
1:A:249:LEU:HD12	1:A:254:PHE:HZ	1.64	0.62
1:A:578:TRP:O	1:A:581:GLN:HB2	2.00	0.61
1:A:214:ARG:HD2	4:A:2027:HOH:O	2.01	0.61
1:A:94:ALA:CB	1:A:95:ARG:HB3	2.25	0.61
1:A:279:GLU:HB3	1:A:282:ARG:HG3	1.83	0.60
1:A:583:ARG:HG3	1:A:584:GLU:N	2.17	0.60
1:A:513:PRO:HB3	1:A:574:MET:CE	2.29	0.59
1:A:426:GLU:HG3	4:A:2067:HOH:O	2.01	0.59
1:A:3:GLU:H	1:A:4:PRO:HD3	1.67	0.59
1:A:60:ARG:NH2	1:A:514:ASP:OD2	2.34	0.58
1:A:24:PRO:HG2	1:A:48:VAL:HG12	1.87	0.56
1:A:28:LEU:HA	1:A:29:THR:HG22	1.44	0.56
1:A:241:MET:HG3	2:A:1646:SAH:N6	2.20	0.56
1:A:634:ILE:CG2	1:A:635:ASP:N	2.65	0.56
1:A:638:LEU:O	1:A:642:ARG:HG2	2.06	0.56
1:A:30:GLY:O	1:A:56:LYS:HE2	2.06	0.56
1:A:633:SER:O	1:A:637:TRP:HD1	1.87	0.56
1:A:513:PRO:CB	1:A:574:MET:HE3	2.31	0.55
1:A:225:PRO:CG	1:A:241:MET:HE3	2.29	0.55
1:A:584:GLU:O	1:A:588:ARG:HG3	2.07	0.54
1:A:44:TYR:CG	1:A:48:VAL:HG11	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:LEU:H	1:A:588:ARG:HB2	1.73	0.54
1:A:168:THR:HG21	4:A:2018:HOH:O	2.08	0.53
1:A:214:ARG:CD	4:A:2027:HOH:O	2.54	0.53
1:A:125:ALA:HB2	1:A:433:ILE:HG21	1.92	0.52
1:A:2:PRO:CG	1:A:453:ARG:HH22	2.15	0.52
1:A:182:MET:HE1	4:A:2042:HOH:O	2.05	0.52
1:A:585:GLN:HE21	1:A:585:GLN:H	1.56	0.52
1:A:313:LYS:NZ	4:A:2045:HOH:O	2.42	0.52
1:A:248:ILE:HG22	1:A:252:MET:HE3	1.92	0.51
1:A:151:TYR:CD2	1:A:393:VAL:HB	2.46	0.51
1:A:249:LEU:HD22	1:A:296:MET:HE3	1.93	0.51
1:A:28:LEU:HB3	1:A:32:GLU:OE2	2.10	0.51
1:A:31:ASP:N	1:A:31:ASP:OD1	2.45	0.50
1:A:376:ARG:HD3	1:A:376:ARG:O	2.12	0.50
1:A:623:LYS:CB	1:A:634:ILE:HD13	2.42	0.50
1:A:157:PRO:HG2	1:A:159:LEU:HD21	1.92	0.50
1:A:530:LEU:HD21	1:A:560:MET:HB3	1.93	0.50
1:A:59:ILE:HD13	1:A:83:LYS:HD3	1.94	0.49
1:A:552:SER:HB3	1:A:614:ASP:HB3	1.95	0.49
1:A:3:GLU:N	1:A:4:PRO:CD	2.70	0.49
1:A:99:MET:O	1:A:103:GLU:HG3	2.14	0.48
1:A:588:ARG:O	1:A:590:LEU:N	2.47	0.48
1:A:341:ARG:HD3	1:A:353:HIS:O	2.14	0.48
1:A:44:TYR:CD2	1:A:48:VAL:HG11	2.49	0.48
1:A:2:PRO:CD	1:A:453:ARG:HH12	2.19	0.48
1:A:248:ILE:HD13	1:A:262:PHE:HE1	1.78	0.48
1:A:177:GLU:HG3	1:A:180:VAL:CG1	2.42	0.47
1:A:461:SER:OG	1:A:569:PHE:HB2	2.14	0.47
1:A:441:ALA:C	1:A:443:LEU:HB2	2.36	0.47
1:A:65:HIS:HE2	1:A:598:ILE:HG21	1.80	0.47
1:A:480:ARG:NH2	1:A:506:PRO:O	2.48	0.46
1:A:225:PRO:HG2	1:A:241:MET:CE	2.29	0.46
1:A:2:PRO:CD	1:A:440:ARG:H	2.15	0.46
1:A:588:ARG:C	1:A:590:LEU:H	2.23	0.46
1:A:551:LEU:HD21	1:A:575:ILE:HD12	1.97	0.46
1:A:583:ARG:O	1:A:587:LEU:HD12	2.15	0.46
1:A:632:ALA:CA	1:A:633:SER:HB2	2.46	0.46
1:A:131:GLU:OE1	1:A:402:SER:HB3	2.15	0.46
1:A:224:ASP:OD2	2:A:1646:SAH:H1'	2.15	0.46
1:A:24:PRO:HG2	1:A:48:VAL:CG1	2.46	0.45
1:A:620:ARG:O	1:A:624:ARG:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:ALA:O	1:A:635:ASP:HB2	2.15	0.45
1:A:28:LEU:O	1:A:29:THR:HG22	2.05	0.45
1:A:184:ASP:C	3:A:1647:GUN:HN21	2.24	0.45
1:A:28:LEU:HA	1:A:32:GLU:OE2	2.16	0.45
1:A:106:ILE:O	1:A:110:ARG:HB2	2.17	0.44
1:A:470:GLY:HA3	1:A:496:ALA:O	2.17	0.44
1:A:249:LEU:HD13	1:A:296:MET:HE2	1.98	0.44
1:A:633:SER:H	1:A:635:ASP:N	2.15	0.44
1:A:196:ILE:HD13	1:A:223:TYR:CD1	2.53	0.44
1:A:576:LEU:HD22	1:A:612:ARG:HG3	2.00	0.43
1:A:581:GLN:HB3	1:A:582:ASN:H	1.56	0.43
1:A:63:ARG:NH1	1:A:67:PHE:O	2.50	0.43
1:A:151:TYR:HD2	1:A:393:VAL:HB	1.83	0.43
1:A:166:ILE:HD12	1:A:369:MET:CG	2.49	0.43
1:A:632:ALA:HB3	1:A:633:SER:OG	2.19	0.43
1:A:556:TYR:CE1	1:A:560:MET:HE3	2.54	0.43
1:A:166:ILE:HD12	1:A:369:MET:HG3	2.00	0.42
1:A:574:MET:HE2	1:A:574:MET:HB2	1.87	0.42
1:A:110:ARG:HH11	1:A:492:ASP:CG	2.26	0.42
1:A:117:PHE:HD2	3:A:1648:GUN:N2	2.17	0.42
1:A:252:MET:HE1	1:A:300:PHE:CE1	2.54	0.42
1:A:453:ARG:HD2	1:A:562:GLY:O	2.19	0.42
1:A:144:ASN:H	1:A:148:HIS:CD2	2.37	0.42
1:A:144:ASN:H	1:A:148:HIS:HD2	1.68	0.42
1:A:635:ASP:HA	1:A:638:LEU:HB2	2.02	0.42
1:A:76:VAL:HG13	1:A:78:LEU:HD13	2.02	0.42
1:A:259:GLU:HG3	1:A:301:SER:HB3	2.00	0.42
1:A:162:GLU:CA	1:A:163:TYR:CB	2.98	0.42
1:A:313:LYS:NZ	4:A:2044:HOH:O	2.53	0.42
1:A:26:TRP:CE2	1:A:28:LEU:HD21	2.55	0.42
1:A:409:LEU:O	2:A:1645:SAH:N	2.53	0.42
1:A:160:TYR:OH	1:A:361:VAL:HA	2.20	0.41
1:A:182:MET:HE3	1:A:337:ARG:HD2	2.02	0.41
1:A:267:SER:HB2	1:A:308:ARG:NH2	2.35	0.41
1:A:24:PRO:CG	1:A:48:VAL:HG12	2.48	0.41
1:A:383:LYS:HG2	3:A:1647:GUN:N2	2.27	0.41
1:A:591:LYS:CA	1:A:592:ARG:HB3	2.50	0.41
1:A:208:LYS:HG3	1:A:215:PHE:CD2	2.56	0.41
1:A:585:GLN:HE21	1:A:585:GLN:N	2.18	0.41
1:A:469:ASP:HB3	1:A:565:VAL:HB	2.02	0.41
1:A:65:HIS:NE2	1:A:598:ILE:HG21	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ALA:HB3	1:A:340:MET:HB2	2.02	0.40
1:A:216:ARG:NH1	1:A:216:ARG:CG	2.70	0.40
1:A:600:TRP:HA	1:A:600:TRP:CE3	2.56	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	605/644 (94%)	554 (92%)	34 (6%)	17 (3%)	4 6

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	32	GLU
1	A	95	ARG
1	A	162	GLU
1	A	163	TYR
1	A	633	SER
1	A	166	ILE
1	A	589	ASP
1	A	632	ALA
1	A	3	GLU
1	A	164	ALA
1	A	442	PRO
1	A	587	LEU
1	A	592	ARG
1	A	630	GLU
1	A	634	ILE
1	A	581	GLN

5.3.2 Protein sidechains ⓘ

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	542/571 (95%)	490 (90%)	52 (10%)	8 17

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	29	THR
1	A	31	ASP
1	A	48	VAL
1	A	78	LEU
1	A	92	GLU
1	A	109	ARG
1	A	110	ARG
1	A	138	GLU
1	A	161	MET
1	A	166	ILE
1	A	175	THR
1	A	180	VAL
1	A	196	ILE
1	A	209	LYS
1	A	210	ARG
1	A	216	ARG
1	A	240	ILE
1	A	249	LEU
1	A	269	ASP
1	A	278	TRP
1	A	287	ARG
1	A	308	ARG
1	A	309	ILE
1	A	324	PHE
1	A	343	ARG
1	A	355	ASP
1	A	361	VAL
1	A	362	VAL
1	A	366	VAL

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Mol	Chain	Res	Type
1	A	376	ARG
1	A	412	LEU
1	A	444	TYR
1	A	466	ARG
1	A	475	LEU
1	A	487	LYS
1	A	515	ILE
1	A	551	LEU
1	A	574	MET
1	A	582	ASN
1	A	583	ARG
1	A	584	GLU
1	A	585	GLN
1	A	587	LEU
1	A	591	LYS
1	A	596	GLU
1	A	598	ILE
1	A	619	LEU
1	A	624	ARG
1	A	633	SER
1	A	641	LEU
1	A	643	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	HIS
1	A	253	ASN
1	A	307	HIS
1	A	338	ASN
1	A	400	HIS
1	A	471	ASN
1	A	585	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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$
2	SAH	A	1646	-	27,28,28	1.13	4 (14%)	36,40,40	2.03	9 (25%)
2	SAH	A	1645	-	27,28,28	1.18	4 (14%)	36,40,40	2.08	10 (27%)
3	GUN	A	1648	-	12,12,12	1.14	1 (8%)	15,17,17	2.70	8 (53%)
3	GUN	A	1647	-	12,12,12	1.29	1 (8%)	15,17,17	2.38	7 (46%)

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
2	SAH	A	1646	-	-	1/15/31/31	0/3/3/3
2	SAH	A	1645	-	-	8/15/31/31	0/3/3/3
3	GUN	A	1648	-	-	-	0/2/2/2
3	GUN	A	1647	-	-	-	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1647	GUN	C5-N7	-2.90	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1645	SAH	C2-N1	2.78	1.38	1.33
2	A	1645	SAH	C2-N3	2.77	1.38	1.33
2	A	1646	SAH	C2-N3	2.68	1.38	1.33
3	A	1648	GUN	C5-N7	-2.66	1.33	1.39
2	A	1645	SAH	C8-N7	2.37	1.36	1.31
2	A	1646	SAH	C2-N1	2.37	1.38	1.33
2	A	1645	SAH	OXT-C	-2.23	1.23	1.30
2	A	1646	SAH	OXT-C	-2.23	1.23	1.30
2	A	1646	SAH	C8-N7	2.15	1.35	1.31

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1646	SAH	N3-C2-N1	-5.88	119.69	128.58
2	A	1645	SAH	N3-C2-N1	-5.49	120.28	128.58
3	A	1648	GUN	N9-C4-N3	5.15	132.25	125.99
3	A	1648	GUN	C2-N3-C4	4.78	121.80	113.36
3	A	1647	GUN	N9-C4-N3	4.58	131.56	125.99
2	A	1645	SAH	C5-C4-N3	-4.55	120.45	126.72
2	A	1646	SAH	C5-C4-N3	-4.27	120.84	126.72
2	A	1645	SAH	C5'-SD-CG	-4.11	90.06	102.26
2	A	1646	SAH	N9-C8-N7	-4.10	108.12	113.94
3	A	1647	GUN	C2-N3-C4	3.77	120.02	113.36
2	A	1645	SAH	N9-C8-N7	-3.73	108.65	113.94
3	A	1647	GUN	C2-N1-C6	-3.66	118.47	125.11
3	A	1648	GUN	C2-N1-C6	-3.64	118.50	125.11
2	A	1646	SAH	C5-N7-C8	3.51	108.97	103.45
2	A	1646	SAH	C2-N3-C4	3.51	120.39	111.83
2	A	1645	SAH	C2-N3-C4	3.44	120.23	111.83
2	A	1645	SAH	C5-N7-C8	3.40	108.79	103.45
3	A	1648	GUN	N9-C8-N7	-3.28	109.17	112.98
2	A	1645	SAH	N3-C4-N9	3.08	132.40	127.17
3	A	1648	GUN	C8-N7-C5	2.98	108.40	104.38
3	A	1647	GUN	N9-C8-N7	-2.98	109.53	112.98
2	A	1646	SAH	C5'-SD-CG	-2.72	94.20	102.26
2	A	1646	SAH	N3-C4-N9	2.71	131.77	127.17
3	A	1647	GUN	C8-N7-C5	2.60	107.90	104.38
2	A	1646	SAH	OXT-C-O	-2.55	118.31	124.08
2	A	1645	SAH	OXT-C-O	-2.51	118.39	124.08
2	A	1646	SAH	C4-C5-N7	-2.50	107.72	110.58
2	A	1645	SAH	O4'-C1'-N9	2.43	112.76	108.09
2	A	1645	SAH	C4-C5-N7	-2.38	107.86	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1648	GUN	C5-C6-N1	2.36	119.25	113.25
3	A	1647	GUN	O6-C6-C5	-2.24	120.61	126.53
3	A	1648	GUN	O6-C6-C5	-2.17	120.79	126.53
3	A	1648	GUN	C4-C5-N7	-2.13	106.84	110.17
3	A	1647	GUN	C5-C6-N1	2.00	118.35	113.25

There are no chirality outliers.

All (9) torsion outliers are listed below:

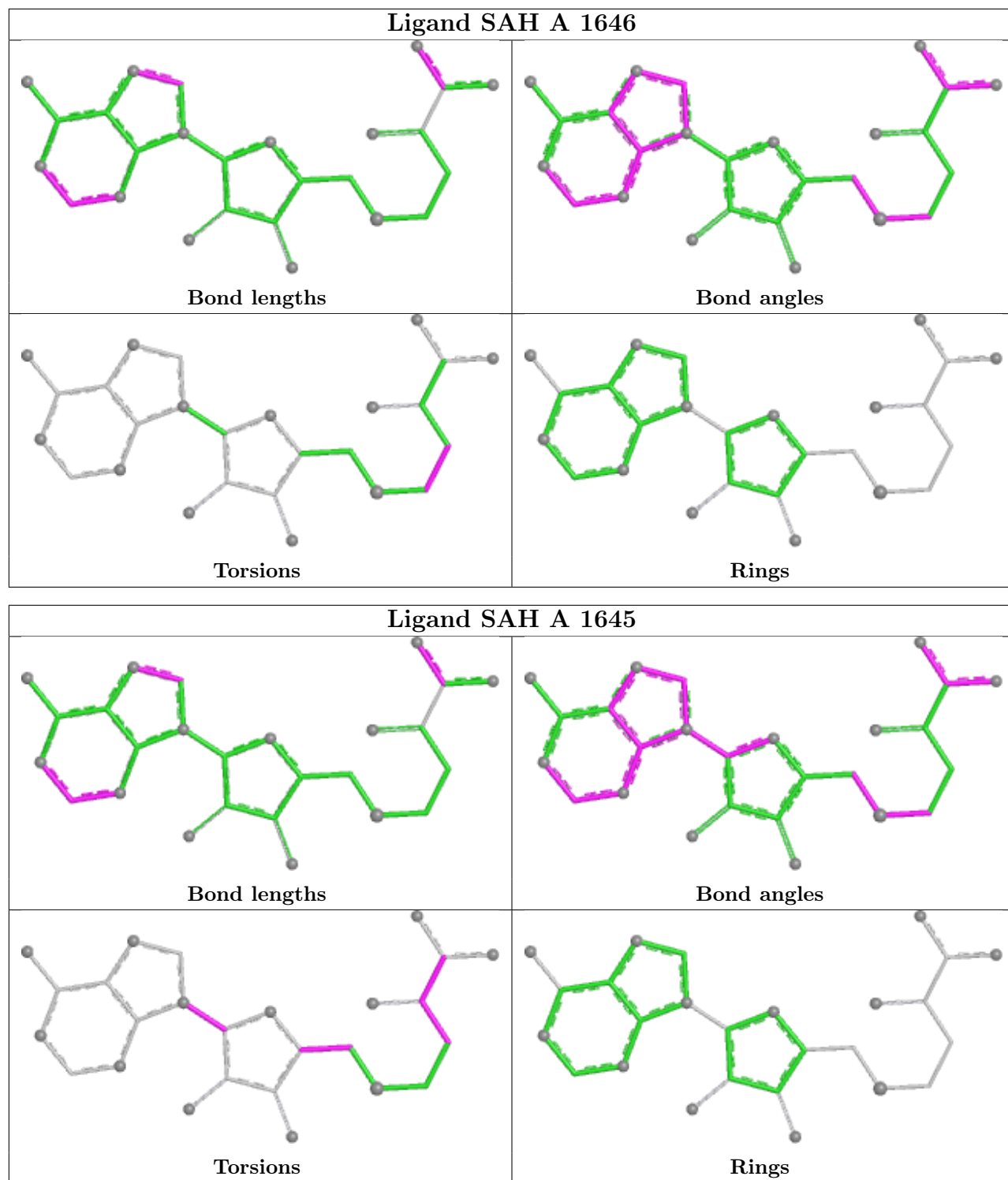
Mol	Chain	Res	Type	Atoms
2	A	1645	SAH	N-CA-CB-CG
2	A	1645	SAH	C-CA-CB-CG
2	A	1645	SAH	O4'-C4'-C5'-SD
2	A	1645	SAH	C3'-C4'-C5'-SD
2	A	1646	SAH	CA-CB-CG-SD
2	A	1645	SAH	OXT-C-CA-CB
2	A	1645	SAH	O-C-CA-CB
2	A	1645	SAH	OXT-C-CA-N
2	A	1645	SAH	C2'-C1'-N9-C8

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1646	SAH	2	0
2	A	1645	SAH	1	0
3	A	1648	GUN	2	0
3	A	1647	GUN	3	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

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	606/644 (94%)	0.99	101 (16%) 4 3	-10, 17, 39, 141	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	TRP	7.7
1	A	163	TYR	6.5
1	A	166	ILE	6.5
1	A	612	ARG	6.3
1	A	588	ARG	6.2
1	A	639	GLU	6.0
1	A	30	GLY	5.5
1	A	633	SER	5.5
1	A	631	GLY	5.3
1	A	644	LEU	5.1
1	A	584	GLU	5.1
1	A	628	MET	5.1
1	A	620	ARG	4.8
1	A	28	LEU	4.8
1	A	635	ASP	4.7
1	A	621	GLU	4.5
1	A	626	MET	4.4
1	A	164	ALA	4.4
1	A	376	ARG	4.2
1	A	624	ARG	4.2
1	A	227	ALA	4.2
1	A	31	ASP	4.0
1	A	579	SER	4.0
1	A	279	GLU	4.0
1	A	92	GLU	3.9
1	A	580	ALA	3.9
1	A	642	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	256	LYS	3.9
1	A	587	LEU	3.9
1	A	616	ILE	3.8
1	A	581	GLN	3.7
1	A	436	ALA	3.6
1	A	29	THR	3.6
1	A	614	ASP	3.4
1	A	442	PRO	3.4
1	A	632	ALA	3.4
1	A	444	TYR	3.3
1	A	622	TYR	3.3
1	A	486	LYS	3.3
1	A	509	ASP	3.3
1	A	255	LEU	3.3
1	A	583	ARG	3.3
1	A	94	ALA	3.3
1	A	162	GLU	3.2
1	A	371	GLU	3.2
1	A	585	GLN	3.2
1	A	445	ASP	3.1
1	A	443	LEU	3.1
1	A	95	ARG	3.1
1	A	617	ALA	3.1
1	A	550	ASP	3.1
1	A	589	ASP	3.1
1	A	508	PRO	3.0
1	A	243	ASP	3.0
1	A	435	THR	2.9
1	A	600	TRP	2.9
1	A	172	ASP	2.8
1	A	269	ASP	2.8
1	A	623	LYS	2.8
1	A	551	LEU	2.7
1	A	314	ASP	2.7
1	A	167	GLY	2.6
1	A	365	ASP	2.6
1	A	352	MET	2.6
1	A	629	ARG	2.6
1	A	575	ILE	2.6
1	A	96	SER	2.6
1	A	483	ASP	2.6
1	A	578	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	175	THR	2.5
1	A	267	SER	2.5
1	A	515	ILE	2.5
1	A	39	LEU	2.5
1	A	576	LEU	2.5
1	A	630	GLU	2.4
1	A	627	GLY	2.4
1	A	355	ASP	2.4
1	A	169	ARG	2.4
1	A	312	SER	2.4
1	A	249	LEU	2.4
1	A	613	ASN	2.4
1	A	504	LYS	2.4
1	A	2	PRO	2.3
1	A	553	GLY	2.3
1	A	100	LYS	2.3
1	A	569	PHE	2.3
1	A	57	TRP	2.2
1	A	637	TRP	2.2
1	A	643	HIS	2.2
1	A	161	MET	2.2
1	A	168	THR	2.2
1	A	433	ILE	2.2
1	A	536	THR	2.2
1	A	315	GLU	2.2
1	A	48	VAL	2.1
1	A	582	ASN	2.1
1	A	216	ARG	2.1
1	A	91	ARG	2.0
1	A	426	GLU	2.0
1	A	311	ASN	2.0
1	A	171	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](#)

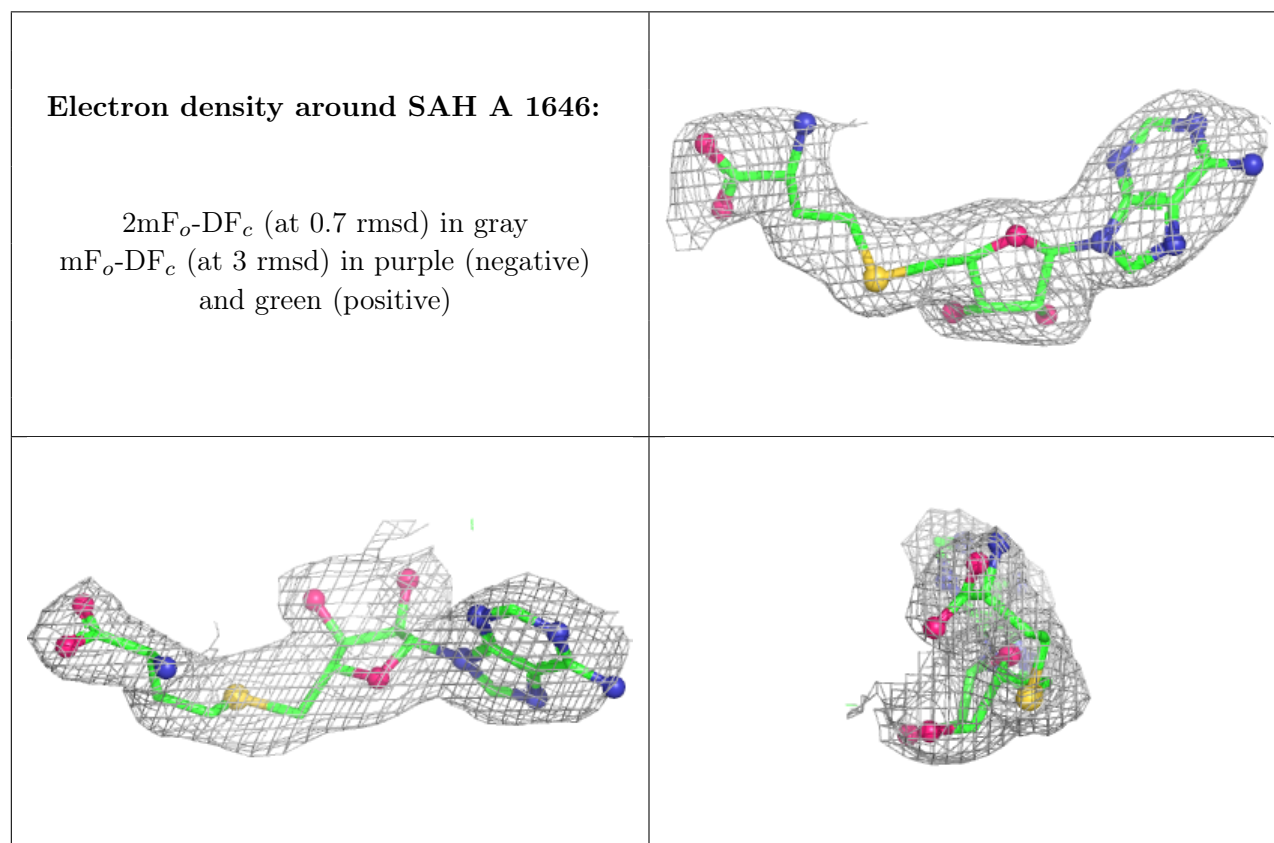
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

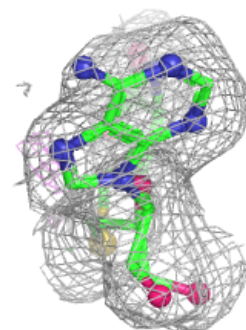
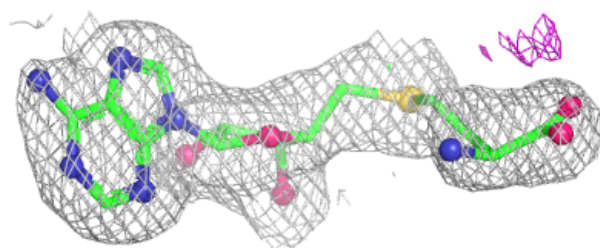
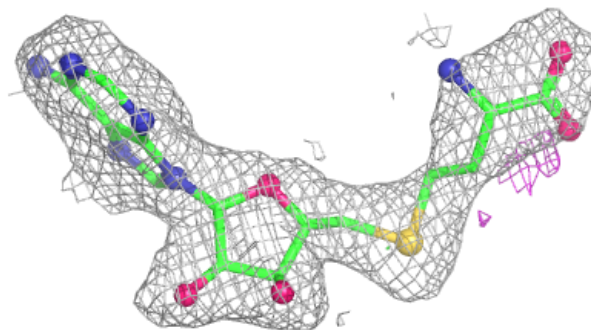
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GUN	A	1648	11/11	0.82	0.18	22,82,119,127	0
2	SAH	A	1646	26/26	0.89	0.10	5,27,49,57	0
3	GUN	A	1647	11/11	0.91	0.12	19,30,50,88	0
2	SAH	A	1645	26/26	0.95	0.10	-7,9,34,48	0

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



Electron density around SAH A 1645:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.