



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:18 AM UTC

PDB ID : 4CKE / pdb_00004cke
Title : Vaccinia virus capping enzyme complexed with SAH in P1 form
Authors : Kyrieleis, O.J.P.; Chang, J.; de la Pena, M.; Shuman, S.; Cusack, S.
Deposited on : 2014-01-03
Resolution : 2.90 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

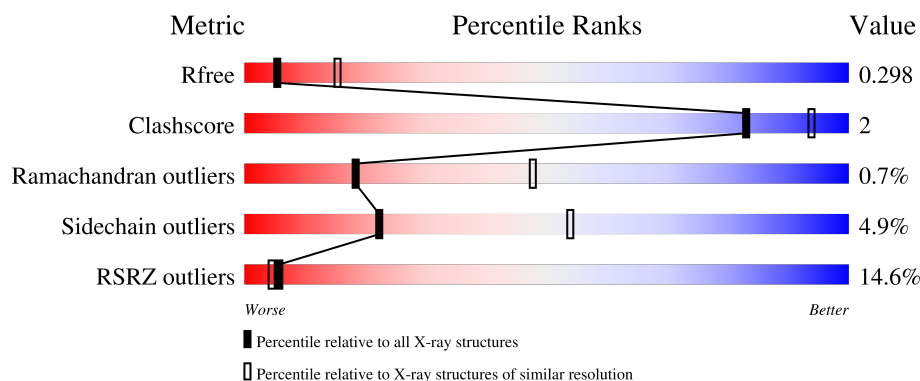
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	844	17% 84% 11% 5%
1	D	844	14% 84% 12% ••
2	B	287	8% 90% 9% •
2	E	287	13% 88% 9% •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17794 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.

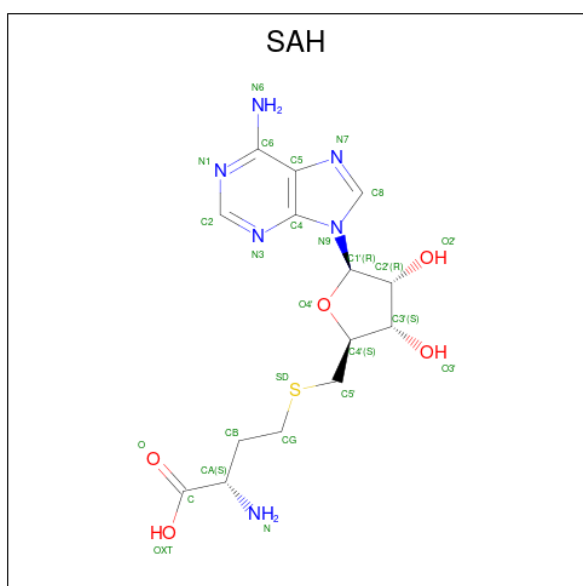
- Molecule 1 is a protein called MRNA-CAPPING ENZYME CATALYTIC SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	802	Total	C	N	O	S	0	1	0
			6485	4181	1060	1226	18			
1	D	813	Total	C	N	O	S	0	1	0
			6583	4245	1080	1239	19			

- Molecule 2 is a protein called MRNA-CAPPING ENZYME REGULATORY SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	284	Total	C	N	O	S	0	0	0
			2320	1492	385	430	13			
2	E	278	Total	C	N	O	S	0	0	0
			2278	1468	375	422	13			

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



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

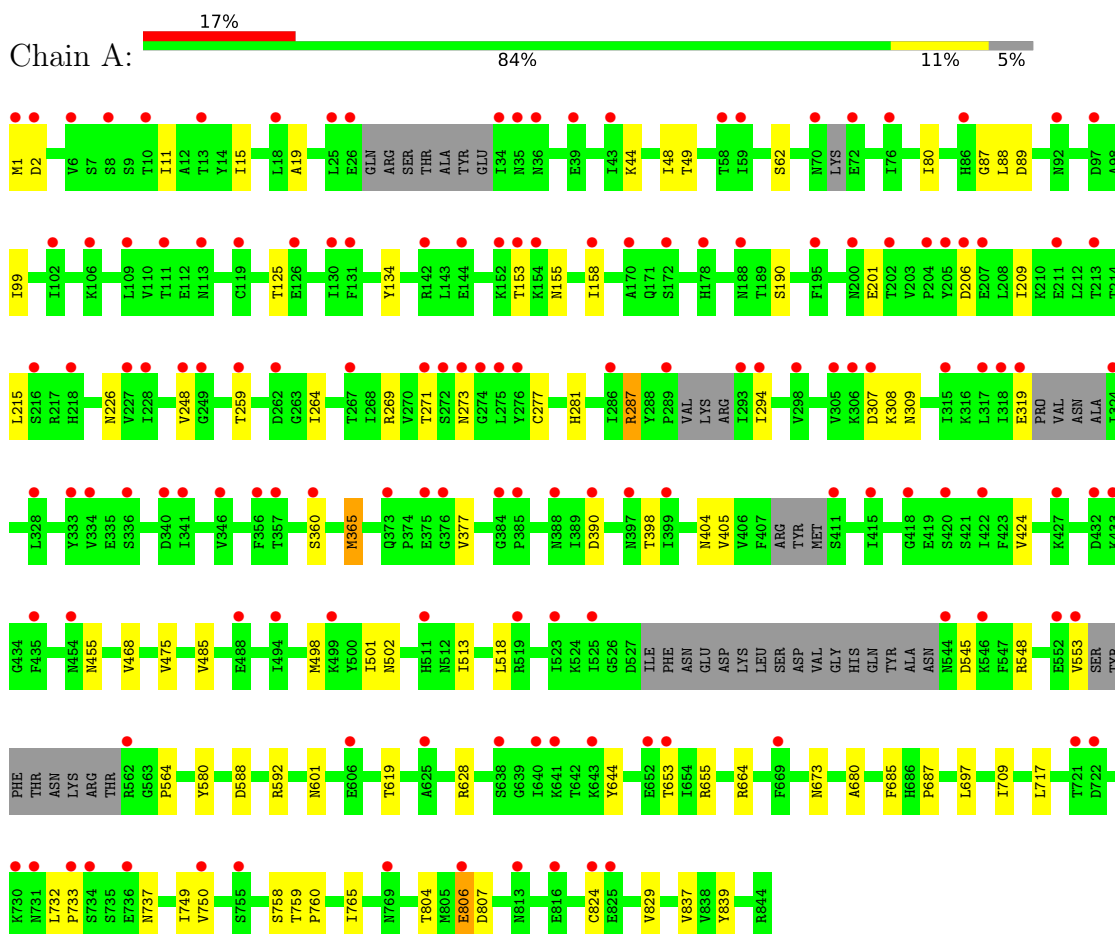
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	11	Total	O	0	0
			11	11		
4	D	37	Total	O	0	0
			37	37		
4	E	5	Total	O	0	0
			5	5		

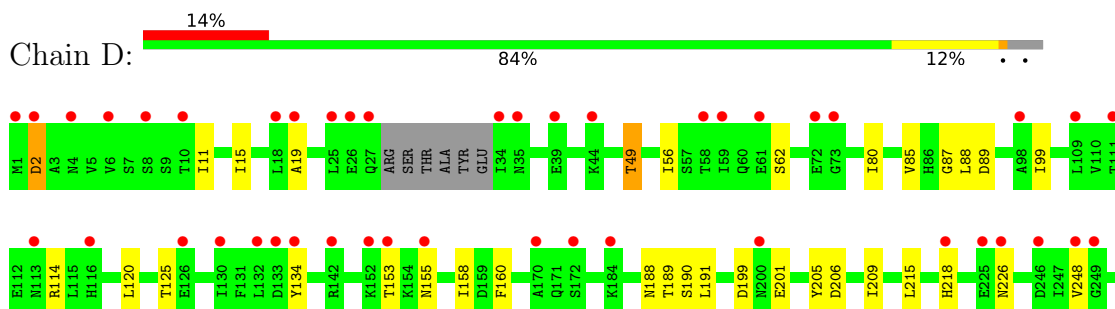
3 Residue-property plots

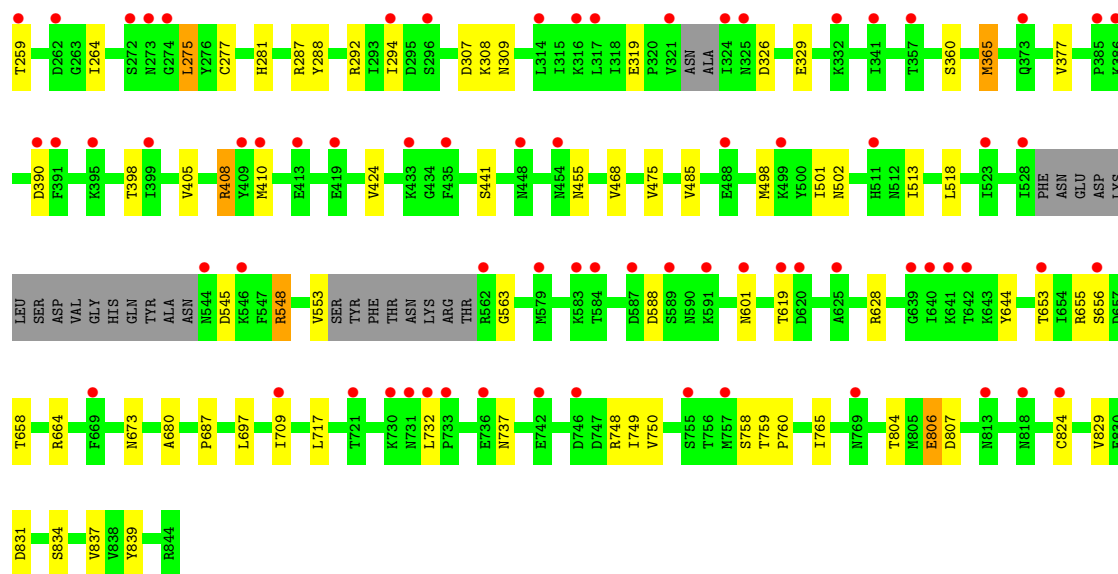
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: MRNA-CAPPING ENZYME CATALYTIC SUBUNIT

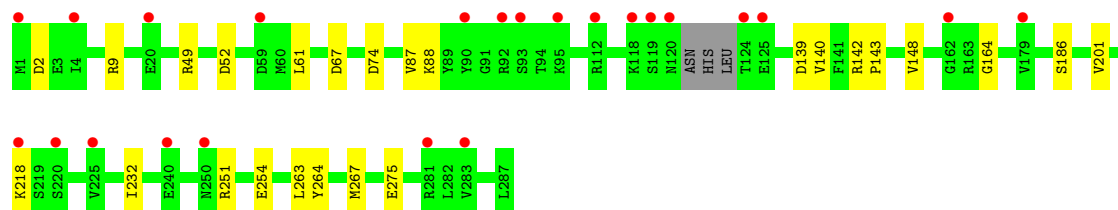
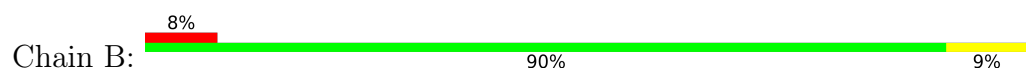


• Molecule 1: MRNA-CAPPING ENZYME CATALYTIC SUBUNIT

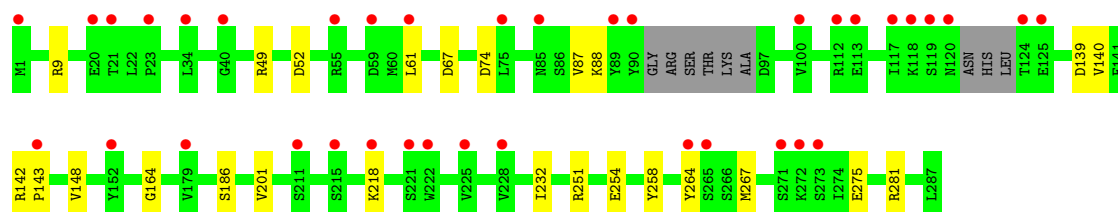
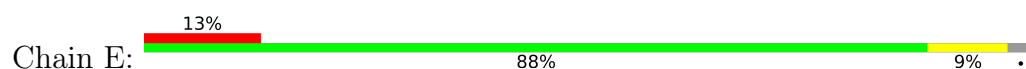




• Molecule 2: MRNA-CAPPING ENZYME REGULATORY SUBUNIT



• Molecule 2: MRNA-CAPPING ENZYME REGULATORY SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.13Å 62.02Å 198.50Å 90.01° 85.53° 71.69°	Depositor
Resolution (Å)	41.81 – 2.90 41.81 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.8 (41.81-2.90) 94.8 (41.81-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.91Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.255 , 0.295 0.260 , 0.298	Depositor DCC
R_{free} test set	2929 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.035 for k,h,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	17794	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.31	0/6612	0.68	2/8936 (0.0%)
1	D	0.31	0/6715	0.68	2/9078 (0.0%)
2	B	0.29	0/2365	0.65	0/3189
2	E	0.29	0/2322	0.65	0/3131
All	All	0.30	0/18014	0.67	4/24334 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	LYS	CA-C-N	5.46	126.01	120.38
1	A	44	LYS	C-N-CA	5.46	126.01	120.38
1	D	563	GLY	CA-C-N	5.16	126.28	119.84
1	D	563	GLY	C-N-CA	5.16	126.28	119.84

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	6485	0	6552	33	0
1	D	6583	0	6669	40	0
2	B	2320	0	2363	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2278	0	2316	7	0
3	A	26	0	19	1	0
3	D	26	0	19	1	0
4	A	23	0	0	1	0
4	B	11	0	0	0	0
4	D	37	0	0	3	0
4	E	5	0	0	0	0
All	All	17794	0	17938	86	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 2.

All (86) 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:87:GLY:O	1:A:89:ASP:N	2.30	0.64
1:D:87:GLY:O	1:D:89:ASP:N	2.30	0.64
1:A:485:VAL:HG11	1:A:518:LEU:HA	1.83	0.61
1:D:99:ILE:O	1:D:134:TYR:OH	2.18	0.61
1:A:99:ILE:O	1:A:134:TYR:OH	2.18	0.60
1:D:485:VAL:HG11	1:D:518:LEU:HA	1.81	0.60
1:D:62:SER:OG	1:D:455:ASN:O	2.19	0.59
1:D:226:ASN:OD1	1:D:287:ARG:NH1	2.38	0.56
1:A:588:ASP:O	1:A:592:ARG:NH2	2.38	0.56
1:D:545:ASP:OD1	1:D:655:ARG:NH1	2.41	0.53
2:B:74:ASP:N	2:B:74:ASP:OD1	2.43	0.52
1:A:545:ASP:OD1	1:A:655:ARG:NH1	2.42	0.52
1:D:548:ARG:NH2	4:D:2020:HOH:O	2.43	0.51
2:B:61:LEU:HD12	2:B:267:MET:HE1	1.92	0.51
1:A:62:SER:OG	1:A:455:ASN:O	2.29	0.51
2:E:74:ASP:N	2:E:74:ASP:OD1	2.44	0.51
1:A:226:ASN:OD1	1:A:287:ARG:NH1	2.46	0.49
2:E:61:LEU:HD12	2:E:267:MET:HE1	1.94	0.49
1:D:498:MET:O	1:D:502:ASN:ND2	2.45	0.49
1:A:19:ALA:HB3	1:A:209:ILE:HD11	1.95	0.49
1:A:685:PHE:N	4:A:2018:HOH:O	2.45	0.49
1:A:201:GLU:N	1:A:201:GLU:OE1	2.46	0.49
1:D:19:ALA:HB3	1:D:209:ILE:HD11	1.94	0.49
1:D:275:LEU:N	1:D:288:TYR:O	2.40	0.49
1:D:709:ILE:HB	1:D:839:TYR:HB2	1.97	0.47
1:D:2:ASP:OD1	1:D:2:ASP:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:MET:HE1	1:A:377:VAL:HG11	1.97	0.47
1:A:709:ILE:HB	1:A:839:TYR:HB2	1.96	0.46
1:A:498:MET:O	1:A:502:ASN:ND2	2.47	0.46
1:D:408:ARG:C	1:D:410:MET:H	2.24	0.46
1:A:759:THR:HB	1:A:760:PRO:HD2	1.98	0.45
1:D:206:ASP:OD1	1:D:206:ASP:N	2.49	0.45
1:A:264:ILE:HD11	1:A:281:HIS:HB3	1.98	0.45
2:B:2:ASP:N	2:B:2:ASP:OD1	2.50	0.45
1:A:271:THR:HG22	1:A:273:ASN:H	1.82	0.45
1:A:307:ASP:O	1:A:309:ASN:N	2.50	0.45
1:A:717:LEU:HD13	1:A:749:ILE:CD1	2.46	0.45
1:D:759:THR:HB	1:D:760:PRO:HD2	1.99	0.44
2:E:52:ASP:HB3	2:E:264:TYR:CE1	2.51	0.44
1:D:717:LEU:HD13	1:D:749:ILE:CD1	2.48	0.44
1:D:601:ASN:OD1	1:D:628:ARG:NH1	2.49	0.44
1:A:601:ASN:OD1	1:A:628:ARG:NH1	2.51	0.43
2:B:87:VAL:HG12	2:B:88:LYS:N	2.33	0.43
2:E:87:VAL:HG12	2:E:88:LYS:N	2.33	0.43
1:A:2:ASP:OD1	1:A:2:ASP:N	2.47	0.43
1:A:806:GLU:HA	2:B:49:ARG:HH12	1.83	0.43
1:A:806:GLU:OE1	1:A:807:ASP:N	2.52	0.43
1:D:153:THR:O	1:D:155:ASN:N	2.43	0.42
2:E:258:TYR:OH	2:E:281:ARG:NH2	2.52	0.42
1:A:749:ILE:HG22	1:A:750:VAL:N	2.34	0.42
1:D:365:MET:HE1	1:D:377:VAL:HG11	2.01	0.42
1:D:748:ARG:NH2	4:D:2019:HOH:O	2.52	0.42
1:D:806:GLU:OE1	1:D:807:ASP:N	2.52	0.42
1:D:205:TYR:CZ	1:D:209:ILE:HG13	2.55	0.42
1:A:1:MET:HE3	1:A:269:ARG:HB2	2.02	0.42
1:A:153:THR:O	1:A:155:ASN:N	2.44	0.41
1:D:56:ILE:HG23	1:D:218:HIS:NE2	2.35	0.41
1:A:206:ASP:OD1	1:A:206:ASP:N	2.53	0.41
1:D:656:SER:HG	1:D:658:THR:HG1	1.58	0.41
1:D:405:VAL:HG13	1:D:424:VAL:HG22	2.02	0.41
1:D:806:GLU:HA	2:E:49:ARG:HH12	1.86	0.41
1:A:732:LEU:HB3	1:A:737:ASN:HB3	2.03	0.41
1:A:749:ILE:HD11	1:A:765:ILE:HG12	2.03	0.41
2:B:263:LEU:HG	2:B:267:MET:HE3	2.03	0.41
1:D:114:ARG:HB2	1:D:120:LEU:HD23	2.02	0.41
1:D:264:ILE:HD11	1:D:281:HIS:HB3	2.03	0.41
1:D:655:ARG:NH2	3:D:1845:SAH:N7	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:TYR:O	1:A:592:ARG:NH1	2.54	0.41
1:A:655:ARG:NH2	3:A:1845:SAH:N7	2.69	0.41
2:B:52:ASP:HB3	2:B:264:TYR:CE1	2.56	0.41
1:D:49:THR:HG21	1:D:191:LEU:HD22	2.03	0.41
1:D:732:LEU:HB3	1:D:737:ASN:HB3	2.02	0.41
1:D:749:ILE:HD11	1:D:765:ILE:HG12	2.02	0.41
1:A:732:LEU:HD23	1:A:733:PRO:HD2	2.03	0.41
2:B:142:ARG:N	2:B:143:PRO:CD	2.84	0.41
1:D:158:ILE:HD11	1:D:215:LEU:HD11	2.01	0.41
1:D:831:ASP:O	1:D:834:SER:OG	2.35	0.40
1:A:405:VAL:HG13	1:A:424:VAL:HG22	2.03	0.40
1:D:158:ILE:CD1	1:D:215:LEU:HD11	2.50	0.40
1:D:307:ASP:O	1:D:309:ASN:N	2.54	0.40
1:D:588:ASP:OD2	4:D:2024:HOH:O	2.22	0.40
1:A:158:ILE:CD1	1:A:215:LEU:HD11	2.52	0.40
1:D:749:ILE:HG22	1:D:750:VAL:N	2.35	0.40
1:D:160:PHE:CZ	1:D:189:THR:HG23	2.56	0.40
1:D:326:ASP:OD2	1:D:329:GLU:N	2.50	0.40
2:E:142:ARG:N	2:E:143:PRO:CD	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	787/844 (93%)	719 (91%)	62 (8%)	6 (1%)	16	44
1	D	804/844 (95%)	734 (91%)	65 (8%)	5 (1%)	21	51
2	B	280/287 (98%)	257 (92%)	21 (8%)	2 (1%)	18	48
2	E	272/287 (95%)	250 (92%)	20 (7%)	2 (1%)	18	48
All	All	2143/2262 (95%)	1960 (92%)	168 (8%)	15 (1%)	18	48

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	LEU
1	D	88	LEU
2	B	164	GLY
2	E	164	GLY
1	A	308	LYS
1	A	680	ALA
1	D	680	ALA
2	B	148	VAL
1	D	308	LYS
2	E	148	VAL
1	A	248	VAL
1	A	564	PRO
1	A	687	PRO
1	D	248	VAL
1	D	687	PRO

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	737/774 (95%)	702 (95%)	35 (5%)	23	56
1	D	748/774 (97%)	707 (94%)	41 (6%)	19	50
2	B	269/272 (99%)	258 (96%)	11 (4%)	27	61
2	E	265/272 (97%)	254 (96%)	11 (4%)	26	60
All	All	2019/2092 (96%)	1921 (95%)	98 (5%)	22	54

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	A	15	ILE
1	A	48	ILE
1	A	49	THR
1	A	80	ILE

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Mol	Chain	Res	Type
1	A	125	THR
1	A	190	SER
1	A	259	THR
1	A	277	CYS
1	A	287	ARG
1	A	294	ILE
1	A	319	GLU
1	A	360	SER
1	A	365	MET
1	A	390	ASP
1	A	398	THR
1	A	404	ASN
1	A	468	VAL
1	A	475	VAL
1	A	501	ILE
1	A	513	ILE
1	A	548	ARG
1	A	553	VAL
1	A	619	THR
1	A	644	TYR
1	A	653	THR
1	A	664	ARG
1	A	673	ASN
1	A	697	LEU
1	A	758	SER
1	A	804	THR
1	A	806	GLU
1	A	824	CYS
1	A	829	VAL
1	A	837	VAL
2	B	9	ARG
2	B	67	ASP
2	B	139	ASP
2	B	140	VAL
2	B	186	SER
2	B	201	VAL
2	B	218	LYS
2	B	232	ILE
2	B	251	ARG
2	B	254	GLU
2	B	275	GLU
1	D	2	ASP

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Mol	Chain	Res	Type
1	D	11	ILE
1	D	15	ILE
1	D	49	THR
1	D	80	ILE
1	D	85	VAL
1	D	125	THR
1	D	188	ASN
1	D	190	SER
1	D	199	ASP
1	D	201	GLU
1	D	259	THR
1	D	275	LEU
1	D	277	CYS
1	D	292	ARG
1	D	294	ILE
1	D	319	GLU
1	D	360	SER
1	D	365	MET
1	D	390	ASP
1	D	398	THR
1	D	408	ARG
1	D	441	SER
1	D	468	VAL
1	D	475	VAL
1	D	501	ILE
1	D	513	ILE
1	D	548	ARG
1	D	553	VAL
1	D	619	THR
1	D	644	TYR
1	D	653	THR
1	D	664	ARG
1	D	673	ASN
1	D	697	LEU
1	D	758	SER
1	D	804	THR
1	D	806	GLU
1	D	824	CYS
1	D	829	VAL
1	D	837	VAL
2	E	9	ARG
2	E	67	ASP

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Mol	Chain	Res	Type
2	E	139	ASP
2	E	140	VAL
2	E	186	SER
2	E	201	VAL
2	E	218	LYS
2	E	232	ILE
2	E	251	ARG
2	E	254	GLU
2	E	275	GLU

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

Mol	Chain	Res	Type
1	A	4	ASN
1	A	36	ASN
1	A	785	ASN
2	B	66	HIS
2	B	278	HIS
1	D	36	ASN
1	D	454	ASN
2	E	66	HIS
2	E	178	ASN
2	E	235	ASN
2	E	278	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 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	SAH	D	1845	-	27,28,28	1.10	4 (14%)	36,40,40	2.11	10 (27%)
3	SAH	A	1845	-	27,28,28	1.12	4 (14%)	36,40,40	2.14	10 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAH	D	1845	-	-	3/15/31/31	0/3/3/3
3	SAH	A	1845	-	-	4/15/31/31	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1845	SAH	C2-N3	2.60	1.38	1.33
3	D	1845	SAH	C2-N3	2.56	1.38	1.33
3	A	1845	SAH	C2-N1	2.55	1.38	1.33
3	D	1845	SAH	C2-N1	2.47	1.38	1.33
3	D	1845	SAH	C5-N7	-2.27	1.34	1.39
3	D	1845	SAH	OXT-C	-2.19	1.23	1.30
3	A	1845	SAH	OXT-C	-2.19	1.23	1.30
3	A	1845	SAH	C5-N7	-2.19	1.35	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1845	SAH	N3-C2-N1	-5.47	120.30	128.58
3	D	1845	SAH	N3-C2-N1	-5.42	120.37	128.58
3	A	1845	SAH	C5-C4-N3	-5.40	119.28	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1845	SAH	C5-C4-N3	-5.37	119.33	126.72
3	D	1845	SAH	N3-C4-N9	3.83	133.68	127.17
3	A	1845	SAH	N9-C8-N7	-3.81	108.53	113.94
3	D	1845	SAH	N9-C8-N7	-3.80	108.55	113.94
3	A	1845	SAH	N3-C4-N9	3.77	133.58	127.17
3	A	1845	SAH	C5-N7-C8	3.69	109.25	103.45
3	D	1845	SAH	C5-N7-C8	3.69	109.25	103.45
3	A	1845	SAH	C2-N3-C4	3.68	120.81	111.83
3	D	1845	SAH	C2-N3-C4	3.60	120.62	111.83
3	A	1845	SAH	C5'-SD-CG	-3.15	92.90	102.26
3	D	1845	SAH	OXT-C-O	-2.56	118.28	124.08
3	A	1845	SAH	OXT-C-O	-2.51	118.38	124.08
3	D	1845	SAH	C6-C5-C4	2.49	120.57	117.18
3	A	1845	SAH	C4-C5-N7	-2.47	107.76	110.58
3	A	1845	SAH	C6-C5-C4	2.43	120.50	117.18
3	D	1845	SAH	C4-C5-N7	-2.35	107.89	110.58
3	D	1845	SAH	C5'-SD-CG	-2.33	95.33	102.26

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1845	SAH	C2'-C1'-N9-C4
3	D	1845	SAH	C2'-C1'-N9-C4
3	D	1845	SAH	C2'-C1'-N9-C8
3	A	1845	SAH	C2'-C1'-N9-C8
3	A	1845	SAH	CB-CG-SD-C5'
3	A	1845	SAH	O4'-C1'-N9-C8
3	D	1845	SAH	O4'-C1'-N9-C8

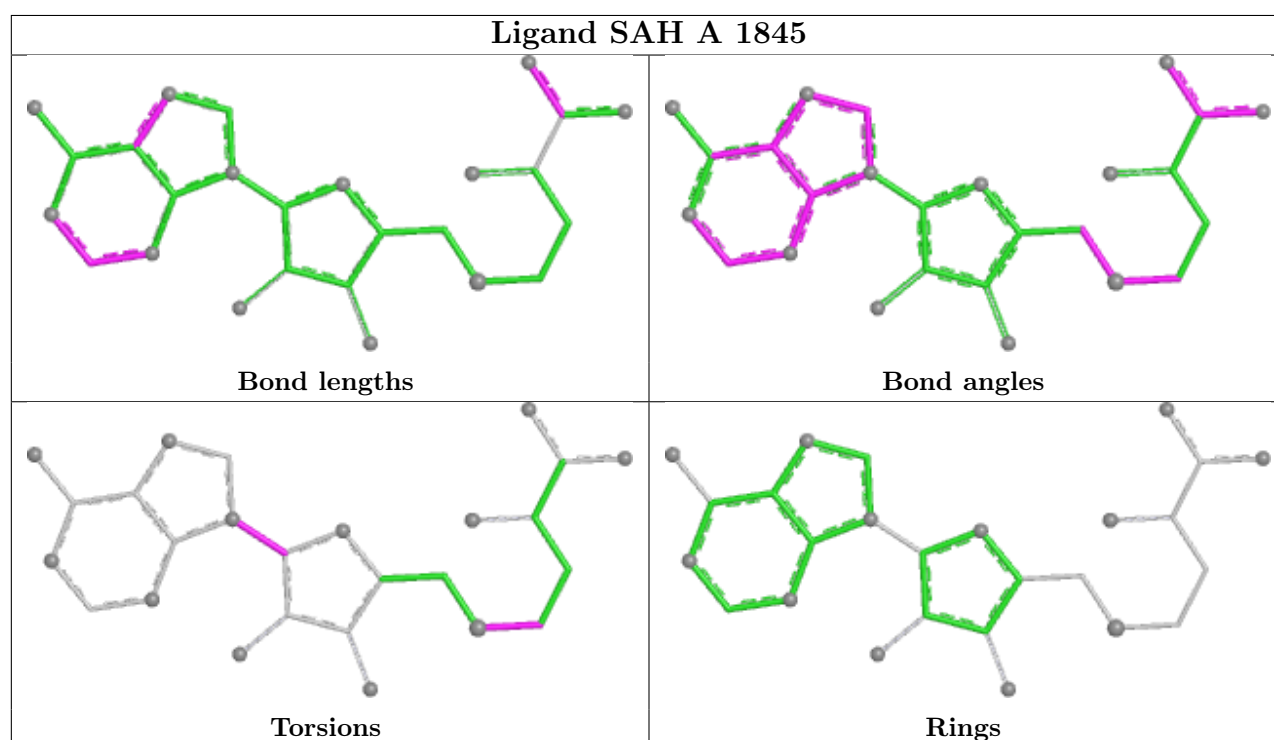
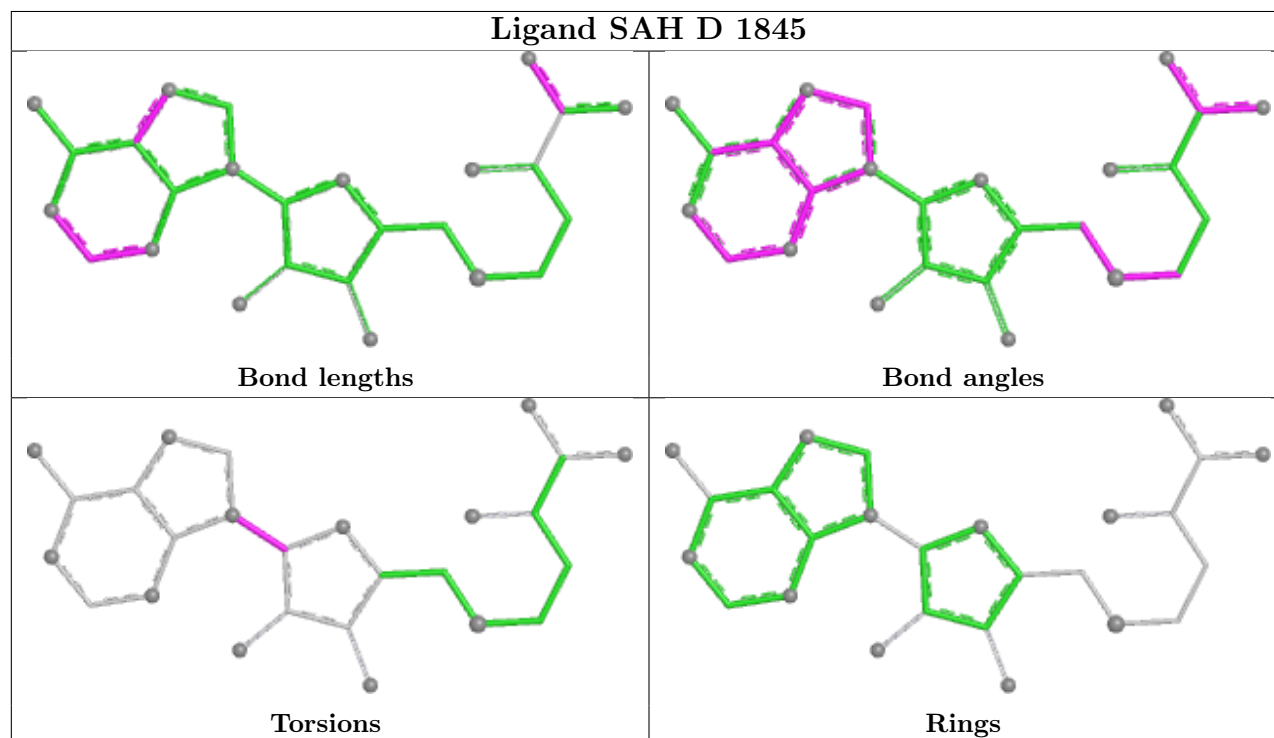
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1845	SAH	1	0
3	A	1845	SAH	1	0

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

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	802/844 (95%)	1.25	143 (17%) 4 3	17, 63, 107, 133	1 (0%)
1	D	813/844 (96%)	1.08	115 (14%) 6 5	22, 49, 88, 114	1 (0%)
2	B	284/287 (98%)	0.79	23 (8%) 18 15	15, 39, 78, 130	0
2	E	278/287 (96%)	1.13	37 (13%) 7 6	23, 54, 89, 131	0
All	All	2177/2262 (96%)	1.11	318 (14%) 6 4	15, 54, 97, 133	2 (0%)

All (318) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	544	ASN	5.2
1	D	653	THR	4.8
1	A	669[A]	PHE	4.8
1	D	669[A]	PHE	4.7
1	A	25	LEU	4.7
1	D	435	PHE	4.5
1	A	488	GLU	4.5
2	E	225	VAL	4.4
1	D	27	GLN	4.3
2	E	89	TYR	4.2
1	A	399	ILE	4.2
1	D	2	ASP	4.1
1	D	249	GLY	4.1
1	D	25	LEU	4.1
1	A	2	ASP	4.0
2	E	90	TYR	4.0
1	D	386	LYS	4.0
2	B	120	ASN	4.0
2	E	222	TRP	3.9
1	A	218	HIS	3.9
2	B	119	SER	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	220	SER	3.9
2	E	211	SER	3.9
1	D	746	ASP	3.9
2	B	59	ASP	3.8
1	A	433	LYS	3.8
1	D	35	ASN	3.8
1	A	72	GLU	3.7
1	A	262	ASP	3.7
1	A	274	GLY	3.6
1	A	641	LYS	3.6
1	D	546	LYS	3.6
2	E	20	GLU	3.6
1	A	59	ILE	3.6
1	D	733	PRO	3.6
1	D	373	GLN	3.6
1	A	126	GLU	3.6
1	D	218	HIS	3.5
1	A	293	ILE	3.5
1	D	34	ILE	3.5
1	D	324	ILE	3.5
1	D	109	LEU	3.5
1	A	454	ASN	3.5
1	A	34	ILE	3.5
2	E	118	LYS	3.5
1	A	153	THR	3.5
1	D	126	GLU	3.5
2	B	1	MET	3.4
1	A	273	ASN	3.4
1	D	113	ASN	3.4
1	A	324	ILE	3.4
1	A	267	THR	3.4
1	D	316	LYS	3.4
2	E	119	SER	3.4
1	D	111	THR	3.4
1	D	6	VAL	3.4
1	D	562	ARG	3.4
1	D	385	PRO	3.4
2	E	124	THR	3.4
1	D	641	LYS	3.3
1	D	391	PHE	3.3
2	E	59	ASP	3.3
1	A	172	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	262	ASP	3.3
1	D	409	TYR	3.3
1	D	226	ASN	3.3
1	A	553	VAL	3.3
2	E	125	GLU	3.2
1	A	113	ASN	3.2
1	A	200	ASN	3.2
1	A	227	VAL	3.2
1	D	1	MET	3.2
1	D	410	MET	3.2
1	A	275	LEU	3.2
1	A	6	VAL	3.2
1	A	204	PRO	3.2
1	D	272	SER	3.2
1	D	296	SER	3.2
1	D	528	ILE	3.2
1	D	813	ASN	3.2
1	D	732	LEU	3.1
1	D	321	VAL	3.1
1	A	319	GLU	3.1
2	E	61	LEU	3.1
1	D	433	LYS	3.1
1	A	35	ASN	3.1
1	A	58	THR	3.1
1	A	154	LYS	3.1
1	A	205	TYR	3.1
2	E	1	MET	3.1
1	A	731	ASN	3.0
1	D	73	GLY	3.0
1	D	325	ASN	3.0
2	B	90	TYR	3.0
1	A	119	CYS	3.0
1	D	8	SER	3.0
1	A	435	PHE	3.0
1	A	519	ARG	2.9
1	A	70	ASN	2.9
1	A	376	GLY	2.9
1	A	26	GLU	2.9
1	A	388	ASN	2.9
2	E	120	ASN	2.9
1	D	583	LYS	2.8
1	A	341	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	357	THR	2.8
1	D	395	LYS	2.8
1	A	333	TYR	2.8
1	D	98	ALA	2.8
1	A	92	ASN	2.8
1	D	200	ASN	2.8
1	D	755	SER	2.8
1	A	248	VAL	2.8
1	A	813	ASN	2.8
1	A	640	ILE	2.8
1	D	314	LEU	2.8
1	A	511	HIS	2.8
1	D	731	ASN	2.8
1	A	546	LYS	2.8
1	A	653	THR	2.8
2	B	162	GLY	2.8
1	A	318	ILE	2.7
1	D	184	LYS	2.7
1	D	601	ASN	2.7
1	A	272	SER	2.7
1	A	39	GLU	2.7
1	A	523	ILE	2.7
1	D	544	ASN	2.7
1	D	399	ILE	2.7
1	D	721	THR	2.7
2	B	92	ARG	2.7
1	A	211	GLU	2.7
2	E	273	SER	2.7
1	A	271	THR	2.6
1	D	153	THR	2.6
1	D	730	LYS	2.6
2	B	218	LYS	2.6
2	B	240	GLU	2.6
1	A	131	PHE	2.6
1	A	384	GLY	2.6
1	D	152	LYS	2.6
1	A	298	VAL	2.6
1	A	525	ILE	2.6
1	D	248	VAL	2.6
1	A	195	PHE	2.6
1	D	133	ASP	2.6
2	E	265	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	118	LYS	2.6
1	A	36	ASN	2.6
1	A	769	ASN	2.6
1	D	511	HIS	2.5
1	D	589	SER	2.5
1	A	76	ILE	2.5
2	E	117	ILE	2.5
1	D	642	THR	2.5
1	A	142	ARG	2.5
1	D	499	LYS	2.5
1	A	158	ILE	2.5
1	D	294	ILE	2.5
1	A	111	THR	2.5
2	B	281	ARG	2.5
1	A	315	ILE	2.5
1	D	640	ILE	2.5
1	D	72	GLU	2.5
2	B	125	GLU	2.5
2	B	112	ARG	2.5
1	A	340	ASP	2.5
2	E	75	LEU	2.5
1	A	305	VAL	2.5
2	E	100	VAL	2.5
2	E	264	TYR	2.5
1	D	142	ARG	2.5
1	A	824	CYS	2.5
1	D	58	THR	2.4
1	A	86	HIS	2.4
1	A	102	ILE	2.4
1	D	639	GLY	2.4
1	A	734	SER	2.4
1	D	419	GLU	2.4
1	A	170	ALA	2.4
1	D	10	THR	2.4
1	D	579	MET	2.4
1	D	273	ASN	2.4
2	B	250	ASN	2.4
1	A	294	ILE	2.4
1	D	59	ILE	2.4
1	A	418	GLY	2.4
1	A	336	SER	2.4
1	A	420	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	638	SER	2.4
1	D	742	GLU	2.4
1	A	733	PRO	2.4
1	D	769	ASN	2.4
1	A	722	ASP	2.4
1	A	730	LYS	2.4
2	E	221	SER	2.4
1	D	357	THR	2.4
1	D	619	THR	2.4
2	E	21	THR	2.4
1	D	523	ILE	2.4
1	A	346	VAL	2.3
2	E	113	GLU	2.3
2	B	124	THR	2.3
1	D	44	LYS	2.3
2	E	55	ARG	2.3
1	D	818	ASN	2.3
1	D	736	GLU	2.3
1	D	317	LEU	2.3
1	A	415	ILE	2.3
1	A	652	GLU	2.3
1	D	488	GLU	2.3
1	A	307	ASP	2.3
1	A	317	LEU	2.3
1	D	332	LYS	2.3
2	B	4	ILE	2.3
2	E	23	PRO	2.3
2	E	40	GLY	2.3
1	D	39	GLU	2.3
1	D	225	GLU	2.3
1	A	373	GLN	2.3
1	D	132	LEU	2.3
2	E	271	SER	2.3
1	A	109	LEU	2.2
1	A	106	LYS	2.2
1	A	228	ILE	2.2
1	D	130	ILE	2.2
1	A	721	THR	2.2
1	A	276	TYR	2.2
1	A	360	SER	2.2
1	A	499	LYS	2.2
2	E	34	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	272	LYS	2.2
1	D	341	ILE	2.2
1	A	178	HIS	2.2
1	A	289	PRO	2.2
1	D	824	CYS	2.2
2	E	143	PRO	2.2
1	D	274	GLY	2.2
1	A	207	GLU	2.2
1	D	625	ALA	2.2
1	D	448	ASN	2.2
1	A	97	ASP	2.2
1	A	10	THR	2.2
2	E	215	SER	2.2
1	A	152	LYS	2.2
1	A	375	GLU	2.2
1	D	19	ALA	2.2
1	D	620	ASP	2.2
2	B	283	VAL	2.2
2	E	152	TYR	2.2
1	A	755	SER	2.2
1	D	18	LEU	2.2
1	D	26	GLU	2.2
1	A	43	ILE	2.1
1	A	494	ILE	2.1
1	D	155	ASN	2.1
1	D	454	ASN	2.1
2	E	179	VAL	2.1
1	A	356	PHE	2.1
2	B	93	SER	2.1
1	A	825	GLU	2.1
1	D	413	GLU	2.1
1	A	130	ILE	2.1
1	A	286	ILE	2.1
1	D	709	ILE	2.1
1	D	4	ASN	2.1
2	B	95	LYS	2.1
1	A	202	THR	2.1
1	D	584	THR	2.1
1	D	134	TYR	2.1
1	A	422	ILE	2.1
1	A	306	LYS	2.1
1	A	397	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	757	MET	2.1
2	E	85	ASN	2.1
2	E	112	ARG	2.1
1	A	144	GLU	2.1
1	A	606	GLU	2.1
1	A	736	GLU	2.1
1	A	411	SER	2.1
1	D	172	SER	2.1
1	D	656	SER	2.1
2	B	179	VAL	2.1
2	B	225	VAL	2.1
1	A	328	LEU	2.1
1	A	249	GLY	2.1
1	A	432	ASP	2.1
1	A	216	SER	2.0
1	D	591	LYS	2.0
1	D	116	HIS	2.0
1	A	385	PRO	2.0
1	A	18	LEU	2.0
1	A	188	ASN	2.0
1	A	562	ARG	2.0
1	A	213	THR	2.0
1	A	259	THR	2.0
1	D	259	THR	2.0
1	A	206	ASP	2.0
1	D	170	ALA	2.0
1	D	390	ASP	2.0
1	D	587	ASP	2.0
1	D	61	GLU	2.0
1	A	427	LYS	2.0
1	A	8	SER	2.0
1	A	334	VAL	2.0
1	A	750	VAL	2.0
2	E	228	VAL	2.0
1	A	13	THR	2.0
1	A	625	ALA	2.0
1	A	390	ASP	2.0
1	A	552	GLU	2.0
1	A	643	LYS	2.0
1	A	806	GLU	2.0
1	A	816	GLU	2.0
1	D	246	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	20	GLU	2.0
2	E	218	LYS	2.0
1	A	1	MET	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](#)

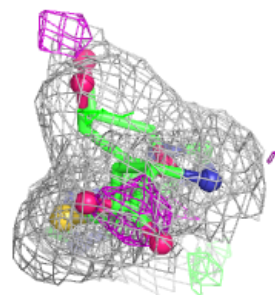
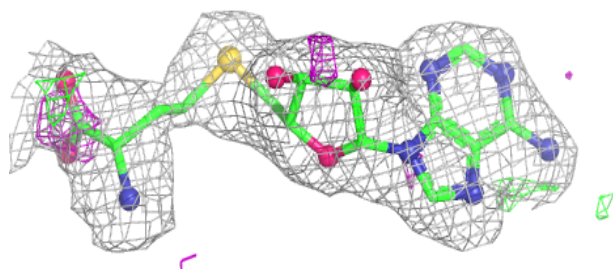
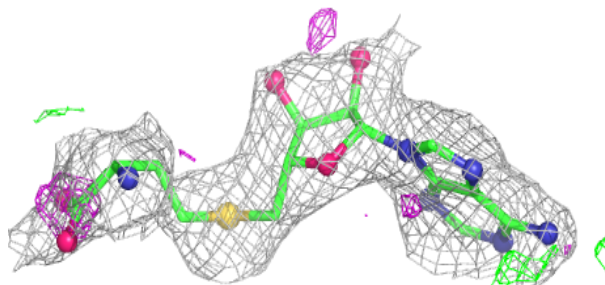
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SAH	D	1845	26/26	0.84	0.14	22,28,32,33	0
3	SAH	A	1845	26/26	0.89	0.11	23,32,38,39	0

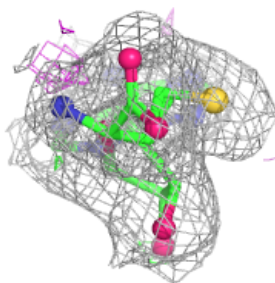
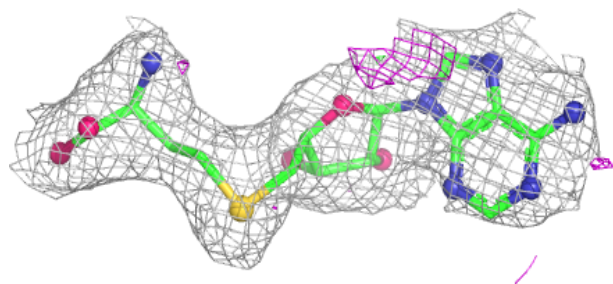
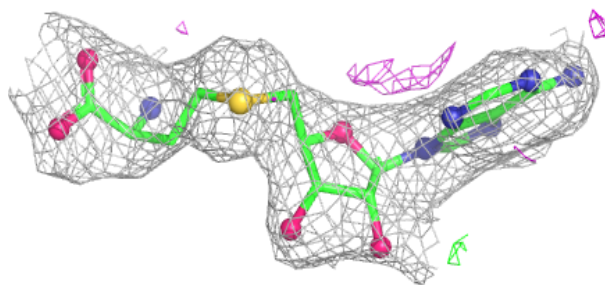
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH D 1845:

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

**Electron density around SAH A 1845:**

$2mF_o-DF_c$ (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.