



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:27 PM UTC

PDB ID : 2VDW / pdb_00002vdw
Title : Guanosine N7 methyl-transferase sub-complex (D1-D12) of the vaccinia virus mRNA capping enzyme
Authors : De la Pena, M.; Kyrieleis, O.J.P.; Cusack, S.
Deposited on : 2007-10-12
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	:	4-5-2 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

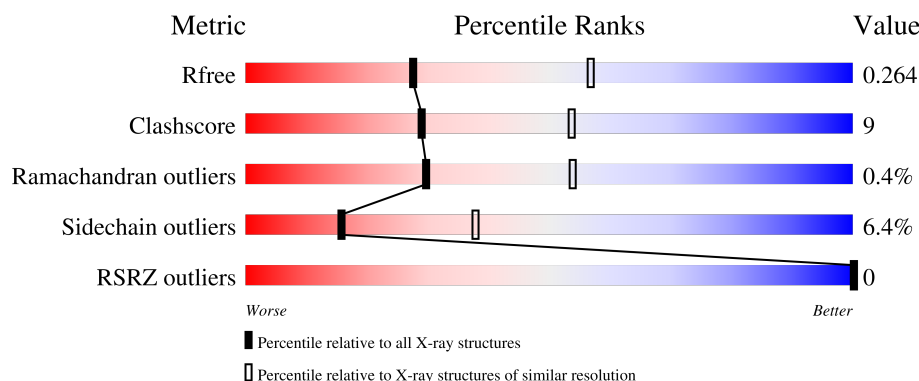
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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	302	 79% 17% ..
1	C	302	 79% 16% ..
1	E	302	 74% 19% • 6%
1	G	302	 71% 20% • 9%
2	B	287	 72% 24% ..

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Mol	Chain	Length	Quality of chain
2	D	287	75% 21% ..
2	F	287	75% 19% ...
2	H	287	76% 20% ...

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18796 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 VACCINIA VIRUS CAPPING ENZYME D1 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2413	1549	399	456	9			
1	C	296	Total	C	N	O	S	0	0	0
			2413	1549	399	456	9			
1	E	283	Total	C	N	O	S	0	0	0
			2317	1492	384	433	8			
1	G	276	Total	C	N	O	S	0	0	0
			2253	1450	374	421	8			

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

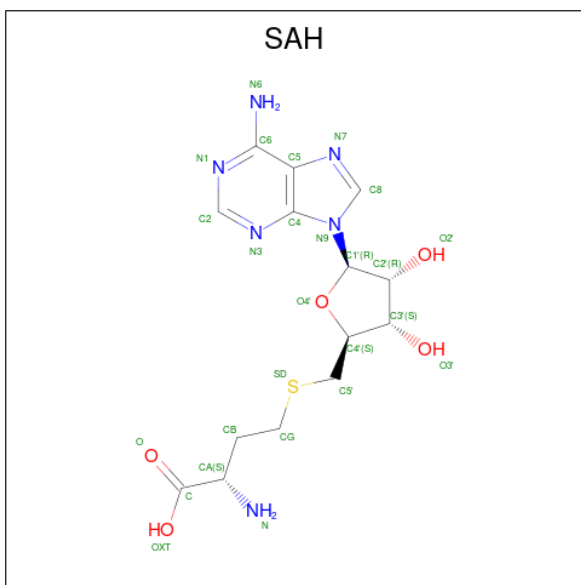
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	283	Total	C	N	O	S	0	0	0
			2312	1488	383	428	13			
2	D	283	Total	C	N	O	S	0	0	0
			2312	1488	383	428	13			
2	F	281	Total	C	N	O	S	0	0	0
			2297	1479	380	425	13			
2	H	284	Total	C	N	O	S	0	0	0
			2320	1492	385	430	13			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).



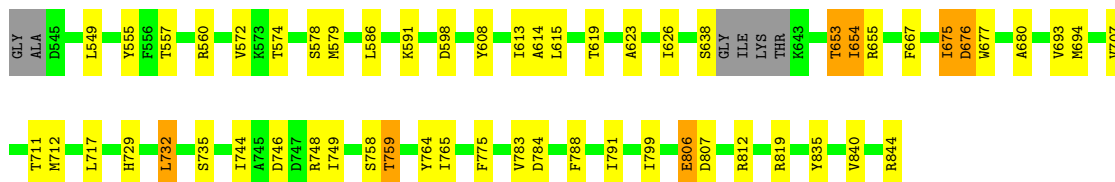
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 26	C 14	N 6	O 5	S 1	0	0
4	C	1	Total 26	C 14	N 6	O 5	S 1	0	0
4	E	1	Total 26	C 14	N 6	O 5	S 1	0	0
4	G	1	Total 26	C 14	N 6	O 5	S 1	0	0

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.

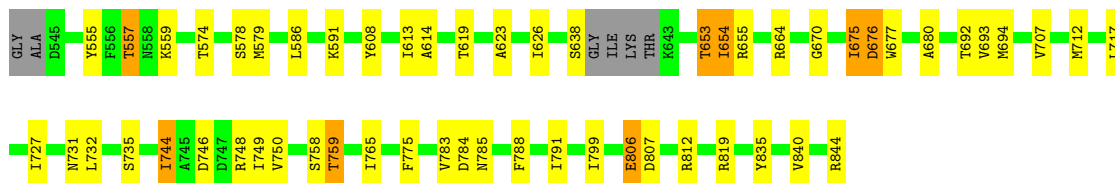
• Molecule 1: VACCINIA VIRUS CAPPING ENZYME D1 SUBUNIT

Chain A: 



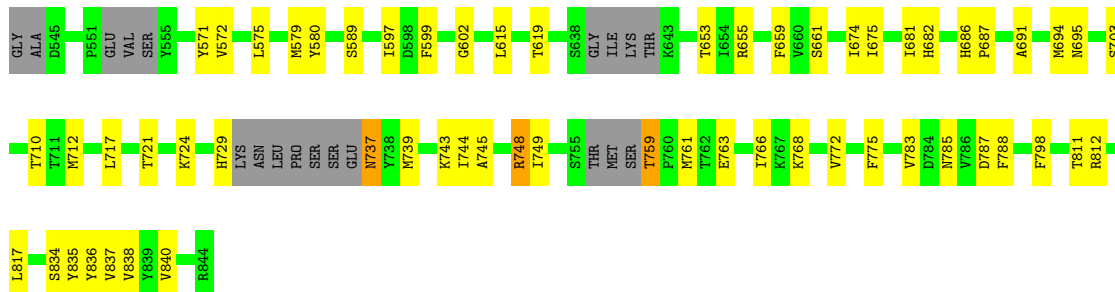
• Molecule 1: VACCINIA VIRUS CAPPING ENZYME D1 SUBUNIT

Chain C: 



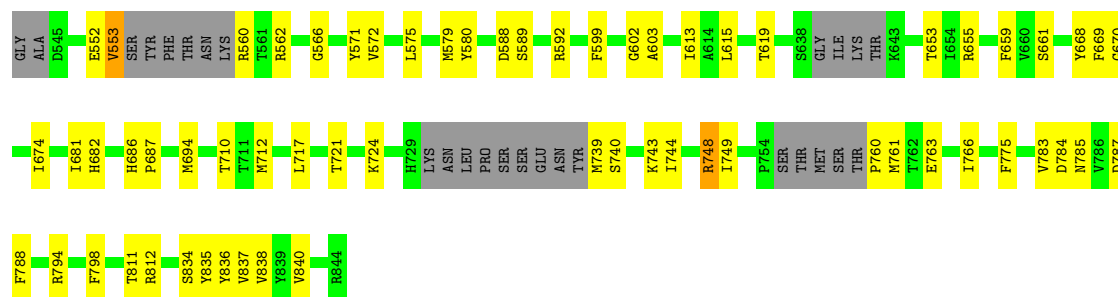
• Molecule 1: VACCINIA VIRUS CAPPING ENZYME D1 SUBUNIT

Chain E: 



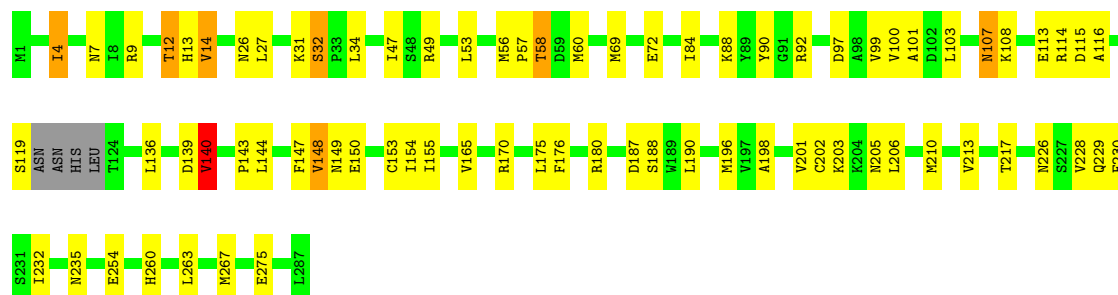
• Molecule 1: VACCINIA VIRUS CAPPING ENZYME D1 SUBUNIT

Chain G: 



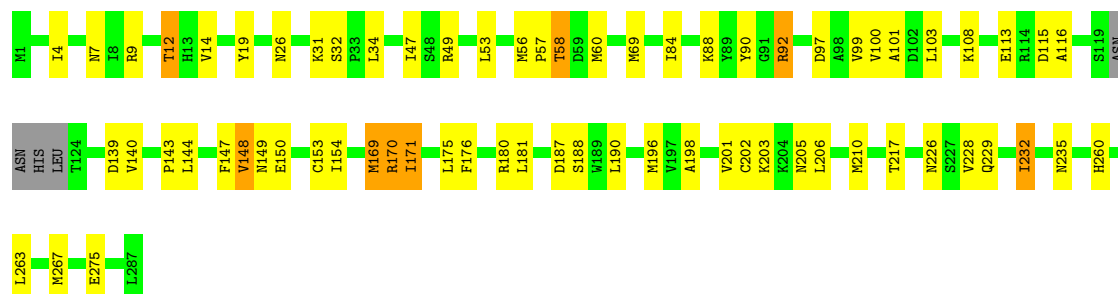
- Molecule 2: MRNA-CAPPING ENZYME SMALL SUBUNIT

Chain B: 72% 24% ..



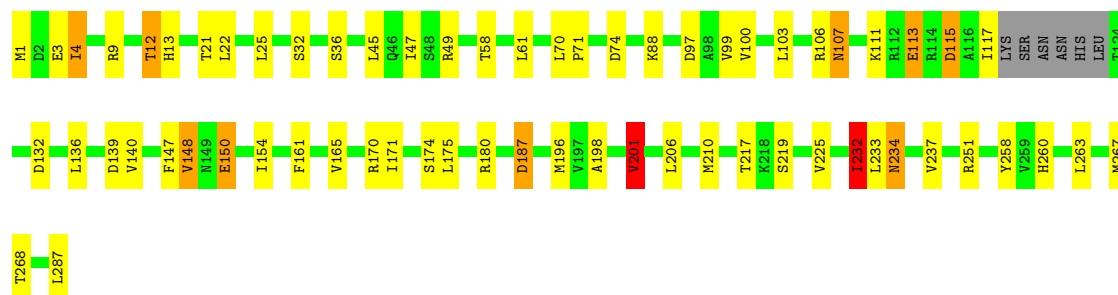
- Molecule 2: MRNA-CAPPING ENZYME SMALL SUBUNIT

Chain D: 75% 21% ..



- Molecule 2: MRNA-CAPPING ENZYME SMALL SUBUNIT

Chain F: 75% 19% ...



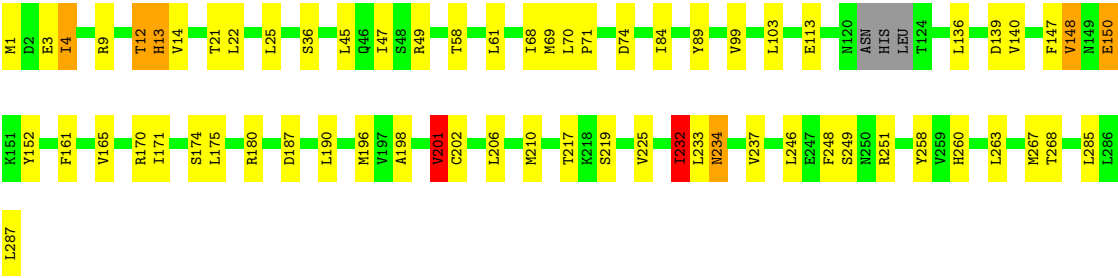
- Molecule 2: MRNA-CAPPING ENZYME SMALL SUBUNIT

Chain H:

76%

20%

...



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.89Å 61.02Å 225.78Å 94.22° 92.95° 108.26°	Depositor
Resolution (Å)	48.39 – 2.70 48.39 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.8 (48.39-2.70) 89.8 (48.39-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.223 , 0.265 0.227 , 0.264	Depositor DCC
R_{free} test set	3818 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 20.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.207 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18796	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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: SAH, SO4

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	0.73	0/2464	0.89	5/3323 (0.2%)
1	C	0.77	3/2464 (0.1%)	0.88	4/3323 (0.1%)
1	E	0.64	0/2364	0.81	3/3183 (0.1%)
1	G	0.64	0/2297	0.81	2/3091 (0.1%)
2	B	0.71	4/2357 (0.2%)	0.85	1/3178 (0.0%)
2	D	0.70	3/2357 (0.1%)	0.83	0/3178
2	F	0.68	1/2342 (0.0%)	0.86	1/3159 (0.0%)
2	H	0.69	1/2365 (0.0%)	0.86	4/3189 (0.1%)
All	All	0.70	12/19010 (0.1%)	0.85	20/25624 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	205	ASN	CG-OD1	5.50	1.33	1.23
2	B	205	ASN	CG-OD1	5.50	1.33	1.23
2	B	149	ASN	CG-OD1	5.42	1.33	1.23
2	F	107	ASN	CG-OD1	5.36	1.33	1.23
2	D	26	ASN	CG-OD1	5.35	1.33	1.23
2	B	107	ASN	CG-OD1	5.29	1.33	1.23
1	C	785	ASN	CG-OD1	5.26	1.33	1.23
1	C	731	ASN	CG-OD1	5.25	1.33	1.23
2	B	26	ASN	CG-OD1	5.25	1.33	1.23
1	C	785	ASN	CG-ND2	-5.10	1.22	1.33
2	H	13	HIS	ND1-CE1	5.04	1.37	1.32
2	D	149	ASN	CG-OD1	5.03	1.33	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	13	HIS	CB-CG-CD2	-6.49	122.76	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	201	VAL	CB-CA-C	-6.37	104.32	111.45
1	G	748	ARG	N-CA-C	6.30	118.12	108.42
1	E	748	ARG	N-CA-C	6.25	118.04	108.42
1	A	748	ARG	N-CA-C	6.20	118.72	108.99
1	E	759	THR	CA-C-N	6.08	126.09	119.89
1	E	759	THR	C-N-CA	6.08	126.09	119.89
1	C	555	TYR	N-CA-C	5.98	117.60	111.14
1	C	748	ARG	N-CA-C	5.92	118.29	108.99
2	F	201	VAL	CB-CA-C	-5.80	104.95	111.45
1	A	555	TYR	N-CA-C	5.73	117.20	111.07
1	C	732	LEU	CA-C-N	5.57	125.88	119.92
1	C	732	LEU	C-N-CA	5.57	125.88	119.92
1	A	560	ARG	N-CA-C	5.51	118.22	109.24
2	H	13	HIS	CB-CG-ND1	5.50	130.96	122.70
2	B	140	VAL	CB-CA-C	-5.47	104.88	112.04
1	G	668	TYR	N-CA-C	5.42	118.23	111.24
2	H	74	ASP	N-CA-C	5.17	116.91	111.28
1	A	732	LEU	CA-C-N	5.05	125.32	119.92
1	A	732	LEU	C-N-CA	5.05	125.32	119.92

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	2413	0	2389	37	0
1	C	2413	0	2389	36	0
1	E	2317	0	2292	37	0
1	G	2253	0	2237	39	0
2	B	2312	0	2357	51	0
2	D	2312	0	2357	46	0
2	F	2297	0	2339	47	0
2	H	2320	0	2363	49	0
3	A	5	0	0	0	0
3	C	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	5	0	0	0	0
3	F	10	0	0	0	0
3	G	5	0	0	1	0
3	H	20	0	0	0	0
4	A	26	0	19	2	0
4	C	26	0	19	2	0
4	E	26	0	19	0	0
4	G	26	0	19	0	0
All	All	18796	0	18799	327	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 9.

All (327) 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)
2:H:232:ILE:HD13	2:H:232:ILE:O	1.57	1.04
2:H:61:LEU:HD12	2:H:267:MET:HE1	1.43	1.01
2:F:232:ILE:O	2:F:232:ILE:HD13	1.62	0.99
2:F:99:VAL:HG23	2:F:150:GLU:HG3	1.43	0.98
2:D:263:LEU:HG	2:D:267:MET:HE2	1.51	0.93
2:H:99:VAL:HG23	2:H:150:GLU:HG3	1.50	0.92
2:F:61:LEU:HD12	2:F:267:MET:HE1	1.50	0.91
2:B:263:LEU:HG	2:B:267:MET:HE2	1.52	0.90
1:C:654:ILE:HG23	1:C:693:VAL:HG22	1.54	0.89
2:F:58:THR:HG21	2:F:113:GLU:HG3	1.57	0.84
2:B:103:LEU:HD21	2:B:139:ASP:HB2	1.59	0.82
1:G:552:GLU:O	1:G:553:VAL:HG23	1.80	0.82
2:F:103:LEU:CD1	2:F:140:VAL:HG13	2.11	0.81
1:A:654:ILE:HG23	1:A:693:VAL:HG22	1.62	0.81
2:D:175:LEU:HD22	2:D:206:LEU:HA	1.64	0.80
1:C:653:THR:HG21	1:C:655:ARG:NH1	1.97	0.79
1:G:717:LEU:HD13	1:G:749:ILE:HD13	1.67	0.77
2:B:175:LEU:HD22	2:B:206:LEU:HA	1.65	0.77
2:H:196:MET:HE3	2:H:198:ALA:HB2	1.64	0.77
1:E:579:MET:HE3	1:E:580:TYR:CE1	2.21	0.76
2:D:103:LEU:HD21	2:D:139:ASP:HB2	1.67	0.74
1:G:653:THR:HG21	1:G:655:ARG:CZ	2.17	0.74
2:F:196:MET:HE3	2:F:198:ALA:HB2	1.69	0.74
2:H:103:LEU:CD1	2:H:140:VAL:HG13	2.17	0.74
1:C:608:TYR:HB3	1:C:613:ILE:HD13	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:THR:HG21	1:A:655:ARG:NH1	2.04	0.72
2:B:210:MET:HE2	2:B:210:MET:HA	1.71	0.71
1:E:653:THR:HG21	1:E:655:ARG:CZ	2.20	0.71
2:D:210:MET:HE2	2:D:210:MET:HA	1.73	0.70
1:E:717:LEU:HD13	1:E:749:ILE:HD13	1.73	0.70
1:C:653:THR:HG21	1:C:655:ARG:CZ	2.21	0.69
1:A:653:THR:HG21	1:A:655:ARG:CZ	2.23	0.69
2:H:103:LEU:HD11	2:H:140:VAL:HG13	1.73	0.69
1:A:788:PHE:HA	1:A:791:ILE:HD12	1.75	0.68
2:B:58:THR:HG21	2:B:113:GLU:HG3	1.76	0.68
2:F:25:LEU:HD22	2:F:232:ILE:CD1	2.22	0.68
2:F:25:LEU:HD22	2:F:232:ILE:HD11	1.76	0.68
1:A:608:TYR:HB3	1:A:613:ILE:HD13	1.76	0.67
2:D:147:PHE:CE2	2:D:201:VAL:HG21	2.30	0.67
2:F:1:MET:HE1	2:F:258:TYR:CE1	2.29	0.67
2:H:196:MET:CE	2:H:198:ALA:HB2	2.25	0.67
1:G:653:THR:HG22	1:G:655:ARG:H	1.60	0.66
1:A:591:LYS:HB3	1:A:614:ALA:HB2	1.76	0.66
2:F:263:LEU:HG	2:F:267:MET:HE3	1.78	0.66
1:G:579:MET:HE3	1:G:580:TYR:CE1	2.31	0.66
1:E:653:THR:HG22	1:E:655:ARG:H	1.61	0.65
2:H:25:LEU:HD22	2:H:232:ILE:HD11	1.79	0.65
1:C:591:LYS:HB3	1:C:614:ALA:HB2	1.78	0.65
1:G:694:MET:HE1	1:G:775:PHE:CE2	2.32	0.65
1:C:608:TYR:OH	1:C:676:ASP:HB2	1.97	0.65
2:H:25:LEU:HD22	2:H:232:ILE:CD1	2.26	0.65
2:D:58:THR:HG21	2:D:113:GLU:HG3	1.77	0.64
1:A:608:TYR:OH	1:A:676:ASP:HB2	1.97	0.64
2:F:21:THR:HG22	2:F:22:LEU:O	1.98	0.64
1:C:579:MET:HE1	2:D:47:ILE:HD12	1.80	0.64
2:H:263:LEU:HG	2:H:267:MET:HE3	1.80	0.63
1:E:619:THR:HG21	1:E:659:PHE:HE1	1.63	0.63
1:G:571:TYR:CE2	1:G:575:LEU:HD11	2.33	0.63
2:B:147:PHE:CE2	2:B:201:VAL:HG21	2.33	0.63
1:C:788:PHE:HA	1:C:791:ILE:HD12	1.81	0.62
1:A:574:THR:O	1:A:578:SER:OG	2.16	0.62
1:C:654:ILE:CG2	1:C:693:VAL:HG22	2.27	0.62
1:G:572:VAL:HG21	1:G:788:PHE:CD2	2.34	0.62
1:A:579:MET:HE1	2:B:47:ILE:HD12	1.80	0.62
2:F:115:ASP:N	2:F:115:ASP:OD1	2.32	0.62
2:D:56:MET:HE2	2:D:56:MET:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:176:PHE:CE2	2:D:201:VAL:HG22	2.35	0.61
1:E:694:MET:HE1	1:E:775:PHE:CE2	2.36	0.61
1:C:784:ASP:HB3	1:C:840:VAL:HB	1.81	0.61
1:G:580:TYR:CE1	1:G:840:VAL:HG21	2.36	0.61
1:G:619:THR:HG21	1:G:659:PHE:HE1	1.66	0.61
2:F:103:LEU:HD21	2:F:139:ASP:HB3	1.81	0.61
1:E:653:THR:HG21	1:E:655:ARG:NH1	2.17	0.60
1:G:710:THR:HG22	1:G:838:VAL:HG22	1.83	0.60
2:F:58:THR:CG2	2:F:113:GLU:HG3	2.30	0.60
1:C:579:MET:HE1	2:D:47:ILE:CD1	2.32	0.59
1:E:710:THR:HG22	1:E:838:VAL:HG22	1.83	0.59
2:H:1:MET:HE1	2:H:258:TYR:CE1	2.38	0.59
2:H:171:ILE:HD11	2:H:232:ILE:HD12	1.84	0.59
2:H:61:LEU:CD1	2:H:267:MET:HE1	2.26	0.59
2:B:90:TYR:CD1	2:D:115:ASP:HB3	2.37	0.59
1:C:574:THR:O	1:C:578:SER:OG	2.19	0.59
2:D:196:MET:HE3	2:D:198:ALA:HB2	1.85	0.59
1:E:579:MET:CE	1:E:580:TYR:CE1	2.86	0.59
2:F:106:ARG:O	2:F:107:ASN:HB2	2.01	0.59
1:G:682:HIS:CG	1:G:763:GLU:OE1	2.56	0.59
1:E:580:TYR:CE1	1:E:840:VAL:HG21	2.38	0.59
2:B:176:PHE:CE2	2:B:201:VAL:HG22	2.37	0.59
2:H:12:THR:HG21	2:H:251:ARG:HD3	1.84	0.58
2:F:268:THR:HG22	2:F:268:THR:O	2.02	0.58
2:B:196:MET:HE3	2:B:198:ALA:HB2	1.85	0.58
2:F:268:THR:O	2:F:268:THR:CG2	2.52	0.58
1:G:743:LYS:HA	1:G:749:ILE:HG22	1.86	0.58
1:E:572:VAL:HG21	1:E:788:PHE:CD2	2.38	0.58
2:F:103:LEU:HD12	2:F:140:VAL:HG13	1.84	0.58
1:A:654:ILE:CG2	1:A:693:VAL:HG22	2.32	0.57
1:A:784:ASP:HB3	1:A:840:VAL:HB	1.86	0.56
2:D:99:VAL:HG23	2:D:150:GLU:HG2	1.86	0.56
1:A:598:ASP:OD1	4:A:1846:SAH:H8	2.05	0.56
2:H:21:THR:HG22	2:H:22:LEU:O	2.05	0.56
2:H:175:LEU:HD22	2:H:206:LEU:HA	1.87	0.56
1:C:654:ILE:HG21	1:C:677:TRP:CH2	2.41	0.56
2:H:171:ILE:HD11	2:H:233:LEU:HD21	1.87	0.56
1:C:694:MET:HE1	1:C:775:PHE:CE2	2.40	0.56
2:D:84:ILE:HG23	2:D:97:ASP:HB2	1.86	0.56
1:C:655:ARG:NH2	4:C:1846:SAH:N7	2.53	0.56
2:F:12:THR:HG21	2:F:251:ARG:HD3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:586:LEU:CD1	2:D:34:LEU:HD22	2.35	0.55
2:F:103:LEU:HD11	2:F:140:VAL:HG13	1.86	0.55
1:G:653:THR:HG21	1:G:655:ARG:NH1	2.21	0.55
1:G:682:HIS:HA	1:G:766:ILE:HD11	1.88	0.55
2:D:153:CYS:HB3	2:D:198:ALA:HB3	1.87	0.54
2:F:171:ILE:HD11	2:F:233:LEU:HD21	1.89	0.54
2:B:99:VAL:HG23	2:B:150:GLU:HG2	1.89	0.54
2:H:103:LEU:HD11	2:H:140:VAL:CG1	2.38	0.54
2:H:69:MET:HE3	2:H:190:LEU:HD22	1.89	0.54
2:H:14:VAL:HG21	2:H:248:PHE:HB2	1.89	0.54
2:H:58:THR:HG21	2:H:113:GLU:HG3	1.89	0.54
2:H:103:LEU:CD1	2:H:140:VAL:CG1	2.86	0.54
1:A:694:MET:HE1	1:A:775:PHE:CE2	2.43	0.54
2:F:171:ILE:HD11	2:F:232:ILE:HD12	1.89	0.53
2:F:103:LEU:CD1	2:F:140:VAL:CG1	2.85	0.53
2:B:90:TYR:CE1	2:D:115:ASP:HB3	2.44	0.53
2:D:53:LEU:CD2	2:D:267:MET:HE1	2.39	0.53
2:B:56:MET:HA	2:B:56:MET:HE2	1.91	0.52
2:B:72:GLU:H	2:B:107:ASN:HD21	1.57	0.52
2:H:147:PHE:CE2	2:H:201:VAL:HG21	2.44	0.52
2:F:103:LEU:HD12	2:F:140:VAL:CG1	2.39	0.52
1:A:653:THR:HG22	1:A:655:ARG:H	1.74	0.52
1:A:654:ILE:HG21	1:A:677:TRP:CH2	2.45	0.52
1:A:608:TYR:O	1:A:613:ILE:HG23	2.10	0.52
1:A:675:ILE:CG2	1:A:707:VAL:HG13	2.40	0.52
2:F:147:PHE:CE2	2:F:201:VAL:HG21	2.45	0.52
2:F:100:VAL:HG22	2:F:154:ILE:HB	1.92	0.52
2:F:217:THR:HG22	2:F:219:SER:HB3	1.92	0.52
1:E:743:LYS:HA	1:E:749:ILE:HG22	1.92	0.52
1:E:579:MET:HE3	1:E:580:TYR:CD1	2.46	0.52
2:D:201:VAL:HG12	2:D:202:CYS:N	2.25	0.51
1:G:572:VAL:HG11	1:G:788:PHE:CZ	2.45	0.51
1:G:579:MET:CE	1:G:580:TYR:CE1	2.92	0.51
2:B:228:VAL:HG22	2:B:229:GLN:N	2.25	0.51
2:B:153:CYS:HB3	2:B:198:ALA:HB3	1.91	0.51
1:A:655:ARG:NH2	4:A:1846:SAH:N7	2.58	0.51
2:B:57:PRO:HD3	2:B:116:ALA:HB2	1.91	0.51
2:D:57:PRO:HG3	2:D:116:ALA:HB2	1.93	0.51
2:B:53:LEU:CD2	2:B:267:MET:HE1	2.41	0.51
2:H:171:ILE:CD1	2:H:232:ILE:HD12	2.39	0.51
2:B:92:ARG:O	2:B:148:VAL:HG21	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:190:LEU:N	2:D:190:LEU:HD12	2.25	0.51
2:F:196:MET:HE3	2:F:198:ALA:CB	2.41	0.51
2:H:210:MET:HE2	2:H:210:MET:HA	1.93	0.51
1:G:798:PHE:CD1	2:H:45:LEU:HD13	2.46	0.51
2:H:196:MET:HE3	2:H:198:ALA:CB	2.37	0.51
2:B:108:LYS:NZ	2:D:108:LYS:NZ	2.59	0.50
1:E:619:THR:HG21	1:E:659:PHE:CE1	2.46	0.50
1:E:571:TYR:CE2	1:E:575:LEU:HD11	2.47	0.50
1:G:562:ARG:HB3	1:G:566:GLY:HA3	1.93	0.50
2:B:190:LEU:N	2:B:190:LEU:HD12	2.26	0.50
1:G:682:HIS:CD2	1:G:763:GLU:OE1	2.64	0.50
2:B:7:ASN:OD1	2:B:12:THR:HG23	2.12	0.50
2:H:49:ARG:HG3	2:H:260:HIS:HB3	1.94	0.50
1:C:675:ILE:CG2	1:C:707:VAL:HG13	2.41	0.50
1:E:712:MET:HE3	1:E:836:TYR:CE1	2.47	0.50
2:F:175:LEU:HD22	2:F:206:LEU:HA	1.94	0.49
2:H:268:THR:O	2:H:268:THR:HG22	2.12	0.49
1:E:759:THR:O	1:E:761:MET:CE	2.59	0.49
2:D:92:ARG:O	2:D:148:VAL:HG21	2.12	0.49
2:F:171:ILE:CD1	2:F:232:ILE:HD12	2.43	0.49
1:C:608:TYR:O	1:C:613:ILE:HG23	2.11	0.49
2:H:69:MET:CE	2:H:190:LEU:HD22	2.42	0.49
2:B:201:VAL:HG12	2:B:202:CYS:N	2.28	0.49
1:E:729:HIS:HB2	1:E:737:ASN:HB2	1.94	0.49
2:H:4:ILE:HD11	2:H:258:TYR:CD1	2.48	0.49
2:B:136:LEU:HD13	2:B:165:VAL:HG22	1.95	0.49
2:H:268:THR:O	2:H:268:THR:CG2	2.60	0.48
1:C:712:MET:CE	1:C:835:TYR:HB3	2.43	0.48
2:D:217:THR:HG23	2:D:226:ASN:HD21	1.77	0.48
2:F:47:ILE:HD11	2:F:161:PHE:CZ	2.47	0.48
1:G:744:ILE:HG23	1:G:748:ARG:HG3	1.95	0.48
2:B:57:PRO:HG3	2:B:116:ALA:HB2	1.93	0.48
1:A:712:MET:CE	1:A:835:TYR:HB3	2.43	0.48
2:H:232:ILE:O	2:H:232:ILE:CD1	2.46	0.48
1:G:603:ALA:HB2	3:G:1845:SO4:O3	2.14	0.48
2:B:84:ILE:HG23	2:B:97:ASP:HB2	1.96	0.48
2:D:169:MET:SD	2:D:181:LEU:HD21	2.54	0.48
1:G:615:LEU:C	1:G:615:LEU:HD12	2.39	0.48
2:F:49:ARG:HG3	2:F:260:HIS:HB3	1.96	0.47
2:H:147:PHE:HE2	2:H:201:VAL:HG21	1.78	0.47
1:E:599:PHE:CE2	1:E:602:GLY:HA2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4:ILE:HD11	2:F:258:TYR:CD1	2.48	0.47
2:B:228:VAL:HG22	2:B:229:GLN:H	1.80	0.47
2:B:53:LEU:HD22	2:B:267:MET:HE1	1.96	0.47
1:C:591:LYS:CB	1:C:614:ALA:HB2	2.45	0.47
1:E:572:VAL:HG11	1:E:788:PHE:CZ	2.49	0.47
1:G:760:PRO:C	1:G:761:MET:HE2	2.39	0.47
2:F:147:PHE:HE2	2:F:201:VAL:HG21	1.79	0.47
1:C:623:ALA:HA	1:C:626:ILE:HD12	1.96	0.47
2:D:57:PRO:CD	2:D:116:ALA:HB2	2.45	0.47
1:A:549:LEU:HD11	1:A:764:TYR:CZ	2.49	0.46
2:D:228:VAL:HG22	2:D:229:GLN:N	2.29	0.46
2:F:232:ILE:O	2:F:232:ILE:CD1	2.51	0.46
1:A:623:ALA:HA	1:A:626:ILE:HD12	1.98	0.46
2:B:13:HIS:O	2:B:14:VAL:HG23	2.15	0.46
1:E:615:LEU:C	1:E:615:LEU:HD12	2.40	0.46
1:G:787:ASP:HA	1:G:837:VAL:HA	1.98	0.46
2:B:57:PRO:CD	2:B:116:ALA:HB2	2.46	0.46
1:C:717:LEU:HD13	1:C:749:ILE:HD13	1.98	0.46
1:E:744:ILE:HG23	1:E:748:ARG:HG3	1.97	0.46
2:H:103:LEU:HD21	2:H:139:ASP:HB3	1.98	0.46
1:A:746:ASP:O	1:A:765:ILE:HD12	2.15	0.46
2:D:57:PRO:HD3	2:D:116:ALA:HB2	1.98	0.46
2:F:111:LYS:NZ	2:F:132:ASP:OD2	2.42	0.46
1:A:806:GLU:OE2	1:A:807:ASP:N	2.49	0.45
2:D:88:LYS:HE2	2:D:99:VAL:HG22	1.98	0.45
1:G:599:PHE:CE2	1:G:602:GLY:HA2	2.50	0.45
1:G:785:ASN:HA	1:G:838:VAL:O	2.16	0.45
1:A:579:MET:HE1	2:B:47:ILE:CD1	2.45	0.45
1:A:758:SER:O	1:A:759:THR:HG22	2.16	0.45
2:D:19:TYR:HB3	2:D:170:ARG:NH2	2.31	0.45
2:F:196:MET:CE	2:F:198:ALA:HB2	2.42	0.45
1:A:591:LYS:CB	1:A:614:ALA:HB2	2.43	0.45
1:E:682:HIS:CG	1:E:763:GLU:OE1	2.69	0.45
2:D:217:THR:HG23	2:D:226:ASN:ND2	2.31	0.45
2:F:136:LEU:HD11	2:F:140:VAL:HG11	1.97	0.45
2:B:100:VAL:HG12	2:B:101:ALA:N	2.31	0.45
2:B:217:THR:HG23	2:B:226:ASN:HD21	1.81	0.45
1:C:557:THR:HG22	1:C:559:LYS:HE2	1.99	0.45
2:F:234:ASN:OD1	2:F:234:ASN:N	2.47	0.45
1:A:711:THR:HG23	1:A:712:MET:O	2.17	0.45
1:A:799:ILE:O	1:A:819:ARG:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:681:ILE:HG23	1:E:766:ILE:CD1	2.46	0.45
1:E:768:LYS:O	1:E:772:VAL:HG23	2.16	0.45
1:G:686:HIS:CD2	1:G:687:PRO:HD2	2.52	0.45
2:D:100:VAL:HG12	2:D:101:ALA:N	2.31	0.45
2:H:136:LEU:HD11	2:H:140:VAL:HG11	1.98	0.45
1:G:592:ARG:HB2	1:G:613:ILE:HG22	1.99	0.45
1:G:580:TYR:O	1:G:592:ARG:NH1	2.50	0.44
2:B:58:THR:HB	2:B:114:ARG:O	2.17	0.44
1:E:682:HIS:HA	1:E:766:ILE:HD11	2.00	0.44
2:D:7:ASN:OD1	2:D:12:THR:HG23	2.17	0.44
1:E:759:THR:O	1:E:761:MET:HE2	2.18	0.44
1:C:758:SER:C	1:C:759:THR:CG2	2.90	0.44
1:E:686:HIS:CD2	1:E:687:PRO:HD2	2.53	0.44
2:H:196:MET:CE	2:H:198:ALA:CB	2.94	0.44
2:H:217:THR:HG22	2:H:219:SER:HB3	2.00	0.44
1:A:758:SER:C	1:A:759:THR:CG2	2.91	0.44
1:G:653:THR:CG2	1:G:655:ARG:CZ	2.94	0.44
1:C:727:ILE:HD11	2:H:89:TYR:HB2	2.00	0.43
2:D:60:MET:HE2	2:D:60:MET:HA	1.99	0.43
2:F:88:LYS:HE2	2:F:99:VAL:HG22	2.00	0.43
1:C:653:THR:HG22	1:C:655:ARG:H	1.82	0.43
2:B:49:ARG:HG2	2:B:260:HIS:HB2	2.01	0.43
1:E:691:ALA:O	1:E:695:ASN:ND2	2.51	0.43
1:G:681:ILE:HG23	1:G:766:ILE:CD1	2.48	0.43
2:B:100:VAL:HA	2:B:154:ILE:O	2.19	0.43
1:C:655:ARG:O	1:C:692:THR:HG21	2.19	0.43
2:F:99:VAL:CG2	2:F:150:GLU:HG3	2.31	0.43
1:A:586:LEU:CD1	2:B:34:LEU:HD22	2.48	0.43
1:A:717:LEU:HD13	1:A:749:ILE:HD13	2.00	0.43
2:B:60:MET:HA	2:B:60:MET:HE2	2.00	0.43
1:E:712:MET:HE2	1:E:835:TYR:HB3	2.00	0.43
2:H:47:ILE:HD11	2:H:161:PHE:CZ	2.54	0.43
2:H:84:ILE:HD11	2:H:152:TYR:CD1	2.54	0.43
1:A:572:VAL:HG11	1:A:788:PHE:CZ	2.54	0.42
1:C:806:GLU:OE2	1:C:807:ASP:N	2.51	0.42
2:D:99:VAL:HG12	2:D:143:PRO:HB3	2.01	0.42
1:A:572:VAL:HG21	1:A:788:PHE:CD2	2.54	0.42
2:B:115:ASP:HB3	2:D:90:TYR:CD1	2.54	0.42
2:B:115:ASP:HB3	2:D:90:TYR:CE1	2.54	0.42
1:C:744:ILE:HD12	1:C:750:VAL:HG23	2.01	0.42
1:E:745:ALA:HB3	1:E:748:ARG:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:817:LEU:HD12	1:E:817:LEU:HA	1.90	0.42
2:H:14:VAL:CG2	2:H:248:PHE:HB2	2.49	0.42
2:B:58:THR:HG21	2:B:113:GLU:CG	2.48	0.42
1:E:798:PHE:CD1	2:F:45:LEU:HD13	2.54	0.42
2:B:144:LEU:HD13	2:B:175:LEU:HD13	2.01	0.42
2:D:100:VAL:HA	2:D:154:ILE:O	2.20	0.42
2:H:246:LEU:HA	2:H:249:SER:HB2	2.00	0.42
4:C:1846:SAH:H2'	4:C:1846:SAH:N3	2.35	0.42
1:E:785:ASN:HA	1:E:838:VAL:O	2.20	0.42
1:G:712:MET:HE3	1:G:836:TYR:CE1	2.54	0.42
2:H:70:LEU:HB3	2:H:71:PRO:HD2	2.01	0.42
2:D:228:VAL:HG22	2:D:229:GLN:H	1.85	0.42
1:A:586:LEU:HD12	1:A:586:LEU:HA	1.89	0.42
2:B:217:THR:HG23	2:B:226:ASN:ND2	2.35	0.42
1:C:586:LEU:HD12	1:C:586:LEU:HA	1.92	0.42
2:F:70:LEU:HB3	2:F:71:PRO:HD2	2.02	0.42
2:D:171:ILE:HD11	2:D:232:ILE:HG23	2.02	0.42
2:F:210:MET:HE2	2:F:210:MET:HA	2.02	0.42
2:B:4:ILE:HG21	2:B:254:GLU:HB3	2.01	0.41
2:B:49:ARG:HG2	2:B:260:HIS:CB	2.50	0.41
2:F:74:ASP:CG	2:F:187:ASP:HB3	2.45	0.41
1:C:712:MET:HE2	1:C:835:TYR:HB3	2.03	0.41
2:D:144:LEU:HD13	2:D:175:LEU:HD13	2.02	0.41
1:G:588:ASP:O	1:G:592:ARG:NH2	2.53	0.41
1:G:619:THR:HG21	1:G:659:PHE:CE1	2.50	0.41
1:G:794:ARG:HD3	2:H:246:LEU:HD13	2.02	0.41
1:C:758:SER:O	1:C:759:THR:HG22	2.20	0.41
1:E:653:THR:CG2	1:E:655:ARG:CZ	2.94	0.41
1:E:787:ASP:HA	1:E:837:VAL:HA	2.01	0.41
2:F:47:ILE:HD11	2:F:161:PHE:HZ	1.85	0.41
1:A:615:LEU:HD21	1:A:667:PHE:HE1	1.86	0.41
2:D:19:TYR:CB	2:D:170:ARG:NH2	2.84	0.41
1:C:712:MET:HE2	1:C:712:MET:HB3	1.99	0.41
1:C:799:ILE:O	1:C:819:ARG:HD3	2.21	0.41
1:G:669:PHE:CG	1:G:670:GLY:N	2.88	0.41
2:B:32:SER:HA	2:B:230:PHE:O	2.19	0.41
2:D:49:ARG:HG2	2:D:260:HIS:HB2	2.03	0.41
2:H:201:VAL:HG12	2:H:202:CYS:N	2.36	0.41
2:H:258:TYR:HE2	2:H:285:LEU:HD22	1.86	0.41
2:H:263:LEU:CG	2:H:267:MET:HE3	2.49	0.41
2:D:201:VAL:CG1	2:D:202:CYS:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:597:ILE:CD1	1:E:675:ILE:HG23	2.51	0.40
1:G:712:MET:HE2	1:G:835:TYR:HB3	2.02	0.40
2:B:27:LEU:HD22	2:B:213:VAL:HG22	2.03	0.40
2:B:99:VAL:HG12	2:B:143:PRO:HB3	2.03	0.40
1:C:664:ARG:NH2	1:C:670:GLY:O	2.54	0.40
2:H:234:ASN:OD1	2:H:234:ASN:N	2.47	0.40
1:A:729:HIS:CG	1:A:732:LEU:HD12	2.57	0.40
2:B:88:LYS:HE2	2:B:99:VAL:HG22	2.03	0.40
2:B:108:LYS:HZ1	2:D:108:LYS:NZ	2.18	0.40
2:B:140:VAL:O	2:B:155:ILE:CD1	2.70	0.40
2:D:92:ARG:HB2	2:D:92:ARG:HH11	1.87	0.40
2:F:1:MET:HE1	2:F:258:TYR:HE1	1.84	0.40
1:A:712:MET:HE2	1:A:712:MET:HB3	1.93	0.40
1:C:746:ASP:O	1:C:765:ILE:HD12	2.21	0.40
1:G:784:ASP:HB3	1:G:840:VAL:HB	2.03	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	292/302 (97%)	280 (96%)	11 (4%)	1 (0%)	36	60
1	C	292/302 (97%)	277 (95%)	14 (5%)	1 (0%)	36	60
1	E	273/302 (90%)	255 (93%)	18 (7%)	0	100	100
1	G	266/302 (88%)	247 (93%)	19 (7%)	0	100	100
2	B	279/287 (97%)	262 (94%)	16 (6%)	1 (0%)	30	54
2	D	279/287 (97%)	260 (93%)	18 (6%)	1 (0%)	30	54
2	F	277/287 (96%)	258 (93%)	17 (6%)	2 (1%)	18	41
2	H	280/287 (98%)	264 (94%)	14 (5%)	2 (1%)	18	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2238/2356 (95%)	2103 (94%)	127 (6%)	8 (0%)	30	54

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	680	ALA
1	C	680	ALA
2	H	148	VAL
2	F	148	VAL
2	B	148	VAL
2	D	148	VAL
2	H	232	ILE
2	F	232	ILE

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	268/271 (99%)	254 (95%)	14 (5%)	21	47
1	C	268/271 (99%)	254 (95%)	14 (5%)	21	47
1	E	255/271 (94%)	243 (95%)	12 (5%)	23	51
1	G	248/271 (92%)	235 (95%)	13 (5%)	21	47
2	B	268/272 (98%)	250 (93%)	18 (7%)	15	36
2	D	268/272 (98%)	248 (92%)	20 (8%)	12	31
2	F	266/272 (98%)	242 (91%)	24 (9%)	9	23
2	H	269/272 (99%)	249 (93%)	20 (7%)	13	32
All	All	2110/2172 (97%)	1975 (94%)	135 (6%)	16	38

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	557	THR
1	A	619	THR

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Mol	Chain	Res	Type
1	A	638	SER
1	A	653	THR
1	A	654	ILE
1	A	675	ILE
1	A	676	ASP
1	A	735	SER
1	A	744	ILE
1	A	759	THR
1	A	783	VAL
1	A	806	GLU
1	A	812	ARG
1	A	844	ARG
2	B	4	ILE
2	B	9	ARG
2	B	12	THR
2	B	14	VAL
2	B	31	LYS
2	B	32	SER
2	B	58	THR
2	B	69	MET
2	B	119	SER
2	B	140	VAL
2	B	170	ARG
2	B	180	ARG
2	B	187	ASP
2	B	188	SER
2	B	203	LYS
2	B	232	ILE
2	B	235	ASN
2	B	275	GLU
1	C	557	THR
1	C	619	THR
1	C	638	SER
1	C	653	THR
1	C	654	ILE
1	C	675	ILE
1	C	676	ASP
1	C	735	SER
1	C	744	ILE
1	C	759	THR
1	C	783	VAL
1	C	806	GLU

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Mol	Chain	Res	Type
1	C	812	ARG
1	C	844	ARG
2	D	4	ILE
2	D	9	ARG
2	D	12	THR
2	D	14	VAL
2	D	31	LYS
2	D	32	SER
2	D	58	THR
2	D	69	MET
2	D	92	ARG
2	D	140	VAL
2	D	169	MET
2	D	170	ARG
2	D	171	ILE
2	D	180	ARG
2	D	187	ASP
2	D	188	SER
2	D	203	LYS
2	D	232	ILE
2	D	235	ASN
2	D	275	GLU
1	E	589	SER
1	E	661	SER
1	E	674	ILE
1	E	703	SER
1	E	721	THR
1	E	724	LYS
1	E	737	ASN
1	E	739	MET
1	E	783	VAL
1	E	811	THR
1	E	812	ARG
1	E	834	SER
2	F	3	GLU
2	F	4	ILE
2	F	9	ARG
2	F	12	THR
2	F	13	HIS
2	F	32	SER
2	F	36	SER
2	F	97	ASP

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Mol	Chain	Res	Type
2	F	113	GLU
2	F	115	ASP
2	F	117	ILE
2	F	148	VAL
2	F	150	GLU
2	F	165	VAL
2	F	170	ARG
2	F	174	SER
2	F	180	ARG
2	F	187	ASP
2	F	201	VAL
2	F	225	VAL
2	F	232	ILE
2	F	234	ASN
2	F	237	VAL
2	F	287	LEU
1	G	553	VAL
1	G	560	ARG
1	G	589	SER
1	G	661	SER
1	G	674	ILE
1	G	721	THR
1	G	724	LYS
1	G	739	MET
1	G	740	SER
1	G	783	VAL
1	G	811	THR
1	G	812	ARG
1	G	834	SER
2	H	3	GLU
2	H	4	ILE
2	H	9	ARG
2	H	12	THR
2	H	13	HIS
2	H	36	SER
2	H	68	ILE
2	H	148	VAL
2	H	150	GLU
2	H	165	VAL
2	H	170	ARG
2	H	174	SER
2	H	180	ARG

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Mol	Chain	Res	Type
2	H	187	ASP
2	H	201	VAL
2	H	225	VAL
2	H	232	ILE
2	H	234	ASN
2	H	237	VAL
2	H	287	LEU

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	731	ASN
1	A	737	ASN
1	A	785	ASN
2	B	229	GLN
2	D	229	GLN
1	E	678	GLN
2	H	54	ASN

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 ⓘ

15 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	SO4	G	1845	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	H	1291	-	4,4,4	0.27	0	6,6,6	0.21	0
3	SO4	H	1289	-	4,4,4	0.25	0	6,6,6	0.13	0
3	SO4	H	1288	-	4,4,4	0.23	0	6,6,6	0.16	0
4	SAH	C	1846	-	27,28,28	1.11	3 (11%)	36,40,40	2.16	11 (30%)
4	SAH	E	1846	-	27,28,28	1.18	4 (14%)	36,40,40	2.08	9 (25%)
3	SO4	C	1847	-	4,4,4	0.28	0	6,6,6	0.15	0
3	SO4	H	1290	-	4,4,4	0.25	0	6,6,6	0.18	0
3	SO4	F	1288	-	4,4,4	0.25	0	6,6,6	0.24	0
3	SO4	C	1845	-	4,4,4	0.25	0	6,6,6	0.21	0
3	SO4	A	1845	-	4,4,4	0.23	0	6,6,6	0.29	0
3	SO4	F	1289	-	4,4,4	0.28	0	6,6,6	0.19	0
3	SO4	E	1845	-	4,4,4	0.23	0	6,6,6	0.10	0
4	SAH	A	1846	-	27,28,28	1.20	3 (11%)	36,40,40	2.27	9 (25%)
4	SAH	G	1846	-	27,28,28	1.21	4 (14%)	36,40,40	2.07	11 (30%)

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
4	SAH	A	1846	-	-	4/15/31/31	0/3/3/3
4	SAH	E	1846	-	-	8/15/31/31	0/3/3/3
4	SAH	G	1846	-	-	5/15/31/31	0/3/3/3
4	SAH	C	1846	-	-	3/15/31/31	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1846	SAH	C2-N3	3.16	1.39	1.33
4	A	1846	SAH	C5-N7	-3.02	1.33	1.39
4	G	1846	SAH	C2-N1	2.97	1.39	1.33
4	E	1846	SAH	C2-N1	2.91	1.39	1.33
4	C	1846	SAH	C5-N7	-2.89	1.33	1.39
4	A	1846	SAH	C2-N1	2.79	1.38	1.33
4	G	1846	SAH	C2-N3	2.76	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1846	SAH	C5-N7	-2.60	1.34	1.39
4	E	1846	SAH	C2-N3	2.54	1.38	1.33
4	C	1846	SAH	C2-N3	2.36	1.38	1.33
4	G	1846	SAH	C5-N7	-2.36	1.34	1.39
4	C	1846	SAH	C2-N1	2.31	1.38	1.33
4	E	1846	SAH	OXT-C	-2.15	1.23	1.30
4	G	1846	SAH	C8-N7	2.10	1.35	1.31

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1846	SAH	C5-C4-N3	-5.81	118.71	126.72
4	G	1846	SAH	N3-C2-N1	-5.44	120.35	128.58
4	C	1846	SAH	N3-C2-N1	-5.28	120.59	128.58
4	A	1846	SAH	C5-N7-C8	5.10	111.46	103.45
4	E	1846	SAH	C5-C4-N3	-5.07	119.73	126.72
4	E	1846	SAH	N3-C2-N1	-5.04	120.95	128.58
4	G	1846	SAH	C5-C4-N3	-4.96	119.89	126.72
4	C	1846	SAH	C5-C4-N3	-4.59	120.40	126.72
4	A	1846	SAH	N9-C8-N7	-4.55	107.48	113.94
4	C	1846	SAH	N9-C8-N7	-4.46	107.61	113.94
4	C	1846	SAH	C5-N7-C8	4.35	110.28	103.45
4	A	1846	SAH	N3-C2-N1	-4.21	122.21	128.58
4	A	1846	SAH	C4-C5-N7	-4.11	105.88	110.58
4	A	1846	SAH	N3-C4-N9	3.98	133.94	127.17
4	E	1846	SAH	C5-N7-C8	3.96	109.67	103.45
4	A	1846	SAH	C6-C5-C4	3.70	122.23	117.18
4	G	1846	SAH	C5-N7-C8	3.64	109.17	103.45
4	C	1846	SAH	C4-C5-N7	-3.52	106.56	110.58
4	E	1846	SAH	N9-C8-N7	-3.48	109.00	113.94
4	E	1846	SAH	C6-C5-C4	3.38	121.79	117.18
4	G	1846	SAH	N9-C8-N7	-3.35	109.18	113.94
4	G	1846	SAH	C2-N3-C4	3.35	120.01	111.83
4	G	1846	SAH	N3-C4-N9	3.30	132.77	127.17
4	A	1846	SAH	C2-N3-C4	3.25	119.77	111.83
4	E	1846	SAH	C2-N3-C4	3.19	119.62	111.83
4	E	1846	SAH	N3-C4-N9	3.12	132.47	127.17
4	E	1846	SAH	OXT-C-O	-3.10	117.06	124.08
4	C	1846	SAH	C2-N3-C4	3.01	119.17	111.83
4	C	1846	SAH	CB-CG-SD	-2.97	106.82	113.45
4	E	1846	SAH	C4-C5-N7	-2.87	107.31	110.58
4	G	1846	SAH	C6-C5-C4	2.76	120.94	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1846	SAH	C6-C5-C4	2.64	120.78	117.18
4	C	1846	SAH	N3-C4-N9	2.59	131.57	127.17
4	G	1846	SAH	OXT-C-O	-2.38	118.69	124.08
4	C	1846	SAH	OXT-C-O	-2.37	118.70	124.08
4	G	1846	SAH	C4-C5-N7	-2.35	107.89	110.58
4	A	1846	SAH	C1'-N9-C8	-2.31	121.97	127.09
4	G	1846	SAH	CB-CG-SD	-2.26	108.40	113.45
4	G	1846	SAH	C5'-SD-CG	-2.06	96.14	102.26
4	C	1846	SAH	C5-C4-N9	2.03	108.03	105.81

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1846	SAH	N-CA-CB-CG
4	E	1846	SAH	C-CA-CB-CG
4	E	1846	SAH	C2'-C1'-N9-C4
4	G	1846	SAH	C2'-C1'-N9-C4
4	E	1846	SAH	C2'-C1'-N9-C8
4	G	1846	SAH	C2'-C1'-N9-C8
4	G	1846	SAH	C-CA-CB-CG
4	A	1846	SAH	C2'-C1'-N9-C8
4	E	1846	SAH	CB-CG-SD-C5'
4	G	1846	SAH	CB-CG-SD-C5'
4	E	1846	SAH	CA-CB-CG-SD
4	C	1846	SAH	C2'-C1'-N9-C8
4	A	1846	SAH	O4'-C1'-N9-C8
4	C	1846	SAH	C2'-C1'-N9-C4
4	C	1846	SAH	O4'-C1'-N9-C8
4	E	1846	SAH	O4'-C1'-N9-C8
4	G	1846	SAH	O4'-C1'-N9-C8
4	A	1846	SAH	CB-CG-SD-C5'
4	A	1846	SAH	C2'-C1'-N9-C4
4	E	1846	SAH	OXT-C-CA-N

There are no ring outliers.

3 monomers are involved in 5 short contacts:

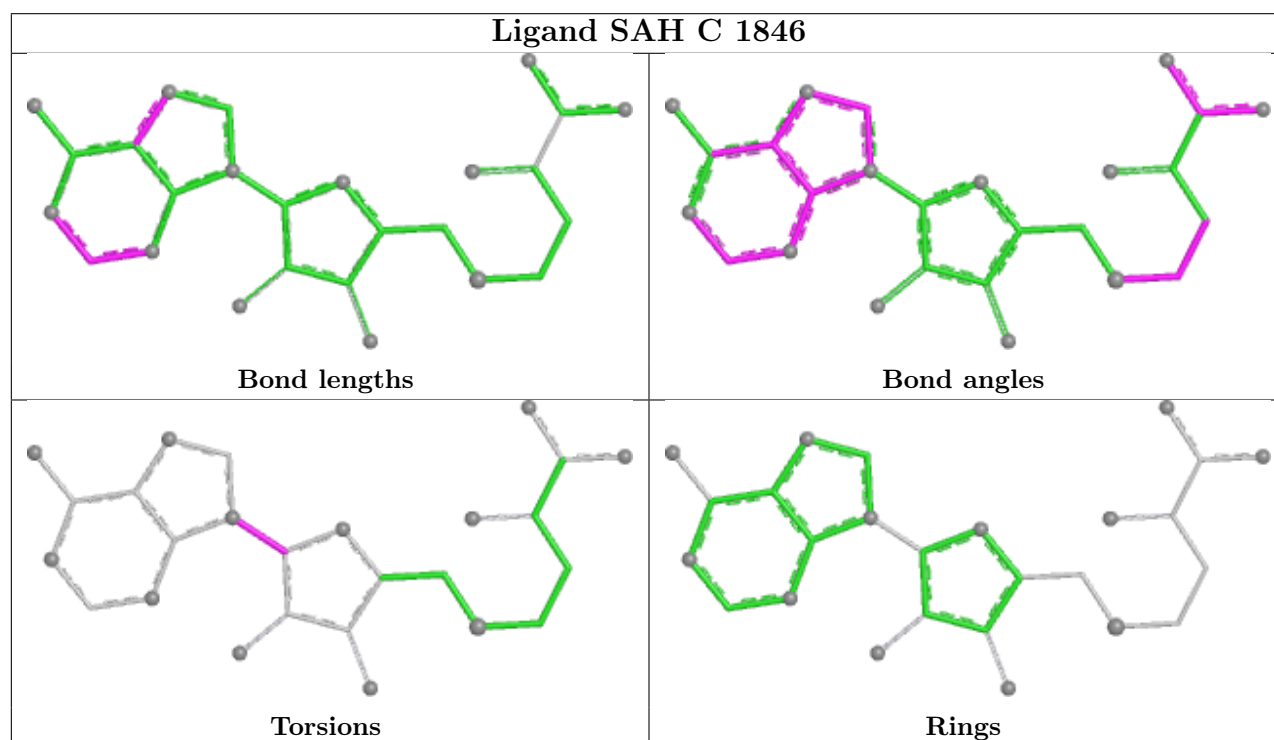
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1845	SO4	1	0
4	C	1846	SAH	2	0

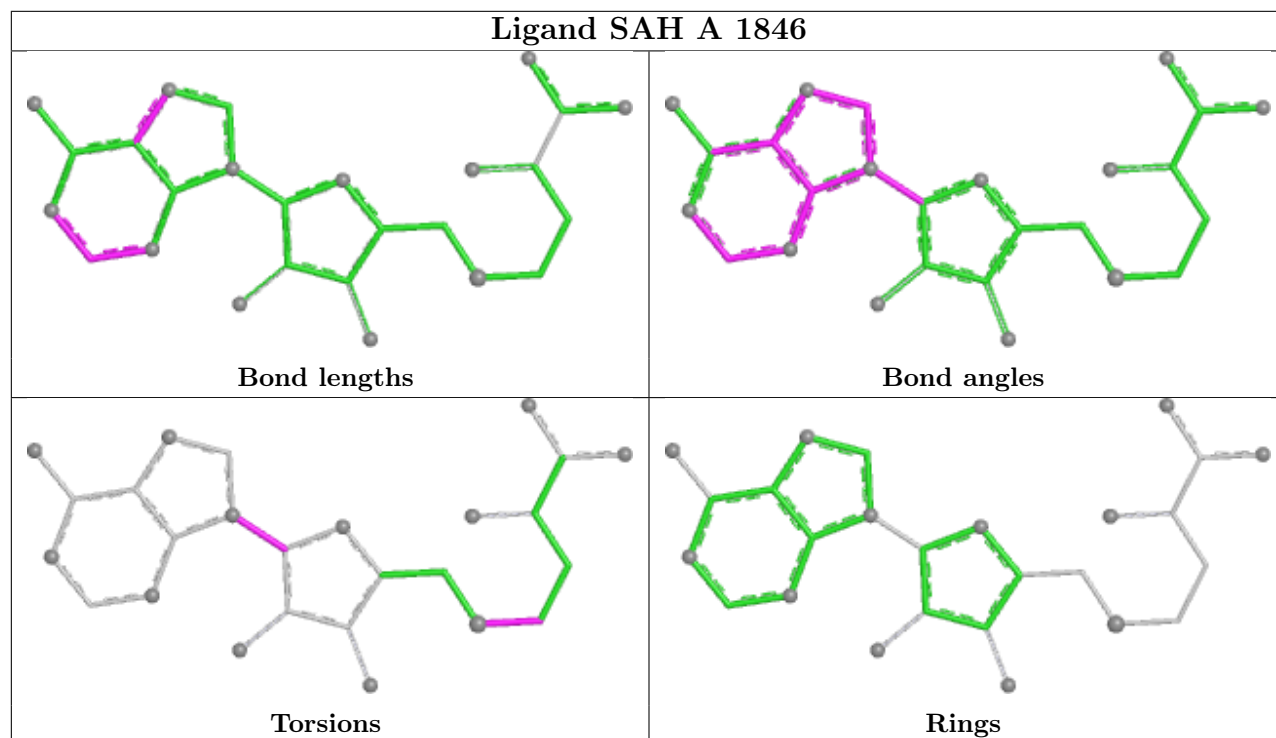
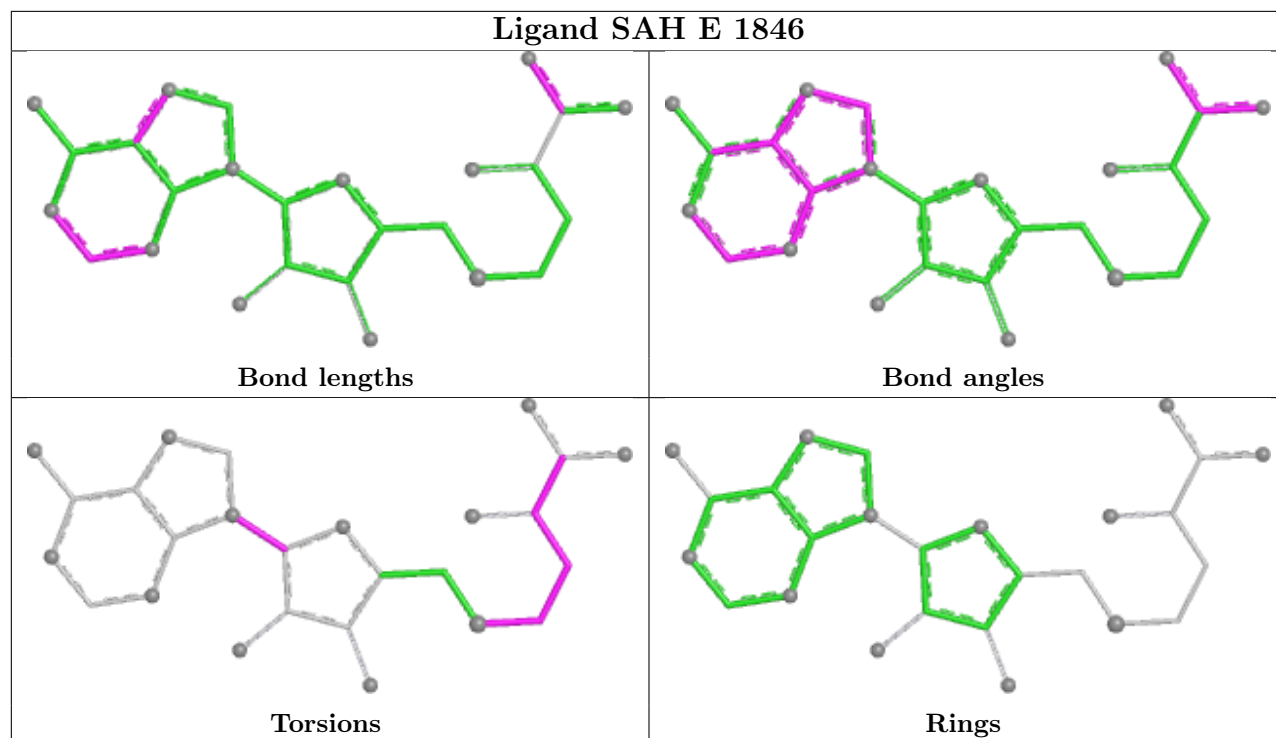
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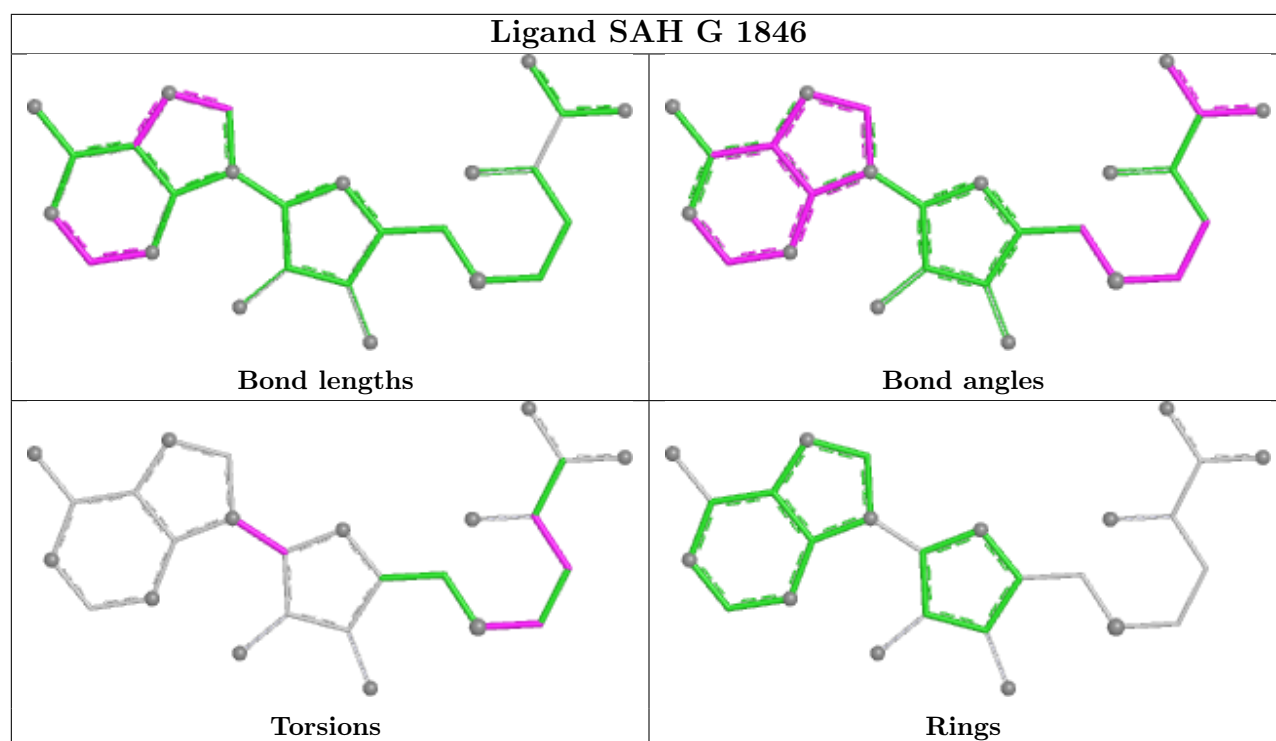
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1846	SAH	2	0

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	296/302 (98%)	-1.77	0 100 100	17, 33, 49, 63	0
1	C	296/302 (98%)	-1.77	0 100 100	18, 33, 47, 60	0
1	E	283/302 (93%)	-1.63	0 100 100	26, 45, 71, 88	0
1	G	276/302 (91%)	-1.62	0 100 100	26, 45, 73, 84	0
2	B	283/287 (98%)	-1.72	0 100 100	23, 42, 60, 69	0
2	D	283/287 (98%)	-1.71	0 100 100	23, 42, 62, 70	0
2	F	281/287 (97%)	-1.74	0 100 100	22, 37, 60, 77	0
2	H	284/287 (98%)	-1.74	0 100 100	22, 37, 60, 75	0
All	All	2282/2356 (96%)	-1.71	0 100 100	17, 38, 64, 88	0

There are no RSRZ outliers to report.

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](#)

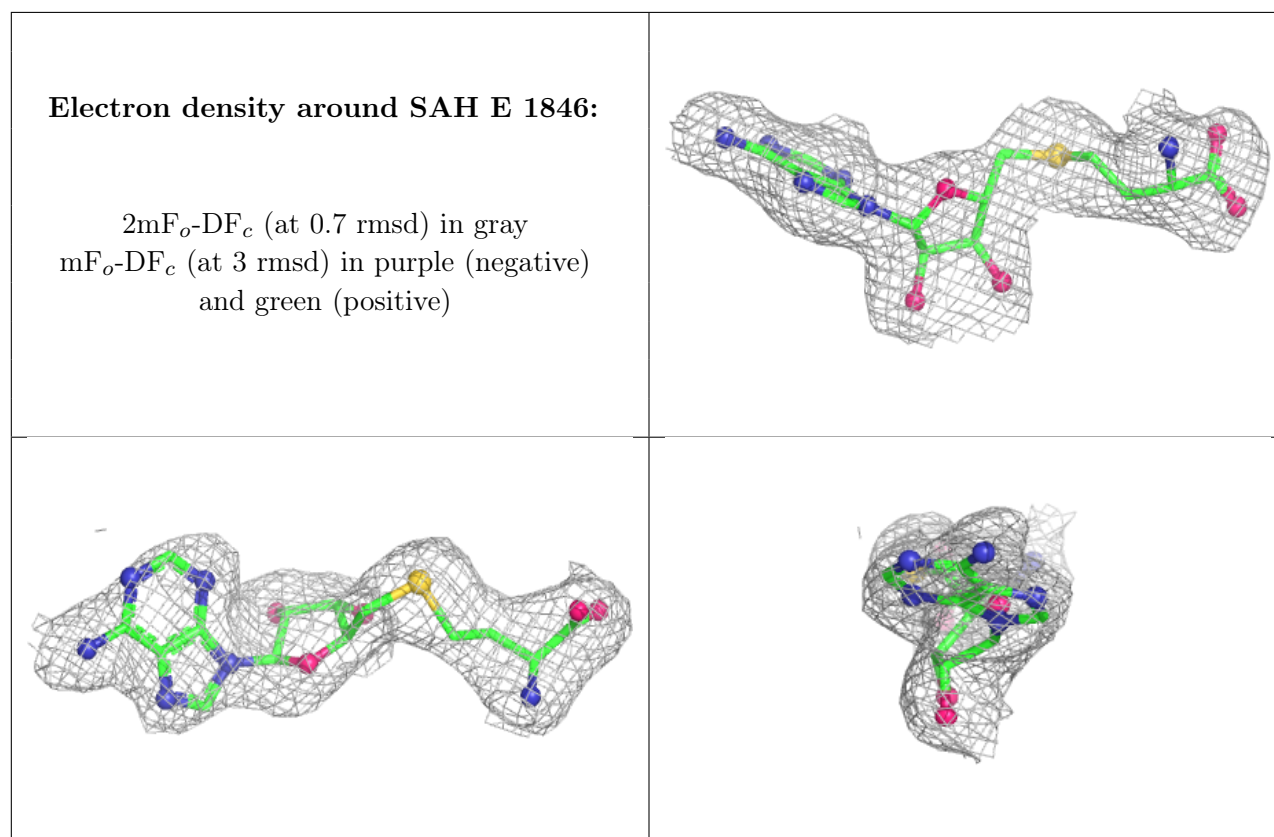
There are no oligosaccharides in this entry.

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.

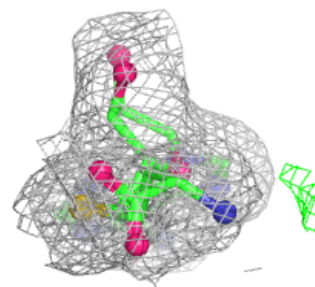
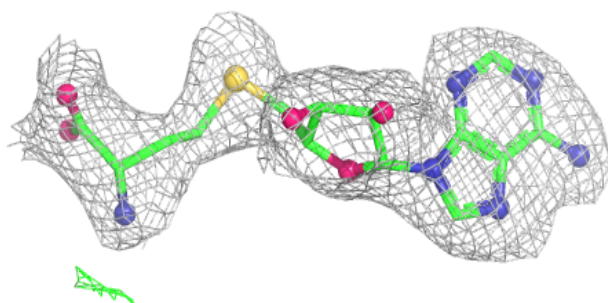
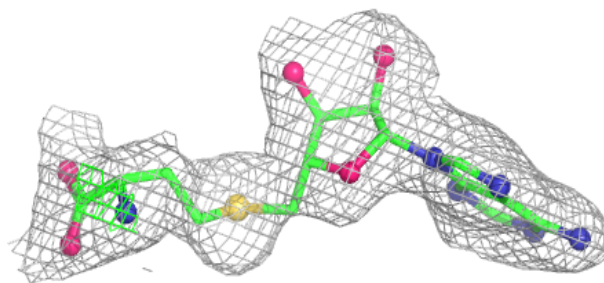
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	C	1847	5/5	0.99	0.03	77,77,77,77	0
3	SO4	E	1845	5/5	0.99	0.04	98,98,99,99	0
3	SO4	F	1288	5/5	0.99	0.07	82,83,83,84	0
3	SO4	G	1845	5/5	0.99	0.03	89,90,90,91	0
3	SO4	H	1288	5/5	0.99	0.06	66,67,67,67	0
3	SO4	H	1290	5/5	0.99	0.03	83,83,83,83	0
3	SO4	H	1291	5/5	0.99	0.03	81,82,82,82	0
4	SAH	E	1846	26/26	0.99	0.02	30,32,36,36	0
4	SAH	G	1846	26/26	0.99	0.03	29,32,35,35	0
3	SO4	F	1289	5/5	1.00	0.04	71,72,72,72	0
3	SO4	C	1845	5/5	1.00	0.02	62,62,63,64	0
4	SAH	A	1846	26/26	1.00	0.02	18,19,20,22	0
4	SAH	C	1846	26/26	1.00	0.02	13,16,18,18	0
3	SO4	A	1845	5/5	1.00	0.02	60,60,61,61	0
3	SO4	H	1289	5/5	1.00	0.03	77,78,78,78	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.

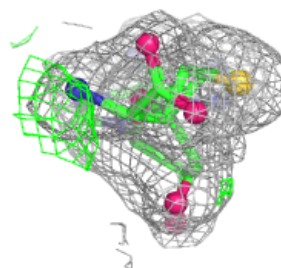
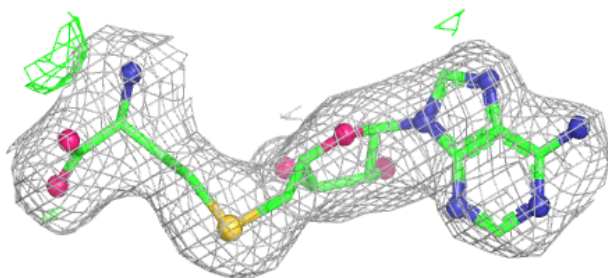
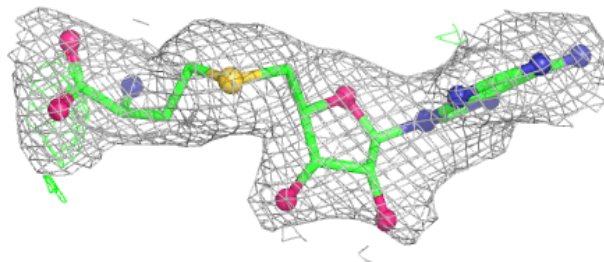


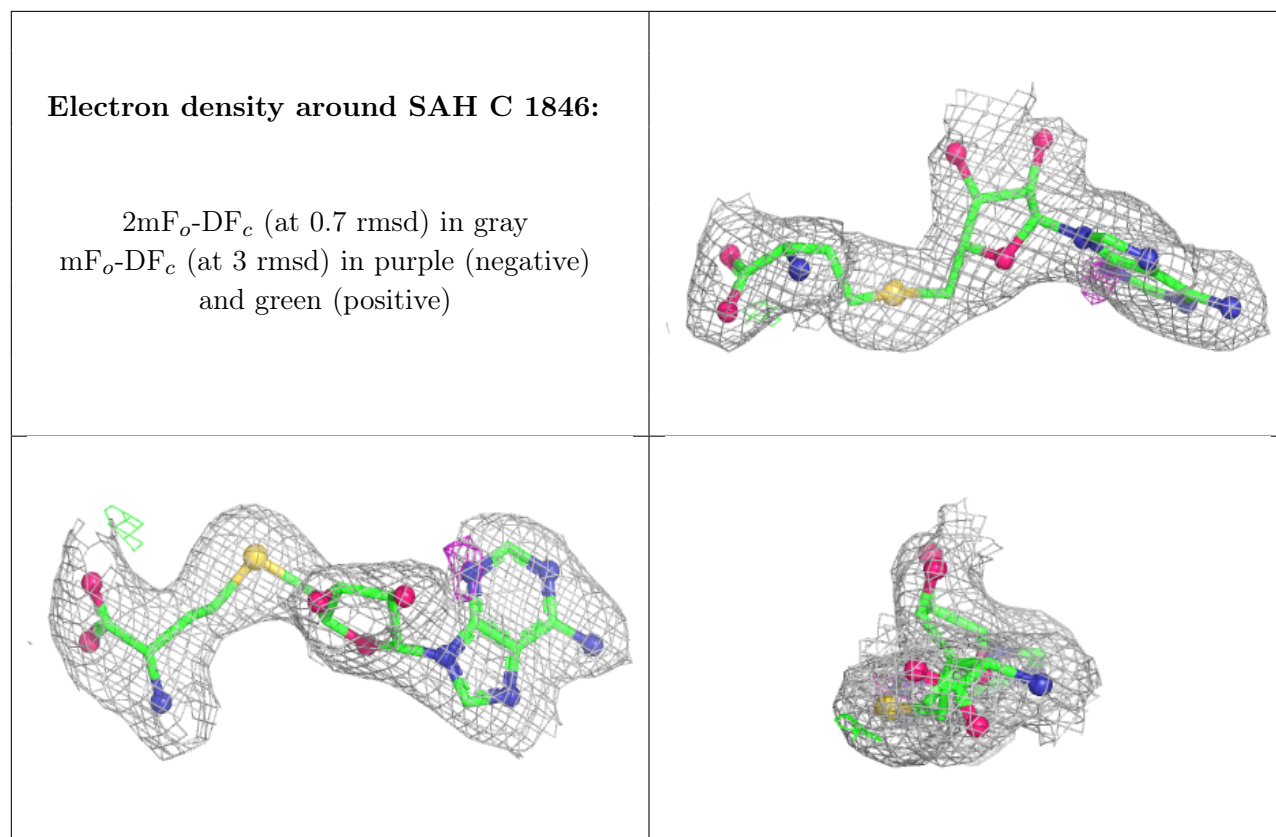
Electron density around SAH G 1846:

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

**Electron density around SAH A 1846:**

$2mF_o-DF_c$ (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.