



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:17 am BST

PDB ID : 2VDW
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

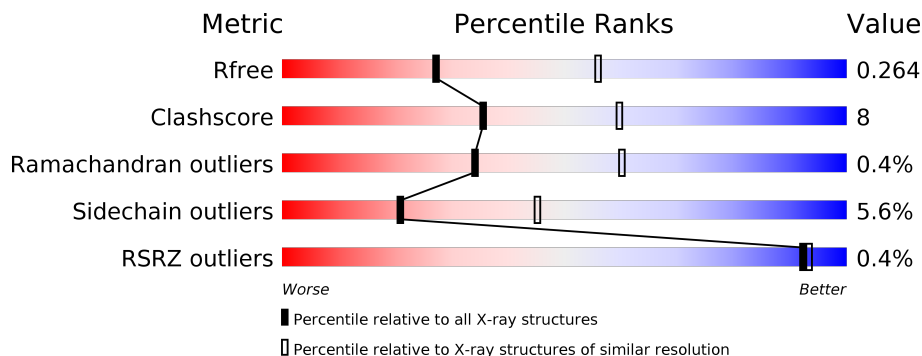
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	
1	C	302	
1	E	302	
1	G	302	
2	B	287	
2	D	287	

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Mol	Chain	Length	Quality of chain
2	F	287	 77% 18% ..
2	H	287	 77% 20% ..

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	296	Total 2413	C 1549	N 399	O 456	S 9	0	0	0
1	C	296	Total 2413	C 1549	N 399	O 456	S 9	0	0	0
1	E	283	Total 2317	C 1492	N 384	O 433	S 8	0	0	0
1	G	276	Total 2253	C 1450	N 374	O 421	S 8	0	0	0

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

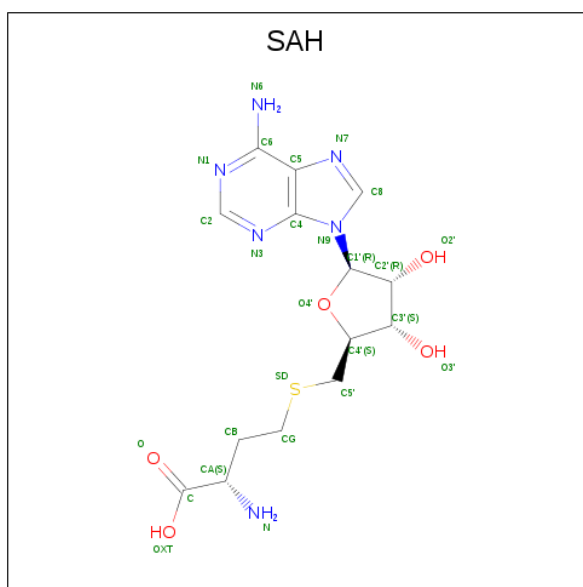
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	283	Total 2312	C 1488	N 383	O 428	S 13	0	0	0
2	D	283	Total 2312	C 1488	N 383	O 428	S 13	0	0	0
2	F	281	Total 2297	C 1479	N 380	O 425	S 13	0	0	0
2	H	284	Total 2320	C 1492	N 385	O 430	S 13	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: 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 (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).

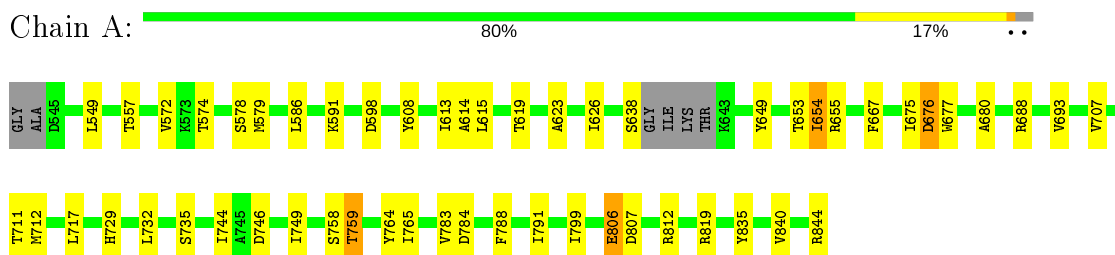


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	S			
4	A	1	Total	26	14	6	5	1	0	0
4	C	1	Total	26	14	6	5	1	0	0
4	E	1	Total	26	14	6	5	1	0	0
4	G	1	Total	26	14	6	5	1	0	0

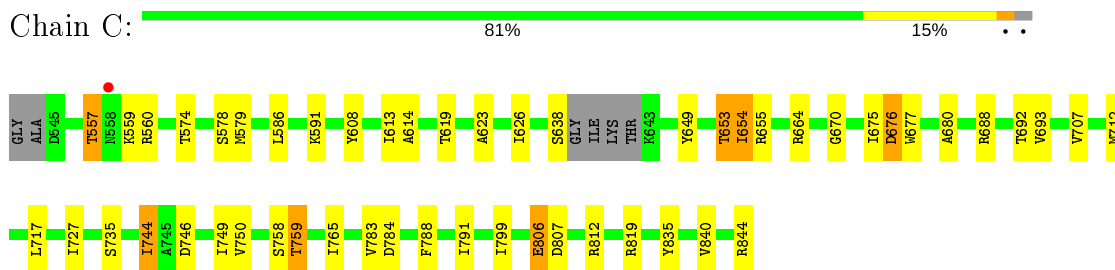
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

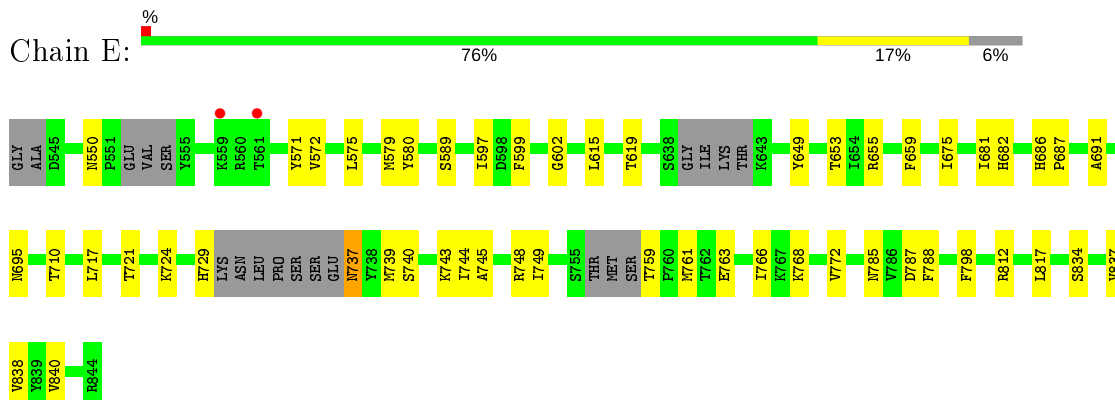
- Molecule 1: VACCINIA VIRUS CAPPING ENZYME D1 SUBUNIT



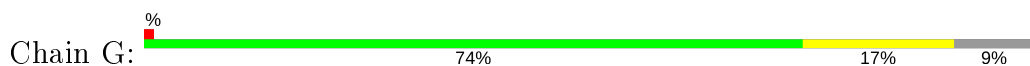
- Molecule 1: VACCINIA VIRUS CAPPING ENZYME D1 SUBUNIT

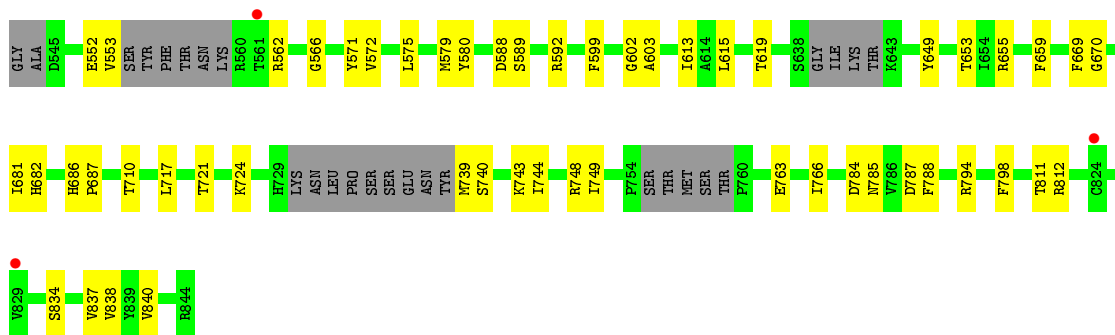


- Molecule 1: VACCINIA VIRUS CAPPING ENZYME D1 SUBUNIT



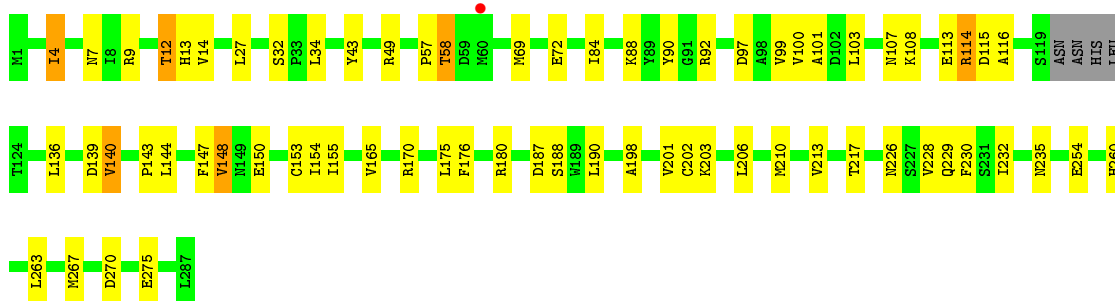
- Molecule 1: VACCINIA VIRUS CAPPING ENZYME D1 SUBUNIT





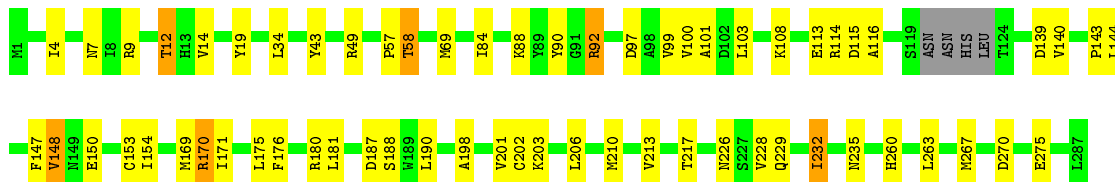
• Molecule 2: MRNA-CAPPING ENZYME SMALL SUBUNIT

Chain B: 75% 22%



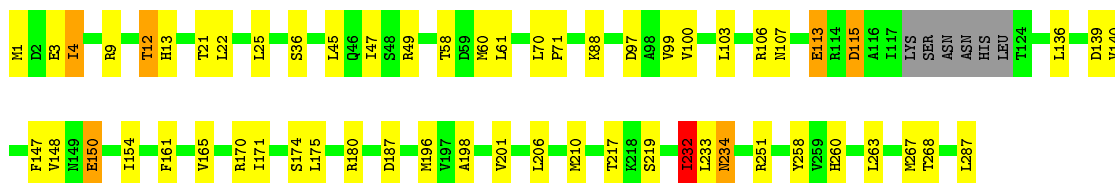
• Molecule 2: MRNA-CAPPING ENZYME SMALL SUBUNIT

Chain D: 77% 20%



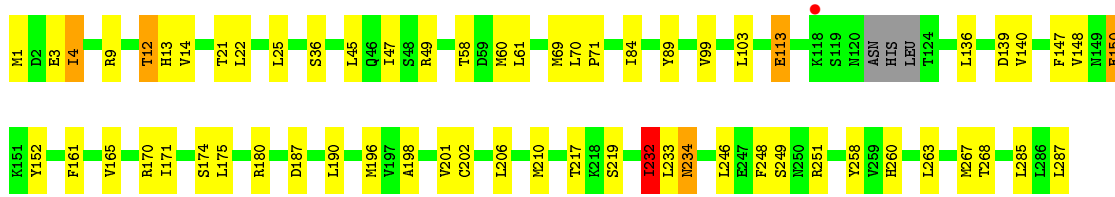
• Molecule 2: MRNA-CAPPING ENZYME SMALL SUBUNIT

Chain F: 77% 18%



• Molecule 2: MRNA-CAPPING ENZYME SMALL SUBUNIT

Chain H: 77% 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 48.37 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.8 (48.39-2.70) 89.8 (48.37-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.69Å)	Xtrriage
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	Xtrriage
Anisotropy	0.148	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 14.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.207 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	18796	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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	0.58	0/2464	0.68	0/3323
1	C	0.61	0/2464	0.68	0/3323
1	E	0.52	0/2364	0.62	0/3183
1	G	0.52	0/2297	0.63	0/3091
2	B	0.58	0/2357	0.65	0/3178
2	D	0.58	0/2357	0.65	0/3178
2	F	0.53	0/2342	0.65	0/3159
2	H	0.54	0/2365	0.64	0/3189
All	All	0.56	0/19010	0.65	0/25624

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2413	0	2389	33	0
1	C	2413	0	2389	31	0
1	E	2317	0	2292	34	0
1	G	2253	0	2237	36	0
2	B	2312	0	2357	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2312	0	2357	43	0
2	F	2297	0	2339	45	0
2	H	2320	0	2363	50	0
3	A	5	0	0	0	0
3	C	10	0	0	0	0
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	306	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 8.

All (306) 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:O	2:H:232:ILE:HD13	1.57	1.04
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:H:99:VAL:HG23	2:H:150:GLU:HG3	1.50	0.92
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: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: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
1:A:653:THR:HG21	1:A:655:ARG:NH1	2.04	0.72
1:E:653:THR:HG21	1:E:655:ARG:CZ	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:H:196:MET:HE3	2:H:198:ALA:HB2	1.76	0.66
1:A:591:LYS:HB3	1:A:614:ALA:HB2	1.76	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: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: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
2:F:115:ASP:OD1	2:F:115:ASP:N	2.32	0.62
2:D:176:PHE:CE2	2:D:201:VAL:HG22	2.35	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
2:H:61:LEU:HD12	2:H:267:MET:CE	2.32	0.59
1:E:710:THR:HG22	1:E:838:VAL:HG22	1.83	0.59
2:H:171:ILE:HD11	2:H:232:ILE:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:579:MET:CE	1:E:580:TYR:CE1	2.86	0.59
2:B:90:TYR:CD1	2:D:115:ASP:HB3	2.37	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:F:268:THR:O	2:F:268:THR:HG22	2.02	0.59
1:E:579:MET:HE3	1:E:580:TYR:CE1	2.37	0.58
2:H:12:THR:HG21	2:H:251:ARG:HD3	1.84	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:175:LEU:HD22	2:H:206:LEU:HA	1.87	0.56
2:H:21:THR:HG22	2:H:22:LEU:O	2.05	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:A:579:MET:HE1	2:B:43:TYR:HD1	1.71	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
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
1:C:579:MET:HE1	2:D:43:TYR:HD1	1.72	0.55
1:E:579:MET:HE3	1:E:580:TYR:CD1	2.42	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:58:THR:HG21	2:H:113:GLU:HG3	1.89	0.54
2:H:14:VAL:HG21	2:H:248:PHE:HB2	1.89	0.54
2:H:103:LEU:CD1	2:H:140:VAL:CG1	2.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:61:LEU:HD12	2:H:267:MET:HE1	1.91	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
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:D:210:MET:HA	2:D:210:MET:HE2	1.93	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
2:D:190:LEU:N	2:D:190:LEU:HD12	2.25	0.51
1:G:798:PHE:CD1	2:H:45:LEU:HD13	2.46	0.51
2:H:210:MET:HA	2:H:210:MET:HE2	1.94	0.50
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:HD12	2:B:190:LEU:N	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
1:C:574:THR:O	1:C:578:SER:OG	2.19	0.50
2:H:49:ARG:HG3	2:H:260:HIS:HB3	1.94	0.50
2:B:263:LEU:HG	2:B:267:MET:CE	2.42	0.50
1:C:675:ILE:CG2	1:C:707:VAL:HG13	2.41	0.50
2:F:196:MET:CE	2:F:198:ALA:HB2	2.42	0.50
2:F:175:LEU:HD22	2:F:206:LEU:HA	1.94	0.49
2:H:268:THR:HG22	2:H:268:THR:O	2.12	0.49
1:E:759:THR:O	1:E:761:MET:CE	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:92:ARG:O	2:D:148:VAL:HG21	2.12	0.49
2:D:263:LEU:HG	2:D:267:MET:CE	2.42	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:210:MET:HE2	2:B:210:MET:HA	1.94	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:69:MET:HE3	2:H:190:LEU:HD22	1.95	0.49
2:F:61:LEU:HD12	2:F:267:MET:CE	2.43	0.48
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
2:F:263:LEU:CD1	2:F:267:MET:HE2	2.44	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
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
2:H:61:LEU:HD12	2:H:267:MET:HE3	1.96	0.47
1:E:599:PHE:CE2	1:E:602:GLY:HA2	2.49	0.47
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:F:263:LEU:HD11	2:F:267:MET:HE2	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
2:F:61:LEU:HD12	2:F:267:MET:HE1	1.97	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
1:G:579:MET:HE3	1:G:580:TYR:CE1	2.49	0.46
2:F:232:ILE:O	2:F:232:ILE:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:ALA:HA	1:A:626:ILE:HD12	1.98	0.46
2:B:100:VAL:HG12	2:B:101:ALA:N	2.31	0.46
2:B:13:HIS:O	2:B:14:VAL:HG23	2.15	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
2:D:210:MET:HE1	2:D:213:VAL:HG11	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:H:263:LEU:CD1	2:H:267:MET:HE2	2.46	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: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
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: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:N	2:F:234:ASN:OD1	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
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
2:H:263:LEU:HD11	2:H:267:MET:HE2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:F:210:MET:HA	2:F:210:MET:HE2	2.01	0.43
1:G:615:LEU:C	1:G:615:LEU:HD12	2.39	0.43
1:A:717:LEU:HD13	1:A:749:ILE:HD13	2.00	0.43
2:B:210:MET:CE	2:B:210:MET:HA	2.49	0.43
1:A:586:LEU:CD1	2:B:34:LEU:HD22	2.48	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
2:D:263:LEU:HG	2:D:267:MET:HE1	1.99	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
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:N3	4:C:1846:SAH:H2'	2.35	0.42
1:E:785:ASN:HA	1:E:838:VAL:O	2.20	0.42
2:H:1:MET:HB3	2:H:1:MET:HE2	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:144:LEU:HD13	2:D:175:LEU:HD13	2.02	0.41
1:E:615:LEU:C	1:E:615:LEU:HD12	2.40	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
2:B:263:LEU:HG	2:B:267:MET:HE1	2.03	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
2:D:210:MET:CE	2:D:210:MET:HA	2.50	0.41
2:F:196:MET:HE3	2:F:198:ALA:HB2	2.03	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: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:D:49:ARG:HG2	2:D:260:HIS:HB2	2.03	0.41
2:F:1:MET:HB3	2:F:1:MET:HE2	1.89	0.41
2:D:201:VAL:CG1	2:D:202:CYS:N	2.84	0.41
1:E:597:ILE:CD1	1:E:675:ILE:HG23	2.51	0.40
2:B:99:VAL:HG12	2:B:143:PRO:HB3	2.03	0.40
2:B:27:LEU:HD22	2:B:213:VAL:HG22	2.03	0.40
1:C:664:ARG:NH2	1:C:670:GLY:O	2.54	0.40
2:H:234:ASN:N	2:H:234:ASN:OD1	2.47	0.40
1:E:579:MET:HE1	1:E:580:TYR:CE1	2.55	0.40
2:H:196:MET:HE1	2:H:198:ALA:HB2	2.00	0.40
1:A:729:HIS:CG	1:A:732:LEU:HD12	2.57	0.40
2:B:140:VAL:O	2:B:155:ILE:CD1	2.70	0.40
2:B:88:LYS:HE2	2:B:99:VAL:HG22	2.03	0.40
2:D:92:ARG:HH11	2:D:92:ARG:HB2	1.87	0.40
1:C:746:ASP:O	1:C:765:ILE:HD12	2.21	0.40
1:G:579:MET:HE3	1:G:580:TYR:CD1	2.56	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 [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	292/302 (97%)	280 (96%)	11 (4%)	1 (0%)	41	66
1	C	292/302 (97%)	277 (95%)	14 (5%)	1 (0%)	41	66
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%)	34	60
2	D	279/287 (97%)	260 (93%)	18 (6%)	1 (0%)	34	60
2	F	277/287 (96%)	258 (93%)	17 (6%)	2 (1%)	22	46
2	H	280/287 (98%)	264 (94%)	14 (5%)	2 (1%)	22	46
All	All	2238/2356 (95%)	2103 (94%)	127 (6%)	8 (0%)	34	60

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	268/271 (99%)	254 (95%)	14 (5%)	23	49
1	C	268/271 (99%)	252 (94%)	16 (6%)	19	42
1	E	255/271 (94%)	245 (96%)	10 (4%)	32	61
1	G	248/271 (92%)	239 (96%)	9 (4%)	35	64
2	B	268/272 (98%)	252 (94%)	16 (6%)	19	42
2	D	268/272 (98%)	250 (93%)	18 (7%)	16	37
2	F	266/272 (98%)	247 (93%)	19 (7%)	14	34
2	H	269/272 (99%)	252 (94%)	17 (6%)	18	40
All	All	2110/2172 (97%)	1991 (94%)	119 (6%)	21	45

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	557	THR
1	A	619	THR
1	A	638	SER
1	A	649	TYR
1	A	654	ILE
1	A	676	ASP
1	A	688	ARG
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	58	THR
2	B	69	MET
2	B	114	ARG
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

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Mol	Chain	Res	Type
2	B	235	ASN
2	B	270	ASP
2	B	275	GLU
1	C	557	THR
1	C	560	ARG
1	C	619	THR
1	C	638	SER
1	C	649	TYR
1	C	653	THR
1	C	654	ILE
1	C	676	ASP
1	C	688	ARG
1	C	735	SER
1	C	744	ILE
1	C	759	THR
1	C	783	VAL
1	C	806	GLU
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	58	THR
2	D	69	MET
2	D	92	ARG
2	D	114	ARG
2	D	140	VAL
2	D	170	ARG
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	270	ASP
2	D	275	GLU
1	E	550	ASN
1	E	589	SER
1	E	649	TYR
1	E	721	THR
1	E	724	LYS

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Mol	Chain	Res	Type
1	E	737	ASN
1	E	739	MET
1	E	740	SER
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	36	SER
2	F	60	MET
2	F	97	ASP
2	F	113	GLU
2	F	115	ASP
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	232	ILE
2	F	234	ASN
2	F	287	LEU
1	G	589	SER
1	G	649	TYR
1	G	721	THR
1	G	724	LYS
1	G	739	MET
1	G	740	SER
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	60	MET
2	H	113	GLU
2	H	150	GLU

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Mol	Chain	Res	Type
2	H	165	VAL
2	H	170	ARG
2	H	174	SER
2	H	180	ARG
2	H	187	ASP
2	H	232	ILE
2	H	234	ASN
2	H	287	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	731	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	H	1288	-	4,4,4	0.12	0	6,6,6	0.17	0
3	SO4	H	1291	-	4,4,4	0.17	0	6,6,6	0.29	0
4	SAH	G	1846	-	21,28,28	1.25	2 (9%)	20,40,40	1.72	5 (25%)
3	SO4	F	1288	-	4,4,4	0.15	0	6,6,6	0.23	0
4	SAH	C	1846	-	21,28,28	1.26	2 (9%)	20,40,40	1.84	4 (20%)
3	SO4	H	1290	-	4,4,4	0.14	0	6,6,6	0.17	0
3	SO4	A	1845	-	4,4,4	0.12	0	6,6,6	0.28	0
4	SAH	E	1846	-	21,28,28	1.23	2 (9%)	20,40,40	1.63	4 (20%)
3	SO4	C	1845	-	4,4,4	0.15	0	6,6,6	0.20	0
4	SAH	A	1846	-	21,28,28	1.40	2 (9%)	20,40,40	1.53	3 (15%)
3	SO4	E	1845	-	4,4,4	0.12	0	6,6,6	0.11	0
3	SO4	H	1289	-	4,4,4	0.15	0	6,6,6	0.18	0
3	SO4	G	1845	-	4,4,4	0.15	0	6,6,6	0.13	0
3	SO4	F	1289	-	4,4,4	0.17	0	6,6,6	0.20	0
3	SO4	C	1847	-	4,4,4	0.18	0	6,6,6	0.17	0

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	-	-	1/7/31/31	0/3/3/3
4	SAH	C	1846	-	-	0/7/31/31	0/3/3/3
4	SAH	E	1846	-	-	4/7/31/31	0/3/3/3
4	SAH	G	1846	-	-	1/7/31/31	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1846	SAH	C2-N3	4.62	1.39	1.32
4	G	1846	SAH	C2-N3	4.18	1.38	1.32
4	E	1846	SAH	C2-N3	3.94	1.38	1.32
4	C	1846	SAH	C2-N3	3.75	1.38	1.32
4	G	1846	SAH	C2-N1	2.85	1.39	1.33
4	E	1846	SAH	C2-N1	2.79	1.39	1.33
4	A	1846	SAH	C2-N1	2.68	1.38	1.33
4	C	1846	SAH	C2-N1	2.22	1.38	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1846	SAH	N3-C2-N1	-5.33	120.35	128.68
4	C	1846	SAH	N3-C2-N1	-5.17	120.59	128.68
4	E	1846	SAH	N3-C2-N1	-4.95	120.95	128.68
4	A	1846	SAH	N3-C2-N1	-4.14	122.21	128.68
4	A	1846	SAH	C4-C5-N7	-3.38	105.88	109.40
4	C	1846	SAH	CB-CG-SD	-2.89	106.82	113.31
4	C	1846	SAH	C4-C5-N7	-2.73	106.56	109.40
4	G	1846	SAH	C3'-C2'-C1'	2.40	104.58	100.98
4	E	1846	SAH	C3'-C2'-C1'	2.31	104.45	100.98
4	C	1846	SAH	O4'-C1'-C2'	-2.30	103.57	106.93
4	E	1846	SAH	C1'-N9-C4	2.29	130.67	126.64
4	G	1846	SAH	CB-CG-SD	-2.19	108.40	113.31
4	G	1846	SAH	C1'-N9-C4	2.05	130.25	126.64
4	G	1846	SAH	C5'-SD-CG	-2.04	96.14	102.27
4	A	1846	SAH	C1'-N9-C4	2.01	130.17	126.64
4	E	1846	SAH	C4-C5-N7	-2.01	107.31	109.40

There are no chirality outliers.

All (6) 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	CB-CG-SD-C5'
4	E	1846	SAH	CA-CB-CG-SD
4	G	1846	SAH	CB-CG-SD-C5'
4	A	1846	SAH	CB-CG-SD-C5'

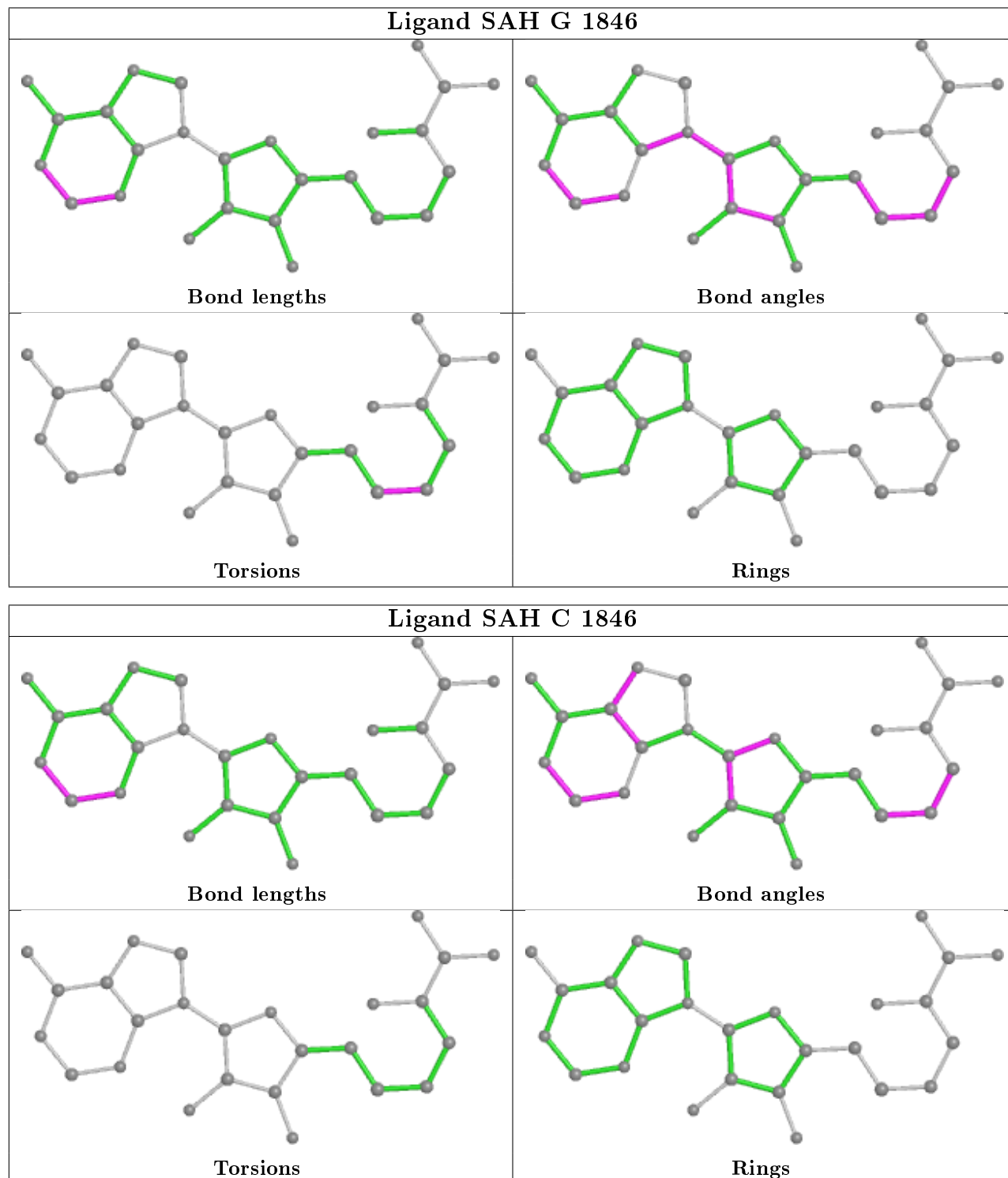
There are no ring outliers.

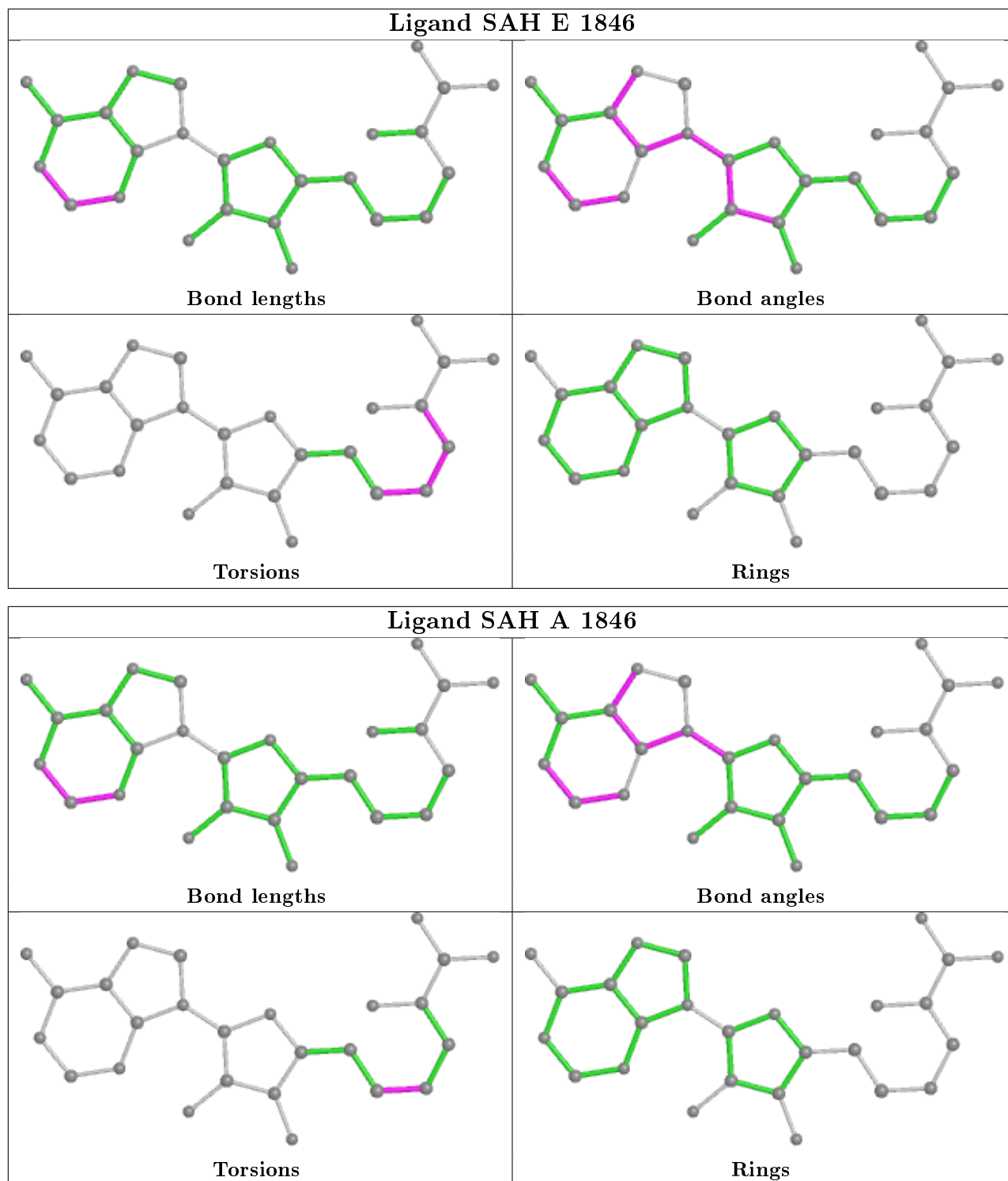
3 monomers are involved in 5 short contacts:

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

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%)	-0.14	0 100 100	17, 33, 49, 63	0
1	C	296/302 (98%)	-0.11	1 (0%) 94 95	18, 33, 47, 60	0
1	E	283/302 (93%)	0.12	2 (0%) 87 89	26, 45, 71, 88	0
1	G	276/302 (91%)	0.13	3 (1%) 80 82	26, 45, 73, 84	0
2	B	283/287 (98%)	-0.00	1 (0%) 92 93	23, 42, 60, 69	0
2	D	283/287 (98%)	-0.02	0 100 100	23, 42, 62, 70	0
2	F	281/287 (97%)	-0.03	0 100 100	22, 37, 60, 77	0
2	H	284/287 (98%)	-0.03	1 (0%) 92 93	22, 37, 60, 75	0
All	All	2282/2356 (96%)	-0.01	8 (0%) 92 93	17, 38, 64, 88	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	561	THR	5.2
1	E	559	LYS	3.6
1	E	561	THR	3.3
1	C	558	ASN	2.8
1	G	824	CYS	2.4
2	B	60	MET	2.4
1	G	829	VAL	2.1
2	H	118	LYS	2.1

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

There are no carbohydrates in this entry.

6.4 Ligands

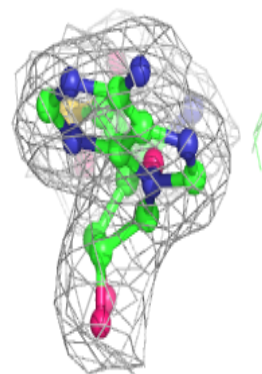
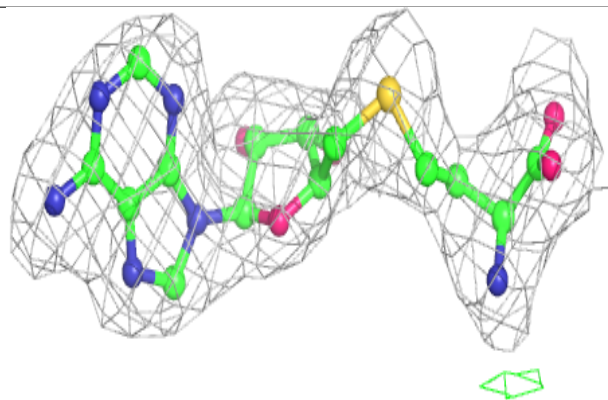
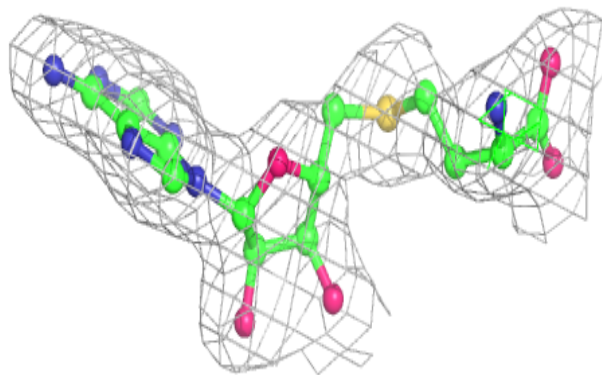
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	H	1291	5/5	0.89	0.12	81,82,82,82	0
3	SO4	H	1290	5/5	0.89	0.17	83,83,83,83	0
3	SO4	F	1288	5/5	0.93	0.33	82,83,83,84	0
3	SO4	E	1845	5/5	0.93	0.14	98,98,99,99	0
3	SO4	C	1847	5/5	0.93	0.13	77,77,77,77	0
3	SO4	H	1288	5/5	0.94	0.22	66,67,67,67	0
3	SO4	G	1845	5/5	0.94	0.17	89,90,90,91	0
3	SO4	F	1289	5/5	0.94	0.15	71,72,72,72	0
4	SAH	G	1846	26/26	0.94	0.13	29,32,35,35	0
3	SO4	H	1289	5/5	0.96	0.17	77,78,78,78	0
4	SAH	E	1846	26/26	0.96	0.14	30,32,36,36	0
4	SAH	A	1846	26/26	0.97	0.15	18,19,20,22	0
4	SAH	C	1846	26/26	0.97	0.16	13,16,18,18	0
3	SO4	C	1845	5/5	0.97	0.12	62,62,63,64	0
3	SO4	A	1845	5/5	0.99	0.10	60,60,61,61	0

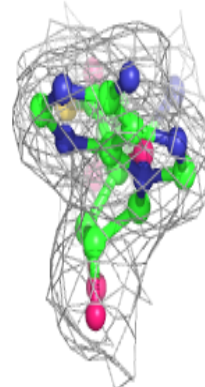
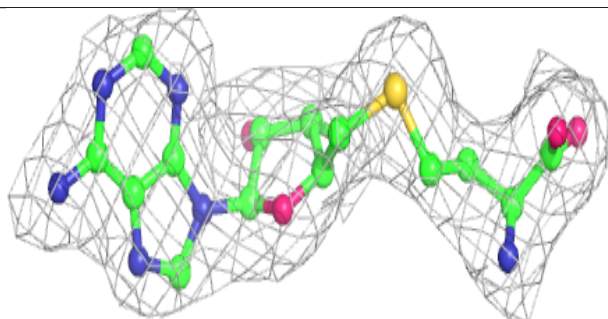
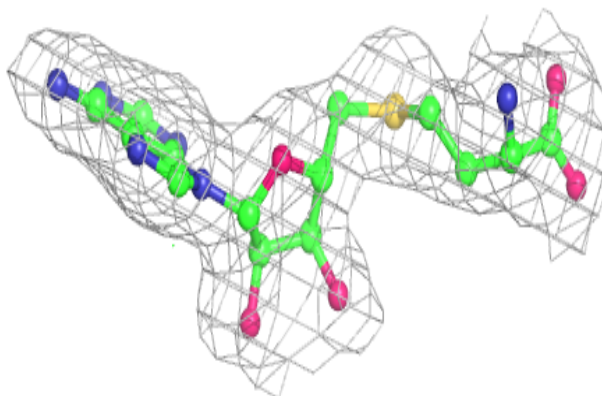
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

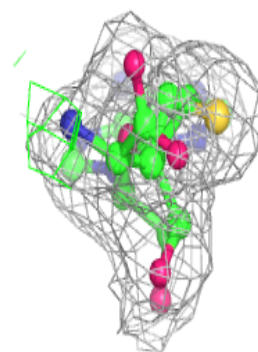
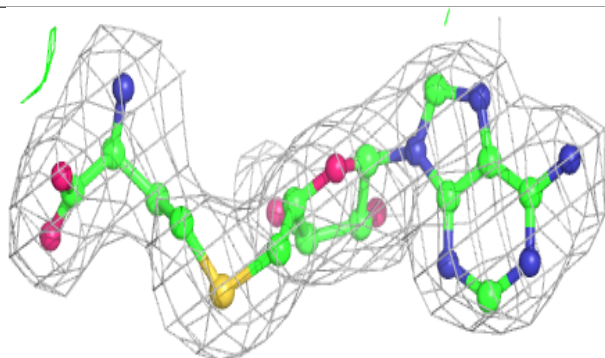
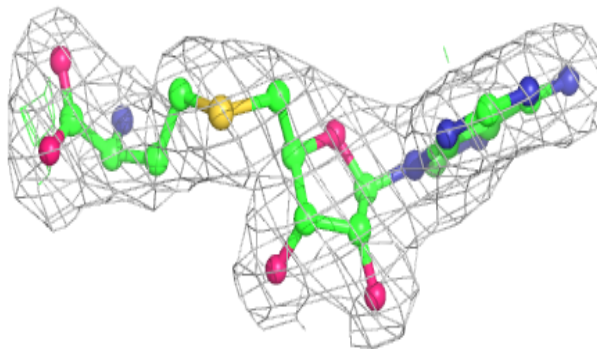
**Electron density around SAH E 1846:**

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

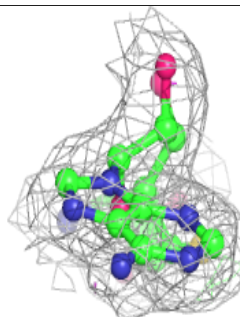
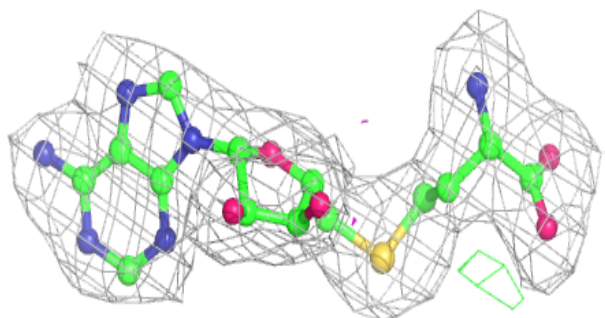
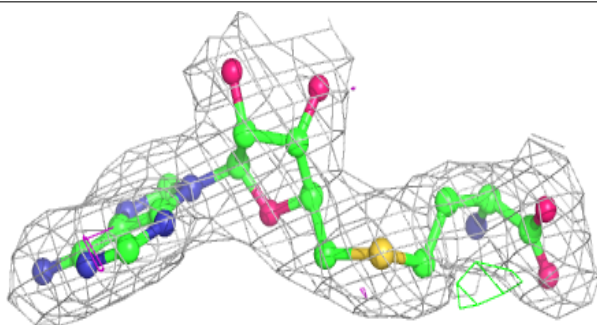


Electron density around SAH A 1846:

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

**Electron density around SAH C 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

There are no such residues in this entry.