



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 05:45 AM BST

PDB ID : 5AB6
Title : Crystal structure of Trypanosoma brucei SCP2-thiolase like protein (TbSLP) in complex with acetoacetyl-CoA.
Authors : Harijan, R.K.; Kiema, T.R.; Wierenga, R.K.
Deposited on : 2015-08-01
Resolution : 1.90 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 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 : 2.13.1
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) : 2.13.1

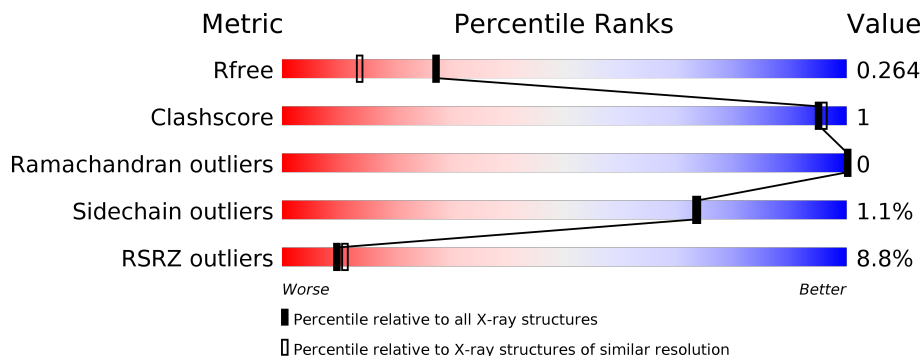
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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	425	
1	B	425	
1	C	425	
1	D	425	
1	E	425	
1	F	425	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 18659 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 SCP2-THIOLASE LIKE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	394	Total 2930	C 1855	N 511	O 539	S 25	0	1	0
1	B	393	Total 2935	C 1858	N 512	O 540	S 25	0	2	0
1	C	394	Total 2923	C 1851	N 511	O 537	S 24	0	0	0
1	D	396	Total 2949	C 1866	N 515	O 543	S 25	0	1	0
1	E	395	Total 2937	C 1858	N 512	O 542	S 25	0	1	0
1	F	396	Total 2960	C 1872	N 519	O 544	S 25	0	3	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	expression tag	UNP C9ZUV7
A	-14	HIS	-	expression tag	UNP C9ZUV7
A	-13	HIS	-	expression tag	UNP C9ZUV7
A	-12	HIS	-	expression tag	UNP C9ZUV7
A	-11	HIS	-	expression tag	UNP C9ZUV7
A	-10	HIS	-	expression tag	UNP C9ZUV7
A	-9	SER	-	expression tag	UNP C9ZUV7
A	-8	SER	-	expression tag	UNP C9ZUV7
A	-7	GLY	-	expression tag	UNP C9ZUV7
A	-6	LEU	-	expression tag	UNP C9ZUV7
A	-5	VAL	-	expression tag	UNP C9ZUV7
A	-4	PRO	-	expression tag	UNP C9ZUV7
A	-3	ARG	-	expression tag	UNP C9ZUV7
A	-2	GLY	-	expression tag	UNP C9ZUV7
A	-1	SER	-	expression tag	UNP C9ZUV7
A	0	HIS	-	expression tag	UNP C9ZUV7
B	-15	HIS	-	expression tag	UNP C9ZUV7

Continued on next page...

Continued from previous page...

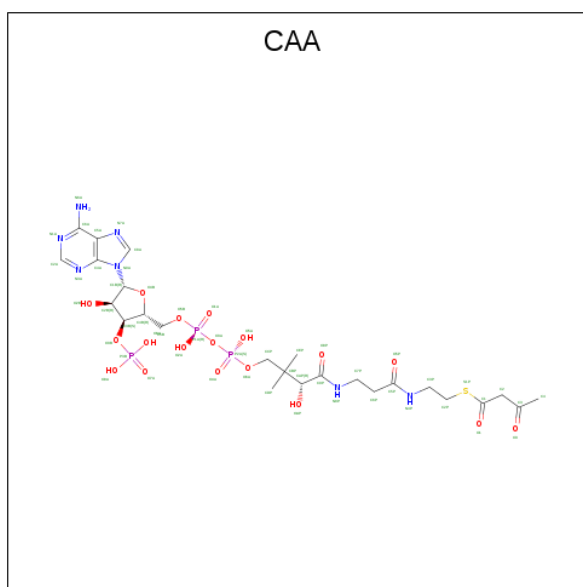
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP C9ZUV7
B	-13	HIS	-	expression tag	UNP C9ZUV7
B	-12	HIS	-	expression tag	UNP C9ZUV7
B	-11	HIS	-	expression tag	UNP C9ZUV7
B	-10	HIS	-	expression tag	UNP C9ZUV7
B	-9	SER	-	expression tag	UNP C9ZUV7
B	-8	SER	-	expression tag	UNP C9ZUV7
B	-7	GLY	-	expression tag	UNP C9ZUV7
B	-6	LEU	-	expression tag	UNP C9ZUV7
B	-5	VAL	-	expression tag	UNP C9ZUV7
B	-4	PRO	-	expression tag	UNP C9ZUV7
B	-3	ARG	-	expression tag	UNP C9ZUV7
B	-2	GLY	-	expression tag	UNP C9ZUV7
B	-1	SER	-	expression tag	UNP C9ZUV7
B	0	HIS	-	expression tag	UNP C9ZUV7
C	-15	HIS	-	expression tag	UNP C9ZUV7
C	-14	HIS	-	expression tag	UNP C9ZUV7
C	-13	HIS	-	expression tag	UNP C9ZUV7
C	-12	HIS	-	expression tag	UNP C9ZUV7
C	-11	HIS	-	expression tag	UNP C9ZUV7
C	-10	HIS	-	expression tag	UNP C9ZUV7
C	-9	SER	-	expression tag	UNP C9ZUV7
C	-8	SER	-	expression tag	UNP C9ZUV7
C	-7	GLY	-	expression tag	UNP C9ZUV7
C	-6	LEU	-	expression tag	UNP C9ZUV7
C	-5	VAL	-	expression tag	UNP C9ZUV7
C	-4	PRO	-	expression tag	UNP C9ZUV7
C	-3	ARG	-	expression tag	UNP C9ZUV7
C	-2	GLY	-	expression tag	UNP C9ZUV7
C	-1	SER	-	expression tag	UNP C9ZUV7
C	0	HIS	-	expression tag	UNP C9ZUV7
D	-15	HIS	-	expression tag	UNP C9ZUV7
D	-14	HIS	-	expression tag	UNP C9ZUV7
D	-13	HIS	-	expression tag	UNP C9ZUV7
D	-12	HIS	-	expression tag	UNP C9ZUV7
D	-11	HIS	-	expression tag	UNP C9ZUV7
D	-10	HIS	-	expression tag	UNP C9ZUV7
D	-9	SER	-	expression tag	UNP C9ZUV7
D	-8	SER	-	expression tag	UNP C9ZUV7
D	-7	GLY	-	expression tag	UNP C9ZUV7
D	-6	LEU	-	expression tag	UNP C9ZUV7
D	-5	VAL	-	expression tag	UNP C9ZUV7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	PRO	-	expression tag	UNP C9ZUV7
D	-3	ARG	-	expression tag	UNP C9ZUV7
D	-2	GLY	-	expression tag	UNP C9ZUV7
D	-1	SER	-	expression tag	UNP C9ZUV7
D	0	HIS	-	expression tag	UNP C9ZUV7
E	-15	HIS	-	expression tag	UNP C9ZUV7
E	-14	HIS	-	expression tag	UNP C9ZUV7
E	-13	HIS	-	expression tag	UNP C9ZUV7
E	-12	HIS	-	expression tag	UNP C9ZUV7
E	-11	HIS	-	expression tag	UNP C9ZUV7
E	-10	HIS	-	expression tag	UNP C9ZUV7
E	-9	SER	-	expression tag	UNP C9ZUV7
E	-8	SER	-	expression tag	UNP C9ZUV7
E	-7	GLY	-	expression tag	UNP C9ZUV7
E	-6	LEU	-	expression tag	UNP C9ZUV7
E	-5	VAL	-	expression tag	UNP C9ZUV7
E	-4	PRO	-	expression tag	UNP C9ZUV7
E	-3	ARG	-	expression tag	UNP C9ZUV7
E	-2	GLY	-	expression tag	UNP C9ZUV7
E	-1	SER	-	expression tag	UNP C9ZUV7
E	0	HIS	-	expression tag	UNP C9ZUV7
F	-15	HIS	-	expression tag	UNP C9ZUV7
F	-14	HIS	-	expression tag	UNP C9ZUV7
F	-13	HIS	-	expression tag	UNP C9ZUV7
F	-12	HIS	-	expression tag	UNP C9ZUV7
F	-11	HIS	-	expression tag	UNP C9ZUV7
F	-10	HIS	-	expression tag	UNP C9ZUV7
F	-9	SER	-	expression tag	UNP C9ZUV7
F	-8	SER	-	expression tag	UNP C9ZUV7
F	-7	GLY	-	expression tag	UNP C9ZUV7
F	-6	LEU	-	expression tag	UNP C9ZUV7
F	-5	VAL	-	expression tag	UNP C9ZUV7
F	-4	PRO	-	expression tag	UNP C9ZUV7
F	-3	ARG	-	expression tag	UNP C9ZUV7
F	-2	GLY	-	expression tag	UNP C9ZUV7
F	-1	SER	-	expression tag	UNP C9ZUV7
F	0	HIS	-	expression tag	UNP C9ZUV7

- Molecule 2 is ACETOACETYL-COENZYME A (three-letter code: CAA) (formula: C₂₅H₄₀N₇O₁₈P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
2	A	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		

- 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	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	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		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	111	Total	O	0	0
			111	111		

Continued on next page...

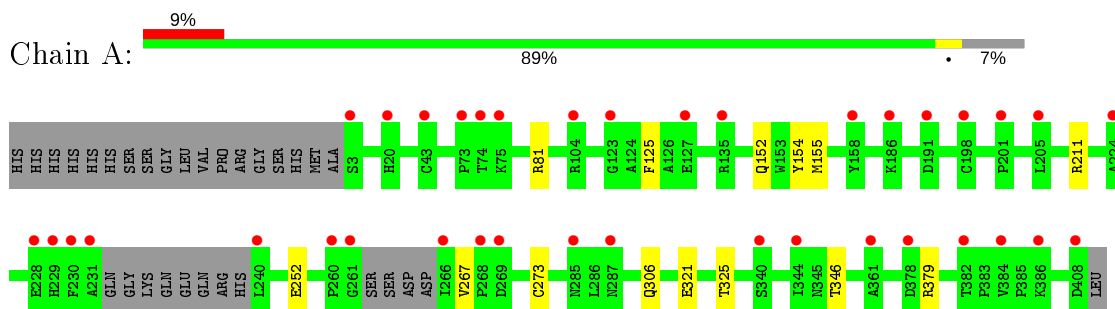
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	90	Total 90	O 90	0	0
4	C	119	Total 119	O 119	0	0
4	D	103	Total 103	O 103	0	0
4	E	119	Total 119	O 119	0	0
4	F	104	Total 104	O 104	0	0

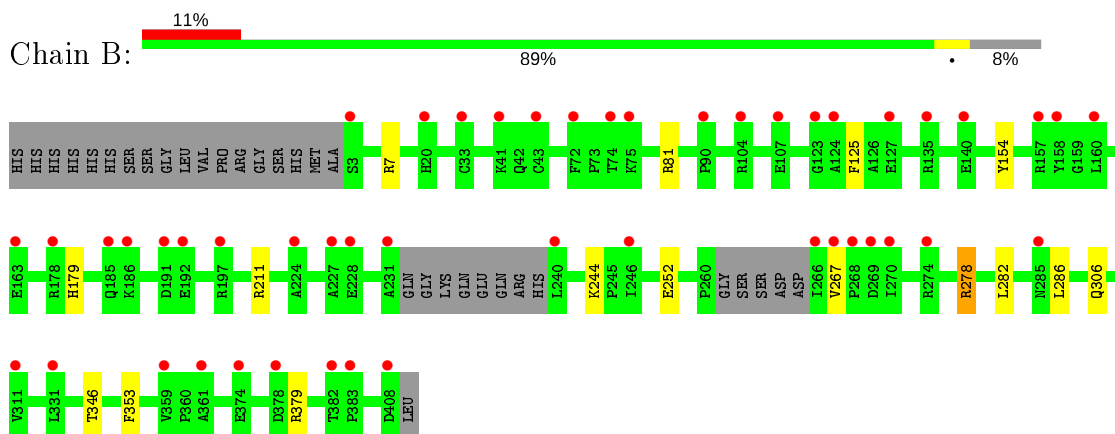
3 Residue-property plots [i](#)

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

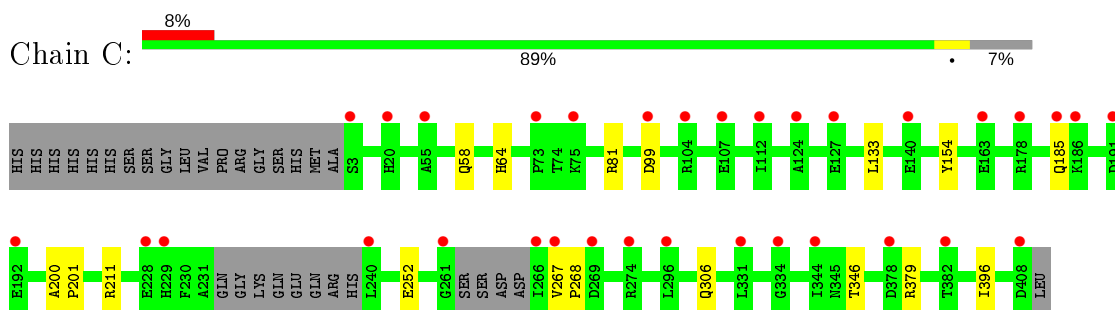
- Molecule 1: SCP2-THIOLASE LIKE PROTEIN



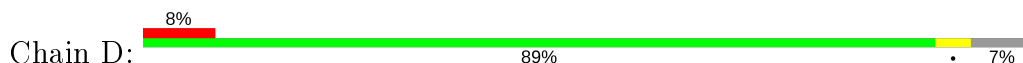
- Molecule 1: SCP2-THIOLASE LIKE PROTEIN

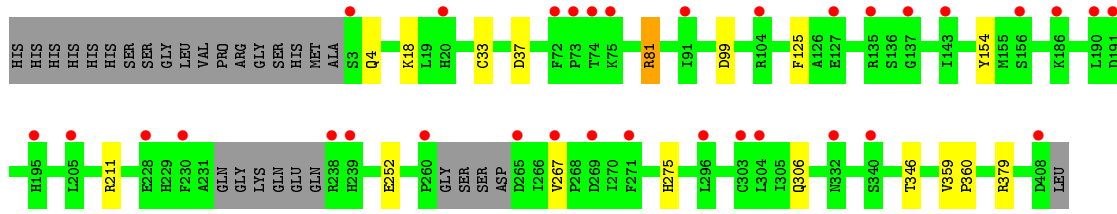


- Molecule 1: SCP2-THIOLASE LIKE PROTEIN

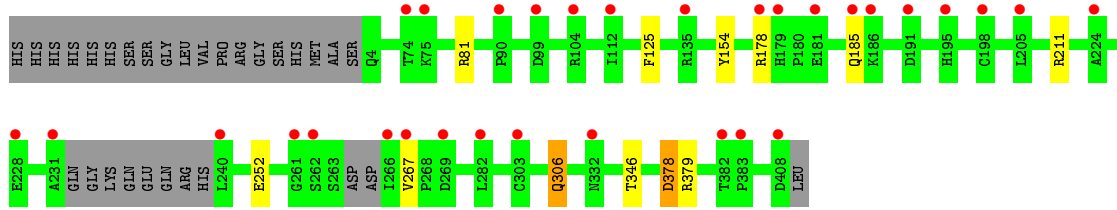
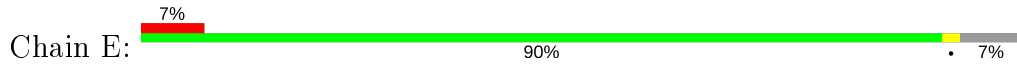


- Molecule 1: SCP2-THIOLASE LIKE PROTEIN

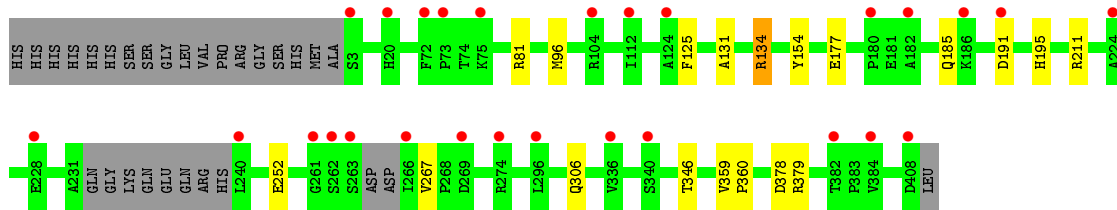
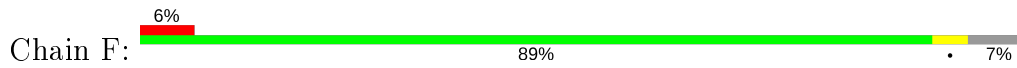




• Molecule 1: SCP2-THIOLASE LIKE PROTEIN



• Molecule 1: SCP2-THIOLASE LIKE PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	116.15Å 65.97Å 156.75Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	29.43 – 1.90 29.41 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (29.43-1.90) 97.9 (29.41-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 1.91Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.248 , 0.264 0.250 , 0.264	Depositor DCC
R_{free} test set	9153 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtrriage
Anisotropy	0.241	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18659	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 68.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4545e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CAA, 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	0.32	0/2993	0.53	0/4061
1	B	0.33	0/2998	0.55	2/4068 (0.0%)
1	C	0.33	0/2983	0.56	1/4048 (0.0%)
1	D	0.33	0/3013	0.53	0/4089
1	E	0.32	0/3000	0.54	0/4070
1	F	0.35	0/3027	0.54	0/4106
All	All	0.33	0/18014	0.54	3/24442 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	211	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	B	278	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	282	LEU	CA-CB-CG	5.04	126.90	115.30

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	2930	0	2929	8	0
1	B	2935	0	2933	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2923	0	2920	8	0
1	D	2949	0	2939	11	0
1	E	2937	0	2937	6	0
1	F	2960	0	2958	13	0
2	A	54	0	36	0	0
2	B	54	0	36	0	0
2	C	54	0	36	0	0
2	D	54	0	36	0	0
2	E	54	0	36	0	0
2	F	54	0	36	0	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
3	E	15	0	0	0	0
3	F	10	0	0	0	0
4	A	111	0	0	0	0
4	B	90	0	0	1	0
4	C	119	0	0	0	0
4	D	103	0	0	3	0
4	E	119	0	0	0	0
4	F	104	0	0	0	0
All	All	18659	0	17832	44	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 1.

All (44) 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:B:278:ARG:NH2	1:F:378:ASP:OD2	1.95	1.00
1:E:178:ARG:HB3	1:E:378:ASP:OD1	1.82	0.80
1:D:306:GLN:NE2	4:D:2075:HOH:O	2.26	0.68
1:F:81:ARG:HD2	1:F:96:MET:CE	2.23	0.68
1:C:267:VAL:HG12	1:C:268:PRO:HD2	1.76	0.66
1:C:99:ASP:OD2	1:D:99:ASP:OD2	2.16	0.64
1:C:58:GLN:HG2	1:C:64:HIS:CG	2.36	0.61
1:B:278:ARG:HD3	1:F:177:GLU:O	2.02	0.59
1:E:252:GLU:OE2	1:F:81:ARG:NH2	2.35	0.59
1:F:131:ALA:O	1:F:134[A]:ARG:HG2	2.02	0.59
1:B:306:GLN:NE2	4:B:2052:HOH:O	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:81:ARG:NH2	1:F:252:GLU:OE2	2.37	0.57
1:B:286:LEU:O	1:F:185:GLN:HG3	2.05	0.56
1:A:325:THR:HG21	1:D:33[A]:CYS:SG	2.46	0.55
1:C:252:GLU:OE2	1:D:81:ARG:NH1	2.40	0.54
1:F:191:ASP:O	1:F:195[A]:HIS:ND1	2.40	0.53
1:A:346:THR:O	1:A:379:ARG:HD2	2.09	0.53
1:F:346:THR:O	1:F:379:ARG:HD2	2.09	0.52
1:B:346:THR:O	1:B:379:ARG:HD2	2.09	0.52
1:E:346:THR:O	1:E:379:ARG:HD2	2.09	0.52
1:D:346:THR:O	1:D:379:ARG:HD2	2.09	0.52
1:C:346:THR:O	1:C:379:ARG:HD2	2.09	0.52
1:A:152:GLN:HA	1:A:155:MET:HE2	1.91	0.52
1:A:273:CYS:HB3	1:A:306:GLN:HE22	1.79	0.47
1:C:81:ARG:NH2	1:D:252:GLU:OE2	2.48	0.46
1:F:81:ARG:HD2	1:F:96:MET:HE3	1.98	0.46
1:A:81:ARG:NH2	1:B:252:GLU:OE2	2.51	0.44
1:A:252:GLU:OE2	1:B:81:ARG:NH2	2.46	0.44
1:A:321:GLU:OE2	1:D:37:ASP:OD1	2.37	0.43
1:E:125:PHE:CD2	1:E:211:ARG:HD3	2.54	0.43
1:B:179:HIS:CD2	1:B:353:PHE:HE1	2.37	0.43
1:D:125:PHE:CD2	1:D:211:ARG:HD3	2.54	0.42
1:B:125:PHE:CD2	1:B:211:ARG:HD3	2.55	0.42
1:F:125:PHE:CD2	1:F:211:ARG:HD3	2.55	0.42
1:A:125:PHE:CD2	1:A:211:ARG:HD3	2.55	0.41
1:D:4:GLN:NE2	4:D:2001:HOH:O	2.53	0.41
1:E:306:GLN:HE21	1:E:306:GLN:HB3	1.69	0.41
1:B:7:ARG:NH1	1:B:244:LYS:O	2.50	0.41
1:C:133:LEU:HD11	1:C:396:ILE:HD11	2.03	0.41
1:F:359:VAL:N	1:F:360:PRO:CD	2.84	0.41
1:C:200:ALA:HB1	1:C:201:PRO:HD2	2.03	0.40
1:D:275:HIS:HD2	4:D:2074:HOH:O	2.04	0.40
1:F:81:ARG:HD2	1:F:96:MET:HE1	1.99	0.40
1:D:359:VAL:N	1:D:360:PRO:CD	2.85	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	389/425 (92%)	383 (98%)	6 (2%)	0	100	100
1	B	389/425 (92%)	383 (98%)	6 (2%)	0	100	100
1	C	388/425 (91%)	382 (98%)	6 (2%)	0	100	100
1	D	391/425 (92%)	385 (98%)	6 (2%)	0	100	100
1	E	390/425 (92%)	384 (98%)	6 (2%)	0	100	100
1	F	393/425 (92%)	387 (98%)	6 (2%)	0	100	100
All	All	2340/2550 (92%)	2304 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	305/332 (92%)	303 (99%)	2 (1%)	84	84
1	B	306/332 (92%)	304 (99%)	2 (1%)	84	84
1	C	303/332 (91%)	300 (99%)	3 (1%)	76	76
1	D	307/332 (92%)	303 (99%)	4 (1%)	69	68
1	E	307/332 (92%)	302 (98%)	5 (2%)	62	60
1	F	309/332 (93%)	304 (98%)	5 (2%)	62	60
All	All	1837/1992 (92%)	1816 (99%)	21 (1%)	73	73

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	TYR
1	A	267	VAL
1	B	154	TYR
1	B	267	VAL
1	C	154	TYR
1	C	185	GLN
1	C	306	GLN
1	D	18	LYS
1	D	81	ARG
1	D	154	TYR
1	D	267	VAL
1	E	154	TYR
1	E	185	GLN
1	E	267	VAL
1	E	306	GLN
1	E	378	ASP
1	F	134[A]	ARG
1	F	134[B]	ARG
1	F	154	TYR
1	F	267	VAL
1	F	306	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	306	GLN
1	B	306	GLN
1	C	4	GLN
1	C	185	GLN
1	D	4	GLN
1	D	275	HIS
1	E	4	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 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	E	1411	-	4,4,4	0.35	0	6,6,6	0.06	0
3	SO4	F	1411	-	4,4,4	0.34	0	6,6,6	0.10	0
2	CAA	E	1409	-	47,56,56	0.94	2 (4%)	60,83,83	1.21	5 (8%)
2	CAA	F	1409	-	47,56,56	0.98	3 (6%)	60,83,83	1.19	6 (10%)
2	CAA	C	1409	-	47,56,56	0.95	2 (4%)	60,83,83	1.20	5 (8%)
2	CAA	D	1409	-	47,56,56	0.95	3 (6%)	60,83,83	1.21	5 (8%)
3	SO4	A	1410	-	4,4,4	0.32	0	6,6,6	0.08	0
3	SO4	B	1411	-	4,4,4	0.35	0	6,6,6	0.05	0
3	SO4	D	1411	-	4,4,4	0.32	0	6,6,6	0.09	0
3	SO4	C	1410	-	4,4,4	0.33	0	6,6,6	0.10	0
3	SO4	E	1410	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	F	1410	-	4,4,4	0.33	0	6,6,6	0.08	0
3	SO4	D	1410	-	4,4,4	0.31	0	6,6,6	0.11	0
3	SO4	E	1412	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	B	1410	-	4,4,4	0.34	0	6,6,6	0.09	0
2	CAA	A	1409	-	47,56,56	0.95	3 (6%)	60,83,83	1.26	6 (10%)
2	CAA	B	1409	-	47,56,56	0.97	2 (4%)	60,83,83	1.23	5 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CAA	E	1409	-	-	3/50/71/71	0/3/3/3
2	CAA	F	1409	-	-	10/50/71/71	0/3/3/3
2	CAA	C	1409	-	-	3/50/71/71	0/3/3/3
2	CAA	D	1409	-	-	9/50/71/71	0/3/3/3
2	CAA	A	1409	-	-	9/50/71/71	0/3/3/3
2	CAA	B	1409	-	-	11/50/71/71	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1409	CAA	C1-S1P	-3.40	1.67	1.76
2	B	1409	CAA	C1-S1P	-3.39	1.67	1.76
2	C	1409	CAA	C1-S1P	-3.34	1.68	1.76
2	E	1409	CAA	C1-S1P	-3.33	1.68	1.76
2	A	1409	CAA	C1-S1P	-3.33	1.68	1.76
2	D	1409	CAA	C1-S1P	-3.08	1.68	1.76
2	D	1409	CAA	C5A-C4A	2.49	1.47	1.40
2	B	1409	CAA	C5A-C4A	2.47	1.47	1.40
2	C	1409	CAA	C5A-C4A	2.47	1.47	1.40
2	E	1409	CAA	C5A-C4A	2.47	1.47	1.40
2	F	1409	CAA	C5A-C4A	2.44	1.47	1.40
2	A	1409	CAA	C5A-C4A	2.38	1.47	1.40
2	F	1409	CAA	O4B-C1B	2.08	1.44	1.41
2	A	1409	CAA	C2A-N3A	2.05	1.35	1.32
2	D	1409	CAA	O4B-C1B	2.03	1.43	1.41

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1409	CAA	C2-C1-S1P	4.92	119.82	113.69
2	B	1409	CAA	C2-C1-S1P	4.32	119.07	113.69
2	D	1409	CAA	C2-C1-S1P	4.10	118.80	113.69
2	C	1409	CAA	C2-C1-S1P	3.79	118.42	113.69
2	E	1409	CAA	C2-C1-S1P	3.74	118.36	113.69
2	E	1409	CAA	N3A-C2A-N1A	-3.69	122.91	128.68
2	B	1409	CAA	N3A-C2A-N1A	-3.68	122.92	128.68
2	C	1409	CAA	N3A-C2A-N1A	-3.68	122.93	128.68
2	D	1409	CAA	N3A-C2A-N1A	-3.65	122.97	128.68
2	F	1409	CAA	C2-C1-S1P	3.61	118.19	113.69
2	A	1409	CAA	N3A-C2A-N1A	-3.59	123.07	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1409	CAA	N3A-C2A-N1A	-3.50	123.20	128.68
2	F	1409	CAA	P2A-O3A-P1A	-3.38	121.22	132.83
2	E	1409	CAA	P2A-O3A-P1A	-3.26	121.63	132.83
2	C	1409	CAA	P2A-O3A-P1A	-3.20	121.83	132.83
2	D	1409	CAA	C4A-C5A-N7A	-2.88	106.39	109.40
2	B	1409	CAA	P2A-O3A-P1A	-2.79	123.25	132.83
2	F	1409	CAA	C4A-C5A-N7A	-2.78	106.50	109.40
2	A	1409	CAA	P2A-O3A-P1A	-2.78	123.29	132.83
2	B	1409	CAA	C4A-C5A-N7A	-2.72	106.57	109.40
2	B	1409	CAA	C3B-C2B-C1B	2.66	105.78	99.89
2	D	1409	CAA	P2A-O3A-P1A	-2.63	123.80	132.83
2	E	1409	CAA	C4A-C5A-N7A	-2.55	106.74	109.40
2	D	1409	CAA	C3B-C2B-C1B	2.51	105.46	99.89
2	A	1409	CAA	C3B-C2B-C1B	2.47	105.36	99.89
2	A	1409	CAA	C4A-C5A-N7A	-2.47	106.83	109.40
2	C	1409	CAA	C4A-C5A-N7A	-2.43	106.86	109.40
2	A	1409	CAA	O1-C1-C2	-2.42	119.17	123.35
2	F	1409	CAA	C3B-C2B-C1B	2.41	105.23	99.89
2	E	1409	CAA	C3B-C2B-C1B	2.24	104.85	99.89
2	C	1409	CAA	C3B-C2B-C1B	2.18	104.72	99.89
2	F	1409	CAA	O1-C1-C2	-2.13	119.67	123.35

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1409	CAA	C1-C2-C3-O3
2	E	1409	CAA	C1-C2-C3-C4
2	F	1409	CAA	C3B-O3B-P3B-O7A
2	F	1409	CAA	C5B-O5B-P1A-O3A
2	F	1409	CAA	C1-C2-C3-O3
2	F	1409	CAA	C1-C2-C3-C4
2	C	1409	CAA	C3B-O3B-P3B-O9A
2	C	1409	CAA	C1-C2-C3-O3
2	C	1409	CAA	C1-C2-C3-C4
2	D	1409	CAA	C4B-C3B-O3B-P3B
2	D	1409	CAA	C3B-O3B-P3B-O8A
2	D	1409	CAA	P2A-O3A-P1A-O5B
2	D	1409	CAA	CCP-O6A-P2A-O4A
2	D	1409	CAA	C1-C2-C3-O3
2	D	1409	CAA	C1-C2-C3-C4
2	A	1409	CAA	C3B-O3B-P3B-O7A

Continued on next page...

Continued from previous page...

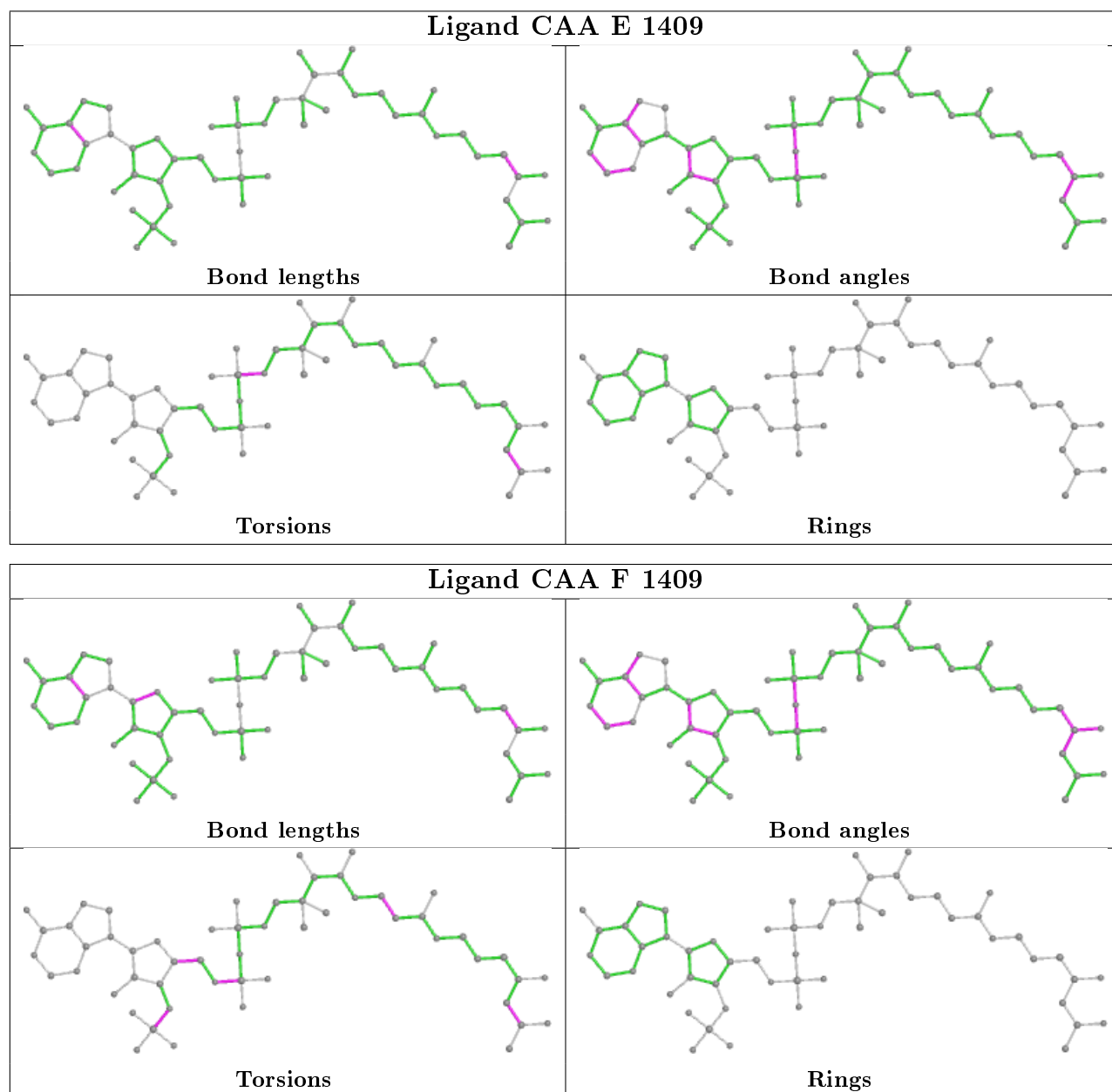
Mol	Chain	Res	Type	Atoms
2	A	1409	CAA	C5B-O5B-P1A-O2A
2	A	1409	CAA	C5B-O5B-P1A-O3A
2	A	1409	CAA	C1-C2-C3-O3
2	A	1409	CAA	C1-C2-C3-C4
2	B	1409	CAA	P2A-O3A-P1A-O5B
2	B	1409	CAA	CCP-O6A-P2A-O4A
2	B	1409	CAA	C1-C2-C3-O3
2	B	1409	CAA	C1-C2-C3-C4
2	B	1409	CAA	C4B-C3B-O3B-P3B
2	F	1409	CAA	C3B-C4B-C5B-O5B
2	F	1409	CAA	O4B-C4B-C5B-O5B
2	A	1409	CAA	C3B-O3B-P3B-O8A
2	F	1409	CAA	C5B-O5B-P1A-O1A
2	F	1409	CAA	C5B-O5B-P1A-O2A
2	D	1409	CAA	CCP-O6A-P2A-O5A
2	B	1409	CAA	CCP-O6A-P2A-O5A
2	B	1409	CAA	O4B-C4B-C5B-O5B
2	A	1409	CAA	C4B-C3B-O3B-P3B
2	F	1409	CAA	C5P-C6P-C7P-N8P
2	D	1409	CAA	C5P-C6P-C7P-N8P
2	A	1409	CAA	O4B-C4B-C5B-O5B
2	B	1409	CAA	C2B-C3B-O3B-P3B
2	B	1409	CAA	C3B-C4B-C5B-O5B
2	F	1409	CAA	C3B-O3B-P3B-O8A
2	D	1409	CAA	CCP-O6A-P2A-O3A
2	B	1409	CAA	C3B-O3B-P3B-O9A
2	B	1409	CAA	CCP-O6A-P2A-O3A
2	A	1409	CAA	C3B-C4B-C5B-O5B
2	E	1409	CAA	CCP-O6A-P2A-O4A

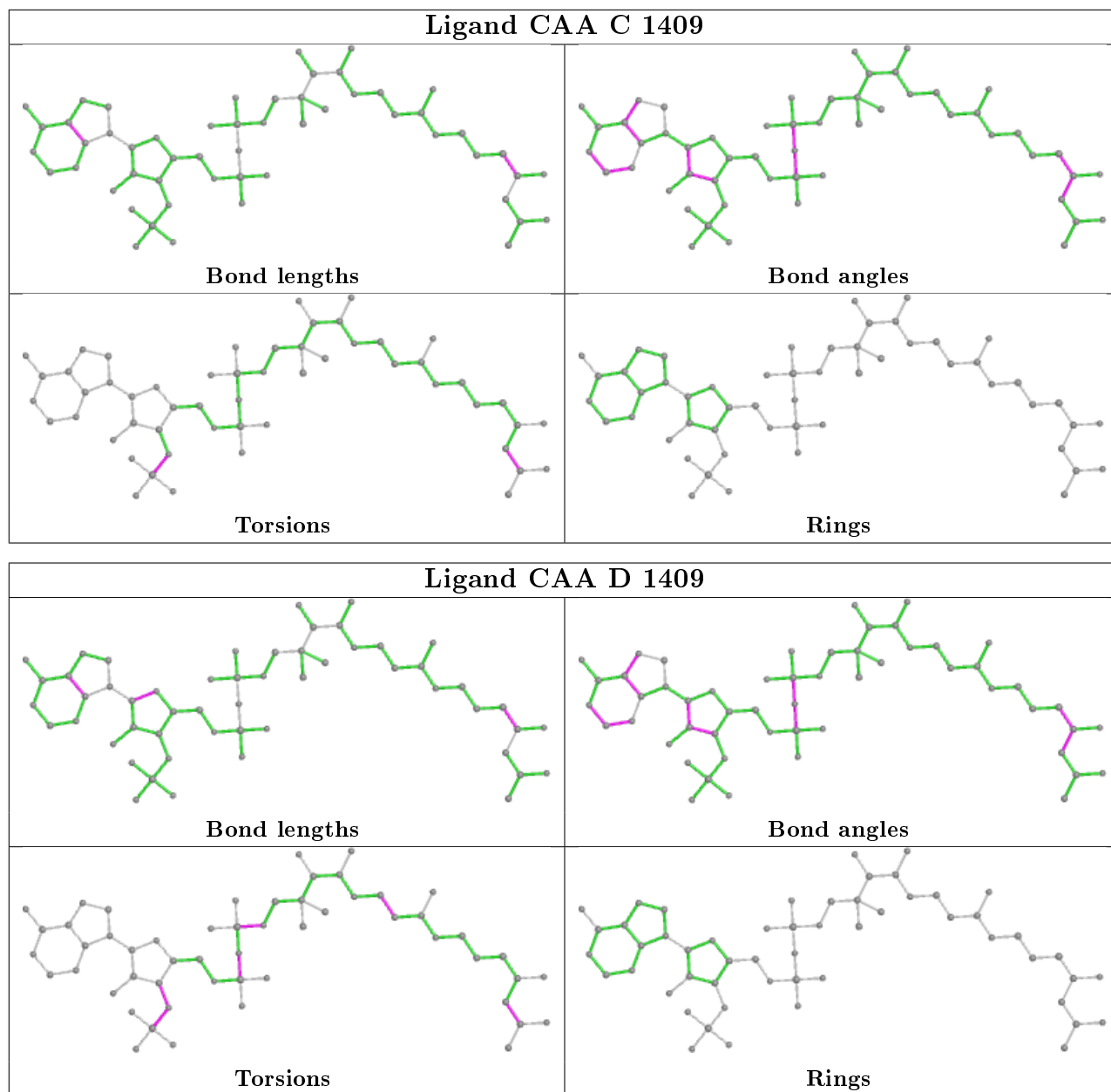
There are no ring outliers.

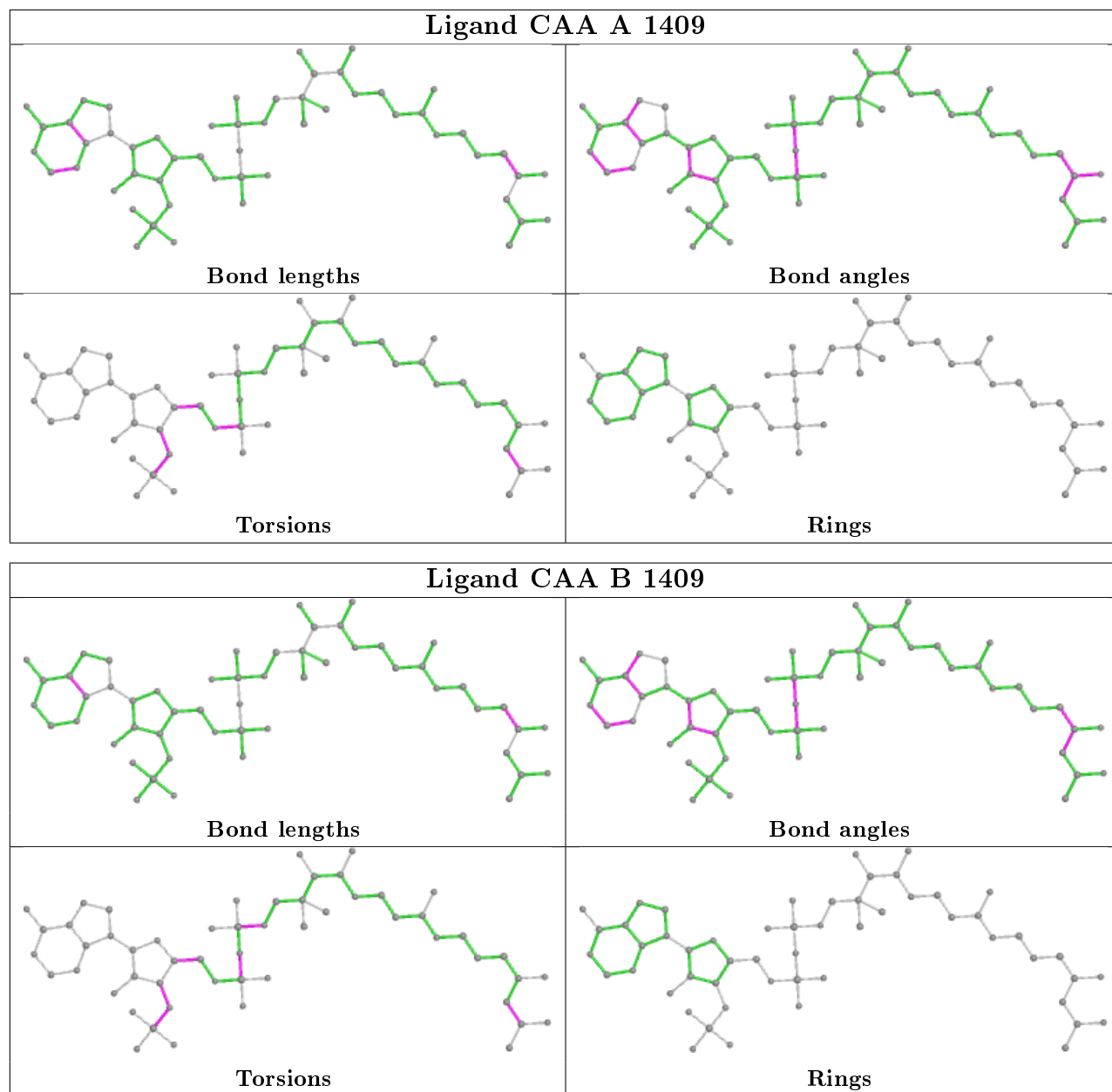
No monomer is involved in short contacts.

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	394/425 (92%)	0.96	37 (9%) 8 9	17, 28, 46, 70	0
1	B	393/425 (92%)	1.01	48 (12%) 4 4	17, 29, 47, 65	0
1	C	394/425 (92%)	0.70	33 (8%) 11 12	16, 26, 45, 60	0
1	D	396/425 (93%)	0.73	33 (8%) 11 13	16, 27, 45, 65	0
1	E	395/425 (92%)	0.70	31 (7%) 13 14	16, 25, 46, 61	0
1	F	396/425 (93%)	0.71	27 (6%) 17 19	16, 25, 44, 67	0
All	All	2368/2550 (92%)	0.80	209 (8%) 10 11	16, 27, 46, 70	0

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	75	LYS	7.2
1	A	240	LEU	6.6
1	E	231	ALA	6.6
1	F	3	SER	6.5
1	E	261	GLY	6.0
1	B	75	LYS	6.0
1	A	75	LYS	5.7
1	F	261	GLY	5.4
1	D	265	ASP	5.4
1	C	266	ILE	5.3
1	C	261	GLY	5.2
1	F	262	SER	5.2
1	E	75	LYS	5.1
1	F	240	LEU	5.1
1	B	127	GLU	5.1
1	B	3	SER	5.1
1	A	269	ASP	5.0
1	A	231	ALA	4.9
1	B	228	GLU	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	20	HIS	4.8
1	E	262	SER	4.8
1	A	230	PHE	4.7
1	A	3	SER	4.4
1	A	20	HIS	4.4
1	D	75	LYS	4.3
1	B	124	ALA	4.2
1	B	224	ALA	4.1
1	B	227	ALA	3.9
1	A	261	GLY	3.9
1	C	75	LYS	3.9
1	B	267	VAL	3.8
1	B	331	LEU	3.8
1	B	382	THR	3.8
1	D	238	ARG	3.8
1	A	228	GLU	3.8
1	B	135	ARG	3.8
1	C	240	LEU	3.7
1	C	186	LYS	3.7
1	A	73	PRO	3.7
1	B	178	ARG	3.7
1	C	267	VAL	3.7
1	C	382	THR	3.7
1	D	205	LEU	3.6
1	C	73	PRO	3.6
1	F	228	GLU	3.6
1	E	382	THR	3.5
1	B	269	ASP	3.5
1	B	185[A]	GLN	3.5
1	D	239	HIS	3.5
1	C	127	GLU	3.5
1	E	267	VAL	3.4
1	E	240	LEU	3.4
1	A	158	TYR	3.4
1	D	3	SER	3.4
1	B	240	LEU	3.4
1	D	137	GLY	3.3
1	C	3	SER	3.3
1	F	73	PRO	3.3
1	A	382	THR	3.3
1	B	74	THR	3.3
1	E	269	ASP	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	185	GLN	3.2
1	A	260	PRO	3.2
1	E	195	HIS	3.2
1	A	408	ASP	3.1
1	A	268	PRO	3.1
1	A	285	ASN	3.1
1	D	74	THR	3.1
1	A	229	HIS	3.1
1	C	334	GLY	3.1
1	A	287	ASN	3.0
1	D	191	ASP	3.0
1	B	266	ILE	3.0
1	B	231	ALA	3.0
1	F	340	SER	3.0
1	D	408	ASP	3.0
1	D	267	VAL	3.0
1	E	191	ASP	3.0
1	E	198	CYS	3.0
1	F	186	LYS	2.9
1	F	408	ASP	2.9
1	E	178	ARG	2.9
1	A	186	LYS	2.9
1	E	185	GLN	2.9
1	E	186	LYS	2.9
1	A	205	LEU	2.9
1	F	269	ASP	2.9
1	B	186	LYS	2.8
1	D	186	LYS	2.8
1	A	127	GLU	2.8
1	A	43	CYS	2.8
1	E	224	ALA	2.8
1	B	361	ALA	2.8
1	A	135	ARG	2.8
1	B	274	ARG	2.8
1	F	382	THR	2.8
1	A	198	CYS	2.8
1	E	104	ARG	2.8
1	D	73	PRO	2.8
1	A	384	VAL	2.8
1	E	282	LEU	2.7
1	B	408	ASP	2.7
1	A	224	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	191	ASP	2.7
1	D	195	HIS	2.7
1	F	296	LEU	2.7
1	E	408	ASP	2.7
1	D	127	GLU	2.7
1	D	230	PHE	2.7
1	D	143	ILE	2.6
1	F	336	VAL	2.6
1	B	20	HIS	2.6
1	A	104	ARG	2.6
1	F	20	HIS	2.6
1	B	107	GLU	2.6
1	F	384	VAL	2.6
1	F	224	ALA	2.5
1	B	191	ASP	2.5
1	C	112	ILE	2.5
1	C	104	ARG	2.5
1	C	229	HIS	2.5
1	C	20	HIS	2.5
1	C	269	ASP	2.5
1	D	269	ASP	2.5
1	B	104	ARG	2.5
1	A	191	ASP	2.5
1	A	386	LYS	2.5
1	B	285	ASN	2.5
1	D	332	ASN	2.5
1	B	192	GLU	2.4
1	F	104	ARG	2.4
1	A	340	SER	2.4
1	B	268	PRO	2.4
1	F	263	SER	2.4
1	B	374	GLU	2.4
1	B	359	VAL	2.4
1	C	408	ASP	2.4
1	A	123	GLY	2.4
1	B	90	PRO	2.4
1	A	378	ASP	2.4
1	D	228	GLU	2.3
1	F	180	PRO	2.3
1	C	124	ALA	2.3
1	B	157	ARG	2.3
1	C	99	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	90	PRO	2.3
1	E	112	ILE	2.3
1	B	140	GLU	2.3
1	E	179	HIS	2.3
1	B	378	ASP	2.3
1	C	191	ASP	2.3
1	A	361	ALA	2.3
1	E	74	THR	2.3
1	E	99	ASP	2.3
1	C	107	GLU	2.2
1	E	332	ASN	2.2
1	B	160	LEU	2.2
1	C	296	LEU	2.2
1	B	123	GLY	2.2
1	A	344	ILE	2.2
1	A	201	PRO	2.2
1	E	303	CYS	2.2
1	D	72	PHE	2.2
1	B	163	GLU	2.2
1	D	135	ARG	2.2
1	D	190	LEU	2.2
1	E	181	GLU	2.2
1	A	74	THR	2.2
1	F	124	ALA	2.2
1	F	274	ARG	2.2
1	E	228	GLU	2.2
1	F	266	ILE	2.2
1	D	340	SER	2.2
1	C	331	LEU	2.2
1	B	43	CYS	2.2
1	D	303	CYS	2.2
1	B	270	ILE	2.1
1	C	378	ASP	2.1
1	F	182	ALA	2.1
1	B	383	PRO	2.1
1	B	33[A]	CYS	2.1
1	D	156	SER	2.1
1	C	178	ARG	2.1
1	E	135	ARG	2.1
1	C	140	GLU	2.1
1	C	344	ILE	2.1
1	E	266	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	274	ARG	2.1
1	D	304	LEU	2.1
1	D	260	PRO	2.1
1	C	192	GLU	2.1
1	D	296	LEU	2.1
1	E	205	LEU	2.1
1	B	41	LYS	2.1
1	B	158	TYR	2.0
1	B	72	PHE	2.0
1	B	311	VAL	2.0
1	D	271	PHE	2.0
1	F	72	PHE	2.0
1	A	266	ILE	2.0
1	B	246	ILE	2.0
1	D	104	ARG	2.0
1	C	55	ALA	2.0
1	E	383	PRO	2.0
1	C	228	GLU	2.0
1	D	91	ILE	2.0
1	F	112	ILE	2.0
1	B	197	ARG	2.0
1	C	163	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

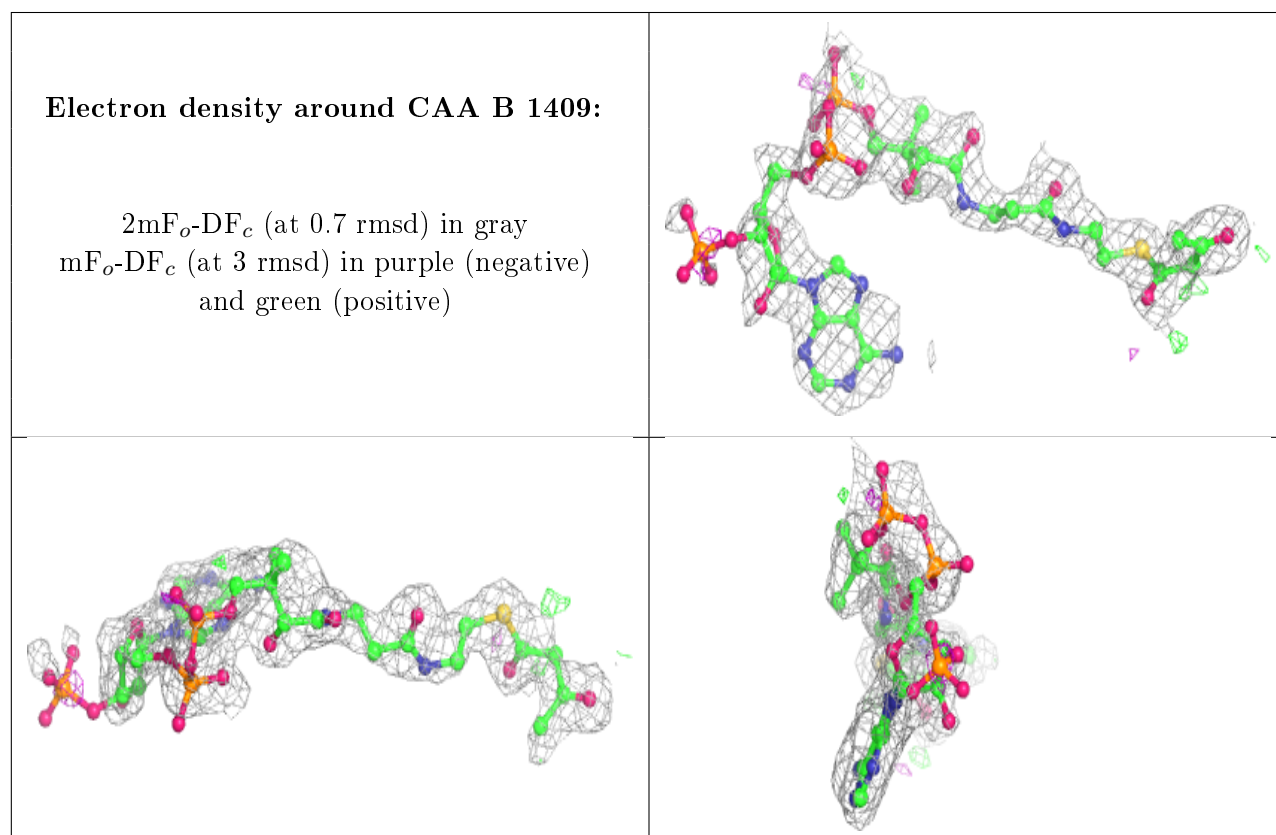
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CAA	B	1409	54/54	0.65	0.24	34,62,89,92	0

Continued on next page...

Continued from previous page...

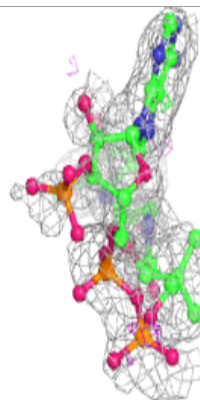
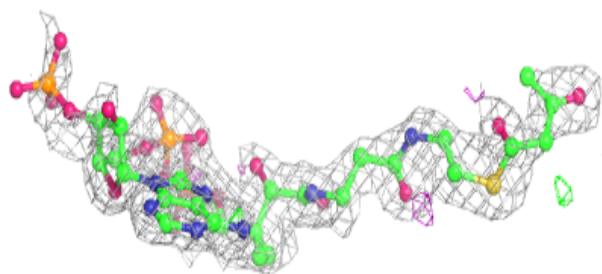
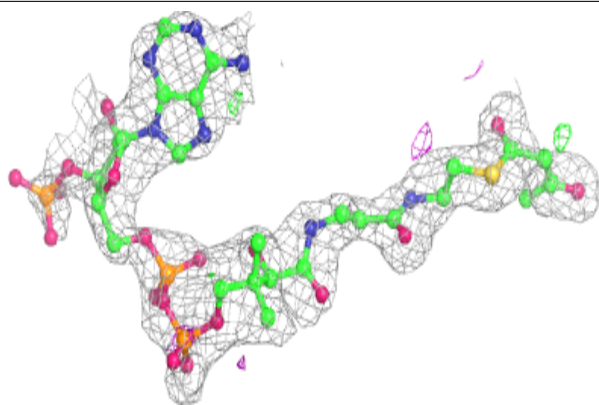
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CAA	C	1409	54/54	0.68	0.23	31,56,82,85	0
3	SO4	D	1411	5/5	0.72	0.22	75,76,78,79	0
2	CAA	A	1409	54/54	0.74	0.25	36,61,86,88	0
2	CAA	D	1409	54/54	0.75	0.23	30,55,81,85	0
2	CAA	F	1409	54/54	0.77	0.21	26,53,76,76	0
2	CAA	E	1409	54/54	0.78	0.20	25,49,67,69	0
3	SO4	E	1412	5/5	0.79	0.36	77,77,79,79	0
3	SO4	F	1411	5/5	0.82	0.21	73,73,75,76	0
3	SO4	E	1410	5/5	0.83	0.26	74,74,76,76	0
3	SO4	A	1410	5/5	0.86	0.28	77,77,79,80	0
3	SO4	B	1411	5/5	0.88	0.33	76,77,77,77	0
3	SO4	B	1410	5/5	0.90	0.33	76,76,77,78	0
3	SO4	E	1411	5/5	0.91	0.23	66,66,66,66	0
3	SO4	D	1410	5/5	0.91	0.21	66,68,68,70	0
3	SO4	C	1410	5/5	0.92	0.28	66,66,67,67	0
3	SO4	F	1410	5/5	0.96	0.18	58,58,60,61	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.

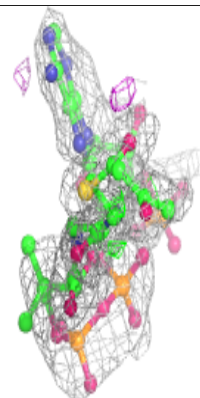
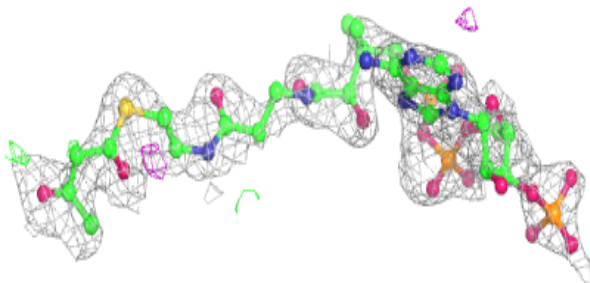
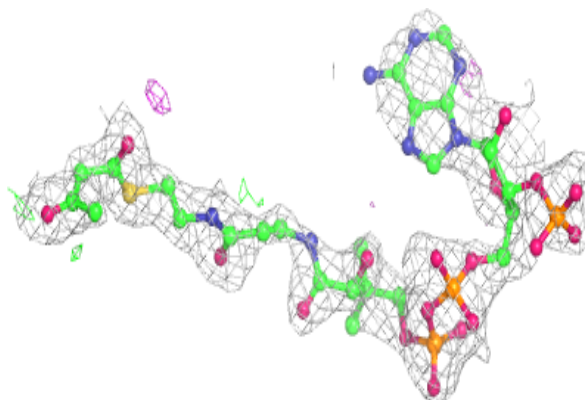


Electron density around CAA C 1409:

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

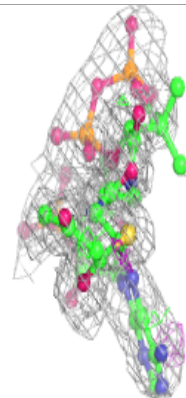
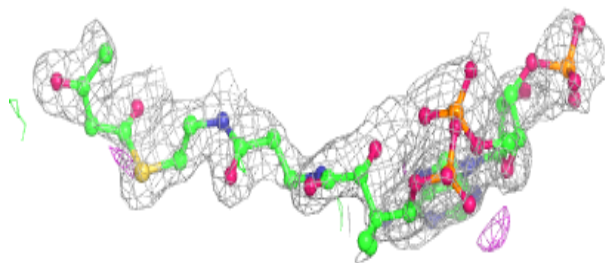
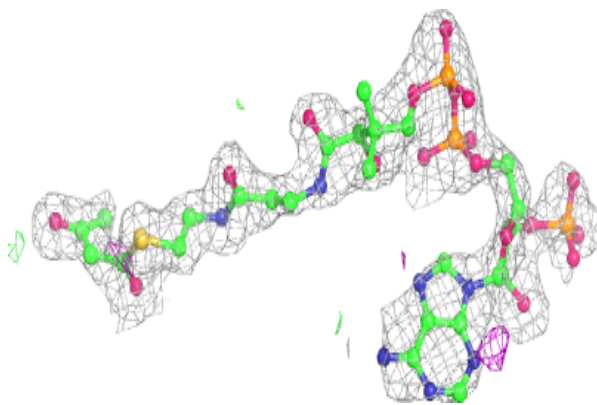
**Electron density around CAA A 1409:**

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

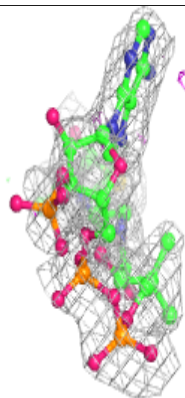
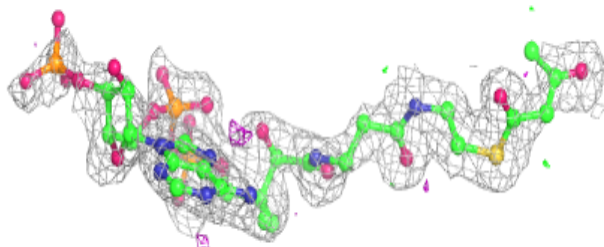
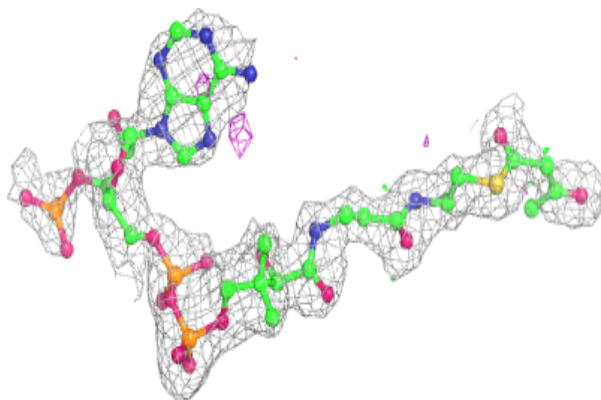


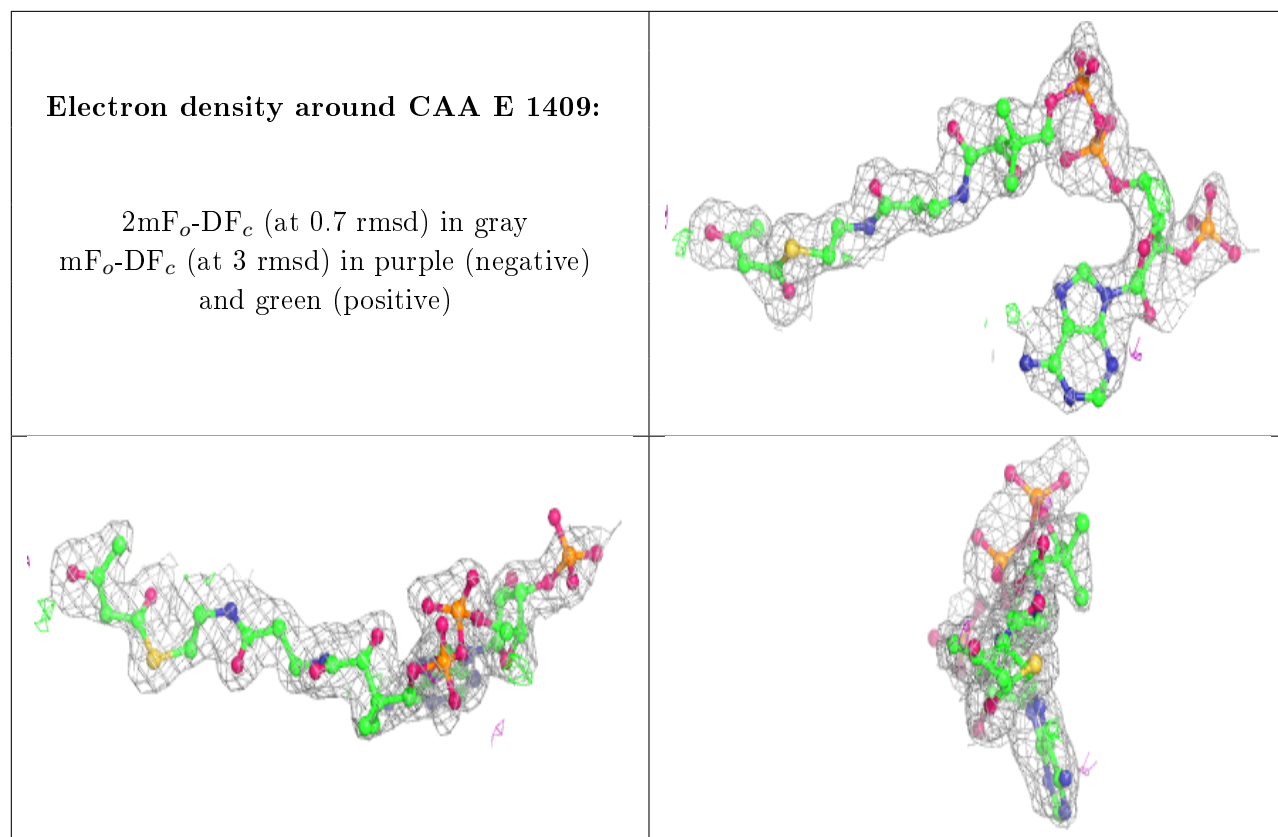
Electron density around CAA D 1409:

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

**Electron density around CAA F 1409:**

$2mF_o-DF_c$ (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.