Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 03:24 PM EDT

PDB ID	:	4ZDB
Title	:	Yeast enoyl-CoA isomerase (ScECI2) complexed with acetoacetyl-CoA
Authors	:	Onwukwe, G.U.; Koski, M.K.; Wierenga, R.K.
Deposited on	:	2015-04-17
Resolution	:	2.14 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 (i) 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 (i)) were used in the production of this report:

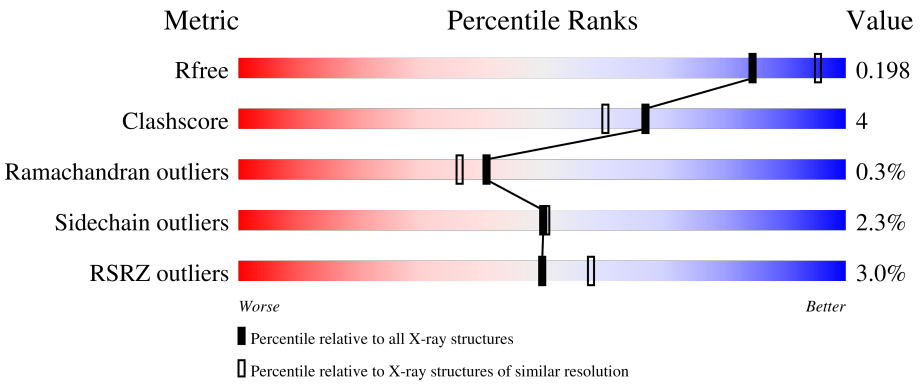
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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 <=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	300	3%, 82%, 6% • 11%
1	B	300	3%, 79%, 7% • 13%
1	C	300	2%, 81%, 6% • 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	307	-	-	X	-
4	GOL	B	305	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7002 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 3,2-trans-enoyl-CoA isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	267	2143	1378	354	400	11	0	2	0
1	B	261	2092	1352	341	388	11	0	2	0
1	C	263	2112	1362	349	390	11	0	2	0

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q05871
A	-18	GLY	-	expression tag	UNP Q05871
A	-17	SER	-	expression tag	UNP Q05871
A	-16	SER	-	expression tag	UNP Q05871
A	-15	HIS	-	expression tag	UNP Q05871
A	-14	HIS	-	expression tag	UNP Q05871
A	-13	HIS	-	expression tag	UNP Q05871
A	-12	HIS	-	expression tag	UNP Q05871
A	-11	HIS	-	expression tag	UNP Q05871
A	-10	HIS	-	expression tag	UNP Q05871
A	-9	SER	-	expression tag	UNP Q05871
A	-8	SER	-	expression tag	UNP Q05871
A	-7	GLY	-	expression tag	UNP Q05871
A	-6	LEU	-	expression tag	UNP Q05871
A	-5	VAL	-	expression tag	UNP Q05871
A	-4	PRO	-	expression tag	UNP Q05871
A	-3	ARG	-	expression tag	UNP Q05871
A	-2	GLY	-	expression tag	UNP Q05871
A	-1	SER	-	expression tag	UNP Q05871
A	0	HIS	-	expression tag	UNP Q05871
A	25	ILE	MET	conflict	UNP Q05871
B	-19	MET	-	initiating methionine	UNP Q05871
B	-18	GLY	-	expression tag	UNP Q05871

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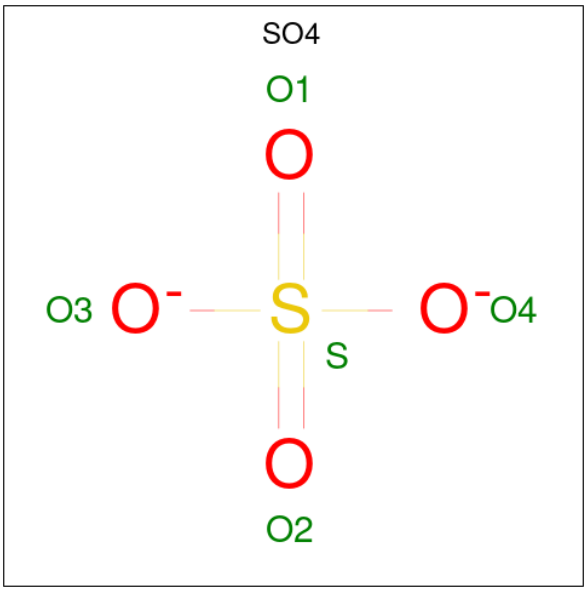
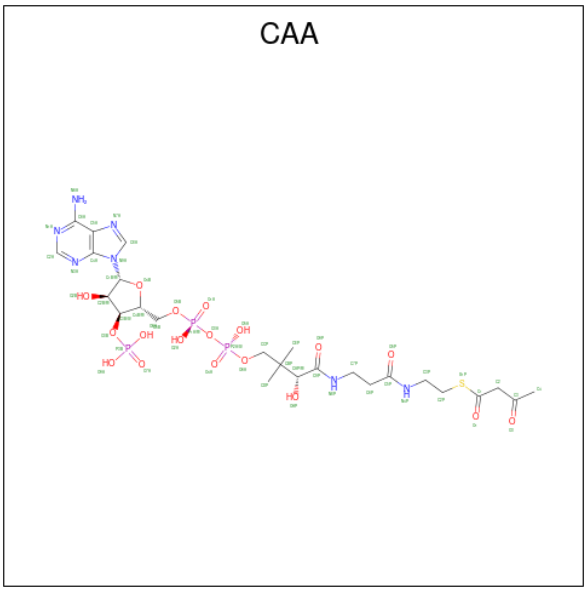
Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP Q05871
B	-16	SER	-	expression tag	UNP Q05871
B	-15	HIS	-	expression tag	UNP Q05871
B	-14	HIS	-	expression tag	UNP Q05871
B	-13	HIS	-	expression tag	UNP Q05871
B	-12	HIS	-	expression tag	UNP Q05871
B	-11	HIS	-	expression tag	UNP Q05871
B	-10	HIS	-	expression tag	UNP Q05871
B	-9	SER	-	expression tag	UNP Q05871
B	-8	SER	-	expression tag	UNP Q05871
B	-7	GLY	-	expression tag	UNP Q05871
B	-6	LEU	-	expression tag	UNP Q05871
B	-5	VAL	-	expression tag	UNP Q05871
B	-4	PRO	-	expression tag	UNP Q05871
B	-3	ARG	-	expression tag	UNP Q05871
B	-2	GLY	-	expression tag	UNP Q05871
B	-1	SER	-	expression tag	UNP Q05871
B	0	HIS	-	expression tag	UNP Q05871
B	25	ILE	MET	conflict	UNP Q05871
C	-19	MET	-	initiating methionine	UNP Q05871
C	-18	GLY	-	expression tag	UNP Q05871
C	-17	SER	-	expression tag	UNP Q05871
C	-16	SER	-	expression tag	UNP Q05871
C	-15	HIS	-	expression tag	UNP Q05871
C	-14	HIS	-	expression tag	UNP Q05871
C	-13	HIS	-	expression tag	UNP Q05871
C	-12	HIS	-	expression tag	UNP Q05871
C	-11	HIS	-	expression tag	UNP Q05871
C	-10	HIS	-	expression tag	UNP Q05871
C	-9	SER	-	expression tag	UNP Q05871
C	-8	SER	-	expression tag	UNP Q05871
C	-7	GLY	-	expression tag	UNP Q05871
C	-6	LEU	-	expression tag	UNP Q05871
C	-5	VAL	-	expression tag	UNP Q05871
C	-4	PRO	-	expression tag	UNP Q05871
C	-3	ARG	-	expression tag	UNP Q05871
C	-2	GLY	-	expression tag	UNP Q05871
C	-1	SER	-	expression tag	UNP Q05871
C	0	HIS	-	expression tag	UNP Q05871
C	25	ILE	MET	conflict	UNP Q05871

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



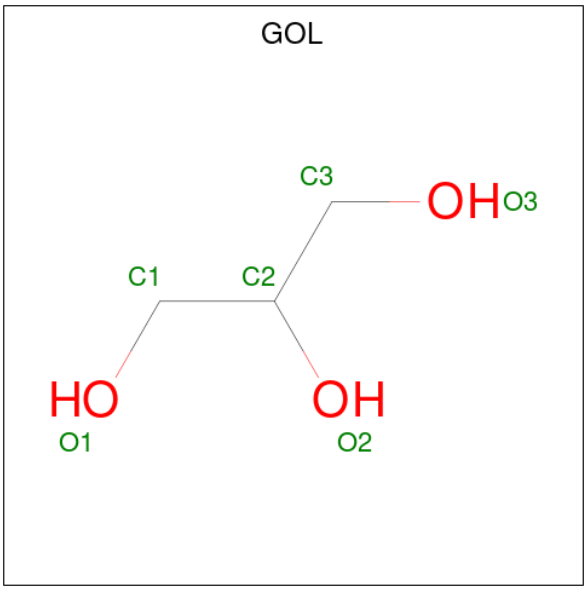
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
2	A	1	5	4	1		0	0
2	A	1	5	4	1		0	0
2	A	1	5	4	1		0	0
2	A	1	5	4	1		0	0
2	B	1	5	4	1		0	0
2	B	1	5	4	1		0	0
2	C	1	5	4	1		0	0
2	C	1	5	4	1		0	0

- Molecule 3 is ACETOACETYL-COENZYME A (three-letter code: CAA) (formula: $C_{25}H_{40}N_7O_{18}P_3S$).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
			Total	C	O		
4	A	1	6	3	3	0	0
			Total	C	O		
4	B	1	6	3	3	0	0
			Total	C	O		
4	B	1	6	3	3	0	0
			Total	C	O		
4	C	1	6	3	3	0	0
			Total	C	O		
4	C	1	6	3	3	0	0

- Molecule 5 is water.

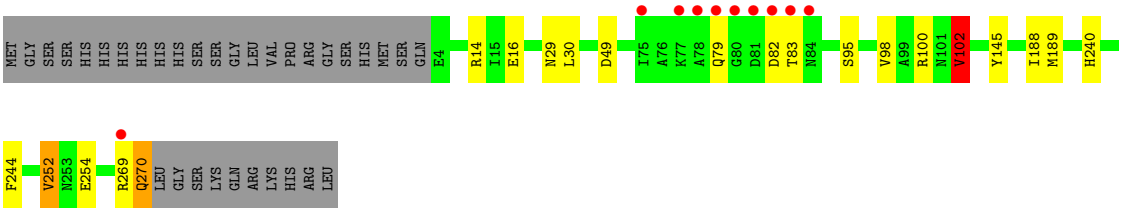
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	155	155	155	0	0
			Total	O		
5	B	123	123	123	0	0
			Total	O		
5	C	133	133	133	0	0

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.

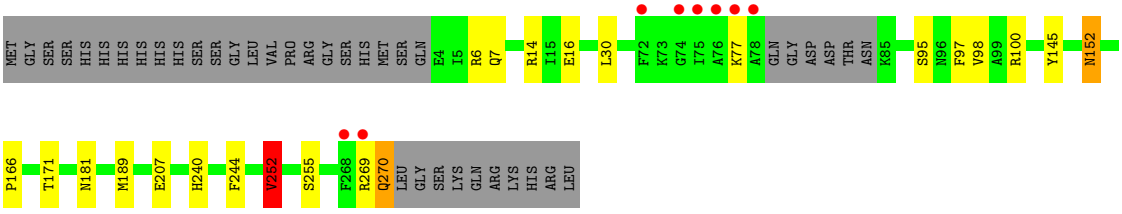
• Molecule 1: 3,2-trans-enoyl-CoA isomerase

Chain A:



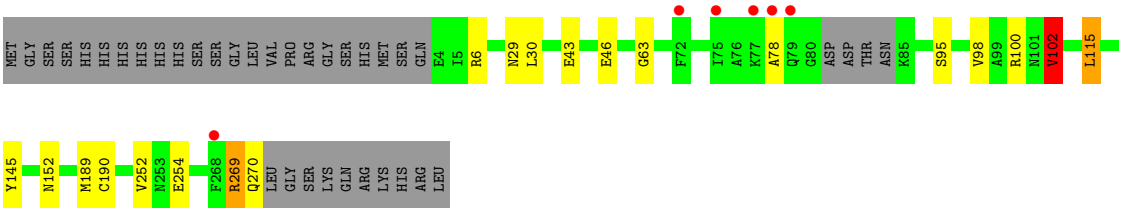
• Molecule 1: 3,2-trans-enoyl-CoA isomerase

Chain B:



• Molecule 1: 3,2-trans-enoyl-CoA isomerase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	116.94Å 116.94Å 218.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	103.10 – 2.14 103.11 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.5 (103.10-2.14) 99.5 (103.11-2.14)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.165 , 0.190 0.174 , 0.198	Depositor DCC
R_{free} test set	4184 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	34.3	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 54.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7002	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, CME, 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	0.90	2/2181 (0.1%)	0.82	3/2945 (0.1%)
1	B	0.67	0/2132	0.75	3/2878 (0.1%)
1	C	0.74	2/2149 (0.1%)	0.76	2/2899 (0.1%)
All	All	0.78	4/6462 (0.1%)	0.78	8/8722 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	GLN	C-O	-23.55	0.78	1.23
1	A	254	GLU	CD-OE1	6.04	1.32	1.25
1	C	46	GLU	CD-OE1	5.63	1.31	1.25
1	C	254	GLU	CD-OE1	5.12	1.31	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	270	GLN	CA-C-O	-8.89	101.44	120.10
1	A	102	VAL	CB-CA-C	-7.45	97.25	111.40
1	C	102	VAL	CB-CA-C	-6.54	98.97	111.40
1	C	115	LEU	CA-CB-CG	6.53	130.31	115.30
1	B	6	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	B	6	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	A	49	ASP	CB-CG-OD1	5.21	122.98	118.30
1	B	252	VAL	CG1-CB-CG2	5.03	118.94	110.90

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	2143	0	2135	17	0
1	B	2092	0	2095	12	0
1	C	2112	0	2113	11	0
2	A	20	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	1	0
3	A	54	0	36	2	0
3	B	54	0	36	1	0
3	C	54	0	36	2	0
4	A	18	0	24	6	0
4	B	12	0	16	5	0
4	C	12	0	16	2	0
5	A	155	0	0	9	0
5	B	123	0	0	6	0
5	C	133	0	0	2	0
All	All	7002	0	6507	51	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 4.

All (51) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLN:O	1:A:270:GLN:CA	1.87	1.22
1:A:270:GLN:O	1:A:270:GLN:C	0.78	0.98
1:A:188:ILE:HD12	5:A:486:HOH:O	1.74	0.87
4:A:307:GOL:H31	5:A:433:HOH:O	1.86	0.76
1:C:63:GLY:N	2:C:302:SO4:O4	2.21	0.74
1:B:98:VAL:HG13	1:B:252:VAL:HG13	1.69	0.72
1:A:98:VAL:HG13	1:A:252:VAL:HG13	1.70	0.72
1:C:29[A]:ASN:OD1	3:C:303:CAA:H1B	1.97	0.65
1:A:270:GLN:O	1:A:270:GLN:HA	1.93	0.64
1:C:269:ARG:O	1:C:269:ARG:HG2	1.99	0.63
1:C:30:LEU:HD12	3:C:303:CAA:H8A	1.83	0.60
1:B:244:PHE:CE2	4:B:305:GOL:H32	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:LEU:HD12	3:B:303:CAA:H8A	1.86	0.58
4:B:305:GOL:H2	5:B:416:HOH:O	2.04	0.57
1:B:207:GLU:HG2	5:B:481:HOH:O	2.05	0.57
1:A:269:ARG:O	1:A:269:ARG:HG2	2.05	0.56
4:A:307:GOL:H2	5:A:483:HOH:O	2.06	0.55
4:C:305:GOL:H32	5:C:407:HOH:O	2.08	0.54
4:A:307:GOL:H12	5:A:415:HOH:O	2.08	0.54
1:A:29[B]:ASN:OD1	3:A:305:CAA:H1B	2.07	0.53
1:C:269:ARG:O	1:C:270:GLN:C	2.47	0.53
1:B:166:PRO:HB3	1:B:171[A]:THR:HG22	1.93	0.51
4:A:307:GOL:C1	5:A:415:HOH:O	2.60	0.50
1:C:269:ARG:O	1:C:269:ARG:CG	2.62	0.48
1:A:240:HIS:HD2	5:A:529:HOH:O	1.97	0.48
1:A:244:PHE:CE2	4:A:307:GOL:H32	2.49	0.48
1:A:82:ASP:N	1:A:83:THR:HA	2.28	0.48
1:C:98:VAL:O	1:C:102:VAL:HG22	2.14	0.47
1:A:98:VAL:O	1:A:102:VAL:HG22	2.15	0.47
1:B:240:HIS:HE1	5:B:507:HOH:O	1.98	0.47
4:B:305:GOL:H11	5:B:403:HOH:O	2.14	0.47
4:B:305:GOL:H31	5:B:421:HOH:O	2.15	0.47
1:C:102:VAL:HG13	1:C:252:VAL:HG21	1.97	0.46
1:A:145:TYR:HA	1:A:189:MET:HE1	1.99	0.45
1:B:270:GLN:NE2	1:B:270:GLN:HA	2.31	0.45
1:A:240:HIS:HE1	5:A:532:HOH:O	2.00	0.44
1:C:6[B]:ARG:HH22	1:C:43:GLU:CD	2.19	0.44
1:B:152:ASN:OD1	1:B:181:ASN:ND2	2.50	0.44
4:C:305:GOL:C3	5:C:407:HOH:O	2.66	0.44
1:A:269:ARG:O	1:A:269:ARG:CG	2.65	0.44
1:B:145:TYR:HA	1:B:189:MET:HE1	2.00	0.43
1:B:77:LYS:HD3	1:B:77:LYS:HA	1.88	0.43
1:C:6[B]:ARG:HE	1:C:6[B]:ARG:HB3	1.23	0.43
1:A:30:LEU:HD12	3:A:305:CAA:H8A	2.00	0.43
1:B:97:PHE:CE2	1:B:255:SER:OG	2.62	0.43
1:B:14:ARG:NE	1:B:16:GLU:OE2	2.39	0.43
1:A:14:ARG:NE	1:A:16:GLU:OE2	2.35	0.42
1:C:145:TYR:HA	1:C:189:MET:HE1	2.01	0.41
4:A:307:GOL:C3	5:A:433:HOH:O	2.59	0.41
4:B:305:GOL:C1	5:B:403:HOH:O	2.68	0.41
1:A:79:GLN:HG3	5:A:465:HOH:O	2.21	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	266/300 (89%)	255 (96%)	11 (4%)	0	100	100
1	B	258/300 (86%)	249 (96%)	8 (3%)	1 (0%)	34	29
1	C	260/300 (87%)	252 (97%)	7 (3%)	1 (0%)	34	29
All	All	784/900 (87%)	756 (96%)	26 (3%)	2 (0%)	41	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	269	ARG
1	C	78	ALA

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	234/261 (90%)	230 (98%)	4 (2%)	60	63
1	B	229/261 (88%)	223 (97%)	6 (3%)	46	45
1	C	230/261 (88%)	224 (97%)	6 (3%)	46	45
All	All	693/783 (88%)	677 (98%)	16 (2%)	50	51

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	SER

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Mol	Chain	Res	Type
1	A	100	ARG
1	A	102	VAL
1	A	252	VAL
1	B	7	GLN
1	B	95	SER
1	B	100	ARG
1	B	152	ASN
1	B	252	VAL
1	B	270	GLN
1	C	95	SER
1	C	100	ARG
1	C	102	VAL
1	C	115	LEU
1	C	152	ASN
1	C	269	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	HIS
1	B	240	HIS
1	C	152	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)

3 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CME	B	190	1	8,9,10	0.82	0	5,9,11	1.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CME	C	190	1	8,9,10	0.98	0	5,9,11	1.51	1 (20%)
1	CME	A	190	1	8,9,10	1.11	0	5,9,11	1.53	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
1	CME	B	190	1	-	2/5/8/10	-
1	CME	C	190	1	-	3/5/8/10	-
1	CME	A	190	1	-	3/5/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	190	CME	CB-SG-SD	2.24	109.62	103.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	190	CME	CE-SD-SG-CB
1	A	190	CME	SD-CE-CZ-OH
1	B	190	CME	CE-SD-SG-CB
1	B	190	CME	SD-CE-CZ-OH
1	C	190	CME	CE-SD-SG-CB
1	C	190	CME	SD-CE-CZ-OH
1	A	190	CME	CZ-CE-SD-SG
1	C	190	CME	CZ-CE-SD-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	301	-	4,4,4	0.35	0	6,6,6	1.04	1 (16%)
2	SO4	A	304	-	4,4,4	0.47	0	6,6,6	0.13	0
3	CAA	A	305	-	47,56,56	0.96	3 (6%)	60,83,83	2.77	12 (20%)
2	SO4	A	303	-	4,4,4	0.41	0	6,6,6	0.89	0
2	SO4	C	301	-	4,4,4	0.37	0	6,6,6	0.44	0
3	CAA	B	303	-	47,56,56	1.01	3 (6%)	60,83,83	1.52	8 (13%)
4	GOL	A	307	-	5,5,5	0.70	0	5,5,5	0.99	0
2	SO4	C	302	-	4,4,4	0.48	0	6,6,6	0.93	0
4	GOL	A	308	-	5,5,5	0.38	0	5,5,5	1.19	0
4	GOL	C	305	-	5,5,5	0.75	0	5,5,5	0.97	0
4	GOL	A	306	-	5,5,5	0.52	0	5,5,5	0.51	0
4	GOL	B	304	-	5,5,5	0.54	0	5,5,5	0.45	0
3	CAA	C	303	-	47,56,56	1.01	4 (8%)	60,83,83	1.90	10 (16%)
2	SO4	B	302	-	4,4,4	0.39	0	6,6,6	0.49	0
4	GOL	C	304	-	5,5,5	0.43	0	5,5,5	0.77	0
2	SO4	B	301	-	4,4,4	0.41	0	6,6,6	0.44	0
4	GOL	B	305	-	5,5,5	0.59	0	5,5,5	0.85	0
2	SO4	A	302	-	4,4,4	0.51	0	6,6,6	0.36	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
3	CAA	A	305	-	-	14/50/71/71	0/3/3/3
3	CAA	B	303	-	-	11/50/71/71	0/3/3/3
4	GOL	A	307	-	-	2/4/4/4	-
4	GOL	C	305	-	-	2/4/4/4	-
4	GOL	A	308	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	306	-	-	2/4/4/4	-
4	GOL	B	304	-	-	2/4/4/4	-
3	CAA	C	303	-	-	22/50/71/71	0/3/3/3
4	GOL	C	304	-	-	2/4/4/4	-
4	GOL	B	305	-	-	1/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	303	CAA	C1-S1P	-3.68	1.67	1.76
3	B	303	CAA	C1-S1P	-3.40	1.67	1.76
3	A	305	CAA	O4B-C1B	2.74	1.44	1.41
3	B	303	CAA	O4B-C1B	2.71	1.44	1.41
3	C	303	CAA	C5A-C4A	2.65	1.47	1.40
3	B	303	CAA	C5A-C4A	2.50	1.47	1.40
3	A	305	CAA	C5A-C4A	2.43	1.47	1.40
3	A	305	CAA	C1-S1P	-2.21	1.70	1.76
3	C	303	CAA	O4B-C1B	2.19	1.44	1.41
3	C	303	CAA	C2A-N3A	2.07	1.35	1.32

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	305	CAA	C2-C1-S1P	15.38	132.85	113.69
3	C	303	CAA	C2-C1-S1P	8.50	124.28	113.69
3	A	305	CAA	O1-C1-C2	-7.87	109.70	123.35
3	B	303	CAA	C2-C1-S1P	5.97	121.13	113.69
3	C	303	CAA	O1-C1-S1P	-5.83	115.05	122.61
3	A	305	CAA	C3-C2-C1	4.43	131.61	113.92
3	A	305	CAA	C2P-C3P-N4P	4.24	121.33	112.42
3	A	305	CAA	O1-C1-S1P	-4.18	117.19	122.61
3	B	303	CAA	O1-C1-S1P	-4.16	117.22	122.61
3	B	303	CAA	N3A-C2A-N1A	-3.91	122.57	128.68
3	C	303	CAA	N3A-C2A-N1A	-3.86	122.64	128.68
3	A	305	CAA	N3A-C2A-N1A	-3.65	122.97	128.68
3	C	303	CAA	C6P-C5P-N4P	2.73	121.01	116.42
3	C	303	CAA	CDP-CBP-CCP	2.72	112.68	108.23
3	A	305	CAA	N6A-C6A-N1A	2.69	124.17	118.57
3	C	303	CAA	O5P-C5P-C6P	-2.67	117.13	122.02
3	C	303	CAA	C4A-C5A-N7A	-2.66	106.63	109.40
3	B	303	CAA	N6A-C6A-N1A	2.64	124.05	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	303	CAA	C2A-N1A-C6A	2.57	123.15	118.75
3	A	305	CAA	C2A-N1A-C6A	2.49	123.02	118.75
3	A	305	CAA	C7P-C6P-C5P	2.48	116.48	112.36
3	A	305	CAA	C4-C3-C2	-2.28	110.00	117.89
3	B	303	CAA	O2A-P1A-O1A	2.25	123.36	112.24
3	B	303	CAA	C4A-C5A-N7A	-2.24	107.07	109.40
3	A	305	CAA	O3-C3-C2	2.20	128.98	121.16
3	B	303	CAA	O9A-P3B-O8A	2.14	115.83	107.64
3	A	305	CAA	O2A-P1A-O1A	2.12	122.73	112.24
2	A	301	SO4	O4-S-O3	2.02	117.70	109.06
3	C	303	CAA	C2A-N1A-C6A	2.02	122.22	118.75
3	C	303	CAA	C7P-N8P-C9P	2.02	126.19	122.59
3	C	303	CAA	CAP-C9P-N8P	2.02	120.59	116.58

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	305	CAA	C5B-O5B-P1A-O3A
3	A	305	CAA	OAP-CAP-CBP-CCP
3	A	305	CAA	C9P-CAP-CBP-CCP
3	A	305	CAA	OAP-CAP-CBP-CDP
3	A	305	CAA	C9P-CAP-CBP-CDP
3	A	305	CAA	OAP-CAP-CBP-CEP
3	A	305	CAA	C9P-CAP-CBP-CEP
3	A	305	CAA	C5P-C6P-C7P-N8P
3	A	305	CAA	S1P-C2P-C3P-N4P
3	A	305	CAA	C1-C2-C3-O3
3	B	303	CAA	C5B-O5B-P1A-O1A
3	B	303	CAA	O1-C1-S1P-C2P
3	B	303	CAA	C2-C1-S1P-C2P
3	B	303	CAA	C1-C2-C3-C4
3	C	303	CAA	C5B-O5B-P1A-O2A
3	C	303	CAA	CDP-CBP-CCP-O6A
3	C	303	CAA	CEP-CBP-CCP-O6A
3	C	303	CAA	CAP-CBP-CCP-O6A
3	C	303	CAA	O9P-C9P-CAP-OAP
3	C	303	CAA	N8P-C9P-CAP-OAP
3	C	303	CAA	CAP-C9P-N8P-C7P
3	C	303	CAA	C2P-C3P-N4P-C5P
3	C	303	CAA	S1P-C2P-C3P-N4P
3	C	303	CAA	C3P-C2P-S1P-C1

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Mol	Chain	Res	Type	Atoms
3	C	303	CAA	O1-C1-S1P-C2P
3	C	303	CAA	C2-C1-S1P-C2P
3	C	303	CAA	C1-C2-C3-O3
3	C	303	CAA	C1-C2-C3-C4
4	A	307	GOL	O1-C1-C2-C3
4	B	304	GOL	C1-C2-C3-O3
3	C	303	CAA	O9P-C9P-N8P-C7P
3	C	303	CAA	O5P-C5P-C6P-C7P
4	A	308	GOL	C1-C2-C3-O3
3	C	303	CAA	N4P-C5P-C6P-C7P
3	B	303	CAA	C5P-C6P-C7P-N8P
4	A	308	GOL	O2-C2-C3-O3
3	B	303	CAA	C1-C2-C3-O3
4	C	305	GOL	O1-C1-C2-C3
3	C	303	CAA	O9P-C9P-CAP-CBP
3	C	303	CAA	N8P-C9P-CAP-CBP
4	B	304	GOL	O2-C2-C3-O3
3	A	305	CAA	C6P-C5P-N4P-C3P
3	B	303	CAA	C3B-O3B-P3B-O8A
3	C	303	CAA	C5B-O5B-P1A-O3A
4	A	306	GOL	O2-C2-C3-O3
4	C	305	GOL	O1-C1-C2-O2
3	B	303	CAA	O1-C1-C2-C3
4	A	306	GOL	C1-C2-C3-O3
4	B	305	GOL	O1-C1-C2-C3
3	A	305	CAA	C5B-O5B-P1A-O1A
3	B	303	CAA	O5P-C5P-C6P-C7P
4	C	304	GOL	C1-C2-C3-O3
4	A	307	GOL	O1-C1-C2-O2
3	B	303	CAA	C5B-O5B-P1A-O3A
3	C	303	CAA	C3B-O3B-P3B-O9A
4	C	304	GOL	O2-C2-C3-O3
3	A	305	CAA	CCP-O6A-P2A-O4A
3	C	303	CAA	C5B-O5B-P1A-O1A
3	A	305	CAA	O5P-C5P-C6P-C7P
3	B	303	CAA	C2P-C3P-N4P-C5P

There are no ring outliers.

7 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	305	CAA	2	0

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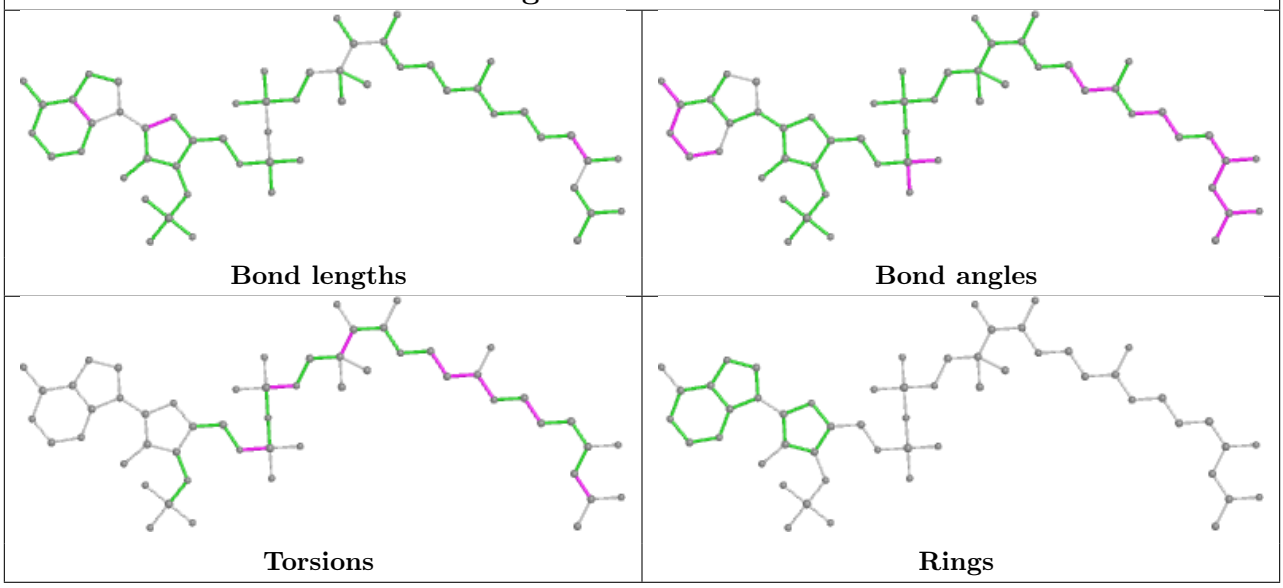
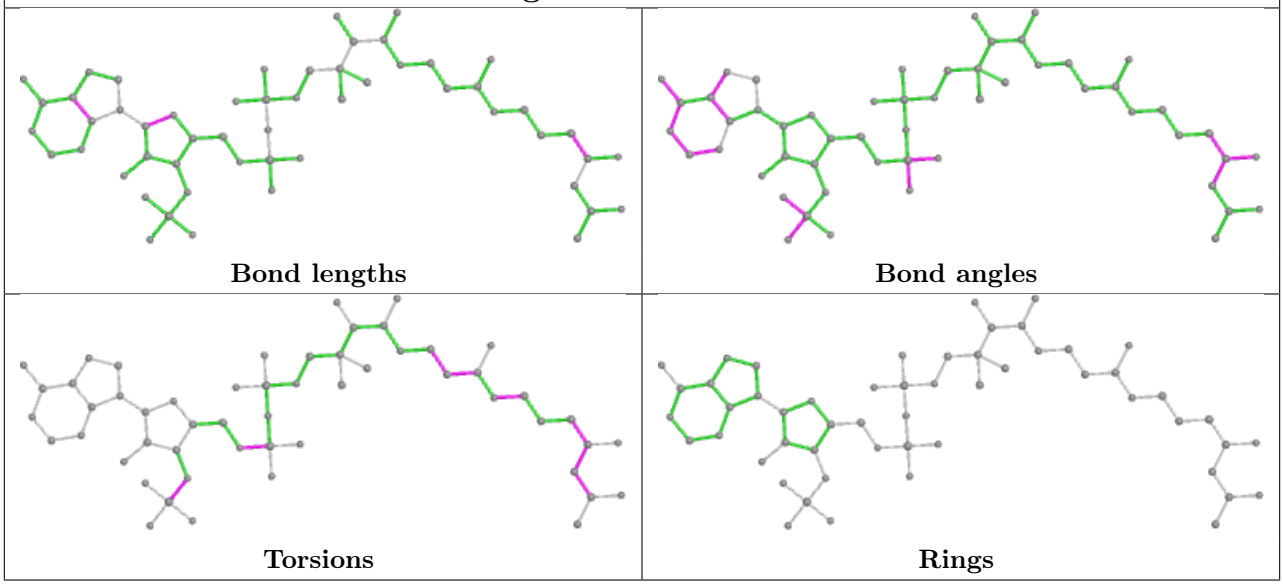
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	303	CAA	1	0
4	A	307	GOL	6	0
2	C	302	SO4	1	0
4	C	305	GOL	2	0
3	C	303	CAA	2	0
4	B	305	GOL	5	0

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 then 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.

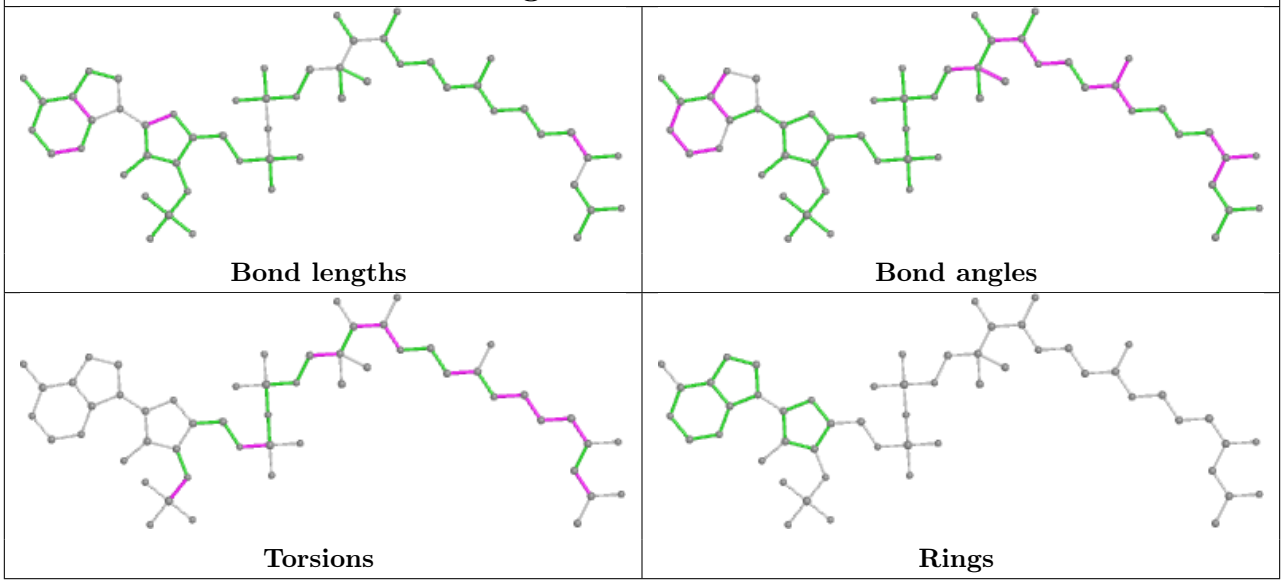
Ligand CAA A 305



Ligand CAA B 303



Ligand CAA C 303



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	266/300 (88%)	0.11	10 (3%) 40 48	20, 31, 79, 134	0
1	B	260/300 (86%)	0.04	8 (3%) 49 57	25, 41, 74, 104	0
1	C	262/300 (87%)	0.04	6 (2%) 60 67	23, 33, 71, 109	0
All	All	788/900 (87%)	0.06	24 (3%) 50 58	20, 34, 74, 134	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	84	ASN	8.0
1	A	83	THR	7.2
1	C	78	ALA	6.2
1	A	78	ALA	5.8
1	C	79	GLN	5.3
1	A	81	ASP	5.3
1	B	78	ALA	5.1
1	A	82	ASP	4.6
1	A	77	LYS	4.5
1	B	72	PHE	4.5
1	B	76	ALA	4.2
1	C	72	PHE	3.8
1	B	77	LYS	3.4
1	A	269	ARG	3.4
1	A	75	ILE	3.1
1	A	79	GLN	3.0
1	C	75	ILE	3.0
1	C	77	LYS	3.0
1	C	268	PHE	2.8
1	B	268	PHE	2.7
1	A	80	GLY	2.6
1	B	75	ILE	2.6
1	B	269	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	74	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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(Å^2)	Q<0.9
1	CME	A	190	10/11	0.89	0.12	32,42,59,60	0
1	CME	B	190	10/11	0.91	0.12	37,52,71,78	0
1	CME	C	190	10/11	0.92	0.12	33,46,67,75	0

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(Å^2)	Q<0.9
3	CAA	C	303	54/54	0.65	0.37	67,90,117,133	54
3	CAA	B	303	54/54	0.67	0.35	70,92,108,111	54
3	CAA	A	305	54/54	0.73	0.30	57,78,98,113	54
4	GOL	A	306	6/6	0.81	0.15	48,50,54,55	0
4	GOL	C	304	6/6	0.82	0.15	49,56,58,63	0
4	GOL	B	304	6/6	0.84	0.19	50,57,58,73	0
4	GOL	A	307	6/6	0.84	0.20	43,59,60,61	0
2	SO4	C	301	5/5	0.85	0.16	81,85,103,107	0
2	SO4	A	304	5/5	0.86	0.14	54,55,56,62	5
2	SO4	A	303	5/5	0.87	0.20	35,43,46,48	5
2	SO4	C	302	5/5	0.87	0.22	40,40,44,46	5
2	SO4	A	302	5/5	0.87	0.29	86,91,107,108	0
4	GOL	B	305	6/6	0.89	0.20	40,53,60,61	0
4	GOL	C	305	6/6	0.89	0.21	37,51,56,59	0

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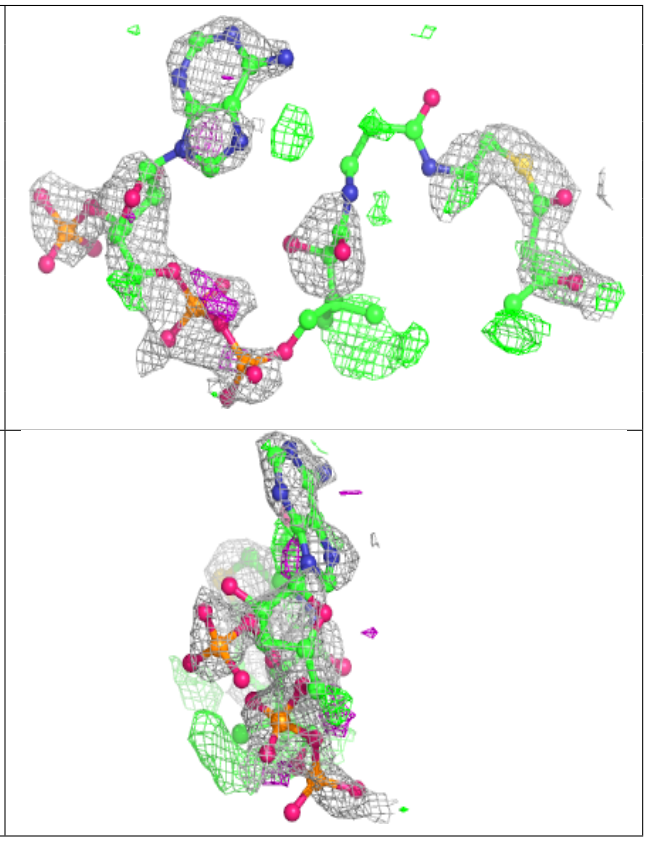
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	302	5/5	0.91	0.16	70,72,80,100	0
4	GOL	A	308	6/6	0.91	0.31	46,49,53,56	0
2	SO4	B	301	5/5	0.92	0.09	72,72,79,82	0
2	SO4	A	301	5/5	0.95	0.16	63,67,73,81	0

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.

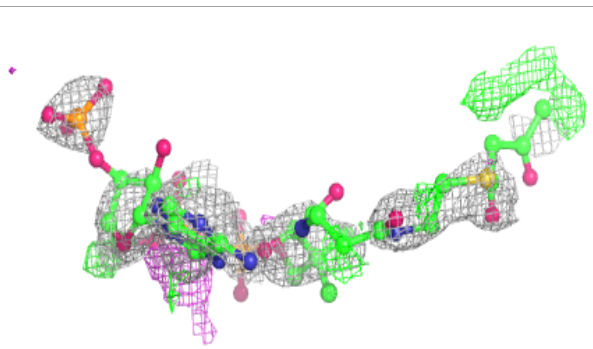
Electron density around CAA C 303:

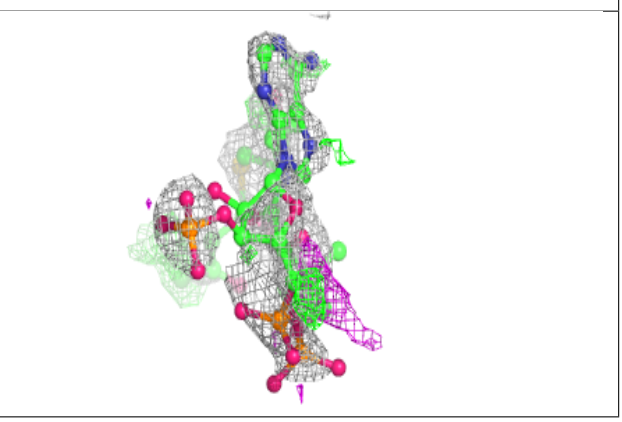
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CAA B 303:

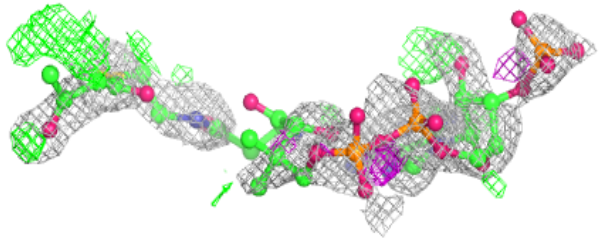
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

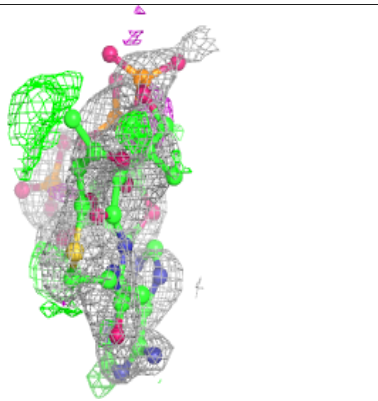




Electron density around CAA A 305:

$2mF_o$-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.