



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:13 PM UTC

PDB ID : 4JAE / pdb_00004jae
Title : STRUCTURAL DETERMINATION OF THE A50T:S279G:S280K:V281
K:K282E:H283N VARIANT OF CITRATE SYNTHASE FROM E. COLI
complexed WITH S-CARBOXYMETHYL-COA
Authors : Maurus, R.; Brayer, G.D.
Deposited on : 2013-02-18
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

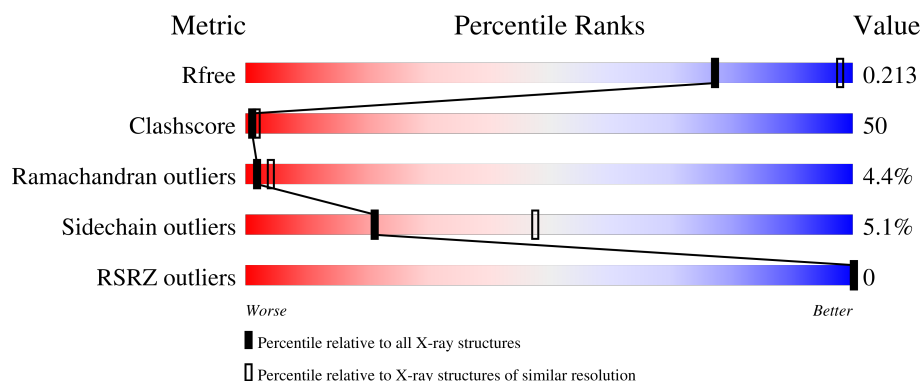
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

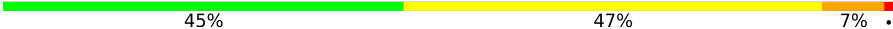
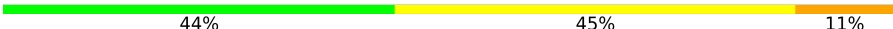
The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	426	
1	B	426	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7081 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 Citrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	0	0
			3365	2132	578	630	25			
1	B	426	Total	C	N	O	S	0	0	0
			3365	2132	578	630	25			

There are 14 discrepancies between the modelled and reference sequences:

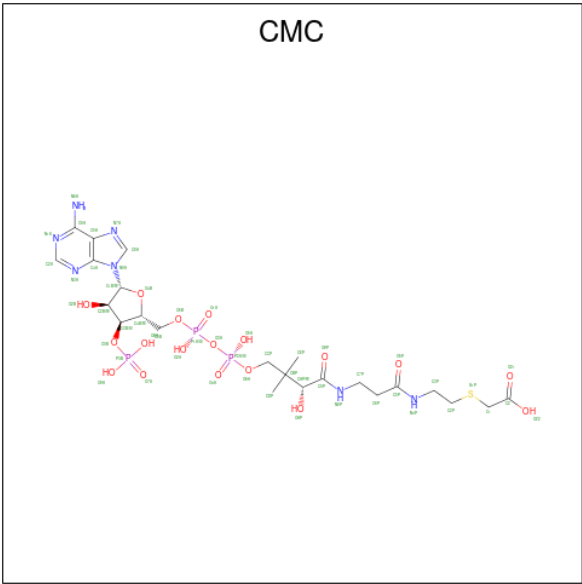
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	ASP	ASN	SEE REMARK 999	UNP P0ABH7
A	50	THR	ALA	engineered mutation	UNP P0ABH7
A	279	GLY	SER	engineered mutation	UNP P0ABH7
A	280	LYS	SER	engineered mutation	UNP P0ABH7
A	281	LYS	VAL	engineered mutation	UNP P0ABH7
A	282	GLU	LYS	engineered mutation	UNP P0ABH7
A	283	ASN	HIS	engineered mutation	UNP P0ABH7
B	1010	ASP	ASN	SEE REMARK 999	UNP P0ABH7
B	1050	THR	ALA	engineered mutation	UNP P0ABH7
B	1279	GLY	SER	engineered mutation	UNP P0ABH7
B	1280	LYS	SER	engineered mutation	UNP P0ABH7
B	1281	LYS	VAL	engineered mutation	UNP P0ABH7
B	1282	GLU	LYS	engineered mutation	UNP P0ABH7
B	1283	ASN	HIS	engineered mutation	UNP P0ABH7

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is CARBOXYMETHYL COENZYME *A (CCD ID: CMC) (formula: C₂₃H₃₈N₇O₁₈P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			52	23	7	18	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			52	23	7	18	3	1		

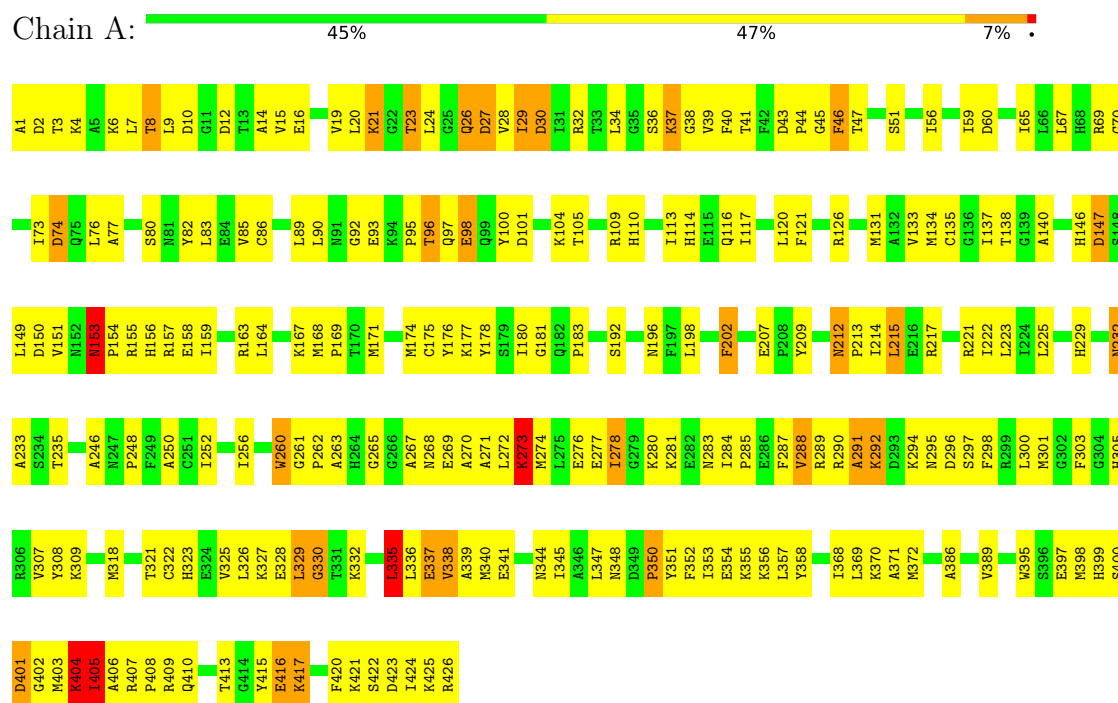
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	104	Total	O	0	0
			104	104		
4	B	123	Total	O	0	0
			123	123		

3 Residue-property plots

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

• Molecule 1: Citrate synthase



• Molecule 1: Citrate synthase



H1247	D1312		H1394
P1248	P1313		W1395
F1249			
	M1318		
I1256	R1319		M1398
A1257	E1320		H1399
S1258	T1321		S1400
L1259			
W1260	E1324		K1404
G1261	V1325		I1405
P1262	L1326		A1406
A1263	R1407		R1407
H1264	K1327		P1408
E1265	E1328		R1409
G1266	L1329		
A1267	G1330		Y1412
N1268	T1331		
E1269	K1332		E1416
A1270	D1333		K1417
L1271	D1334		R1418
L1272	L1335		D1419
K1273	L1336		F1420
M1274	V1337		
L1275	A1338		K1425
E1276	M1340		R1426
E1277	E1341		
I1278	L1342		
G1279	E1343		
K1280	N1344		
K1281	I1345		
E1282	A1346		
N1283			
I1284	D1349		
P1285	P1350		
E1286	Y1351		
F1287	F1352		
V1288			
R1289	K1355		
R1290	K1356		
A1291	L1357		
K1292	Y1358		
D1293			
K1294	F1363		
N1295	Y1364		
D1296			
S1297	I1367		
F1298	I1368		
R1299	L1369		
L1300	K1370		
M1301	A1371		
G1302			
F1303	M1378		
G1304	F1379		
H1305	T1380		
R1306	V1381		
V1307			
Y1308	T1388		
K1309			
N1310	I1392		
Y1311	A1393		

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	164.49Å 164.49Å 157.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.70 30.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.1 (30.00-2.70) 98.2 (30.00-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.177 , 0.216 0.176 , 0.213	Depositor DCC
R_{free} test set	2093 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.467 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7081	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CMC

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	0.50	0/3441	1.03	15/4649 (0.3%)
1	B	0.50	0/3441	1.04	23/4649 (0.5%)
All	All	0.50	0/6882	1.04	38/9298 (0.4%)

There are no bond length outliers.

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	GLU	N-CA-C	-11.07	98.46	113.18
1	B	1355	LYS	CA-C-N	-7.89	110.48	122.08
1	B	1355	LYS	C-N-CA	-7.89	110.48	122.08
1	B	1416	GLU	N-CA-C	-7.40	100.98	110.53
1	A	332	LYS	N-CA-C	-7.39	103.22	114.16

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3365	0	3315	359	0
1	B	3365	0	3312	366	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	52	0	33	15	0
3	B	52	0	33	15	0
4	A	104	0	0	7	0
4	B	123	0	0	10	0
All	All	7081	0	6693	673	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 50.

The worst 5 of 673 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:1283:ASN:O	1:B:1288:VAL:HG21	1.18	1.27
1:A:352:PHE:HA	1:A:357:LEU:HD23	1.31	1.10
1:A:404:LYS:H	1:A:404:LYS:HD3	1.20	1.05
1:B:1289:ARG:HA	1:B:1292:LYS:HB3	1.36	1.04
1:A:284:ILE:HG12	1:A:289:ARG:HH11	1.18	1.02

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	424/426 (100%)	346 (82%)	61 (14%)	17 (4%)	2	5
1	B	424/426 (100%)	341 (80%)	63 (15%)	20 (5%)	2	3
All	All	848/852 (100%)	687 (81%)	124 (15%)	37 (4%)	2	4

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	401	ASP
1	A	405	ILE
1	A	30	ASP
1	A	37	LYS
1	A	147	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	361/361 (100%)	339 (94%)	22 (6%)	17	40
1	B	361/361 (100%)	346 (96%)	15 (4%)	26	55
All	All	722/722 (100%)	685 (95%)	37 (5%)	21	48

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1134	MET
1	B	1398	MET
1	B	1153	ASN
1	B	1292	LYS
1	A	212	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1097	GLN
1	B	1129	HIS
1	B	1323	HIS
1	B	1122	HIS
1	B	1146	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	CMC	B	2003	-	52,54,54	1.01	3 (5%)	75,80,80	1.45	12 (16%)
2	SO4	B	2002	-	4,4,4	0.79	0	6,6,6	0.43	0
2	SO4	A	502	-	4,4,4	0.79	0	6,6,6	0.47	0
2	SO4	A	501	-	4,4,4	0.78	0	6,6,6	0.45	0
3	CMC	A	503	-	52,54,54	0.99	3 (5%)	75,80,80	1.44	9 (12%)
2	SO4	B	2001	-	4,4,4	0.87	0	6,6,6	0.39	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	CMC	B	2003	-	-	14/52/68/68	0/3/3/3
3	CMC	A	503	-	-	15/52/68/68	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	CMC	C5A-N7A	-3.15	1.33	1.39
3	B	2003	CMC	C5A-N7A	-3.07	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2003	CMC	C8A-N9A	-2.33	1.33	1.37
3	A	503	CMC	C8A-N9A	-2.28	1.33	1.37
3	B	2003	CMC	C4A-N9A	-2.08	1.33	1.37

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2003	CMC	C5A-C4A-N3A	-5.42	119.25	126.72
3	A	503	CMC	C5A-C4A-N3A	-5.21	119.54	126.72
3	B	2003	CMC	N3A-C2A-N1A	-4.69	121.48	128.58
3	A	503	CMC	N3A-C2A-N1A	-4.63	121.57	128.58
3	B	2003	CMC	N3A-C4A-N9A	3.92	133.84	127.17

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

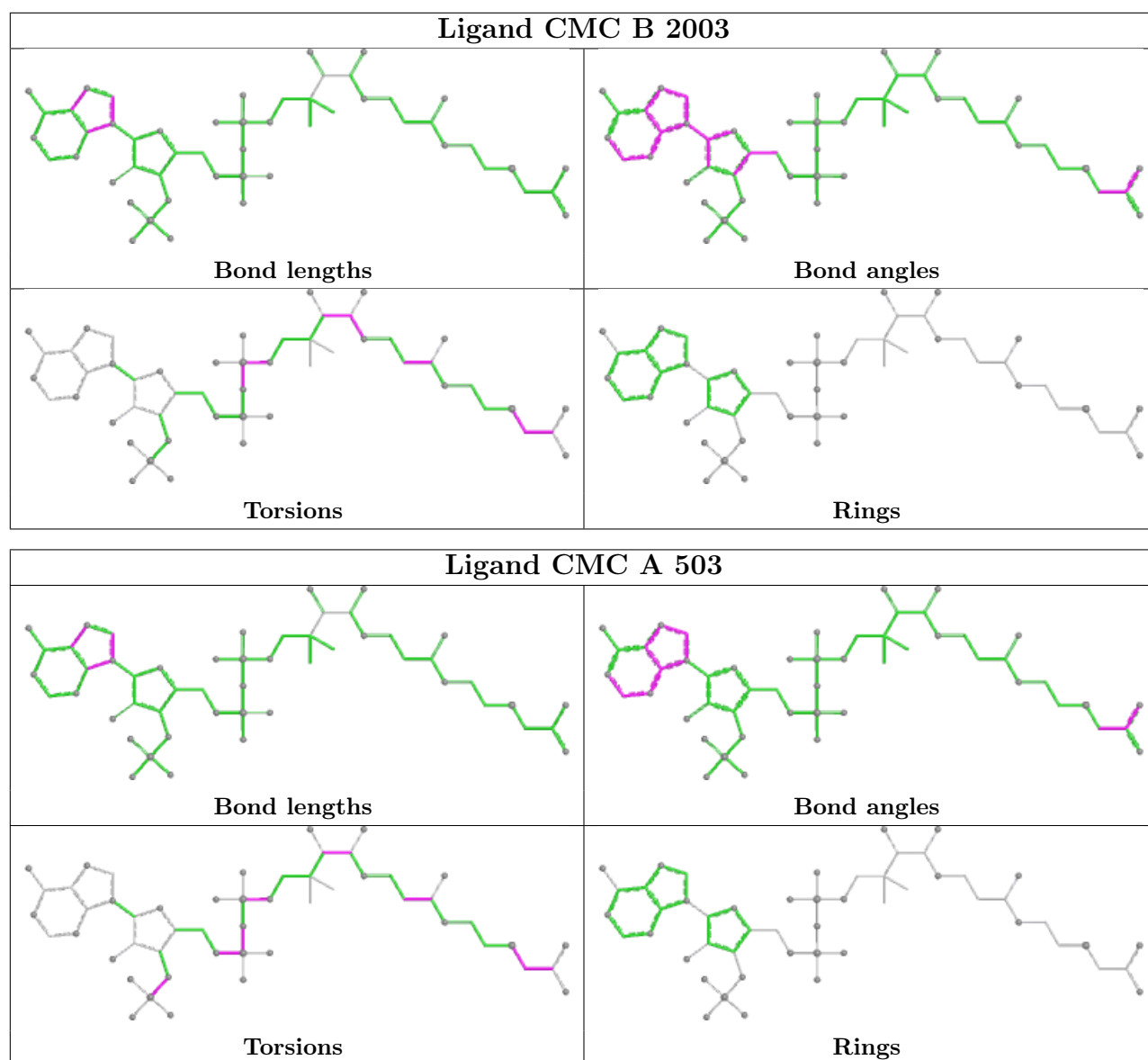
Mol	Chain	Res	Type	Atoms
3	A	503	CMC	C5B-O5B-P1A-O1A
3	A	503	CMC	C5B-O5B-P1A-O3A
3	A	503	CMC	CCP-O6A-P2A-O3A
3	A	503	CMC	O9P-C9P-CAP-CBP
3	A	503	CMC	N8P-C9P-CAP-CBP

There are no ring outliers.

2 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2003	CMC	15	0
3	A	503	CMC	15	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	426/426 (100%)	-1.63	0 100 100	19, 41, 98, 117	0
1	B	426/426 (100%)	-1.61	0 100 100	21, 39, 105, 111	0
All	All	852/852 (100%)	-1.62	0 100 100	19, 40, 104, 117	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

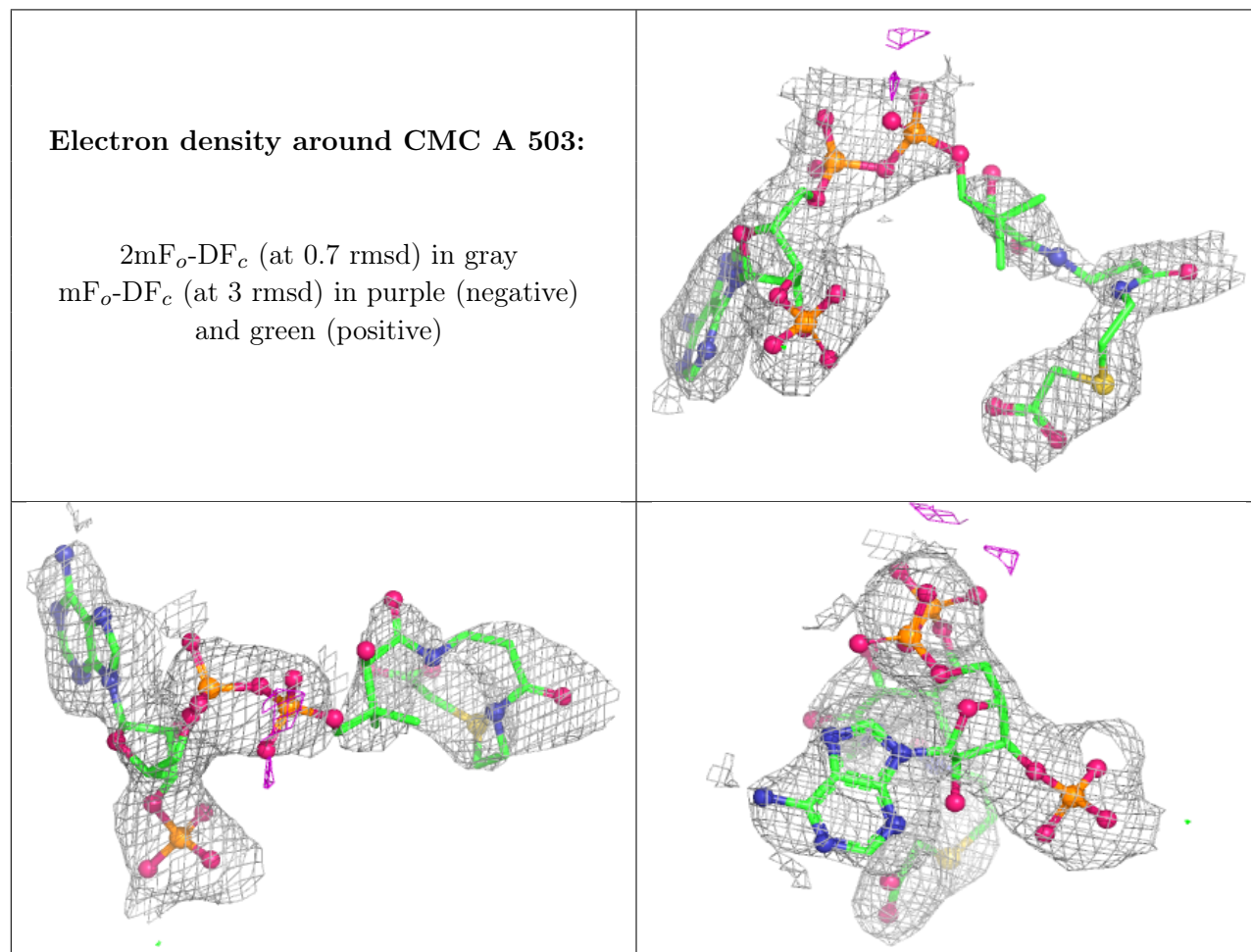
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

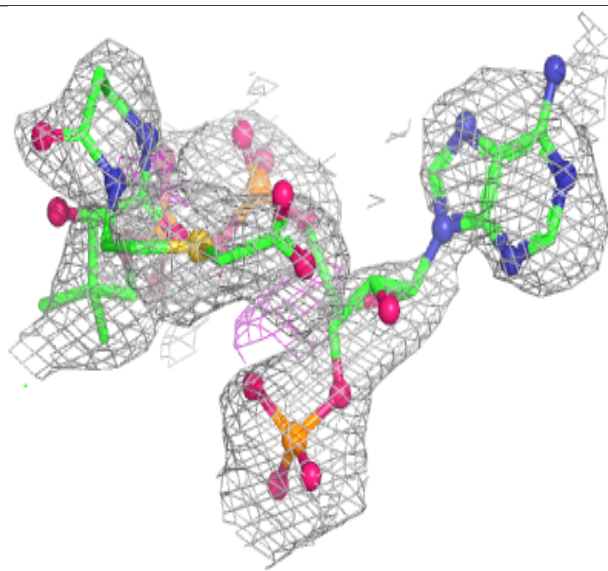
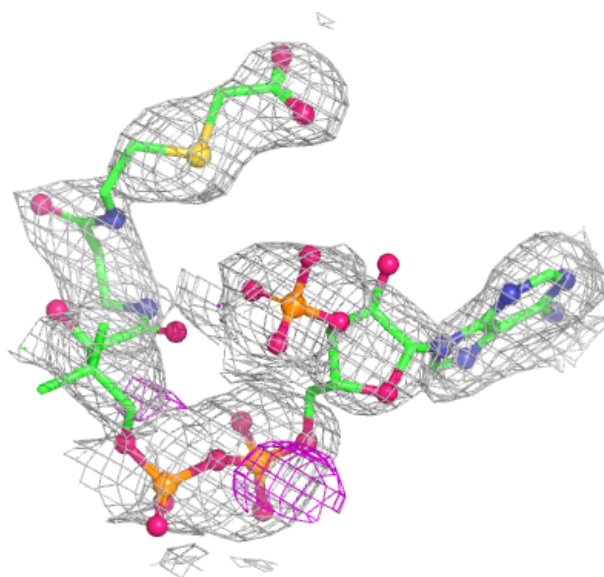
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	502	5/5	0.99	0.04	80,80,81,81	0
2	SO4	B	2002	5/5	0.99	0.03	63,63,64,64	0
3	CMC	A	503	52/52	0.99	0.04	69,74,78,78	0
3	CMC	B	2003	52/52	0.99	0.05	67,73,76,77	0
2	SO4	B	2001	5/5	1.00	0.03	43,43,43,44	0
2	SO4	A	501	5/5	1.00	0.03	53,53,54,54	0

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 CMC B 2003:

$2mF_o-DF_c$ (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.