



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 12:05 PM EDT

PDB ID : 8CSB / pdb_00008csb
Title : WbbB D232N in complex with CMP-beta-Kdo
Authors : Forrester, T.J.B.; Kimber, M.S.
Deposited on : 2022-05-12
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

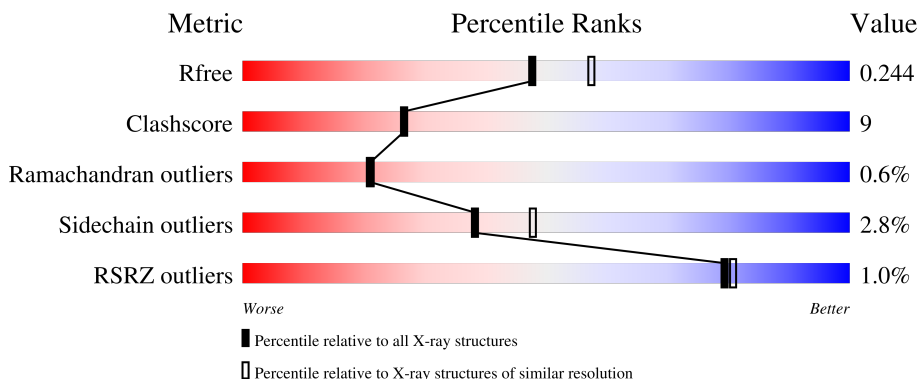
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	410	
1	B	410	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6518 atoms, of which 72 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 N-acetyl glucosaminyl transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	394	3127	2004	515	596	12	0	0	0
1	B	391	3100	1987	510	591	12	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

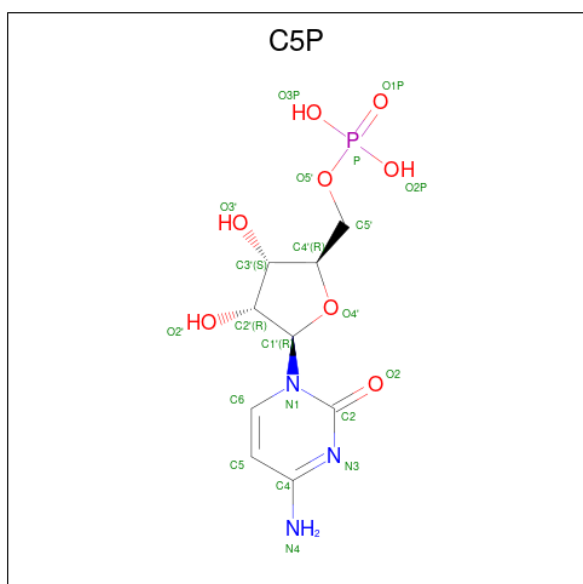
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP Q6U8B0
A	1	GLY	-	expression tag	UNP Q6U8B0
A	232	ASN	ASP	engineered mutation	UNP Q6U8B0
A	402	LEU	-	expression tag	UNP Q6U8B0
A	403	GLU	-	expression tag	UNP Q6U8B0
A	404	HIS	-	expression tag	UNP Q6U8B0
A	405	HIS	-	expression tag	UNP Q6U8B0
A	406	HIS	-	expression tag	UNP Q6U8B0
A	407	HIS	-	expression tag	UNP Q6U8B0
A	408	HIS	-	expression tag	UNP Q6U8B0
A	409	HIS	-	expression tag	UNP Q6U8B0
B	0	MET	-	expression tag	UNP Q6U8B0
B	1	GLY	-	expression tag	UNP Q6U8B0
B	232	ASN	ASP	engineered mutation	UNP Q6U8B0
B	402	LEU	-	expression tag	UNP Q6U8B0
B	403	GLU	-	expression tag	UNP Q6U8B0
B	404	HIS	-	expression tag	UNP Q6U8B0
B	405	HIS	-	expression tag	UNP Q6U8B0
B	406	HIS	-	expression tag	UNP Q6U8B0
B	407	HIS	-	expression tag	UNP Q6U8B0
B	408	HIS	-	expression tag	UNP Q6U8B0
B	409	HIS	-	expression tag	UNP Q6U8B0

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



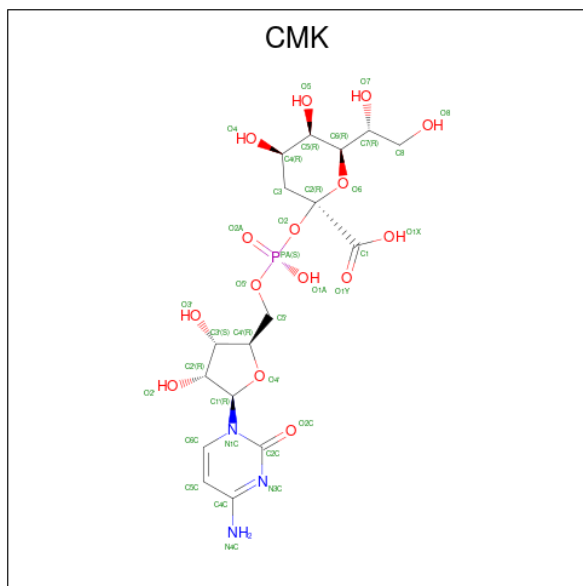
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is CYTIDINE-5'-MONOPHOSPHATE (CCD ID: C5P) (formula: $C_9H_{14}N_3O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	H	N	O	P	0	1
			33	9	12	3	8	1		
3	B	1	Total	C	H	N	O	P	0	1
			33	9	12	3	8	1		

- Molecule 4 is CYTIDINE 5'-MONOPHOSPHATE 3-DEOXY-BETA-D-GULO-OCT-2-UL O-PYRANOSONIC ACID (CCD ID: CMK) (formula: $C_{17}H_{26}N_3O_{15}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total	C	H	N	O	P	0	1
			60	17	24	3	15	1		
4	B	1	Total	C	H	N	O	P	0	1
			60	17	24	3	15	1		

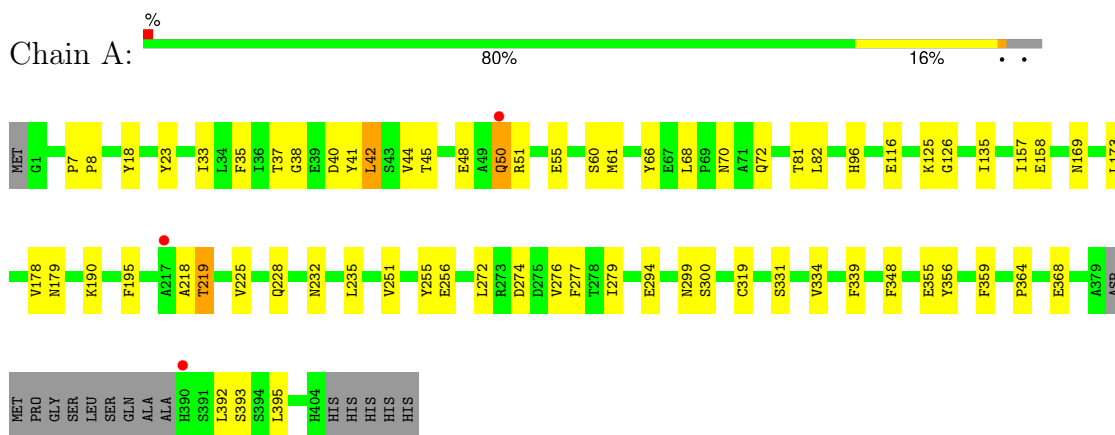
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	44	Total	O	0	0
			44	44		
5	B	41	Total	O	0	0
			41	41		

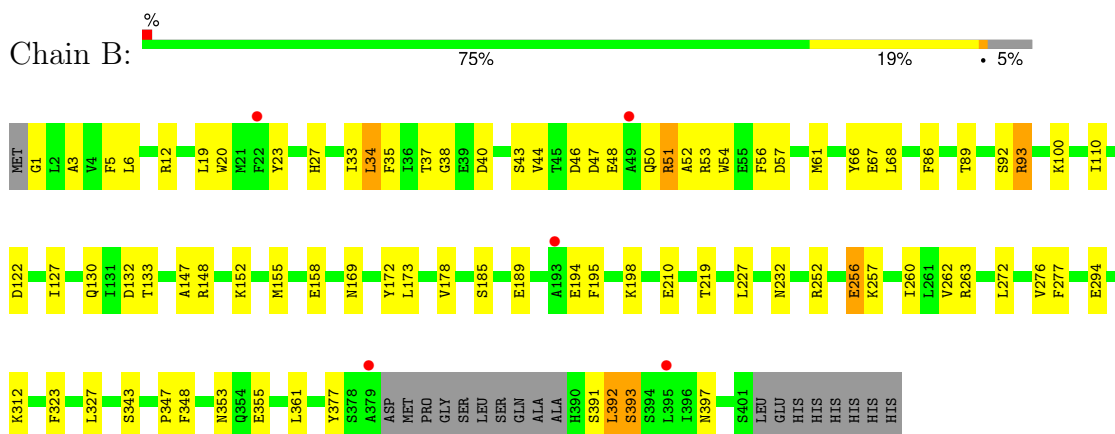
3 Residue-property plots [i](#)

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: N-acetyl glucosaminyl transferase



- Molecule 1: N-acetyl glucosaminyl transferase



4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	92.71Å 157.44Å 120.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.99 – 2.25 47.99 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.99-2.25) 99.8 (47.99-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 1.91Å)	Xtrriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.203 , 0.244 0.203 , 0.244	Depositor DCC
R_{free} test set	3258 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	62.3	Xtrriage
Anisotropy	0.213	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.004 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6518	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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: C5P, CMK, CSO, PO4

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	0.67	0/3197	0.76	0/4343
1	B	0.64	0/3169	0.76	0/4305
All	All	0.65	0/6366	0.76	0/8648

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3127	0	3018	54	0
1	B	3100	0	2994	60	0
2	A	15	0	0	2	0
2	B	5	0	0	1	0
3	A	21	12	12	0	0
3	B	21	12	12	1	0
4	A	36	24	24	4	0
4	B	36	24	24	6	0
5	A	44	0	0	1	0
5	B	41	0	0	3	0
All	All	6446	72	6084	116	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (116) 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:232:ASN:ND2	2:B:501:PO4:O2	2.01	0.93
4:B:502[A]:CMK:O5	4:B:502[A]:CMK:O7	1.93	0.84
1:B:27:HIS:HD2	1:B:66:TYR:HA	1.42	0.83
1:B:27:HIS:CD2	1:B:66:TYR:HA	2.15	0.81
1:B:155:MET:HE3	1:B:361:LEU:HG	1.64	0.79
1:B:257:LYS:HD2	1:B:257:LYS:H	1.47	0.78
1:B:232:ASN:HD21	4:B:502[A]:CMK:H5	1.52	0.75
1:A:48:GLU:HG3	1:A:51:ARG:HH12	1.50	0.74
1:A:61:MET:HE1	1:A:68:LEU:HG	1.70	0.72
1:A:232:ASN:ND2	4:A:505[A]:CMK:H3C2	2.09	0.68
1:B:169:ASN:HB3	1:B:348:PHE:HB2	1.76	0.68
1:A:40:ASP:O	1:A:44:VAL:HG13	1.94	0.68
1:A:33:ILE:HD11	1:A:35:PHE:CZ	2.30	0.67
1:A:44:VAL:HG12	1:A:50:GLN:HE22	1.58	0.67
1:A:33:ILE:HD11	1:A:35:PHE:CE1	2.31	0.65
1:B:391:SER:O	1:B:393:SER:N	2.29	0.65
1:B:198:LYS:HD3	1:B:397:ASN:HD21	1.62	0.65
1:B:51:ARG:HA	1:B:56:PHE:CD2	2.32	0.64
1:B:130:GLN:O	1:B:130:GLN:HG3	1.97	0.64
1:A:169:ASN:HB3	1:A:348:PHE:CB	2.27	0.64
1:A:61:MET:CE	1:A:68:LEU:HG	2.29	0.62
1:A:256:GLU:HA	1:A:256:GLU:OE1	2.00	0.62
1:B:252:ARG:HD3	1:B:257:LYS:NZ	2.15	0.61
1:B:173:LEU:C	1:B:173:LEU:HD23	2.26	0.61
1:B:198:LYS:HD3	1:B:397:ASN:ND2	2.15	0.61
1:B:169:ASN:HB3	1:B:348:PHE:CB	2.30	0.61
1:A:51:ARG:HB2	1:A:51:ARG:NH1	2.17	0.60
1:B:227:LEU:HD11	1:B:272:LEU:HD11	1.82	0.59
1:B:158:GLU:HB3	1:B:178:VAL:HG21	1.85	0.58
1:A:225:VAL:HG22	1:A:251:VAL:HG21	1.86	0.57
1:B:37:THR:HG23	1:B:38:GLY:N	2.19	0.57
1:B:54:TRP:HA	1:B:57:ASP:OD2	2.06	0.56
1:A:23:TYR:OH	1:A:45:THR:HG22	2.05	0.56
1:B:148:ARG:NH1	5:B:602:HOH:O	2.34	0.56
1:A:70:ASN:OD1	1:A:72:GLN:HG3	2.05	0.56
1:B:19:LEU:HD11	1:B:23:TYR:CZ	2.41	0.56
1:A:48:GLU:HA	1:A:51:ARG:HH22	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:GLU:OE1	1:B:48:GLU:HA	2.05	0.55
1:B:155:MET:CE	1:B:361:LEU:HG	2.35	0.55
1:B:5:PHE:O	1:B:6:LEU:HD23	2.06	0.55
1:A:96:HIS:NE2	2:A:502:PO4:O1	2.39	0.55
1:A:51:ARG:HB2	1:A:51:ARG:CZ	2.38	0.54
1:A:135:ILE:HG23	1:A:157:ILE:HD12	1.90	0.54
1:A:135:ILE:CG2	1:A:157:ILE:HD12	2.39	0.53
1:A:44:VAL:HG12	1:A:50:GLN:NE2	2.23	0.52
1:A:276:VAL:HG13	1:A:277:PHE:CD2	2.45	0.52
1:A:81:THR:HG22	5:A:624:HOH:O	2.10	0.51
1:A:8:PRO:HB3	1:A:38:GLY:HA3	1.92	0.51
1:B:232:ASN:OD1	4:B:502[A]:CMK:H6	2.11	0.51
1:A:169:ASN:HB3	1:A:348:PHE:HB2	1.91	0.50
1:A:48:GLU:HA	1:A:51:ARG:NH2	2.26	0.50
1:A:44:VAL:HA	1:A:50:GLN:HE21	1.77	0.50
1:A:228:GLN:HG2	1:A:300:SER:HB2	1.94	0.50
1:A:190:LYS:NZ	1:B:122:ASP:OD2	2.32	0.49
1:B:48:GLU:HB3	1:B:51:ARG:NE	2.28	0.49
1:A:44:VAL:HA	1:A:50:GLN:NE2	2.27	0.49
1:B:27:HIS:CE1	1:B:67:GLU:OE1	2.66	0.49
1:B:262:VAL:HG11	1:B:272:LEU:HD11	1.96	0.48
1:B:86:PHE:CZ	1:B:110:ILE:HG21	2.48	0.48
1:B:276:VAL:HG13	1:B:277:PHE:N	2.29	0.48
1:B:347:PRO:HG3	1:B:377:TYR:CZ	2.49	0.47
1:B:3:ALA:HA	1:B:34:LEU:O	2.14	0.47
1:B:89:THR:O	1:B:93:ARG:HG2	2.14	0.47
1:A:274:ASP:OD1	1:A:274:ASP:N	2.41	0.47
1:B:20:TRP:HB3	1:B:54:TRP:CH2	2.49	0.47
1:A:42:LEU:HD23	1:A:42:LEU:N	2.30	0.47
1:B:86:PHE:HZ	1:B:110:ILE:HG21	1.80	0.47
1:B:252:ARG:HD3	1:B:257:LYS:HZ2	1.78	0.47
1:A:195:PHE:CZ	1:A:339:PHE:HB2	2.50	0.47
1:B:50:GLN:C	1:B:52:ALA:H	2.23	0.46
1:A:125:LYS:HD3	1:A:126:GLY:N	2.29	0.46
1:B:50:GLN:O	1:B:53:ARG:HG2	2.15	0.46
1:A:339:PHE:CD2	1:A:339:PHE:C	2.94	0.46
1:A:364:PRO:HB2	1:A:368:GLU:OE1	2.15	0.46
1:B:232:ASN:ND2	4:B:502[A]:CMK:H3C2	2.31	0.46
1:A:82:LEU:HD23	1:A:116:GLU:HG2	1.99	0.45
1:A:279:ILE:O	1:A:279:ILE:HG13	2.15	0.45
1:B:263:ARG:HE	3:B:503[B]:C5P:C2	2.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:THR:CG2	1:B:361:LEU:HD11	2.46	0.45
1:B:46:ASP:OD1	1:B:47:ASP:N	2.50	0.45
1:B:61:MET:HE1	1:B:68:LEU:HG	1.98	0.45
1:A:173:LEU:C	1:A:173:LEU:HD23	2.42	0.44
1:B:185:SER:HB3	1:B:323:PHE:HB3	1.99	0.44
1:A:55:GLU:O	1:A:66:TYR:OH	2.32	0.44
1:A:218:ALA:O	1:A:219:THR:CB	2.65	0.44
1:A:232:ASN:OD1	4:A:505[A]:CMK:H6	2.18	0.43
1:B:1:GLY:N	1:B:132:ASP:OD2	2.51	0.43
1:B:27:HIS:O	1:B:27:HIS:ND1	2.51	0.43
1:A:255:TYR:OH	1:A:294:GLU:OE2	2.37	0.43
1:B:327:LEU:HD23	1:B:327:LEU:HA	1.72	0.43
1:A:48:GLU:CG	1:A:51:ARG:HH12	2.27	0.43
4:B:502[A]:CMK:O5'	4:B:502[A]:CMK:H6C	2.18	0.43
2:A:501:PO4:O1	4:A:505[A]:CMK:H8C1	2.19	0.42
1:B:33:ILE:HG21	1:B:35:PHE:CZ	2.54	0.42
1:B:232:ASN:HD21	4:B:502[A]:CMK:C5	2.27	0.42
1:A:169:ASN:HB3	1:A:348:PHE:HB3	1.98	0.42
1:A:356:TYR:O	1:A:359:PHE:HB3	2.20	0.42
1:B:147:ALA:HB1	1:B:152:LYS:O	2.20	0.42
1:A:37:THR:HG23	1:A:38:GLY:N	2.35	0.42
1:B:12:ARG:HD3	5:B:638:HOH:O	2.19	0.42
1:A:178:VAL:O	1:A:179:ASN:HB2	2.20	0.41
1:B:34:LEU:C	1:B:34:LEU:CD2	2.93	0.41
1:A:276:VAL:HG13	1:A:277:PHE:N	2.35	0.41
1:A:392:LEU:O	1:A:392:LEU:HD23	2.21	0.41
1:B:172:TYR:HA	5:B:608:HOH:O	2.20	0.41
1:B:294:GLU:OE1	1:B:312:LYS:HE3	2.20	0.41
1:A:37:THR:OG1	1:A:41:TYR:CD1	2.73	0.41
1:A:392:LEU:HA	1:A:395:LEU:HD12	2.03	0.41
1:A:299:ASN:HB2	1:A:319:CYS:HB3	2.03	0.41
1:B:256:GLU:O	1:B:260:ILE:HG13	2.21	0.41
1:A:7:PRO:HG2	1:A:18:TYR:HE2	1.86	0.40
1:B:195:PHE:CE1	1:B:392:LEU:HD21	2.56	0.40
1:B:353:ASN:OD1	1:B:355:GLU:HB2	2.21	0.40
1:A:158:GLU:HG2	4:A:505[A]:CMK:O8	2.21	0.40
1:B:40:ASP:O	1:B:44:VAL:HG13	2.22	0.40
1:B:194:GLU:HB2	1:B:392:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	389/410 (95%)	372 (96%)	15 (4%)	2 (0%)	24	24
1	B	386/410 (94%)	372 (96%)	11 (3%)	3 (1%)	16	14
All	All	775/820 (94%)	744 (96%)	26 (3%)	5 (1%)	21	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	392	LEU
1	A	219	THR
1	B	219	THR
1	A	50	GLN
1	B	51	ARG

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	335/348 (96%)	327 (98%)	8 (2%)	43	54
1	B	332/348 (95%)	321 (97%)	11 (3%)	33	42
All	All	667/696 (96%)	648 (97%)	19 (3%)	38	48

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	60	SER
1	A	235	LEU
1	A	272	LEU
1	A	331	SER
1	A	334	VAL
1	A	355	GLU
1	A	393	SER
1	B	34	LEU
1	B	43	SER
1	B	92	SER
1	B	93	ARG
1	B	100	LYS
1	B	127	ILE
1	B	189	GLU
1	B	210	GLU
1	B	256	GLU
1	B	343	SER
1	B	393	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	50	GLN
1	A	94	HIS
1	A	240	HIS
1	A	290	ASN
1	B	94	HIS
1	B	293	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](#)

2 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	CSO	B	28	1	3,6,7	0.70	0	1,6,8	0.78	0
1	CSO	A	28	1	3,6,7	0.69	0	1,6,8	1.29	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	CSO	B	28	1	-	0/1/5/7	-
1	CSO	A	28	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	C5P	B	503[B]	-	22,22,22	3.32	10 (45%)	32,33,33	1.54	6 (18%)
4	CMK	B	502[A]	-	38,38,38	3.06	15 (39%)	51,58,58	1.86	13 (25%)
3	C5P	A	504[B]	-	22,22,22	3.37	11 (50%)	32,33,33	1.51	7 (21%)
4	CMK	A	505[A]	-	38,38,38	2.95	17 (44%)	51,58,58	1.65	13 (25%)
2	PO4	A	502	-	4,4,4	0.80	0	6,6,6	0.70	0
2	PO4	A	501	-	4,4,4	1.08	0	6,6,6	0.53	0
2	PO4	B	501	-	4,4,4	1.04	0	6,6,6	0.47	0
2	PO4	A	503	-	4,4,4	1.01	0	6,6,6	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CMK	A	505[A]	-	-	10/24/62/62	0/3/3/3
3	C5P	A	504[B]	-	-	2/10/26/26	0/2/2/2
4	CMK	B	502[A]	-	-	11/24/62/62	0/3/3/3
3	C5P	B	503[B]	-	-	1/10/26/26	0/2/2/2

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	504[B]	C5P	P-O5'	11.25	1.95	1.60
3	B	503[B]	C5P	P-O5'	10.68	1.94	1.60
4	B	502[A]	CMK	O4'-C1'	7.59	1.59	1.42
4	B	502[A]	CMK	C3'-C2'	-7.19	1.33	1.53
4	A	505[A]	CMK	C3'-C2'	-7.16	1.34	1.53
4	B	502[A]	CMK	O6-C2	6.72	1.51	1.42
4	A	505[A]	CMK	O6-C2	6.18	1.50	1.42
4	A	505[A]	CMK	O4'-C1'	6.14	1.56	1.42
4	A	505[A]	CMK	O4'-C4'	-5.97	1.31	1.45
4	B	502[A]	CMK	O4'-C4'	-5.71	1.32	1.45
3	B	503[B]	C5P	C4-N4	5.51	1.47	1.33
4	B	502[A]	CMK	C4C-N4C	5.33	1.46	1.33
4	A	505[A]	CMK	C4C-N4C	5.13	1.46	1.33
3	A	504[B]	C5P	C4-N4	5.01	1.46	1.33
3	B	503[B]	C5P	C2-N3	4.99	1.46	1.36
4	A	505[A]	CMK	C1'-N1C	-4.69	1.34	1.47
3	A	504[B]	C5P	C2-N3	4.57	1.45	1.36
4	B	502[A]	CMK	C3'-C4'	4.47	1.64	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	505[A]	CMK	C3'-C4'	4.41	1.64	1.53
4	B	502[A]	CMK	C1'-N1C	-4.34	1.35	1.47
4	B	502[A]	CMK	C3-C4	-3.89	1.47	1.53
4	A	505[A]	CMK	O2'-C2'	3.70	1.52	1.43
4	B	502[A]	CMK	O2'-C2'	3.62	1.51	1.43
3	B	503[B]	C5P	C1'-N1	3.62	1.57	1.47
4	A	505[A]	CMK	C3-C4	-3.55	1.47	1.53
4	B	502[A]	CMK	PA-O2	3.53	1.69	1.59
3	A	504[B]	C5P	C1'-N1	3.31	1.56	1.47
3	A	504[B]	C5P	C5-C4	3.29	1.50	1.42
3	A	504[B]	C5P	C3'-C4'	3.25	1.61	1.53
4	A	505[A]	CMK	PA-O2	3.20	1.68	1.59
3	B	503[B]	C5P	C5'-C4'	3.15	1.61	1.51
4	A	505[A]	CMK	PA-O5'	3.08	1.71	1.59
3	B	503[B]	C5P	C3'-C4'	2.98	1.60	1.53
3	A	504[B]	C5P	C2-N1	2.97	1.46	1.40
3	B	503[B]	C5P	C5-C4	2.90	1.49	1.42
4	A	505[A]	CMK	O6-C6	2.87	1.48	1.44
3	B	503[B]	C5P	O5'-C5'	-2.76	1.34	1.44
4	B	502[A]	CMK	C5C-C4C	-2.70	1.36	1.42
3	A	504[B]	C5P	O5'-C5'	-2.69	1.34	1.44
4	B	502[A]	CMK	O2C-C2C	-2.69	1.18	1.23
4	A	505[A]	CMK	O2C-C2C	-2.65	1.18	1.23
4	B	502[A]	CMK	PA-O5'	2.61	1.69	1.59
4	B	502[A]	CMK	O6-C6	2.56	1.47	1.44
3	B	503[B]	C5P	C2-N1	2.56	1.45	1.40
3	A	504[B]	C5P	C5'-C4'	2.40	1.58	1.51
4	B	502[A]	CMK	C2-C1	-2.35	1.49	1.54
4	A	505[A]	CMK	C5C-C4C	-2.32	1.37	1.42
4	A	505[A]	CMK	C4-C5	-2.27	1.49	1.52
3	A	504[B]	C5P	C2'-C1'	2.16	1.60	1.53
4	A	505[A]	CMK	C2-C1	-2.13	1.49	1.54
3	B	503[B]	C5P	C6-C5	2.13	1.40	1.35
3	A	504[B]	C5P	C6-C5	2.07	1.39	1.35
4	A	505[A]	CMK	C2C-N1C	-2.03	1.35	1.40

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	502[A]	CMK	C3-C4-C5	4.43	115.13	110.84
4	B	502[A]	CMK	C2'-C1'-N1C	4.13	124.74	113.25
4	B	502[A]	CMK	O6-C6-C5	4.13	114.27	108.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	502[A]	CMK	C5'-C4'-C3'	-3.88	101.24	115.21
4	A	505[A]	CMK	O6-C6-C5	3.71	113.69	108.50
4	A	505[A]	CMK	C2'-C1'-N1C	3.71	123.58	113.25
3	A	504[B]	C5P	O5'-P-O1P	-3.38	97.30	106.44
4	B	502[A]	CMK	O2'-C2'-C1'	-3.37	98.51	110.10
4	A	505[A]	CMK	O1Y-C1-C2	-3.21	114.12	123.79
4	B	502[A]	CMK	C3'-C2'-C1'	3.15	107.42	101.46
4	A	505[A]	CMK	C3'-C2'-C1'	3.04	107.21	101.46
4	A	505[A]	CMK	C5'-C4'-C3'	-2.96	104.56	115.21
4	A	505[A]	CMK	O2C-C2C-N3C	-2.93	117.71	122.33
3	B	503[B]	C5P	O3'-C3'-C4'	2.92	119.46	111.08
4	B	502[A]	CMK	O4'-C4'-C5'	2.91	118.64	109.33
3	B	503[B]	C5P	C4-N3-C2	2.91	124.84	120.26
4	B	502[A]	CMK	O6-C2-C3	2.87	115.20	111.35
3	A	504[B]	C5P	C4-N3-C2	2.84	124.74	120.26
3	B	503[B]	C5P	O2P-P-O5'	-2.83	99.30	106.67
4	B	502[A]	CMK	O1A-PA-O2	2.66	117.22	106.27
3	A	504[B]	C5P	O3'-C3'-C4'	2.54	118.37	111.08
4	A	505[A]	CMK	O5'-C5'-C4'	2.38	117.10	108.99
3	A	504[B]	C5P	O3P-P-O5'	-2.38	100.47	106.67
3	A	504[B]	C5P	O2P-P-O3P	2.37	116.68	107.80
3	A	504[B]	C5P	O4'-C4'-C5'	2.36	116.89	109.33
4	A	505[A]	CMK	O4'-C1'-N1C	-2.32	103.09	108.36
3	B	503[B]	C5P	O4'-C4'-C5'	2.30	116.70	109.33
4	A	505[A]	CMK	O4'-C4'-C5'	2.28	116.63	109.33
3	A	504[B]	C5P	C5'-C4'-C3'	-2.27	107.03	115.21
3	B	503[B]	C5P	C5'-C4'-C3'	-2.27	107.04	115.21
4	B	502[A]	CMK	O2C-C2C-N3C	-2.20	118.86	122.33
3	B	503[B]	C5P	O2'-C2'-C3'	-2.19	104.80	111.82
4	A	505[A]	CMK	O4'-C4'-C3'	2.18	109.49	105.15
4	B	502[A]	CMK	O3'-C3'-C4'	2.18	117.35	111.08
4	A	505[A]	CMK	O2'-C2'-C1'	-2.12	102.82	110.10
4	A	505[A]	CMK	C8-C7-C6	-2.10	107.87	112.05
4	A	505[A]	CMK	O3'-C3'-C2'	2.06	118.43	111.82
4	B	502[A]	CMK	C4-C5-C6	2.02	114.58	110.51
4	B	502[A]	CMK	O4'-C1'-N1C	-2.00	103.82	108.36

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	504[B]	C5P	C5'-O5'-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	505[A]	CMK	C5'-O5'-PA-O1A
4	A	505[A]	CMK	O6-C6-C7-C8
4	A	505[A]	CMK	O6-C6-C7-O7
4	B	502[A]	CMK	C5'-O5'-PA-O1A
4	B	502[A]	CMK	C5'-O5'-PA-O2
4	B	502[A]	CMK	O1X-C1-C2-O6
4	B	502[A]	CMK	O6-C6-C7-C8
4	B	502[A]	CMK	O6-C6-C7-O7
4	B	502[A]	CMK	C5-C6-C7-C8
4	B	502[A]	CMK	C5-C6-C7-O7
4	B	502[A]	CMK	O7-C7-C8-O8
4	B	502[A]	CMK	C6-C7-C8-O8
4	A	505[A]	CMK	O1Y-C1-C2-O2
4	B	502[A]	CMK	O1Y-C1-C2-O2
4	A	505[A]	CMK	C5-C6-C7-C8
4	A	505[A]	CMK	C5'-O5'-PA-O2A
4	A	505[A]	CMK	C5'-O5'-PA-O2
4	A	505[A]	CMK	O7-C7-C8-O8
4	A	505[A]	CMK	O1X-C1-C2-O6
3	A	504[B]	C5P	C5'-O5'-P-O3P
4	A	505[A]	CMK	C2-O2-PA-O2A
4	B	502[A]	CMK	C2-O2-PA-O2A
3	B	503[B]	C5P	O4'-C4'-C5'-O5'

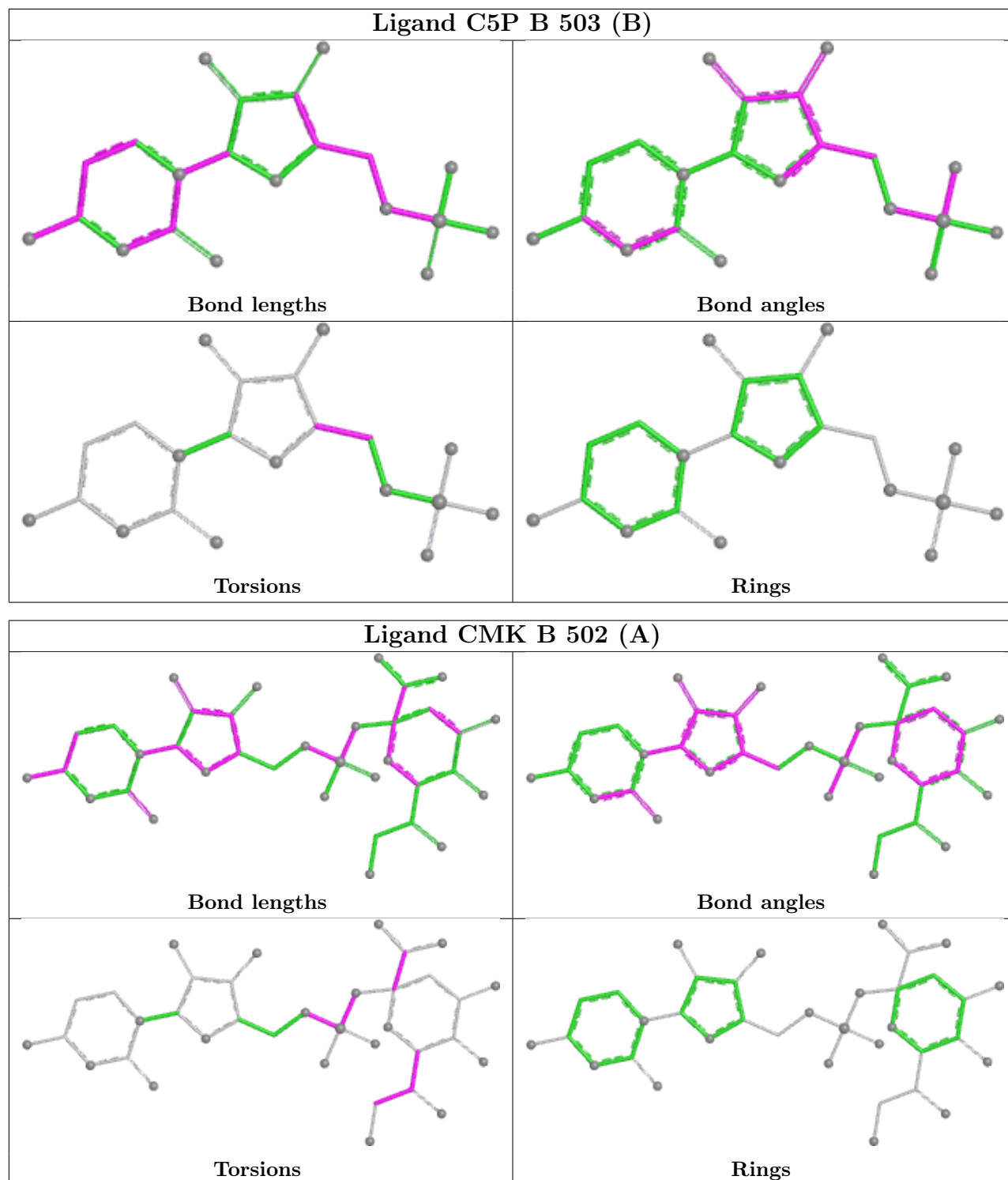
There are no ring outliers.

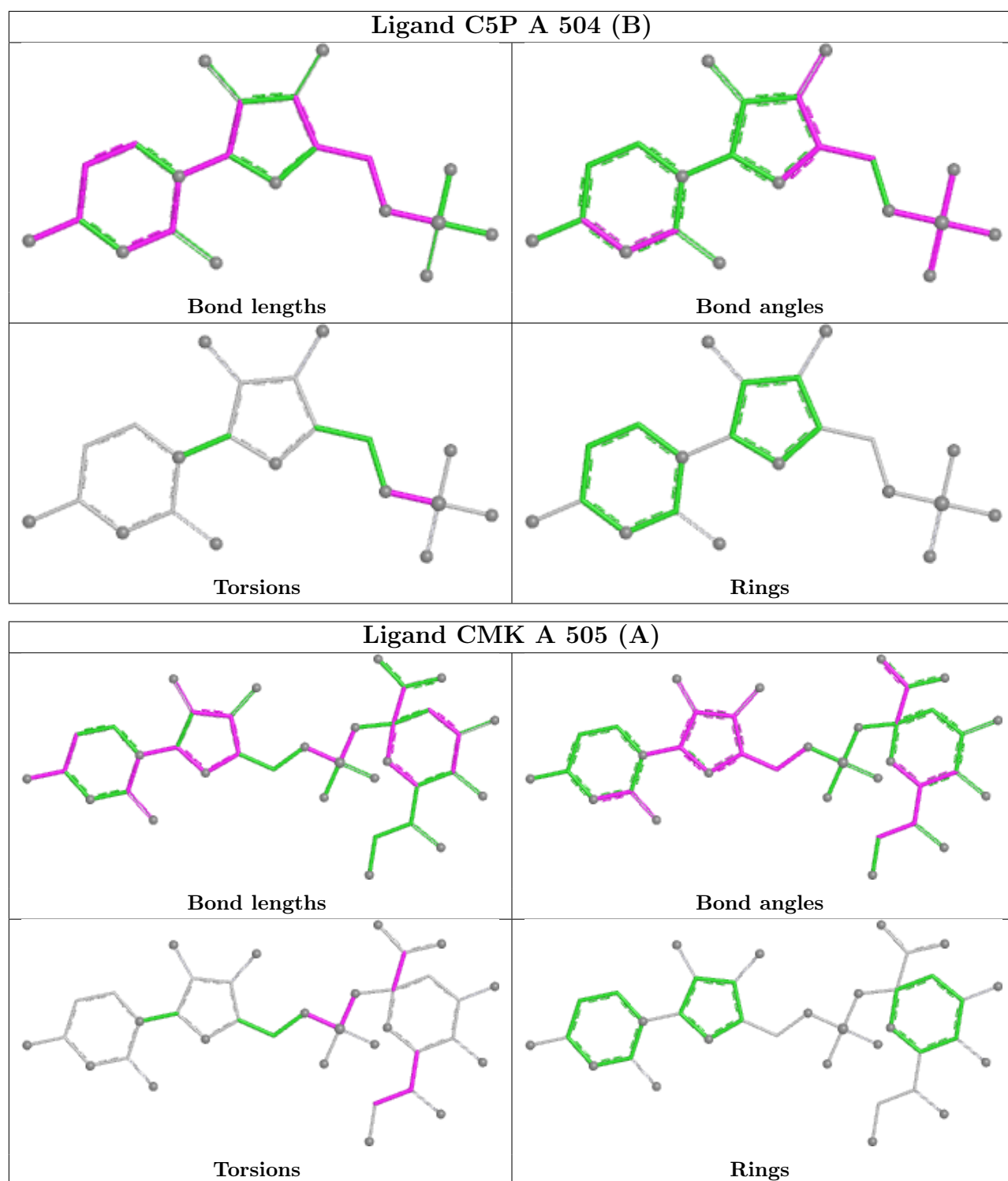
6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	503[B]	C5P	1	0
4	B	502[A]	CMK	6	0
4	A	505[A]	CMK	4	0
2	A	502	PO4	1	0
2	A	501	PO4	1	0
2	B	501	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	393/410 (95%)	0.05	3 (0%) 82 84	48, 67, 117, 191	0
1	B	390/410 (95%)	0.10	5 (1%) 75 76	47, 73, 128, 204	0
All	All	783/820 (95%)	0.08	8 (1%) 79 81	47, 69, 125, 204	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	217	ALA	3.6
1	A	390	HIS	3.1
1	B	379	ALA	3.0
1	B	22	PHE	2.1
1	B	395	LEU	2.1
1	B	49	ALA	2.0
1	B	193	ALA	2.0
1	A	50	GLN	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	CSO	A	28	7/8	0.94	0.07	81,85,95,95	0
1	CSO	B	28	7/8	0.94	0.07	94,98,101,105	0

6.3 Carbohydrates [i](#)

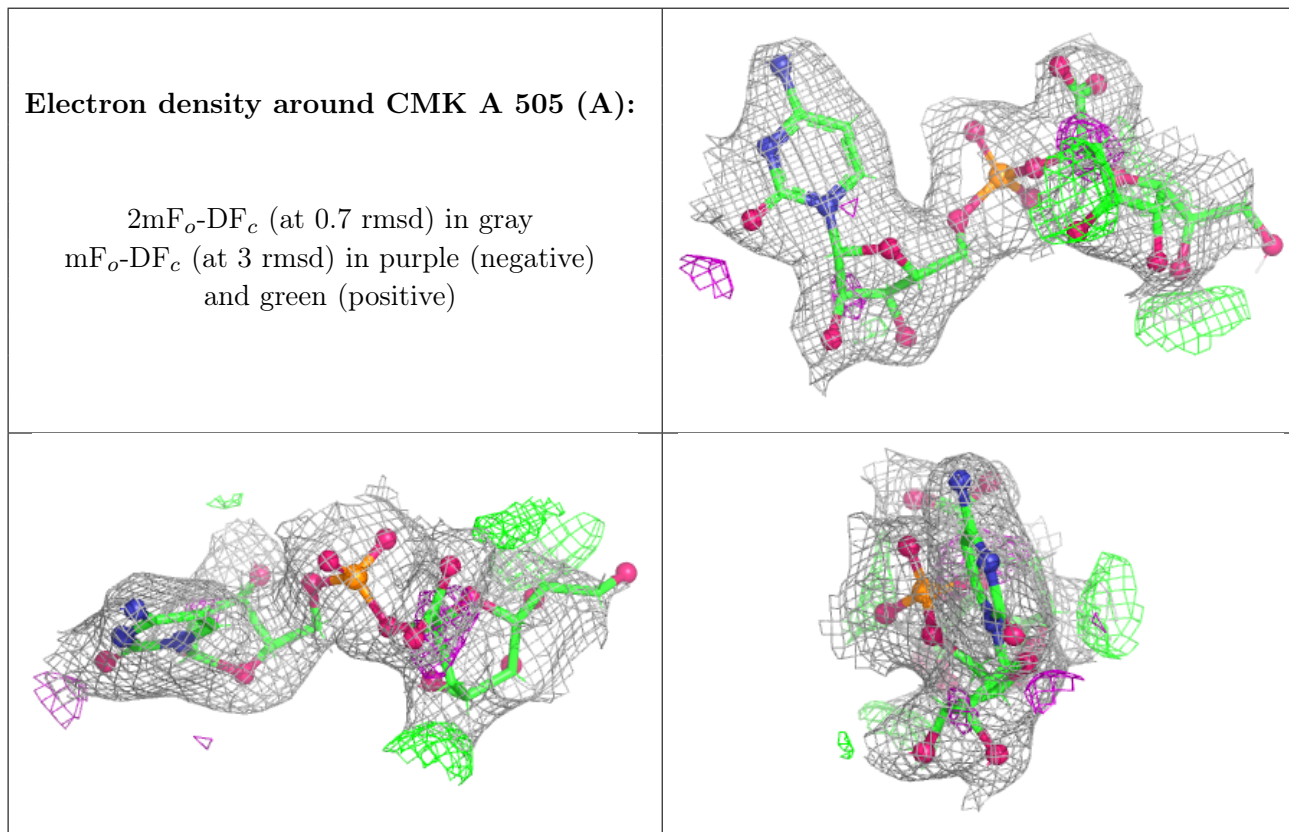
There are no oligosaccharides in this entry.

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.

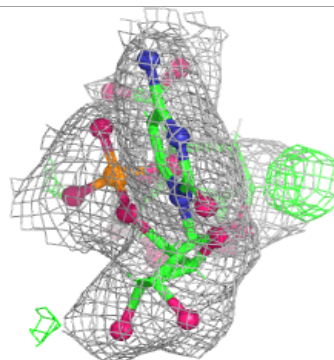
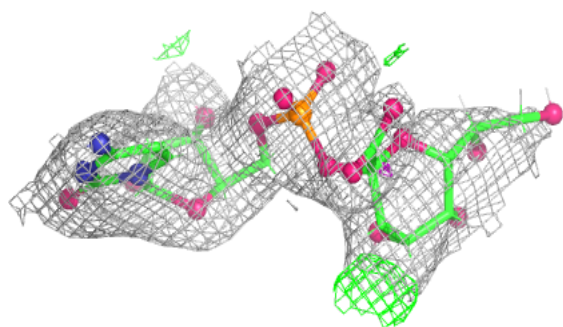
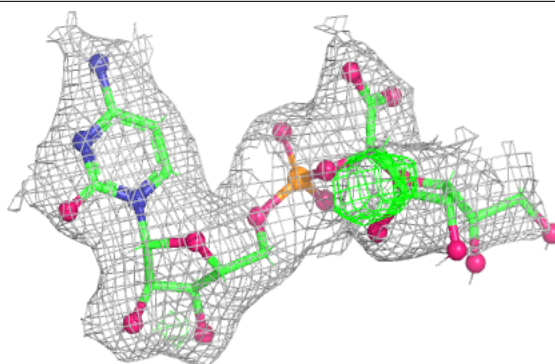
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PO4	A	502	5/5	0.67	0.07	122,132,132,133	0
2	PO4	B	501	5/5	0.71	0.15	139,147,150,151	0
2	PO4	A	503	5/5	0.77	0.13	154,154,155,157	0
2	PO4	A	501	5/5	0.82	0.12	129,129,130,130	0
4	CMK	A	505[A]	36/36	0.87	0.10	56,69,94,95	60
4	CMK	B	502[A]	36/36	0.91	0.09	58,71,101,108	60
3	C5P	B	503[B]	21/21	0.93	0.06	58,60,73,74	33
3	C5P	A	504[B]	21/21	0.95	0.07	55,59,72,72	33

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.



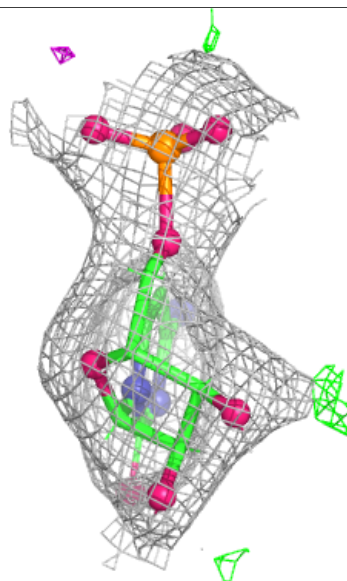
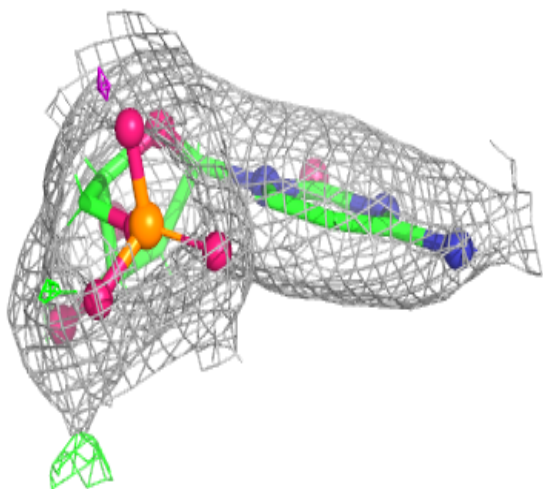
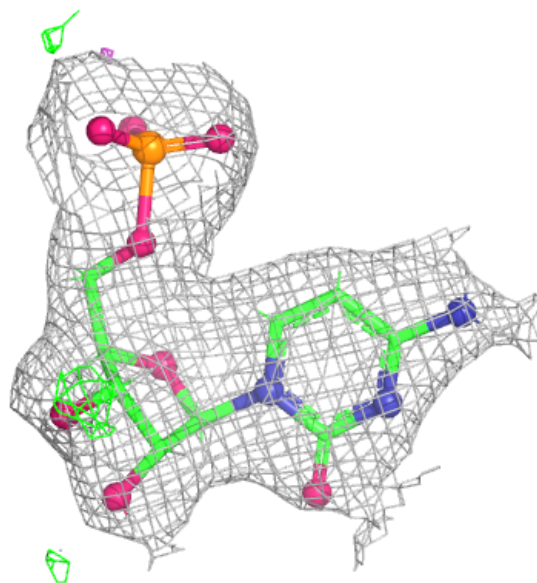
Electron density around CMK B 502 (A):

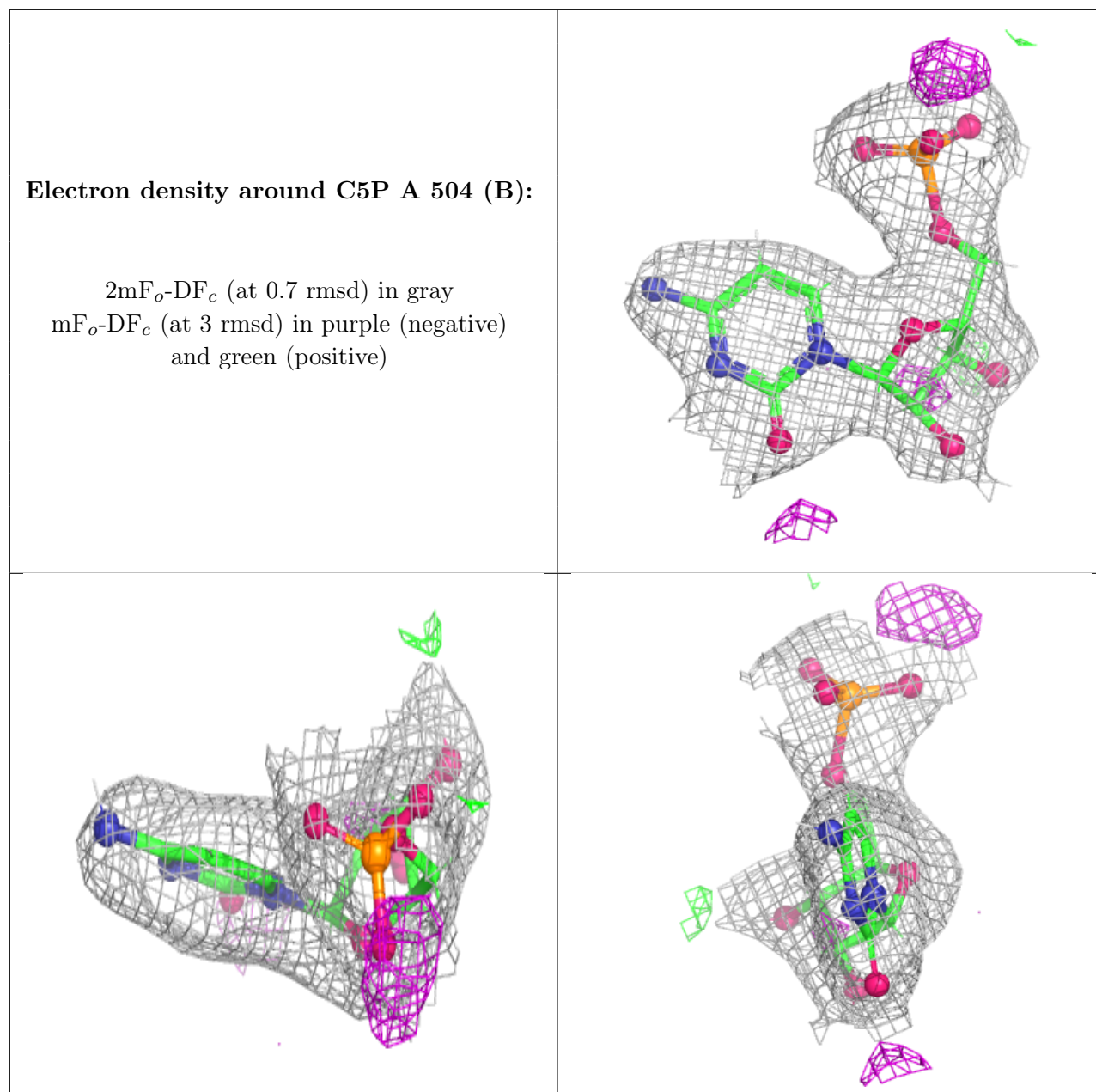
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around C5P B 503 (B):

$2mF_o-DF_c$ (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.