



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:24 PM UTC

PDB ID : 1RO7 / pdb_00001ro7
Title : Structural analysis of the sialyltransferase CstII from *Campylobacter jejuni* in complex with a substrate analogue, CMP-3FNeuAc.
Authors : Chiu, C.P.; Watts, A.G.; Lairson, L.L.; Gilbert, M.; Lim, D.; Wakarchuk, W.W.; Withers, S.G.; Strynadka, N.C.
Deposited on : 2003-12-01
Resolution : 1.80 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

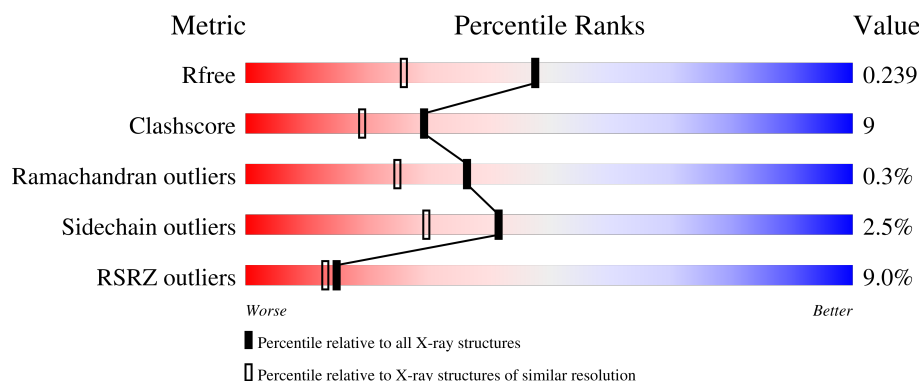
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	259	13% 80% 18% .
1	B	259	6% 71% 19% . 8%
1	C	259	7% 77% 14% . 6%
1	D	259	8% 81% 10% . 8%

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
3	CSF	C	1001	X	-	-	-
3	CSF	C	2001	X	-	-	-
3	CSF	C	3001	X	-	-	-
3	CSF	C	4001	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8668 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.

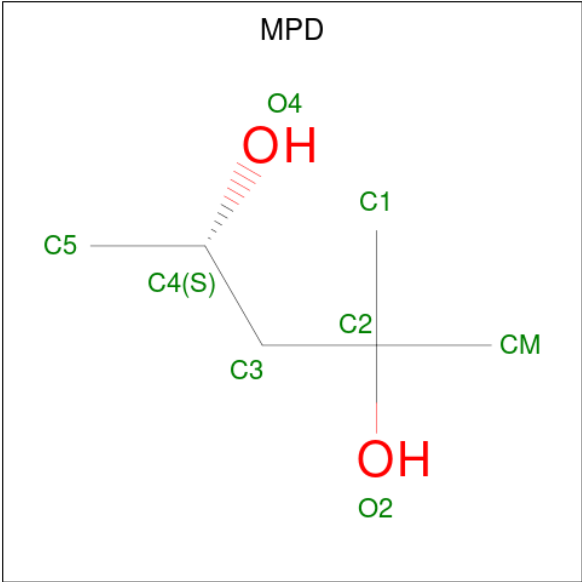
- Molecule 1 is a protein called alpha-2,3/8-sialyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	Se	0	0	0
			2155	1410	340	396	6	3			
1	B	237	Total	C	N	O	S	Se	0	0	0
			1985	1305	311	360	6	3			
1	C	243	Total	C	N	O	S	Se	0	0	0
			2032	1335	317	371	6	3			
1	D	238	Total	C	N	O	S	Se	0	0	0
			1990	1309	311	361	6	3			

There are 16 discrepancies between the modelled and reference sequences:

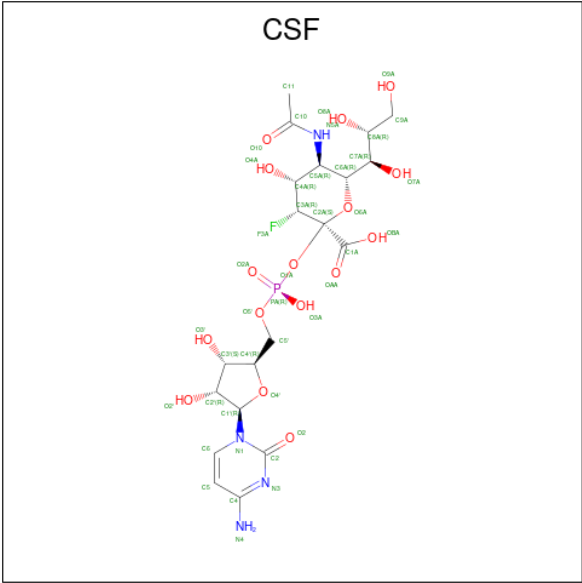
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q9LAK3
A	53	SER	ILE	engineered mutation	UNP Q9LAK3
A	77	MSE	MET	modified residue	UNP Q9LAK3
A	136	MSE	MET	modified residue	UNP Q9LAK3
B	1	MSE	MET	modified residue	UNP Q9LAK3
B	53	SER	ILE	engineered mutation	UNP Q9LAK3
B	77	MSE	MET	modified residue	UNP Q9LAK3
B	136	MSE	MET	modified residue	UNP Q9LAK3
C	1	MSE	MET	modified residue	UNP Q9LAK3
C	53	SER	ILE	engineered mutation	UNP Q9LAK3
C	77	MSE	MET	modified residue	UNP Q9LAK3
C	136	MSE	MET	modified residue	UNP Q9LAK3
D	1	MSE	MET	modified residue	UNP Q9LAK3
D	53	SER	ILE	engineered mutation	UNP Q9LAK3
D	77	MSE	MET	modified residue	UNP Q9LAK3
D	136	MSE	MET	modified residue	UNP Q9LAK3

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is CYTIDINE-5'-MONOPHOSPHATE-3-FLUORO-N-ACETYL-NEURAMINI C ACID (CCD ID: CSF) (formula: C₂₀H₃₀FN₄O₁₆P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	C	1	Total	C	F	N	O	P	0	0
			42	20	1	4	16	1		
3	C	1	Total	C	F	N	O	P	0	0
			42	20	1	4	16	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	C	1	Total	C	F	N	O	P	0	0
			42	20	1	4	16	1		
3	C	1	Total	C	F	N	O	P	0	0
			42	20	1	4	16	1		

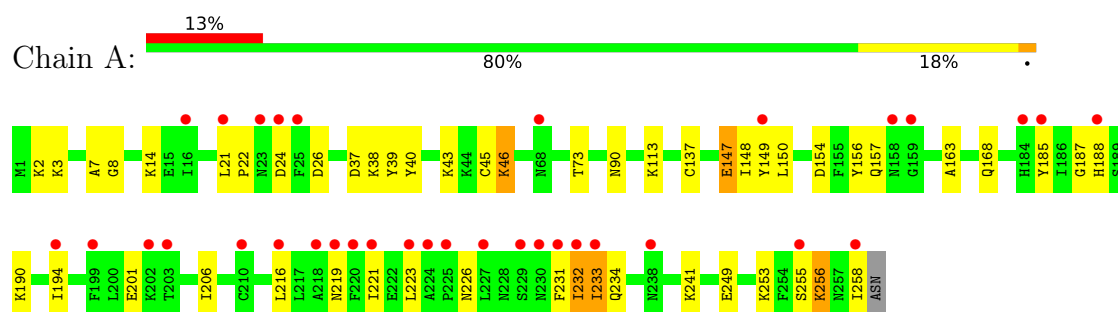
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	89	Total	O	0	0
			89	89		
4	B	85	Total	O	0	0
			85	85		
4	C	83	Total	O	0	0
			83	83		
4	D	73	Total	O	0	0
			73	73		

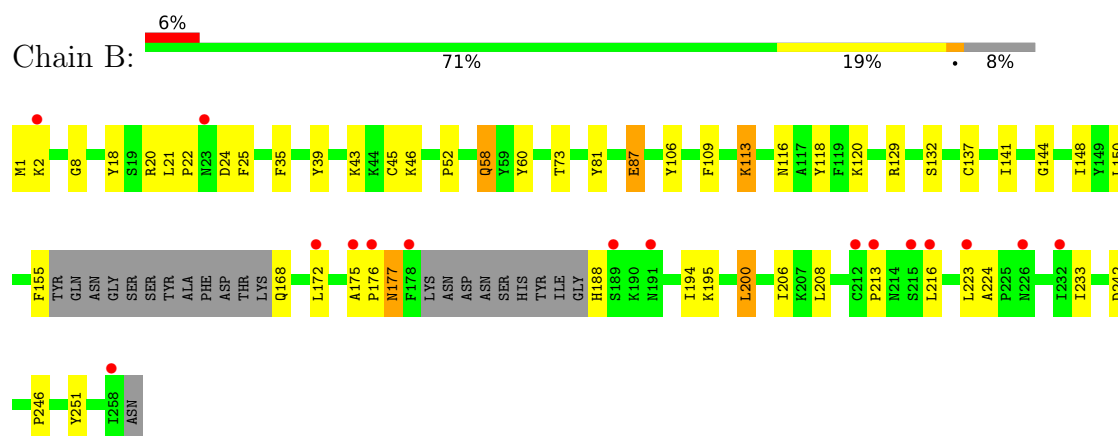
3 Residue-property plots [i](#)

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.

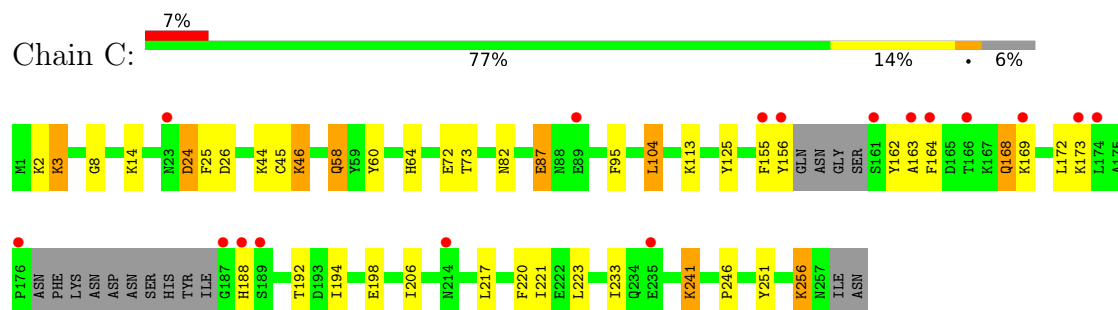
- Molecule 1: alpha-2,3/8-sialyltransferase



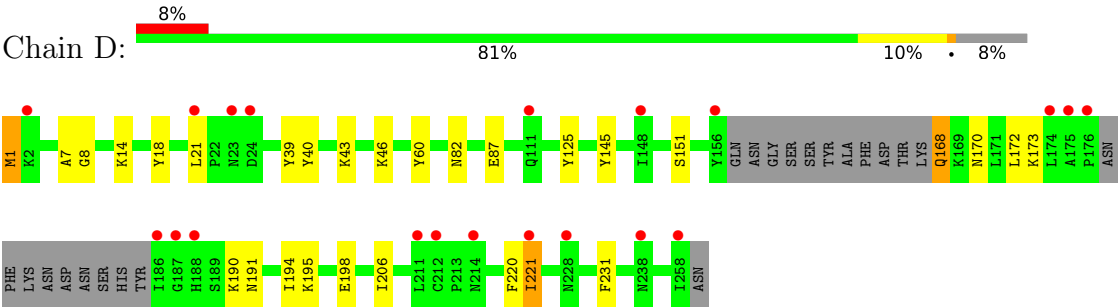
- Molecule 1: alpha-2,3/8-sialyltransferase



- Molecule 1: alpha-2,3/8-sialyltransferase



- Molecule 1: alpha-2,3/8-sialyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.66Å 66.03Å 99.17Å 90.00° 94.42° 90.00°	Depositor
Resolution (Å)	29.64 – 1.80 29.64 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.64-1.80) 99.6 (29.64-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 1.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.248 0.211 , 0.239	Depositor DCC
R_{free} test set	5034 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8668	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.34	0/2213	0.82	5/2982 (0.2%)
1	B	0.34	0/2036	0.82	2/2740 (0.1%)
1	C	0.35	0/2085	0.81	2/2806 (0.1%)
1	D	0.35	0/2041	0.83	2/2747 (0.1%)
All	All	0.34	0/8375	0.82	11/11275 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	8	GLY	N-CA-C	-8.23	100.07	112.41
1	C	8	GLY	N-CA-C	-8.17	100.16	112.41
1	B	8	GLY	N-CA-C	-7.60	100.97	112.60
1	A	8	GLY	N-CA-C	-7.03	101.87	112.41
1	C	46	LYS	N-CA-C	-6.37	103.86	111.69
1	D	46	LYS	N-CA-C	-6.35	103.88	111.69
1	B	46	LYS	N-CA-C	-6.15	104.13	111.69
1	A	255	SER	N-CA-C	6.11	118.72	111.33
1	A	46	LYS	N-CA-C	-5.50	104.93	111.69
1	A	148	ILE	N-CA-C	5.47	115.73	107.80
1	A	7	ALA	N-CA-C	5.03	117.11	108.90

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	2155	0	2087	41	0
1	B	1985	0	1938	40	0
1	C	2032	0	1976	39	0
1	D	1990	0	1946	22	0
2	B	8	0	14	0	0
3	C	168	0	112	6	0
4	A	89	0	0	0	0
4	B	85	0	0	0	0
4	C	83	0	0	3	0
4	D	73	0	0	0	0
All	All	8668	0	8073	141	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 (141) 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:C:256:LYS:HD2	1:C:256:LYS:H	1.40	0.86
1:C:44:LYS:HD2	1:C:72:GLU:HG3	1.62	0.82
1:C:14:LYS:HG3	1:C:163:ALA:HB1	1.62	0.81
1:D:168:GLN:HE21	1:D:168:GLN:N	1.82	0.76
1:A:154:ASP:HB3	1:A:157:GLN:HE21	1.51	0.75
1:C:14:LYS:HD2	1:C:163:ALA:O	1.87	0.74
1:B:1:MSE:HG3	1:B:144:GLY:O	1.89	0.73
1:C:246:PRO:HG2	1:C:251:TYR:CE1	2.25	0.71
1:A:256:LYS:NZ	1:A:256:LYS:H	1.88	0.70
1:A:14:LYS:HG3	1:A:163:ALA:HB1	1.73	0.69
1:C:194:ILE:O	1:C:198:GLU:HG3	1.93	0.69
1:B:118:TYR:OH	1:B:195:LYS:HG2	1.94	0.68
1:A:185:TYR:HB3	1:A:188:HIS:CD2	2.29	0.67
1:D:170:ASN:O	1:D:173:LYS:HG2	1.96	0.66
1:A:233:ILE:HD12	1:A:233:ILE:N	2.10	0.65
1:D:194:ILE:O	1:D:198:GLU:HG3	1.96	0.65
1:D:168:GLN:O	1:D:172:LEU:HD23	1.97	0.65
1:D:168:GLN:N	1:D:168:GLN:NE2	2.44	0.64
1:B:129:ARG:HH21	1:B:188:HIS:HE1	1.47	0.62
1:D:221:ILE:N	1:D:221:ILE:HD12	2.14	0.62
1:B:58:GLN:HA	1:B:58:GLN:HE21	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:HIS:O	1:C:192:THR:HB	2.00	0.61
1:C:155:PHE:CZ	1:C:194:ILE:HD11	2.35	0.61
1:A:2:LYS:HG2	1:A:24:ASP:OD2	2.01	0.60
1:D:14:LYS:HG2	1:D:40:TYR:CZ	2.36	0.60
1:A:256:LYS:H	1:A:256:LYS:HD2	1.64	0.60
1:A:190:LYS:HE2	1:A:216:LEU:HD21	1.82	0.60
1:A:256:LYS:H	1:A:256:LYS:HZ3	1.50	0.59
1:C:256:LYS:H	1:C:256:LYS:CD	2.14	0.59
1:D:39:TYR:CE2	1:D:43:LYS:HG2	2.38	0.59
1:A:231:PHE:O	1:A:232:ILE:HB	2.03	0.58
1:C:58:GLN:HE21	1:C:58:GLN:HA	1.68	0.58
1:C:241:LYS:HD3	4:C:4084:HOH:O	2.04	0.57
1:B:206:ILE:HD12	1:B:206:ILE:C	2.29	0.57
1:B:81:TYR:N	1:B:87:GLU:OE1	2.35	0.57
1:B:155:PHE:CZ	1:B:194:ILE:HD11	2.40	0.57
1:C:188:HIS:HA	4:C:4048:HOH:O	2.04	0.57
1:D:1:MSE:HB2	1:D:145:TYR:CE1	2.39	0.56
1:A:256:LYS:H	1:A:256:LYS:CD	2.19	0.56
1:B:18:TYR:CE2	1:B:233:ILE:HD11	2.39	0.56
1:B:2:LYS:HE2	1:B:25:PHE:C	2.30	0.56
1:A:206:ILE:C	1:A:206:ILE:HD12	2.31	0.56
1:B:35:PHE:CE2	1:B:168:GLN:HG2	2.40	0.56
1:A:216:LEU:HD12	1:A:219:ASN:HD22	1.71	0.55
1:A:37:ASP:OD2	1:A:38:LYS:HG3	2.07	0.55
1:C:2:LYS:HE2	1:C:25:PHE:C	2.32	0.55
1:B:2:LYS:HE3	1:B:24:ASP:CG	2.32	0.54
1:A:253:LYS:O	1:A:256:LYS:HE2	2.07	0.54
1:B:52:PRO:HG2	1:B:87:GLU:HG2	1.89	0.53
1:A:258:ILE:HG13	1:A:258:ILE:O	2.06	0.53
1:C:44:LYS:CD	1:C:72:GLU:HG3	2.38	0.53
3:C:3001:CSF:H3'	3:C:3001:CSF:O3A	2.09	0.52
1:D:206:ILE:C	1:D:206:ILE:HD12	2.33	0.52
1:D:170:ASN:HA	1:D:173:LYS:HE3	1.91	0.52
1:D:190:LYS:O	1:D:194:ILE:HG12	2.10	0.52
1:C:221:ILE:HD12	1:C:221:ILE:N	2.24	0.52
1:B:129:ARG:HH21	1:B:188:HIS:CE1	2.27	0.52
1:B:137:CYS:SG	1:B:150:LEU:HD21	2.50	0.52
1:C:241:LYS:O	1:C:241:LYS:HG2	2.10	0.51
1:D:191:ASN:HB3	1:D:195:LYS:NZ	2.24	0.51
1:A:39:TYR:CE2	1:A:43:LYS:HG2	2.45	0.51
1:B:206:ILE:HD12	1:B:206:ILE:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:LYS:HE3	1:C:24:ASP:OD1	2.10	0.51
1:A:256:LYS:HD2	1:A:256:LYS:N	2.26	0.50
1:D:220:PHE:HB2	1:D:221:ILE:HD12	1.93	0.50
1:A:14:LYS:HG2	1:A:40:TYR:CZ	2.46	0.50
1:A:21:LEU:HD12	1:A:22:PRO:HD2	1.94	0.50
1:A:233:ILE:HD12	1:A:233:ILE:H	1.74	0.50
1:A:256:LYS:NZ	1:A:256:LYS:N	2.59	0.50
1:A:201:GLU:HG3	1:A:206:ILE:O	2.11	0.49
1:A:45:CYS:O	1:A:73:THR:HA	2.12	0.49
1:A:185:TYR:CE1	1:A:187:GLY:HA3	2.47	0.49
1:C:156:TYR:OH	3:C:3001:CSF:H3A	2.13	0.49
1:C:156:TYR:HA	3:C:3001:CSF:H41	1.77	0.49
1:B:60:TYR:HB2	1:D:125:TYR:CE2	2.46	0.49
1:C:256:LYS:HD2	1:C:256:LYS:N	2.19	0.48
1:B:216:LEU:HD22	1:B:216:LEU:N	2.29	0.48
1:A:156:TYR:HA	3:C:1001:CSF:H41	1.77	0.48
1:C:206:ILE:C	1:C:206:ILE:HD12	2.39	0.48
1:B:177:ASN:ND2	1:B:177:ASN:C	2.72	0.47
1:C:168:GLN:O	1:C:172:LEU:HG	2.13	0.47
1:B:113:LYS:HB3	1:B:113:LYS:NZ	2.29	0.47
1:A:190:LYS:O	1:A:194:ILE:HG12	2.15	0.47
1:B:177:ASN:C	1:B:177:ASN:HD22	2.23	0.47
1:B:216:LEU:HD22	1:B:216:LEU:H	1.80	0.46
1:A:3:LYS:HE3	1:A:147:GLU:OE1	2.16	0.46
1:B:116:ASN:HD21	1:B:120:LYS:NZ	2.14	0.46
1:B:246:PRO:HG2	1:B:251:TYR:CE2	2.51	0.45
1:A:43:LYS:HE3	1:A:234:GLN:OE1	2.16	0.45
1:D:21:LEU:HD12	1:D:231:PHE:HB2	1.99	0.45
1:B:1:MSE:HA	1:B:1:MSE:HE2	1.98	0.45
1:A:216:LEU:HD12	1:A:219:ASN:ND2	2.32	0.45
1:B:21:LEU:HD12	1:B:22:PRO:HD2	1.99	0.45
1:B:168:GLN:HB3	1:B:242:ASP:OD2	2.17	0.45
1:D:190:LYS:HD3	1:D:220:PHE:CE2	2.52	0.45
1:A:221:ILE:HD12	1:A:221:ILE:N	2.32	0.45
1:C:162:TYR:C	1:C:164:PHE:H	2.26	0.44
1:B:141:ILE:HD12	1:B:200:LEU:HG	1.98	0.44
1:A:26:ASP:HB3	1:A:46:LYS:HB2	2.00	0.44
1:A:3:LYS:HD3	1:A:149:TYR:CE2	2.53	0.44
1:B:148:ILE:HB	1:B:208:LEU:HD23	1.99	0.44
1:C:217:LEU:CD1	1:C:221:ILE:HD13	2.48	0.44
1:B:39:TYR:CZ	1:B:43:LYS:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:TYR:CE2	1:C:64:HIS:HE1	2.36	0.43
1:D:7:ALA:HA	1:D:151:SER:O	2.18	0.43
1:B:168:GLN:O	1:B:172:LEU:HG	2.17	0.43
1:A:137:CYS:SG	1:A:150:LEU:HD21	2.59	0.43
1:A:223:LEU:HD12	1:A:223:LEU:N	2.33	0.43
1:C:95:PHE:CG	1:C:104:LEU:HD13	2.53	0.43
1:C:95:PHE:CD2	1:C:104:LEU:HD13	2.52	0.43
1:C:168:GLN:HE21	1:C:241:LYS:NZ	2.16	0.43
1:B:106:TYR:HA	1:B:109:PHE:HB3	2.01	0.43
1:C:3:LYS:H	1:C:3:LYS:HD2	1.84	0.43
1:B:45:CYS:O	1:B:73:THR:HA	2.18	0.43
1:C:82:ASN:N	1:C:87:GLU:OE1	2.52	0.42
1:C:45:CYS:O	1:C:73:THR:HA	2.19	0.42
1:B:2:LYS:HE2	1:B:25:PHE:O	2.18	0.42
1:C:113:LYS:HD2	4:C:4028:HOH:O	2.19	0.42
1:B:113:LYS:NZ	1:B:113:LYS:CB	2.83	0.42
1:B:213:PRO:HB3	1:B:223:LEU:HD21	2.02	0.42
1:A:39:TYR:CZ	1:A:43:LYS:HG2	2.54	0.42
1:B:216:LEU:H	1:B:216:LEU:CD2	2.33	0.41
1:A:156:TYR:HA	3:C:1001:CSF:N4	2.36	0.41
1:A:190:LYS:HE2	1:A:216:LEU:CD2	2.49	0.41
1:A:168:GLN:HG3	1:A:241:LYS:O	2.20	0.41
1:A:43:LYS:CE	1:A:234:GLN:HE22	2.34	0.41
1:C:26:ASP:HB3	1:C:46:LYS:HB2	2.03	0.41
1:C:104:LEU:HD12	1:C:104:LEU:HA	1.87	0.41
1:C:125:TYR:CE2	1:D:60:TYR:HB2	2.55	0.41
1:C:220:PHE:HB2	1:C:221:ILE:HD12	2.03	0.41
1:D:82:ASN:N	1:D:87:GLU:OE2	2.48	0.41
1:A:201:GLU:HA	1:A:206:ILE:CD1	2.51	0.41
1:B:20:ARG:HD3	1:B:224:ALA:O	2.21	0.41
1:C:233:ILE:N	1:C:233:ILE:HD12	2.36	0.40
1:D:39:TYR:CZ	1:D:43:LYS:HG2	2.56	0.40
1:B:35:PHE:CZ	1:B:168:GLN:HG2	2.57	0.40
1:C:168:GLN:HG2	1:C:241:LYS:O	2.22	0.40
1:D:18:TYR:HD2	1:D:21:LEU:HD11	1.85	0.40
1:B:132:SER:H	3:C:2001:CSF:HO3'	1.68	0.40
1:B:175:ALA:HA	1:B:176:PRO:HD2	1.96	0.40
1:C:169:LYS:O	1:C:173:LYS:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	256/259 (99%)	239 (93%)	15 (6%)	2 (1%)	16	6
1	B	231/259 (89%)	225 (97%)	6 (3%)	0	100	100
1	C	237/259 (92%)	229 (97%)	7 (3%)	1 (0%)	30	19
1	D	232/259 (90%)	225 (97%)	7 (3%)	0	100	100
All	All	956/1036 (92%)	918 (96%)	35 (4%)	3 (0%)	36	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	24	ASP
1	A	226	ASN
1	A	232	ILE

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	234/232 (101%)	228 (97%)	6 (3%)	40	28
1	B	216/232 (93%)	211 (98%)	5 (2%)	44	33
1	C	220/232 (95%)	212 (96%)	8 (4%)	31	18
1	D	216/232 (93%)	213 (99%)	3 (1%)	59	52
All	All	886/928 (96%)	864 (98%)	22 (2%)	42	30

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	113	LYS
1	A	147	GLU
1	A	233	ILE
1	A	249	GLU
1	A	256	LYS
1	B	58	GLN
1	B	87	GLU
1	B	113	LYS
1	B	177	ASN
1	B	200	LEU
1	C	3	LYS
1	C	58	GLN
1	C	87	GLU
1	C	104	LEU
1	C	168	GLN
1	C	223	LEU
1	C	241	LYS
1	C	256	LYS
1	D	1	MSE
1	D	168	GLN
1	D	221	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	58	GLN
1	A	67	GLN
1	A	69	GLN
1	A	128	GLN
1	A	157	GLN
1	A	158	ASN
1	A	177	ASN
1	A	180	ASN
1	A	219	ASN
1	A	257	ASN
1	B	32	GLN
1	B	51	ASN
1	B	69	GLN
1	B	111	GLN
1	B	116	ASN
1	B	177	ASN

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Mol	Chain	Res	Type
1	B	188	HIS
1	C	32	GLN
1	C	58	GLN
1	C	67	GLN
1	C	68	ASN
1	C	83	GLN
1	C	90	ASN
1	C	168	GLN
1	D	83	GLN
1	D	116	ASN
1	D	128	GLN
1	D	170	ASN
1	D	188	HIS
1	D	219	ASN
1	D	238	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 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	CSF	C	2001	-	42,44,44	2.35	15 (35%)	54,67,67	2.22	15 (27%)
3	CSF	C	1001	-	42,44,44	2.26	15 (35%)	54,67,67	2.12	14 (25%)
3	CSF	C	4001	-	42,44,44	2.37	17 (40%)	54,67,67	2.16	15 (27%)
3	CSF	C	3001	-	42,44,44	2.32	14 (33%)	54,67,67	2.30	16 (29%)
2	MPD	B	401	-	7,7,7	0.47	0	9,10,10	0.47	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	CSF	C	2001	-	1/1/14/15	3/30/75/75	0/3/3/3
3	CSF	C	1001	-	1/1/14/15	0/30/75/75	0/3/3/3
3	CSF	C	4001	-	1/1/14/15	2/30/75/75	0/3/3/3
3	CSF	C	3001	-	1/1/14/15	3/30/75/75	0/3/3/3
2	MPD	B	401	-	-	0/5/5/5	-

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2001	CSF	C3A-C4A	6.98	1.58	1.52
3	C	3001	CSF	C3A-C4A	6.75	1.58	1.52
3	C	4001	CSF	C3A-C4A	6.66	1.58	1.52
3	C	1001	CSF	C3A-C4A	6.07	1.58	1.52
3	C	2001	CSF	C2-N3	5.93	1.48	1.36
3	C	3001	CSF	C2-N3	5.72	1.47	1.36
3	C	4001	CSF	C2-N3	5.54	1.47	1.36
3	C	1001	CSF	C2-N3	5.47	1.47	1.36
3	C	4001	CSF	C5-C4	4.55	1.53	1.42
3	C	2001	CSF	C5-C4	4.22	1.52	1.42
3	C	1001	CSF	C5-C4	4.20	1.52	1.42
3	C	3001	CSF	C5-C4	4.06	1.52	1.42
3	C	1001	CSF	O1A-C2A	4.00	1.51	1.43
3	C	4001	CSF	C6-N1	3.81	1.47	1.38
3	C	3001	CSF	PA-O3A	-3.75	1.38	1.55
3	C	2001	CSF	C4-N3	3.67	1.41	1.34
3	C	2001	CSF	C6-N1	3.64	1.46	1.38
3	C	3001	CSF	C4-N3	3.63	1.41	1.34
3	C	4001	CSF	PA-O3A	-3.62	1.38	1.55
3	C	2001	CSF	PA-O3A	-3.57	1.38	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3001	CSF	C6-N1	3.56	1.46	1.38
3	C	1001	CSF	C6-N1	3.56	1.46	1.38
3	C	4001	CSF	C2-N1	3.52	1.47	1.40
3	C	1001	CSF	C4-N3	3.47	1.41	1.34
3	C	3001	CSF	O1A-C2A	3.36	1.50	1.43
3	C	4001	CSF	C4-N3	3.35	1.41	1.34
3	C	3001	CSF	C2-N1	3.34	1.47	1.40
3	C	3001	CSF	O2-C2	3.28	1.29	1.23
3	C	2001	CSF	O2-C2	3.25	1.29	1.23
3	C	2001	CSF	C2-N1	3.17	1.46	1.40
3	C	4001	CSF	O6A-C2A	3.16	1.46	1.41
3	C	1001	CSF	PA-O3A	-3.15	1.40	1.55
3	C	4001	CSF	C1'-N1	3.14	1.56	1.47
3	C	1001	CSF	C2-N1	3.00	1.46	1.40
3	C	1001	CSF	C1'-N1	3.00	1.56	1.47
3	C	4001	CSF	O2-C2	2.99	1.29	1.23
3	C	1001	CSF	O2-C2	2.98	1.29	1.23
3	C	4001	CSF	O1A-C2A	2.96	1.49	1.43
3	C	2001	CSF	C1'-N1	2.95	1.55	1.47
3	C	2001	CSF	O1A-C2A	2.89	1.49	1.43
3	C	2001	CSF	C6A-C5A	2.83	1.57	1.53
3	C	4001	CSF	C6-C5	2.78	1.41	1.35
3	C	3001	CSF	C1'-N1	2.75	1.55	1.47
3	C	1001	CSF	O6A-C2A	2.63	1.45	1.41
3	C	4001	CSF	C6A-C5A	2.55	1.57	1.53
3	C	2001	CSF	F3A-C3A	-2.42	1.36	1.40
3	C	3001	CSF	PA-O1A	2.39	1.66	1.59
3	C	2001	CSF	C6-C5	2.37	1.40	1.35
3	C	3001	CSF	C6A-C5A	2.31	1.56	1.53
3	C	3001	CSF	O6A-C2A	2.30	1.44	1.41
3	C	3001	CSF	C6-C5	2.29	1.40	1.35
3	C	1001	CSF	PA-O1A	2.29	1.66	1.59
3	C	1001	CSF	C5A-N5A	-2.26	1.42	1.45
3	C	4001	CSF	C5A-N5A	-2.24	1.42	1.45
3	C	1001	CSF	C6-C5	2.24	1.40	1.35
3	C	2001	CSF	PA-O1A	2.19	1.65	1.59
3	C	4001	CSF	PA-O1A	2.10	1.65	1.59
3	C	2001	CSF	O6A-C2A	2.06	1.44	1.41
3	C	1001	CSF	C8A-C7A	-2.04	1.49	1.53
3	C	4001	CSF	O6A-C6A	2.02	1.47	1.44
3	C	4001	CSF	O4'-C1'	2.02	1.46	1.42

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2001	CSF	C2A-O6A-C6A	8.85	125.59	114.17
3	C	3001	CSF	C2A-O6A-C6A	8.84	125.59	114.17
3	C	4001	CSF	C2A-O6A-C6A	8.68	125.38	114.17
3	C	1001	CSF	C2A-O6A-C6A	8.43	125.06	114.17
3	C	2001	CSF	O6A-C6A-C7A	-5.62	97.89	106.65
3	C	3001	CSF	O6A-C6A-C7A	-5.53	98.03	106.65
3	C	1001	CSF	O6A-C6A-C7A	-5.11	98.68	106.65
3	C	4001	CSF	O6A-C6A-C7A	-4.89	99.03	106.65
3	C	4001	CSF	O6A-C2A-C1A	4.82	124.92	107.67
3	C	3001	CSF	O6A-C2A-C1A	4.81	124.88	107.67
3	C	2001	CSF	O6A-C2A-C1A	4.61	124.19	107.67
3	C	1001	CSF	O6A-C2A-C1A	4.54	123.94	107.67
3	C	3001	CSF	O5'-C5'-C4'	4.53	124.43	108.99
3	C	4001	CSF	C8A-C7A-C6A	4.40	121.32	113.05
3	C	1001	CSF	C8A-C7A-C6A	4.39	121.30	113.05
3	C	3001	CSF	C3A-C4A-C5A	4.35	114.96	109.87
3	C	4001	CSF	C3A-C4A-C5A	4.30	114.91	109.87
3	C	2001	CSF	C8A-C7A-C6A	4.18	120.91	113.05
3	C	2001	CSF	C3A-C4A-C5A	3.96	114.51	109.87
3	C	3001	CSF	C8A-C7A-C6A	3.83	120.25	113.05
3	C	1001	CSF	C3A-C4A-C5A	3.16	113.57	109.87
3	C	1001	CSF	C4A-C5A-N5A	3.07	116.28	110.62
3	C	2001	CSF	C4A-C5A-N5A	2.97	116.09	110.62
3	C	3001	CSF	O1A-PA-O2A	2.93	118.70	109.64
3	C	2001	CSF	O8A-C8A-C9A	-2.79	102.68	109.03
3	C	3001	CSF	C4A-C5A-N5A	2.77	115.72	110.62
3	C	1001	CSF	O6A-C6A-C5A	2.77	112.38	109.84
3	C	3001	CSF	O6A-C6A-C5A	2.77	112.38	109.84
3	C	4001	CSF	O8A-C8A-C9A	-2.71	102.88	109.03
3	C	3001	CSF	C5A-N5A-C10	2.68	129.39	123.11
3	C	3001	CSF	O8A-C8A-C9A	-2.65	103.00	109.03
3	C	4001	CSF	C5A-N5A-C10	2.59	129.18	123.11
3	C	4001	CSF	C4A-C5A-N5A	2.59	115.39	110.62
3	C	1001	CSF	O8A-C8A-C9A	-2.58	103.16	109.03
3	C	1001	CSF	C5A-N5A-C10	2.52	129.00	123.11
3	C	2001	CSF	C3'-C2'-C1'	2.51	106.21	101.46
3	C	1001	CSF	C6A-C5A-N5A	-2.51	106.91	110.91
3	C	3001	CSF	O2-C2-N1	2.39	123.58	118.90
3	C	4001	CSF	O2-C2-N1	2.38	123.56	118.90
3	C	3001	CSF	O3A-PA-O2A	-2.36	101.47	112.44
3	C	2001	CSF	C5A-N5A-C10	2.35	128.62	123.11
3	C	2001	CSF	O5'-PA-O2A	-2.25	100.01	108.94
3	C	2001	CSF	C2'-C1'-N1	2.23	119.46	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1001	CSF	O2-C2-N1	2.22	123.25	118.90
3	C	2001	CSF	O2-C2-N1	2.20	123.20	118.90
3	C	2001	CSF	O6A-C6A-C5A	2.19	111.85	109.84
3	C	4001	CSF	O5'-PA-O2A	-2.19	100.27	108.94
3	C	2001	CSF	C6A-C5A-N5A	-2.18	107.42	110.91
3	C	4001	CSF	O4A-C4A-C5A	-2.18	105.25	109.58
3	C	2001	CSF	C9A-C8A-C7A	2.17	116.60	112.17
3	C	1001	CSF	C3'-C2'-C1'	2.14	105.52	101.46
3	C	4001	CSF	C6A-C5A-N5A	-2.13	107.50	110.91
3	C	1001	CSF	O4A-C4A-C5A	-2.12	105.37	109.58
3	C	1001	CSF	O5'-PA-O2A	-2.11	100.58	108.94
3	C	3001	CSF	C6A-C5A-N5A	-2.11	107.54	110.91
3	C	4001	CSF	C9A-C8A-C7A	2.10	116.45	112.17
3	C	4001	CSF	O6A-C6A-C5A	2.07	111.74	109.84
3	C	4001	CSF	O5'-C5'-C4'	2.07	116.03	108.99
3	C	3001	CSF	C2'-C1'-N1	2.06	118.98	113.25
3	C	3001	CSF	O4A-C4A-C5A	-2.02	105.57	109.58

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	1001	CSF	C2A
3	C	2001	CSF	C2A
3	C	3001	CSF	C2A
3	C	4001	CSF	C2A

All (8) torsion outliers are listed below:

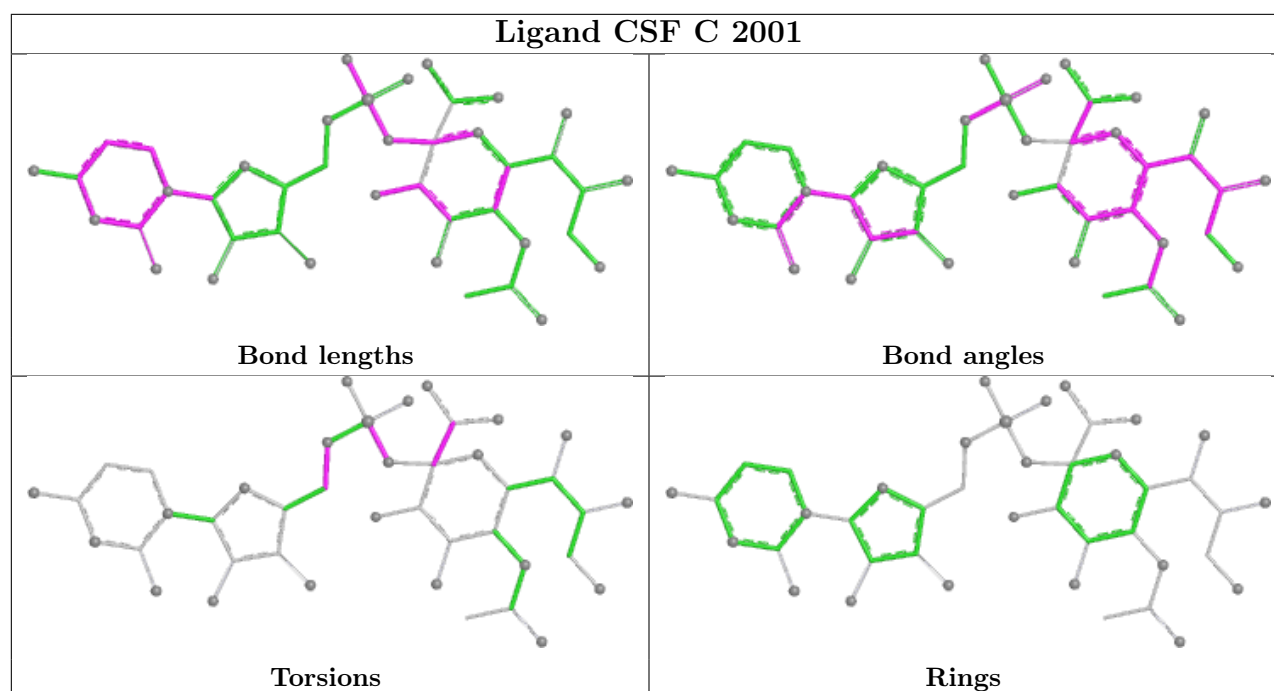
Mol	Chain	Res	Type	Atoms
3	C	2001	CSF	OAA-C1A-C2A-C3A
3	C	3001	CSF	OAA-C1A-C2A-C3A
3	C	3001	CSF	C4'-C5'-O5'-PA
3	C	4001	CSF	C7A-C8A-C9A-O9A
3	C	4001	CSF	O8A-C8A-C9A-O9A
3	C	3001	CSF	OAA-C1A-C2A-O6A
3	C	2001	CSF	C2A-O1A-PA-O2A
3	C	2001	CSF	C4'-C5'-O5'-PA

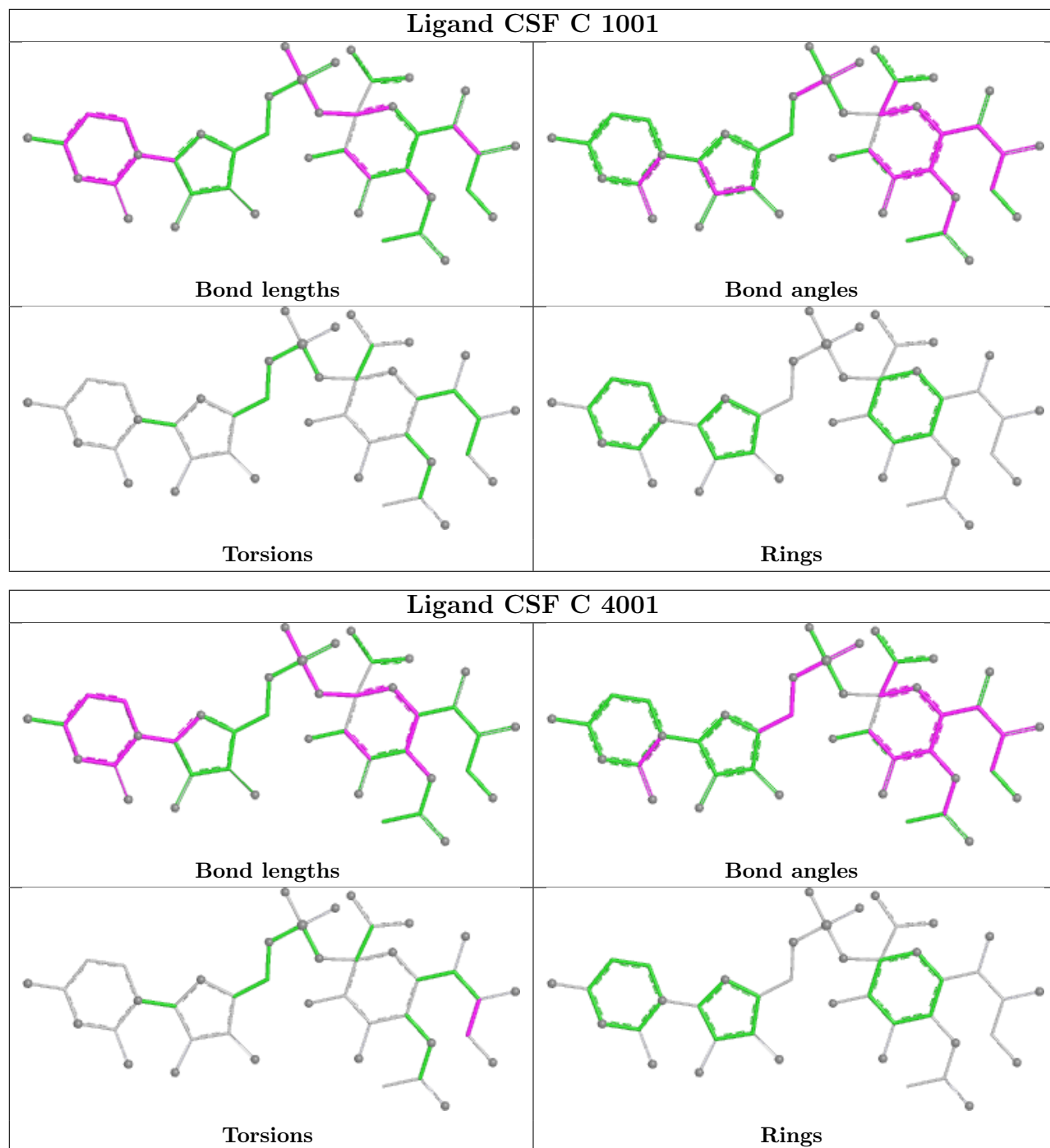
There are no ring outliers.

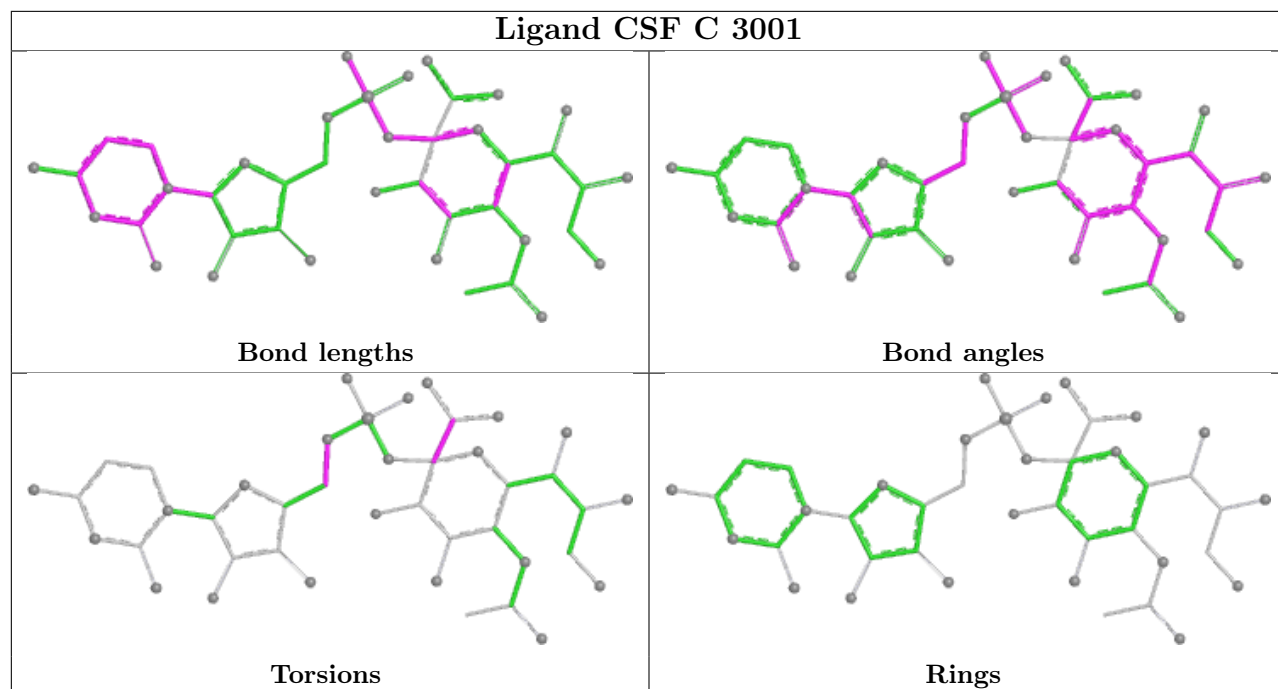
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2001	CSF	1	0
3	C	1001	CSF	2	0
3	C	3001	CSF	3	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

6.1 Protein, DNA and RNA chains

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	255/259 (98%)	0.75	34 (13%) 7 6	17, 34, 63, 77	0
1	B	234/259 (90%)	0.38	16 (6%) 23 22	18, 29, 51, 63	0
1	C	240/259 (92%)	0.49	17 (7%) 22 20	21, 30, 56, 73	0
1	D	235/259 (90%)	0.56	20 (8%) 16 14	20, 32, 53, 65	0
All	All	964/1036 (93%)	0.55	87 (9%) 15 13	17, 31, 57, 77	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	156	TYR	7.0
1	A	258	ILE	6.0
1	D	186	ILE	4.9
1	C	163	ALA	4.5
1	A	231	PHE	4.4
1	C	187	GLY	4.3
1	A	221	ILE	4.2
1	A	232	ILE	4.1
1	C	156	TYR	4.1
1	A	229	SER	4.0
1	B	191	ASN	4.0
1	D	176	PRO	4.0
1	D	238	ASN	3.9
1	A	218	ALA	3.9
1	A	223	LEU	3.8
1	C	188	HIS	3.8
1	B	178	PHE	3.8
1	A	220	PHE	3.6
1	C	164	PHE	3.6
1	B	23	ASN	3.6
1	A	224	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	158	ASN	3.5
1	A	233	ILE	3.5
1	A	184	HIS	3.4
1	D	2	LYS	3.4
1	B	176	PRO	3.4
1	D	23	ASN	3.3
1	B	212	CYS	3.3
1	C	169	LYS	3.2
1	A	23	ASN	3.1
1	D	21	LEU	3.0
1	A	230	ASN	3.0
1	A	219	ASN	3.0
1	C	166	THR	3.0
1	D	214	ASN	2.9
1	D	258	ILE	2.8
1	C	161	SER	2.8
1	A	185	TYR	2.7
1	C	173	LYS	2.7
1	B	232	ILE	2.7
1	D	188	HIS	2.7
1	D	175	ALA	2.6
1	D	187	GLY	2.6
1	C	155	PHE	2.6
1	A	227	LEU	2.5
1	D	221	ILE	2.5
1	B	189	SER	2.5
1	C	176	PRO	2.5
1	D	212	CYS	2.4
1	B	172	LEU	2.4
1	B	2	LYS	2.4
1	A	159	GLY	2.4
1	A	194	ILE	2.4
1	B	175	ALA	2.3
1	D	148	ILE	2.3
1	B	223	LEU	2.3
1	C	174	LEU	2.3
1	D	111	GLN	2.3
1	A	68	ASN	2.3
1	A	225	PRO	2.3
1	A	199	PHE	2.2
1	A	238	ASN	2.2
1	A	203	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	211	LEU	2.2
1	C	214	ASN	2.2
1	C	89	GLU	2.2
1	C	235	GLU	2.2
1	B	215	SER	2.2
1	C	189	SER	2.2
1	D	174	LEU	2.2
1	B	258	ILE	2.1
1	D	24	ASP	2.1
1	A	202	LYS	2.1
1	B	213	PRO	2.1
1	B	226	ASN	2.1
1	A	188	HIS	2.1
1	A	216	LEU	2.1
1	B	216	LEU	2.1
1	A	16	ILE	2.1
1	A	24	ASP	2.1
1	C	23	ASN	2.1
1	A	210	CYS	2.1
1	A	25	PHE	2.0
1	A	149	TYR	2.0
1	A	21	LEU	2.0
1	A	255	SER	2.0
1	D	228	ASN	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](#)

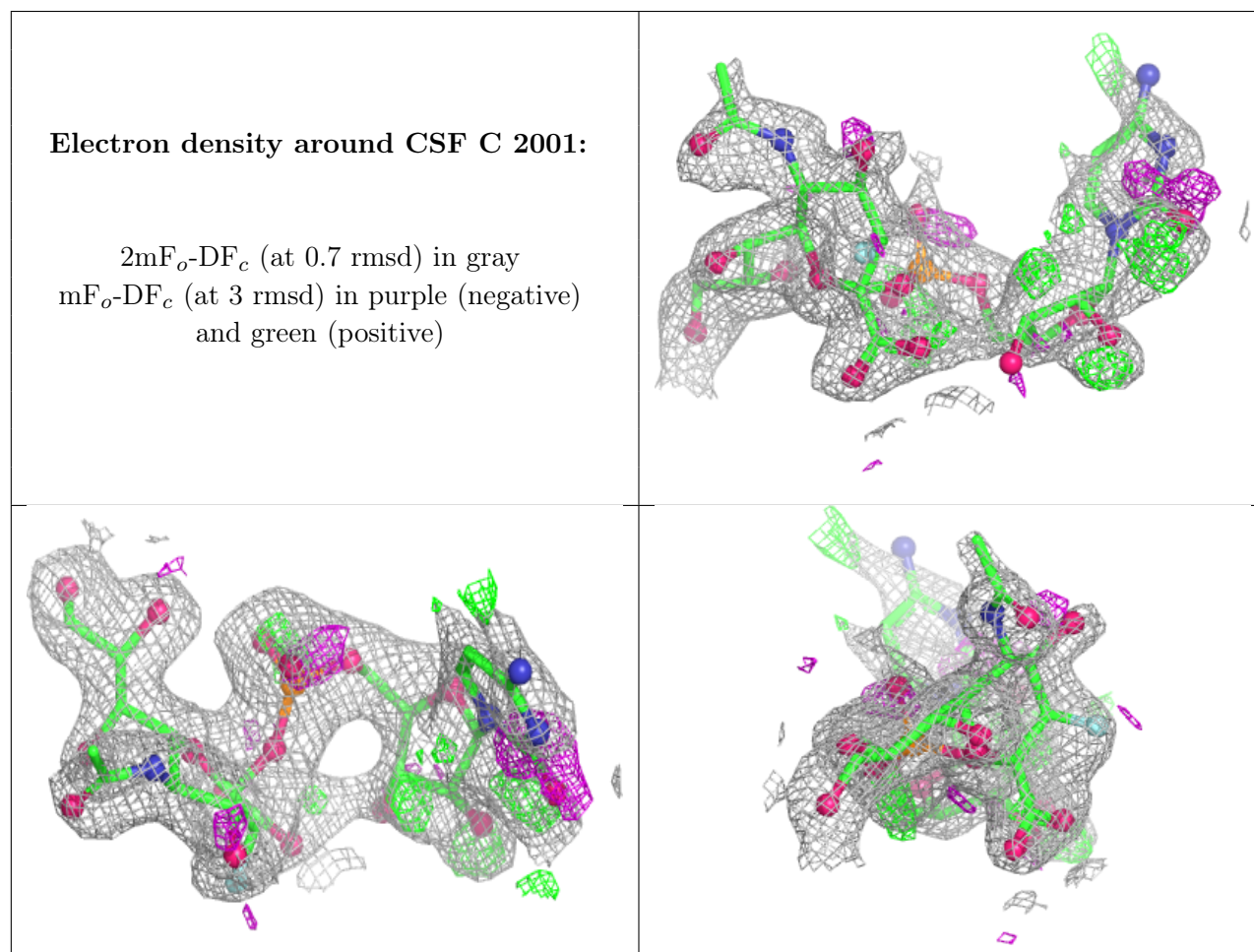
There are no oligosaccharides in this entry.

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.

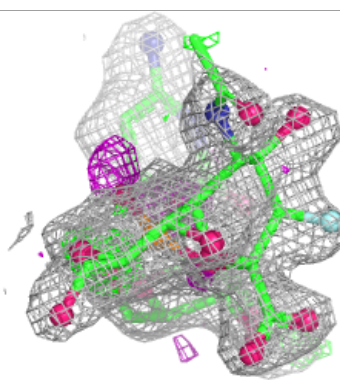
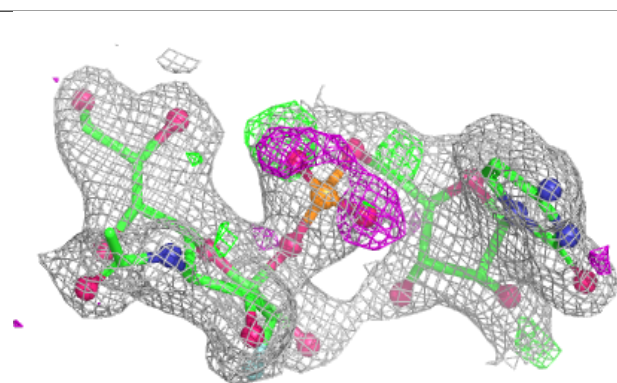
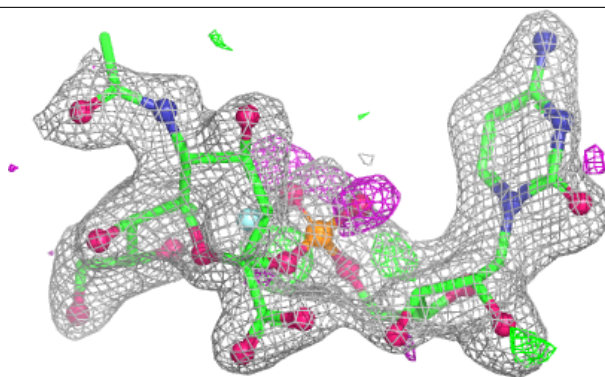
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MPD	B	401	8/8	0.80	0.18	40,46,47,48	0
3	CSF	C	2001	42/42	0.82	0.16	39,49,60,61	0
3	CSF	C	3001	42/42	0.83	0.14	36,43,48,49	0
3	CSF	C	4001	42/42	0.86	0.12	37,41,45,49	0
3	CSF	C	1001	42/42	0.93	0.09	21,29,37,40	0

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.



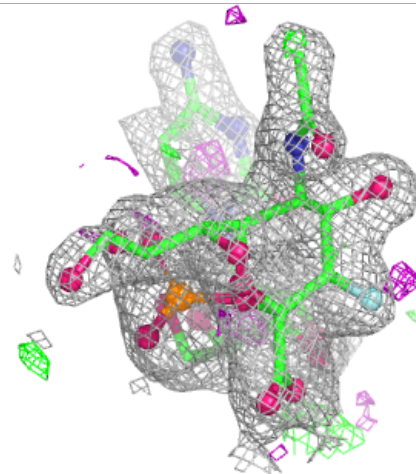
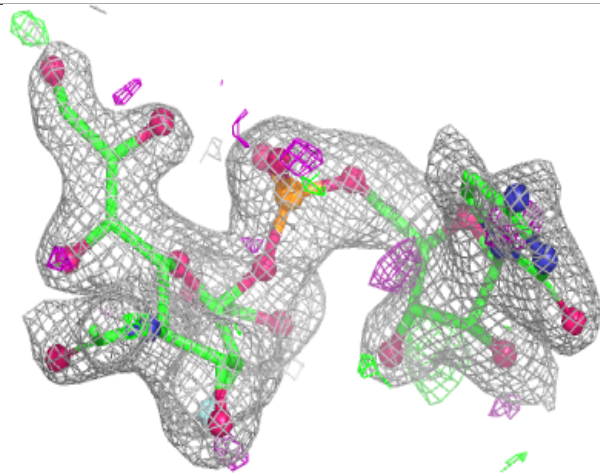
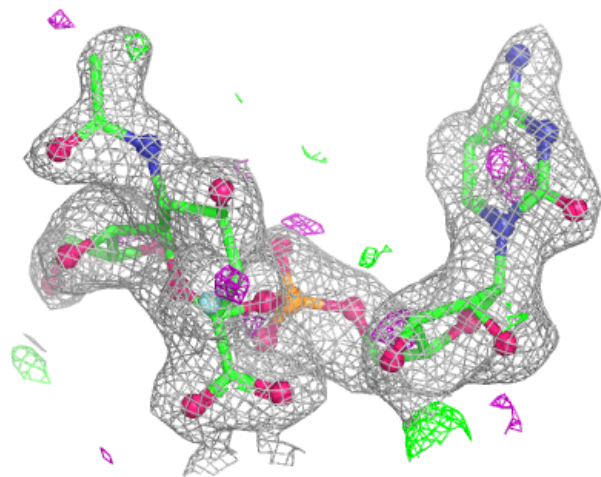
Electron density around CSF C 3001:

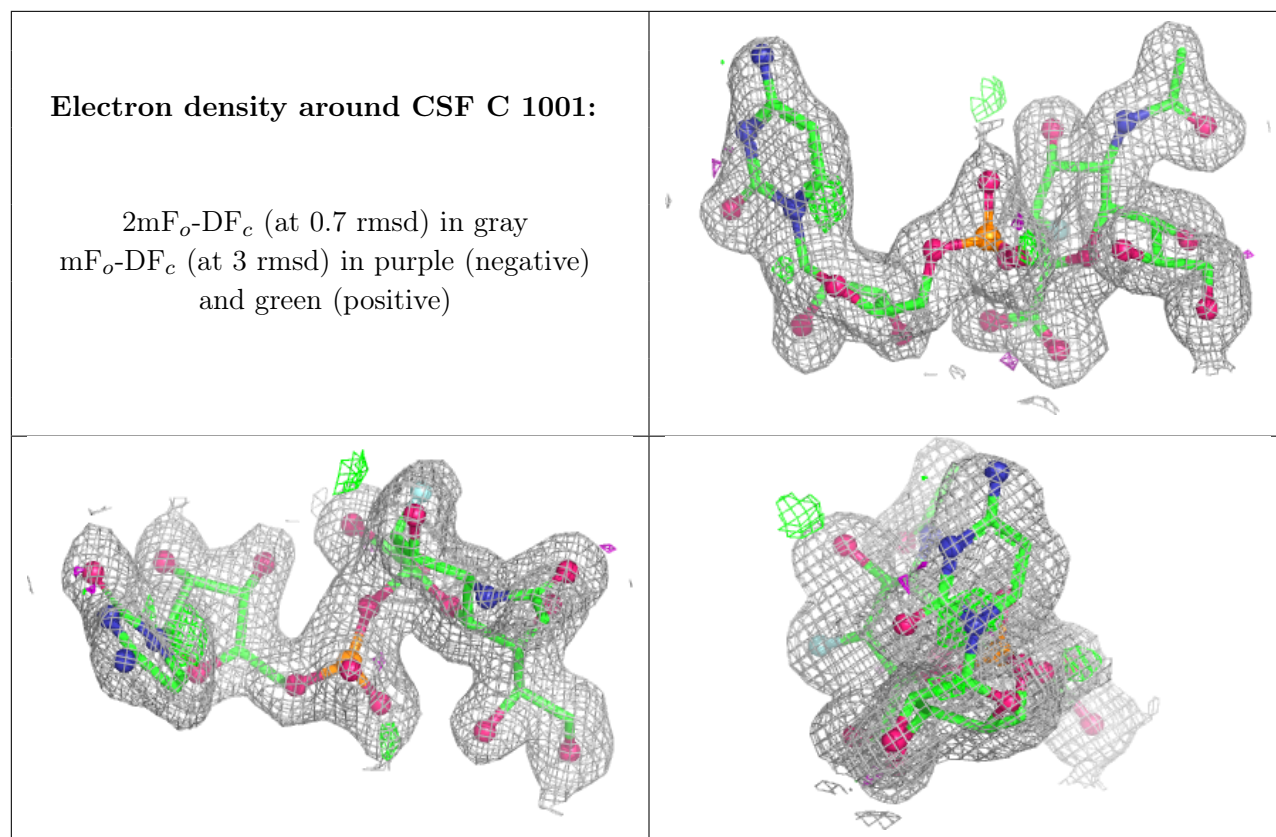
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CSF C 4001:

$2mF_o-DF_c$ (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.