Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:36 pm BST

PDB ID	:	6CBO
Title	:	X-ray structure of GenB1 from micromonospora echinospora in complex with neamine and PLP (as the external aldimine)
Authors	:	Dow, G.T.; Thoden, J.B.; Holden, H.M.
Deposited on	:	2018-02-03
Resolution	:	1.60 Å(reported)

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

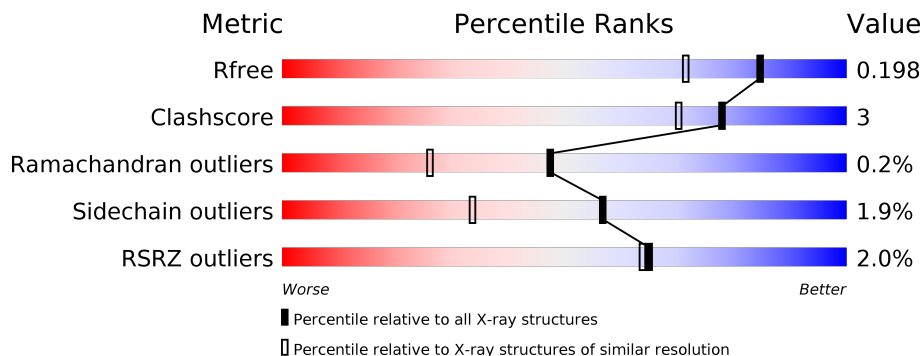|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.60 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	Percentile Ranks	Value
Rfree		0.198
Clashscore		3
Ramachandran outliers		0.2%
Sidechain outliers		1.9%
RSRZ outliers		2.0%

Worse　　　　　*Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	439	% — 86% 8% 7%
1	B	439	2% — 87% 5% · 7%
1	C	439	3% — 85% 8% · 6%
1	D	439	% — 89% · 7%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14374 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 C-6' aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total 3132	C 1962	N 554	O 604	S 12	0	5	0
1	B	408	Total 3132	C 1963	N 556	O 601	S 12	0	6	0
1	C	411	Total 3138	C 1964	N 554	O 608	S 12	0	4	0
1	D	409	Total 3145	C 1971	N 553	O 609	S 12	0	7	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q70KD9
A	-20	GLY	-	expression tag	UNP Q70KD9
A	-19	SER	-	expression tag	UNP Q70KD9
A	-18	SER	-	expression tag	UNP Q70KD9
A	-17	HIS	-	expression tag	UNP Q70KD9
A	-16	HIS	-	expression tag	UNP Q70KD9
A	-15	HIS	-	expression tag	UNP Q70KD9
A	-14	HIS	-	expression tag	UNP Q70KD9
A	-13	HIS	-	expression tag	UNP Q70KD9
A	-12	HIS	-	expression tag	UNP Q70KD9
A	-11	SER	-	expression tag	UNP Q70KD9
A	-10	SER	-	expression tag	UNP Q70KD9
A	-9	GLU	-	expression tag	UNP Q70KD9
A	-8	ASN	-	expression tag	UNP Q70KD9
A	-7	LEU	-	expression tag	UNP Q70KD9
A	-6	TYR	-	expression tag	UNP Q70KD9
A	-5	PHE	-	expression tag	UNP Q70KD9
A	-4	GLN	-	expression tag	UNP Q70KD9
A	-3	GLY	-	expression tag	UNP Q70KD9
A	-2	GLY	-	expression tag	UNP Q70KD9
A	-1	GLY	-	expression tag	UNP Q70KD9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP Q70KD9
B	-21	MET	-	initiating methionine	UNP Q70KD9
B	-20	GLY	-	expression tag	UNP Q70KD9
B	-19	SER	-	expression tag	UNP Q70KD9
B	-18	SER	-	expression tag	UNP Q70KD9
B	-17	HIS	-	expression tag	UNP Q70KD9
B	-16	HIS	-	expression tag	UNP Q70KD9
B	-15	HIS	-	expression tag	UNP Q70KD9
B	-14	HIS	-	expression tag	UNP Q70KD9
B	-13	HIS	-	expression tag	UNP Q70KD9
B	-12	HIS	-	expression tag	UNP Q70KD9
B	-11	SER	-	expression tag	UNP Q70KD9
B	-10	SER	-	expression tag	UNP Q70KD9
B	-9	GLU	-	expression tag	UNP Q70KD9
B	-8	ASN	-	expression tag	UNP Q70KD9
B	-7	LEU	-	expression tag	UNP Q70KD9
B	-6	TYR	-	expression tag	UNP Q70KD9
B	-5	PHE	-	expression tag	UNP Q70KD9
B	-4	GLN	-	expression tag	UNP Q70KD9
B	-3	GLY	-	expression tag	UNP Q70KD9
B	-2	GLY	-	expression tag	UNP Q70KD9
B	-1	GLY	-	expression tag	UNP Q70KD9
B	0	HIS	-	expression tag	UNP Q70KD9
C	-21	MET	-	initiating methionine	UNP Q70KD9
C	-20	GLY	-	expression tag	UNP Q70KD9
C	-19	SER	-	expression tag	UNP Q70KD9
C	-18	SER	-	expression tag	UNP Q70KD9
C	-17	HIS	-	expression tag	UNP Q70KD9
C	-16	HIS	-	expression tag	UNP Q70KD9
C	-15	HIS	-	expression tag	UNP Q70KD9
C	-14	HIS	-	expression tag	UNP Q70KD9
C	-13	HIS	-	expression tag	UNP Q70KD9
C	-12	HIS	-	expression tag	UNP Q70KD9
C	-11	SER	-	expression tag	UNP Q70KD9
C	-10	SER	-	expression tag	UNP Q70KD9
C	-9	GLU	-	expression tag	UNP Q70KD9
C	-8	ASN	-	expression tag	UNP Q70KD9
C	-7	LEU	-	expression tag	UNP Q70KD9
C	-6	TYR	-	expression tag	UNP Q70KD9
C	-5	PHE	-	expression tag	UNP Q70KD9
C	-4	GLN	-	expression tag	UNP Q70KD9
C	-3	GLY	-	expression tag	UNP Q70KD9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP Q70KD9
C	-1	GLY	-	expression tag	UNP Q70KD9
C	0	HIS	-	expression tag	UNP Q70KD9
D	-21	MET	-	initiating methionine	UNP Q70KD9
D	-20	GLY	-	expression tag	UNP Q70KD9
D	-19	SER	-	expression tag	UNP Q70KD9
D	-18	SER	-	expression tag	UNP Q70KD9
D	-17	HIS	-	expression tag	UNP Q70KD9
D	-16	HIS	-	expression tag	UNP Q70KD9
D	-15	HIS	-	expression tag	UNP Q70KD9
D	-14	HIS	-	expression tag	UNP Q70KD9
D	-13	HIS	-	expression tag	UNP Q70KD9
D	-12	HIS	-	expression tag	UNP Q70KD9
D	-11	SER	-	expression tag	UNP Q70KD9
D	-10	SER	-	expression tag	UNP Q70KD9
D	-9	GLU	-	expression tag	UNP Q70KD9
D	-8	ASN	-	expression tag	UNP Q70KD9
D	-7	LEU	-	expression tag	UNP Q70KD9
D	-6	TYR	-	expression tag	UNP Q70KD9
D	-5	PHE	-	expression tag	UNP Q70KD9
D	-4	GLN	-	expression tag	UNP Q70KD9
D	-3	GLY	-	expression tag	UNP Q70KD9
D	-2	GLY	-	expression tag	UNP Q70KD9
D	-1	GLY	-	expression tag	UNP Q70KD9
D	0	HIS	-	expression tag	UNP Q70KD9

- Molecule 2 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: $C_7H_{15}NO_4S$).

MPO
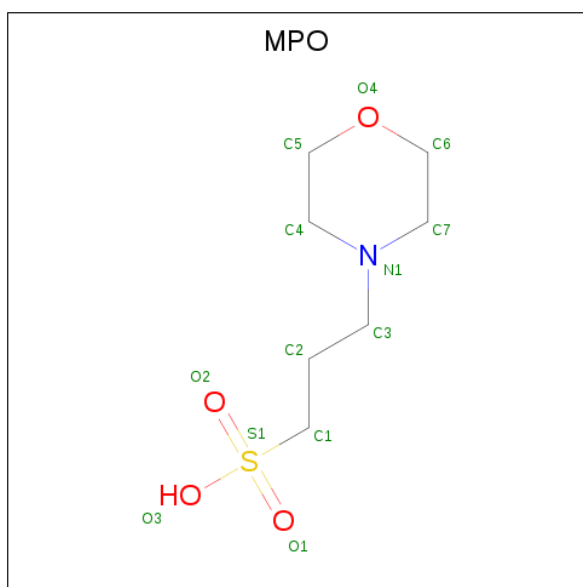
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO
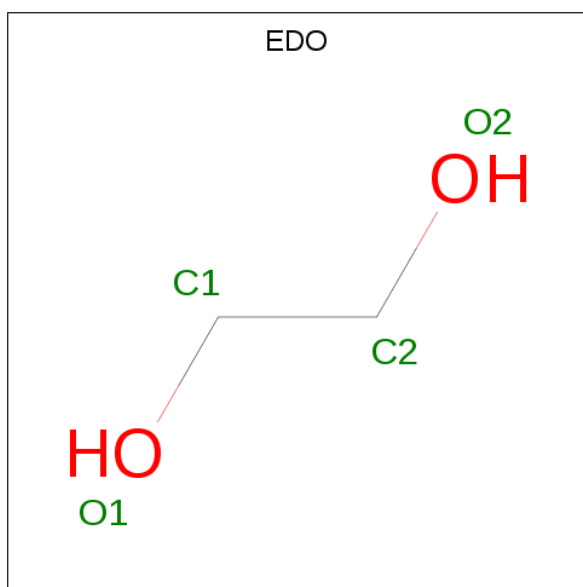
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0

- Molecule 4 is (1R,2R,3S,4R,6S)-4,6-diamino-2,3-dihydroxycyclohexyl 2-amino-2,6-dideoxy-6 -[({3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methyl)amino]-alpha-D-gluc opyranoside (three-letter code: DOW) (formula: $C_{20}H_{36}N_5O_{11}P$).
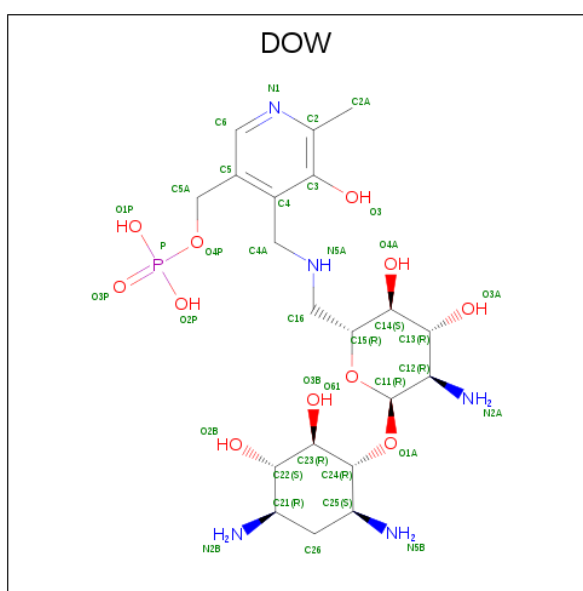
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 37	C 20	N 5	O 11	P 1	0	0
4	B	1	Total 37	C 20	N 5	O 11	P 1	0	0
4	C	1	Total 37	C 20	N 5	O 11	P 1	0	0
4	D	1	Total 37	C 20	N 5	O 11	P 1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
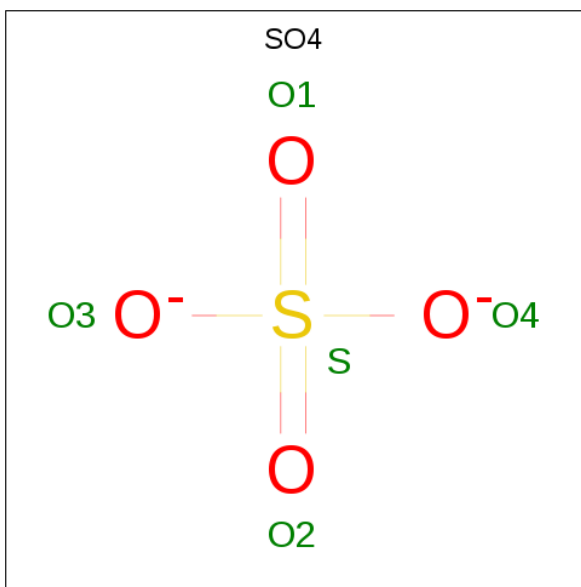
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total 5	O 4	S 1	0	0
5	D	1	Total 5	O 4	S 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	416	Total 416	O 416	0	0
6	B	381	Total 381	O 381	0	0
6	C	420	Total 420	O 420	0	0
6	D	397	Total 397	O 397	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: C-6' aminotransferase

Chain A:

- Molecule 1: C-6' aminotransferase

Chain B:

- Molecule 1: C-6' aminotransferase

Chain C:

- Molecule 1: C-6' aminotransferase

Chain D:

F353 R367 T377 D378 R379 E380 P401 R404 W415 GLU ASP
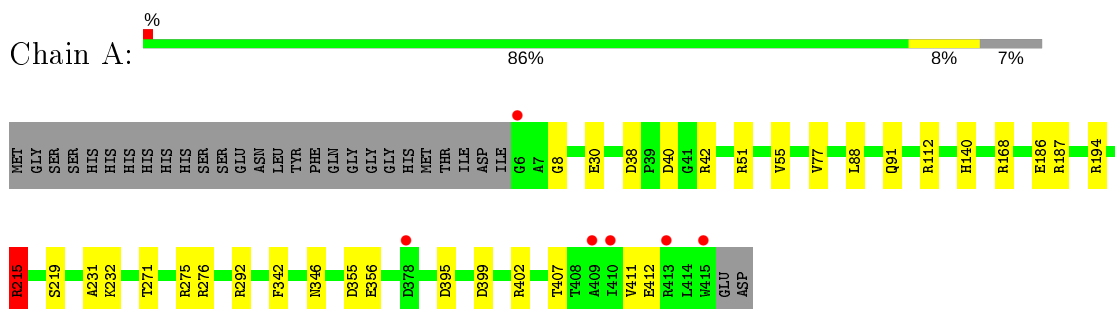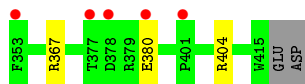
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.89Å 59.98Å 210.69Å 90.00° 95.19° 90.00°	Depositor
Resolution (Å)	50.00 – 1.60 31.52 – 1.60	Depositor EDS
% Data completeness (in resolution range)	92.2 (50.00-1.60) 92.2 (31.52-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$<I/\sigma(I)>$ [1]	12.84 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.155 , 0.188 0.168 , 0.198	Depositor DCC
R_{free} test set	10040 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	12.4	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 60.6	EDS
L-test for twinning[2]	$<\|L\|> = 0.45, <L^2> = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14374	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: MPO, EDO, DOW, 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	0.55	0/3217	0.89	8/4386 (0.2%)
1	B	0.54	0/3221	0.94	9/4391 (0.2%)
1	C	0.58	0/3220	0.92	9/4391 (0.2%)
1	D	0.56	0/3237	0.92	8/4413 (0.2%)
All	All	0.56	0/12895	0.92	34/17581 (0.2%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	287	ARG	NE-CZ-NH2	-12.75	113.92	120.30
1	A	276	ARG	NE-CZ-NH1	-9.01	115.80	120.30
1	D	276	ARG	NE-CZ-NH1	-8.96	115.82	120.30
1	D	309	ASP	CB-CG-OD1	8.42	125.87	118.30
1	B	287	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	C	287	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	D	287	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	C	24	ARG	NE-CZ-NH1	-7.40	116.60	120.30
1	B	267	MET	CA-CB-CG	-6.83	101.69	113.30
1	A	112	ARG	NE-CZ-NH2	6.23	123.42	120.30
1	B	119	ARG	NE-CZ-NH1	-6.21	117.20	120.30
1	B	360	ASP	CB-CG-OD1	6.05	123.75	118.30
1	C	404	ARG	NE-CZ-NH2	5.89	123.24	120.30
1	C	292	ARG	NE-CZ-NH2	5.87	123.23	120.30
1	C	24	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	B	119	ARG	NE-CZ-NH2	5.83	123.21	120.30
1	D	72	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	42	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	112	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	B	168	ARG	NE-CZ-NH2	5.42	123.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	168	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	215	ARG	NE-CZ-NH2	5.25	122.93	120.30
1	A	399	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	D	276	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	D	309	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	C	276	ARG	CA-CB-CG	-5.17	102.02	113.40
1	B	69	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	168	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	C	215	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	C	287	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	48	ASP	CB-CG-OD1	5.09	122.88	118.30
1	D	367	ARG	NE-CZ-NH2	5.07	122.84	120.30
1	D	112	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	A	38	ASP	CB-CG-OD2	-5.02	113.79	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3132	0	3017	22	0
1	B	3132	0	3021	19	0
1	C	3138	0	3014	25	1
1	D	3145	0	3021	6	1
2	A	13	0	15	3	0
2	B	13	0	14	0	0
2	C	13	0	14	2	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
3	C	4	0	6	0	0
3	D	4	0	6	0	0
4	A	37	0	0	3	0
4	B	37	0	0	0	0
4	C	37	0	0	0	0
4	D	37	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	10	0	0	0	0
6	A	416	0	0	6	0
6	B	381	0	0	5	0
6	C	420	0	0	4	1
6	D	397	0	0	2	1
All	All	14374	0	12140	71	2

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 3.

All (71) 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:91:GLN:HE22	1:B:271[B]:THR:HG23	1.14	1.10
1:B:84:VAL:HG23	6:B:826:HOH:O	1.53	1.06
1:C:91:GLN:HE22	1:C:271[B]:THR:HG23	1.24	0.98
1:B:91:GLN:NE2	1:B:271[B]:THR:HG23	1.82	0.94
1:C:91:GLN:NE2	1:C:271[B]:THR:HG23	1.89	0.86
1:B:55:VAL:HG22	6:B:841:HOH:O	1.76	0.85
1:B:221:PRO:HD3	6:B:880:HOH:O	1.75	0.84
1:C:373[A]:THR:HG21	6:C:742:HOH:O	1.77	0.83
1:B:186:GLU:HG2	6:B:848:HOH:O	1.80	0.81
1:C:304:ALA:HB1	1:C:373[A]:THR:HG22	1.64	0.80
1:A:232:LYS:NZ	4:A:503:DOW:N5A	2.29	0.80
1:D:7:ALA:N	6:D:601:HOH:O	2.21	0.73
1:B:91:GLN:OE1	1:B:275[B]:ARG:HG3	1.88	0.72
1:A:395:ASP:OD1	6:A:602:HOH:O	2.09	0.70
1:B:271[B]:THR:HG22	1:B:275[B]:ARG:CZ	2.23	0.69
1:C:220:THR:HG22	1:C:222:LEU:H	1.59	0.67
1:C:304:ALA:HB1	1:C:373[A]:THR:CG2	2.25	0.66
1:A:232:LYS:HZ1	4:A:503:DOW:C4A	2.08	0.66
1:A:8:GLY:O	2:A:501:MPO:C3	2.44	0.66
1:A:91[A]:GLN:OE1	1:A:271[A]:THR:HG23	1.95	0.65
1:A:292:ARG:NH1	1:A:355:ASP:OD1	2.28	0.65
1:B:91:GLN:HE22	1:B:271[B]:THR:CG2	1.99	0.65
1:A:55[B]:VAL:HG22	6:A:801:HOH:O	1.96	0.64
1:C:8:GLY:O	2:C:501:MPO:H31	1.97	0.64
1:A:30:GLU:OE1	1:B:74:ARG:NH2	2.29	0.64
1:A:8:GLY:O	2:A:501:MPO:H31	1.98	0.64
1:C:331:HIS:CE1	1:C:343:GLU:HG3	2.35	0.62
1:D:194:ARG:NH1	6:D:602:HOH:O	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271[B]:THR:HG22	1:B:275[B]:ARG:NE	2.20	0.57
1:C:128[B]:LEU:HD12	1:C:153:VAL:HB	1.86	0.57
1:B:271[B]:THR:CG2	1:B:275[B]:ARG:NH2	2.69	0.56
1:A:88:LEU:HB2	1:A:271[B]:THR:HG22	1.87	0.55
1:C:220:THR:HG23	1:C:221:PRO:HD2	1.87	0.54
1:C:91:GLN:OE1	1:C:275:ARG:HG3	2.07	0.54
1:B:377:THR:HG23	6:B:617:HOH:O	2.08	0.54
1:C:91:GLN:HE22	1:C:271[B]:THR:CG2	2.10	0.54
1:C:271[B]:THR:HG22	1:C:275:ARG:CZ	2.37	0.54
1:D:30:GLU:HG3	1:D:37:THR:HB	1.88	0.54
1:C:284:GLN:OE1	1:C:287:ARG:NE	2.33	0.52
1:A:395:ASP:CG	6:A:602:HOH:O	2.48	0.51
1:C:197:LYS:HE2	1:C:224:ASP:OD1	2.11	0.51
1:B:271[B]:THR:HG21	1:B:275[B]:ARG:NH2	2.25	0.51
1:B:220:THR:HG22	1:B:222:LEU:H	1.76	0.51
1:A:232:LYS:NZ	4:A:503:DOW:C4A	2.70	0.50
1:C:8:GLY:O	2:C:501:MPO:C3	2.59	0.50
1:A:8:GLY:O	2:A:501:MPO:H32	2.12	0.49
1:C:220:THR:CG2	1:C:222:LEU:H	2.24	0.49
1:A:194:ARG:NH1	6:A:604:HOH:O	2.31	0.49
1:C:187:ARG:NH1	6:C:604:HOH:O	2.47	0.47
1:C:370:ALA:O	1:C:373[A]:THR:OG1	2.32	0.47
1:A:88:LEU:HB2	1:A:271[B]:THR:CG2	2.46	0.46
1:A:140:HIS:HE1	6:A:861:HOH:O	1.99	0.46
1:C:62:GLU:OE2	1:C:276:ARG:HD3	2.16	0.45
4:D:502:DOW:N5A	4:D:502:DOW:O3	2.50	0.44
1:A:77:VAL:HG21	1:B:36:LEU:HD22	1.99	0.44
1:B:220:THR:HG22	1:B:221:PRO:HD2	2.00	0.43
1:A:215:ARG:NH1	1:A:219:SER:O	2.52	0.43
1:B:17:CYS:HB2	1:B:18:PRO:HD2	1.99	0.43
1:A:275:ARG:NH2	6:A:611:HOH:O	2.43	0.42
1:B:304:ALA:HB1	1:B:373:THR:HG23	2.01	0.42
6:C:955:HOH:O	1:D:78:GLY:HA3	2.19	0.42
1:C:186:GLU:HG3	6:C:854:HOH:O	2.18	0.42
1:D:30:GLU:CG	1:D:37:THR:HB	2.49	0.42
1:A:186:GLU:HG3	1:A:186:GLU:H	1.62	0.42
1:C:369:SER:O	1:C:373[A]:THR:HG23	2.20	0.42
1:A:407:THR:O	1:A:411:VAL:HG23	2.20	0.42
1:C:89:LEU:HD22	1:C:101:VAL:HG23	2.01	0.41
1:C:276:ARG:HD3	1:C:276:ARG:HH21	1.72	0.41
1:C:38:ASP:HB2	1:C:39:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:VAL:HB	1:D:152:ILE:HD13	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:GLU:OE2	1:D:186:GLU:OE1[1_455]	1.97	0.23
6:C:958:HOH:O	6:D:602:HOH:O[1_455]	2.16	0.04

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	413/439 (94%)	407 (98%)	5 (1%)	1 (0%)	47	26
1	B	412/439 (94%)	405 (98%)	7 (2%)	0	100	100
1	C	413/439 (94%)	407 (98%)	5 (1%)	1 (0%)	47	26
1	D	414/439 (94%)	406 (98%)	7 (2%)	1 (0%)	47	26
All	All	1652/1756 (94%)	1625 (98%)	24 (2%)	3 (0%)	47	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	ALA
1	D	231	ALA
1	C	231	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	317/337 (94%)	308 (97%)	9 (3%)	43	18
1	B	318/337 (94%)	311 (98%)	7 (2%)	52	27
1	C	317/337 (94%)	313 (99%)	4 (1%)	69	50
1	D	319/337 (95%)	315 (99%)	4 (1%)	69	50
All	All	1271/1348 (94%)	1247 (98%)	24 (2%)	57	34

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	51	ARG
1	A	187	ARG
1	A	215	ARG
1	A	342	PHE
1	A	346	ASN
1	A	356	GLU
1	A	402	ARG
1	A	412	GLU
1	B	51	ARG
1	B	186	GLU
1	B	220	THR
1	B	342	PHE
1	B	346	ASN
1	B	377	THR
1	B	384	GLU
1	C	51	ARG
1	C	187	ARG
1	C	342	PHE
1	C	346	ASN
1	D	51	ARG
1	D	346	ASN
1	D	380	GLU
1	D	404	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	HIS
1	B	91	GLN
1	B	284	GLN
1	C	91	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

13 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	$\#|Z| > 2$
5	SO4	D	504	-	4,4,4	0.40	0	6,6,6	0.48	0
3	EDO	C	502	-	3,3,3	0.51	0	2,2,2	0.24	0
2	MPO	B	501	-	13,13,13	2.77	2 (15%)	17,17,17	4.43	7 (41%)
3	EDO	B	502	-	3,3,3	0.57	0	2,2,2	0.30	0
3	EDO	A	502	-	3,3,3	0.46	0	2,2,2	0.81	0
4	DOW	A	503	-	39,39,39	1.70	4 (10%)	53,58,58	1.50	9 (16%)
4	DOW	C	503	-	39,39,39	1.63	4 (10%)	53,58,58	1.51	10 (18%)
2	MPO	C	501	-	13,13,13	2.97	2 (15%)	17,17,17	4.60	12 (70%)
2	MPO	A	501	-	13,13,13	2.36	2 (15%)	17,17,17	2.00	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
4	DOW	D	502	-	39,39,39	1.67	4 (10%)	53,58,58	1.57	9 (16%)
4	DOW	B	503	-	39,39,39	1.58	4 (10%)	53,58,58	1.47	11 (20%)
5	SO4	D	503	-	4,4,4	0.46	0	6,6,6	0.57	0
3	EDO	D	501	-	3,3,3	0.45	0	2,2,2	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
3	EDO	C	502	-	-	0/1/1/1	-
2	MPO	B	501	-	-	3/7/15/15	0/1/1/1
3	EDO	B	502	-	-	0/1/1/1	-
3	EDO	A	502	-	-	0/1/1/1	-
4	DOW	A	503	-	-	7/16/56/56	0/3/3/3
4	DOW	C	503	-	-	6/16/56/56	0/3/3/3
2	MPO	C	501	-	-	4/7/15/15	0/1/1/1
2	MPO	A	501	-	-	3/7/15/15	0/1/1/1
4	DOW	D	502	-	-	6/16/56/56	0/3/3/3
4	DOW	B	503	-	-	6/16/56/56	0/3/3/3
3	EDO	D	501	-	-	0/1/1/1	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	MPO	C1-S1	-9.06	1.64	1.77
2	B	501	MPO	C1-S1	-7.78	1.66	1.77
2	A	501	MPO	C1-S1	-7.18	1.67	1.77
4	D	502	DOW	C3-C2	6.94	1.47	1.40
4	A	503	DOW	C3-C2	6.93	1.47	1.40
4	C	503	DOW	C3-C2	6.91	1.47	1.40
4	B	503	DOW	C3-C2	5.93	1.46	1.40
2	B	501	MPO	O1-S1	5.84	1.62	1.45
4	A	503	DOW	C5-C4	5.54	1.48	1.40
2	C	501	MPO	O2-S1	5.29	1.60	1.45
4	D	502	DOW	C5-C4	5.00	1.47	1.40
4	C	503	DOW	C5-C4	4.66	1.47	1.40
4	B	503	DOW	C5-C4	4.60	1.46	1.40
2	A	501	MPO	O3-S1	4.41	1.63	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	DOW	C4A-C4	-3.48	1.47	1.51
4	D	502	DOW	C4A-C4	-3.36	1.47	1.51
4	D	502	DOW	C4A-N5A	-3.20	1.31	1.46
4	B	503	DOW	C4A-C4	-3.18	1.47	1.51
4	C	503	DOW	C4A-C4	-3.14	1.47	1.51
4	A	503	DOW	C4A-N5A	-3.09	1.31	1.46
4	B	503	DOW	C4A-N5A	-2.77	1.33	1.46
4	C	503	DOW	C4A-N5A	-2.60	1.33	1.46

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	MPO	O2-S1-C1	-12.19	92.23	106.92
2	C	501	MPO	C2-C1-S1	-11.90	95.01	113.25
2	B	501	MPO	O1-S1-C1	11.17	120.36	106.92
2	B	501	MPO	O3-S1-C1	6.24	115.85	105.77
2	C	501	MPO	C5-C4-N1	-6.15	100.78	110.10
2	C	501	MPO	O2-S1-C1	6.15	114.32	106.92
2	C	501	MPO	O1-S1-C1	-5.77	99.97	106.92
4	D	502	DOW	O61-C15-C16	5.44	116.11	105.96
4	C	503	DOW	O61-C15-C16	5.24	115.74	105.96
2	C	501	MPO	C3-N1-C7	4.87	123.68	111.23
4	A	503	DOW	O61-C15-C16	4.58	114.51	105.96
2	A	501	MPO	O2-S1-C1	4.18	111.95	106.92
2	C	501	MPO	C2-C3-N1	-4.04	103.64	113.84
2	C	501	MPO	O4-C5-C4	-4.01	102.97	111.80
4	A	503	DOW	C11-O61-C15	3.82	121.19	113.69
2	C	501	MPO	C3-C2-C1	-3.72	100.15	113.14
4	B	503	DOW	O1A-C24-C25	3.51	117.55	109.18
4	D	502	DOW	C6-N1-C2	3.38	125.43	119.17
2	C	501	MPO	C6-C7-N1	-3.35	105.03	110.10
4	D	502	DOW	O1A-C24-C25	3.33	117.13	109.18
4	B	503	DOW	O61-C15-C16	3.28	112.08	105.96
2	A	501	MPO	C2-C1-S1	-3.26	108.24	113.25
2	C	501	MPO	C7-N1-C4	3.23	116.11	108.83
4	C	503	DOW	C4-C4A-N5A	3.23	117.62	111.58
4	A	503	DOW	C6-N1-C2	2.98	124.68	119.17
4	B	503	DOW	C6-C5-C4	2.97	120.22	118.12
4	B	503	DOW	C4A-C4-C3	2.85	123.10	120.04
4	C	503	DOW	O1A-C24-C25	2.83	115.94	109.18
4	D	502	DOW	C6-C5-C4	2.81	120.11	118.12
4	C	503	DOW	C11-O61-C15	2.76	119.10	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	502	DOW	C4A-C4-C3	2.69	122.92	120.04
2	A	501	MPO	C6-C7-N1	-2.69	106.02	110.10
4	D	502	DOW	C11-O61-C15	2.60	118.80	113.69
4	B	503	DOW	C3-C4-C5	-2.58	116.24	118.72
4	C	503	DOW	C11-O1A-C24	2.57	124.33	117.96
4	A	503	DOW	O1P-P-O2P	2.57	117.45	107.64
4	A	503	DOW	C4-C4A-N5A	2.55	116.34	111.58
4	B	503	DOW	C6-N1-C2	2.54	123.88	119.17
4	D	502	DOW	C5-C6-N1	-2.53	119.61	123.82
4	B	503	DOW	C11-O61-C15	2.50	118.60	113.69
2	C	501	MPO	C6-O4-C5	2.48	118.18	109.89
2	A	501	MPO	C5-C4-N1	-2.42	106.43	110.10
4	C	503	DOW	O61-C15-C14	-2.42	105.30	109.69
4	A	503	DOW	C5-C6-N1	-2.41	119.81	123.82
4	C	503	DOW	O3-C3-C4	2.41	125.19	118.13
4	B	503	DOW	C11-O1A-C24	2.39	123.87	117.96
2	A	501	MPO	O3-S1-O2	-2.37	105.48	111.27
2	C	501	MPO	O3-S1-C1	-2.37	101.93	105.77
4	A	503	DOW	C4A-C4-C3	2.36	122.56	120.04
2	A	501	MPO	O3-S1-C1	2.34	109.56	105.77
2	B	501	MPO	C2-C3-N1	-2.32	108.00	113.84
4	B	503	DOW	C3-C2-N1	-2.31	117.78	120.77
4	C	503	DOW	C4A-N5A-C16	2.27	122.41	113.60
4	A	503	DOW	O1A-C24-C25	2.25	114.55	109.18
4	A	503	DOW	O1A-C24-C23	2.24	113.23	107.28
4	D	502	DOW	C3-C2-N1	-2.16	117.98	120.77
2	B	501	MPO	O2-S1-O1	-2.14	106.53	113.95
2	B	501	MPO	C6-C7-N1	2.13	113.33	110.10
4	D	502	DOW	O2P-P-O4P	-2.10	101.14	106.73
4	C	503	DOW	O1A-C11-C12	-2.09	104.62	108.22
4	B	503	DOW	C4A-N5A-C16	2.05	121.57	113.60
2	B	501	MPO	C2-C1-S1	-2.04	110.13	113.25
4	B	503	DOW	C4-C4A-N5A	2.04	115.38	111.58
4	C	503	DOW	C6-N1-C2	2.03	122.93	119.17

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	DOW	C5-C4-C4A-N5A
4	A	503	DOW	C15-C16-N5A-C4A
4	C	503	DOW	C5-C4-C4A-N5A

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Mol	Chain	Res	Type	Atoms
4	C	503	DOW	C15-C16-N5A-C4A
4	C	503	DOW	C25-C24-O1A-C11
2	C	501	MPO	C1-C2-C3-N1
4	D	502	DOW	C5-C4-C4A-N5A
4	D	502	DOW	C15-C16-N5A-C4A
4	D	502	DOW	C25-C24-O1A-C11
4	B	503	DOW	C5-C4-C4A-N5A
4	B	503	DOW	C15-C16-N5A-C4A
4	B	503	DOW	C25-C24-O1A-C11
2	B	501	MPO	C2-C3-N1-C7
2	B	501	MPO	C2-C3-N1-C4
2	C	501	MPO	C2-C3-N1-C7
2	C	501	MPO	C2-C3-N1-C4
2	C	501	MPO	S1-C1-C2-C3
2	A	501	MPO	C1-C2-C3-N1
4	D	502	DOW	C4-C4A-N5A-C16
4	A	503	DOW	C23-C24-O1A-C11
2	B	501	MPO	C2-C1-S1-O1
2	A	501	MPO	C2-C1-S1-O1
4	A	503	DOW	C4-C4A-N5A-C16
2	A	501	MPO	C2-C3-N1-C7
4	D	502	DOW	C23-C24-O1A-C11
4	B	503	DOW	C4-C4A-N5A-C16
4	A	503	DOW	O61-C11-O1A-C24
4	C	503	DOW	C4-C4A-N5A-C16
4	C	503	DOW	C23-C24-O1A-C11
4	A	503	DOW	C3-C4-C4A-N5A
4	C	503	DOW	C3-C4-C4A-N5A
4	D	502	DOW	C3-C4-C4A-N5A
4	B	503	DOW	C3-C4-C4A-N5A
4	B	503	DOW	C23-C24-O1A-C11
4	A	503	DOW	C25-C24-O1A-C11

There are no ring outliers.

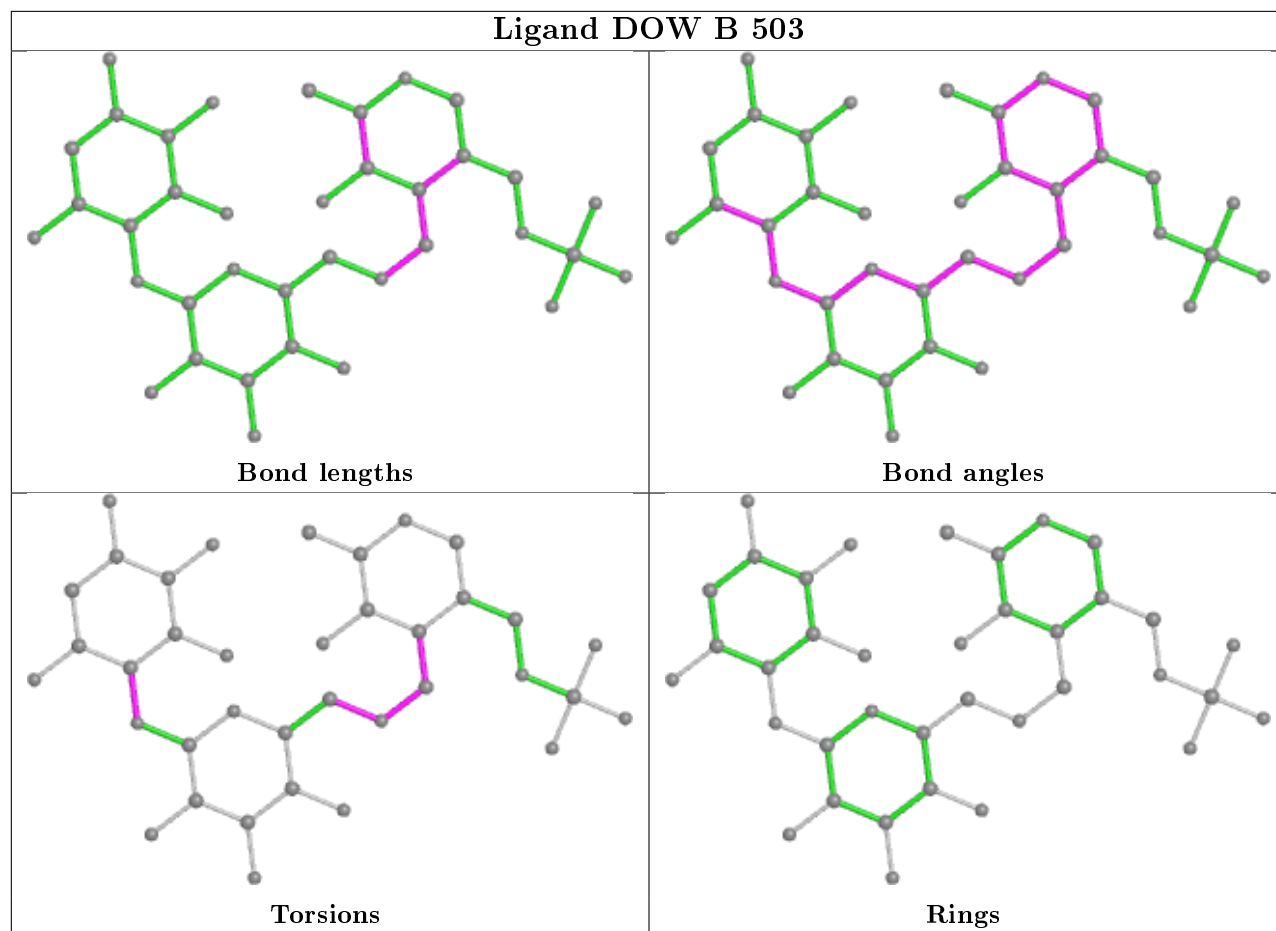4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	DOW	3	0
2	C	501	MPO	2	0
2	A	501	MPO	3	0
4	D	502	DOW	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 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 DOW A 503

Bond lengths

Bond angles

Torsions

Rings

Ligand DOW C 503

Bond lengths

Bond angles

Torsions

Rings

Ligand DOW D 502

Bond lengths

Bond angles

Torsions

Rings

Ligand DOW B 503

Bond lengths

Bond angles

Torsions

Rings
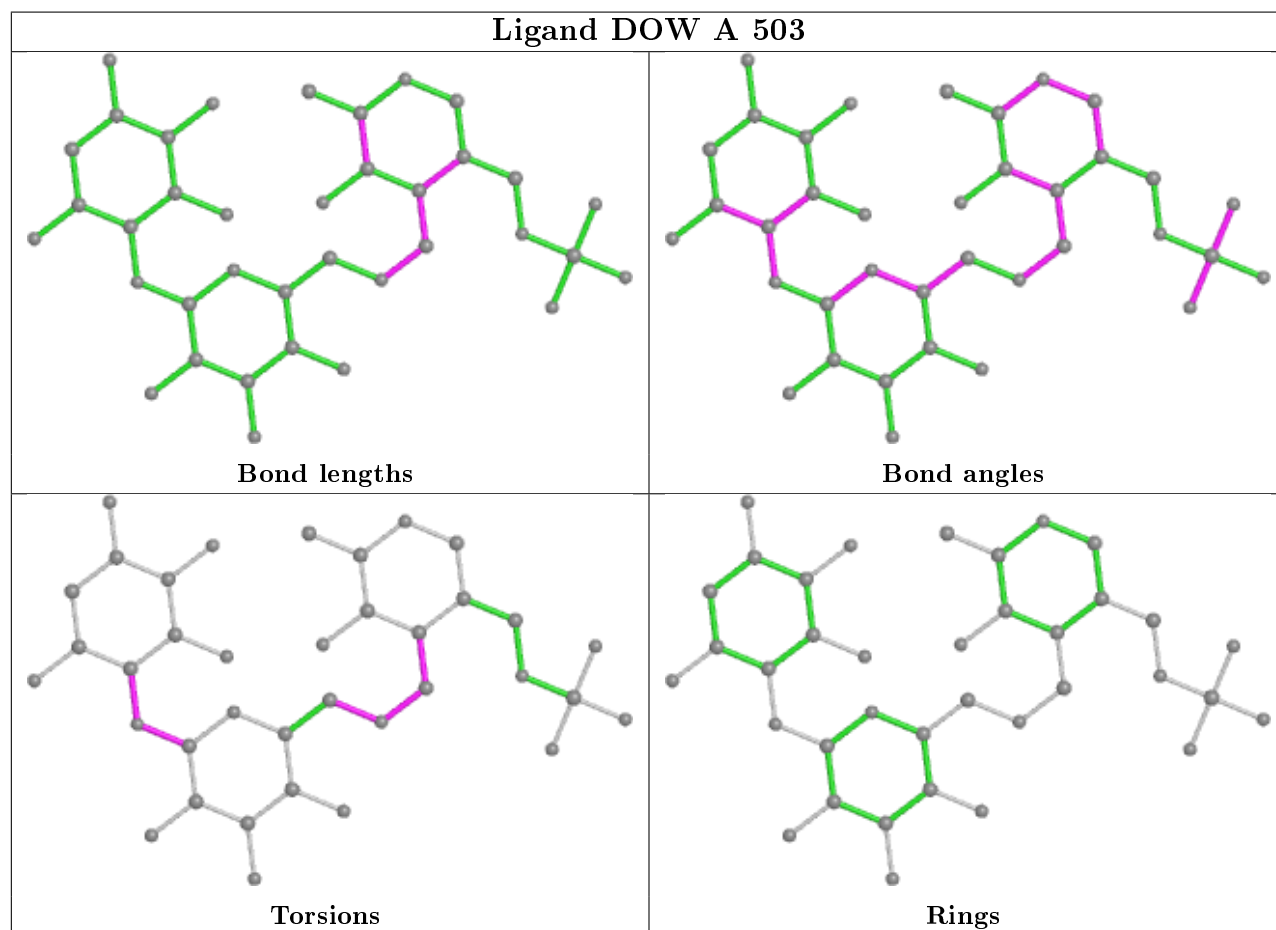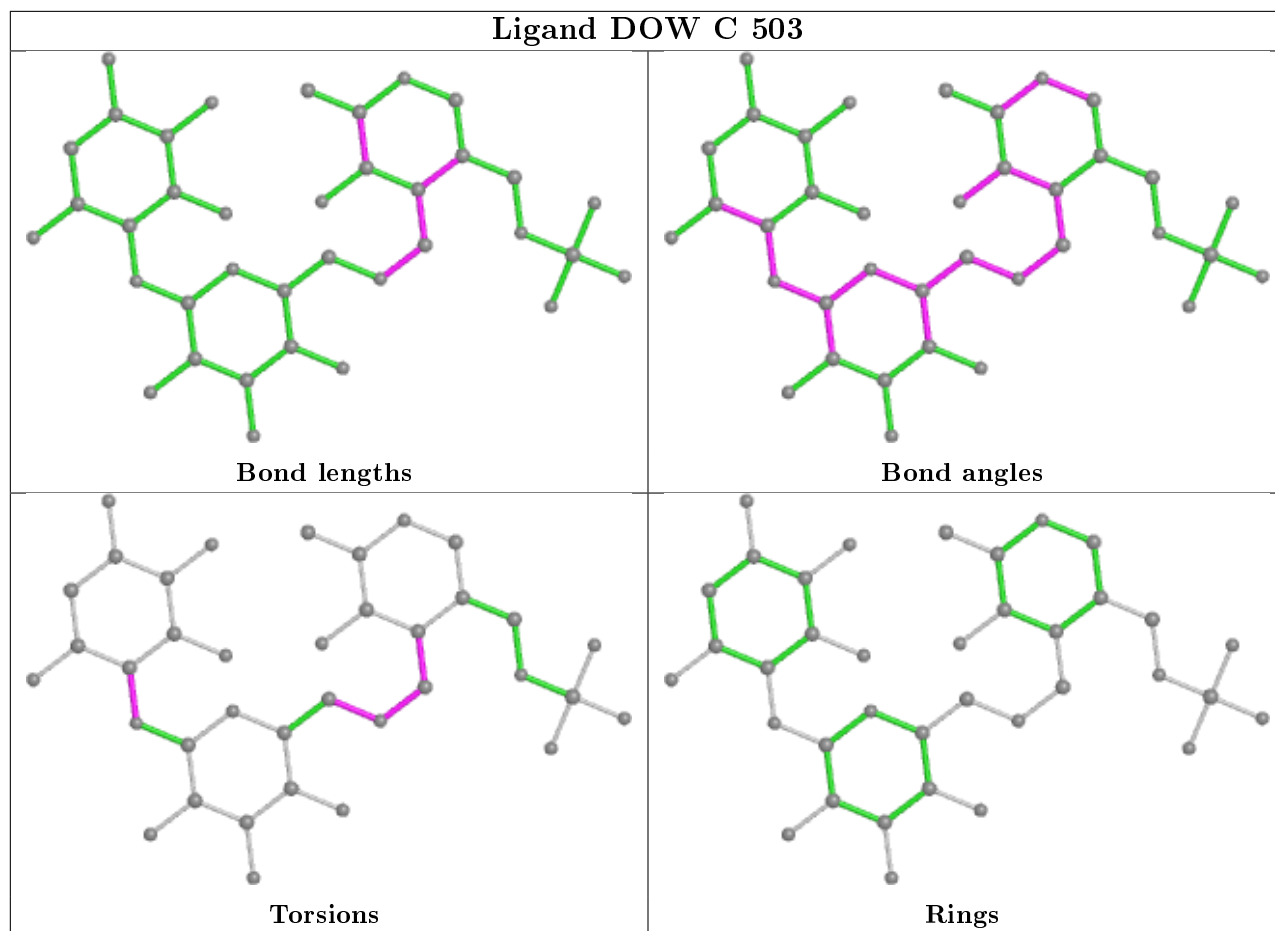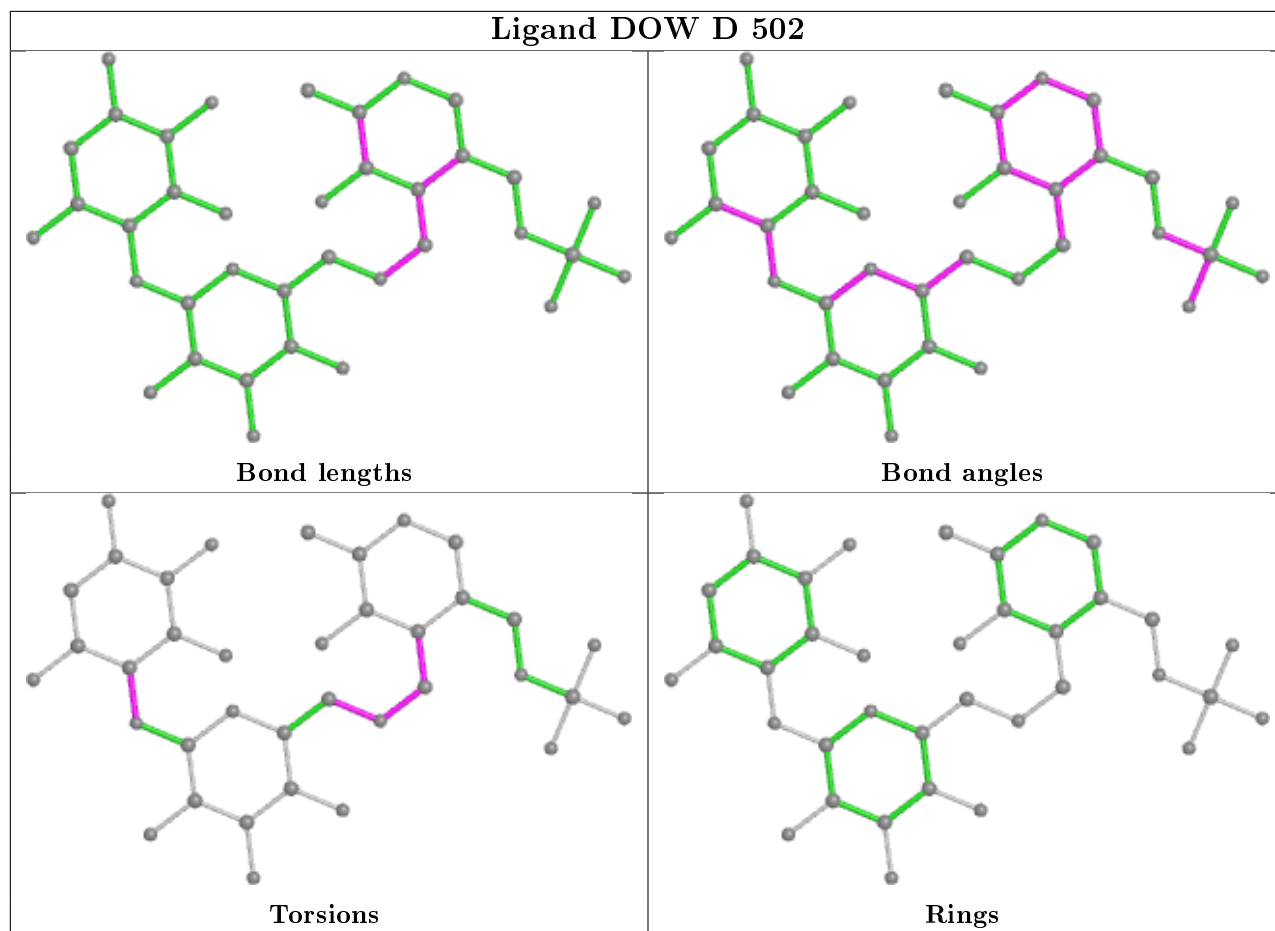
5.7 Other polymers (i)

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	410/439 (93%)	-0.14	6 (1%)	73	73	6, 14, 35, 59	0
1	B	408/439 (92%)	-0.19	9 (2%)	62	60	6, 15, 35, 56	0
1	C	411/439 (93%)	-0.24	11 (2%)	54	52	6, 14, 30, 51	0
1	D	409/439 (93%)	-0.24	6 (1%)	73	73	6, 13, 29, 55	0
All	All	1638/1756 (93%)	-0.20	32 (1%)	65	64	6, 14, 32, 59	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	GLY	5.0
1	C	378	ASP	4.6
1	B	378	ASP	4.3
1	D	378	ASP	3.0
1	D	401	PRO	3.0
1	C	380	GLU	3.0
1	A	415	TRP	2.9
1	A	409	ALA	2.9
1	C	6	GLY	2.9
1	C	416	GLU	2.8
1	C	302	ALA	2.7
1	B	380	GLU	2.7
1	A	378	ASP	2.6
1	B	9	LYS	2.6
1	C	7	ALA	2.6
1	B	377	THR	2.6
1	B	22	ASP	2.5
1	B	222	LEU	2.5
1	C	9	LYS	2.4
1	D	7	ALA	2.4
1	B	299	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	22	ASP	2.2
1	B	302	ALA	2.2
1	C	377	THR	2.2
1	B	381	LEU	2.2
1	A	413	ARG	2.2
1	D	380	GLU	2.1
1	D	353[A]	PHE	2.1
1	C	381	LEU	2.1
1	C	303	ASN	2.1
1	A	410	ILE	2.1
1	D	377	THR	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 carbohydrates 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
5	SO4	D	504	5/5	0.87	0.22	32,33,37,46	0
2	MPO	A	501	13/13	0.90	0.22	36,42,48,50	0
2	MPO	B	501	13/13	0.91	0.24	26,39,56,58	0
5	SO4	D	503	5/5	0.93	0.22	32,32,37,46	0
3	EDO	B	502	4/4	0.94	0.08	20,21,21,22	0
3	EDO	A	502	4/4	0.94	0.09	17,17,20,23	0
3	EDO	D	501	4/4	0.94	0.08	19,21,21,24	0
4	DOW	D	502	37/37	0.96	0.12	6,24,46,48	0
3	EDO	C	502	4/4	0.97	0.05	19,19,20,20	0
4	DOW	A	503	37/37	0.97	0.10	7,25,45,47	0
4	DOW	B	503	37/37	0.97	0.10	6,17,35,37	0
4	DOW	C	503	37/37	0.97	0.09	7,17,35,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MPO	C	501	13/13	0.97	0.15	21,24,25,27	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.
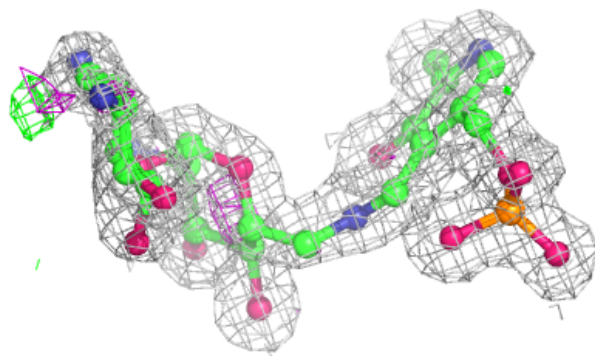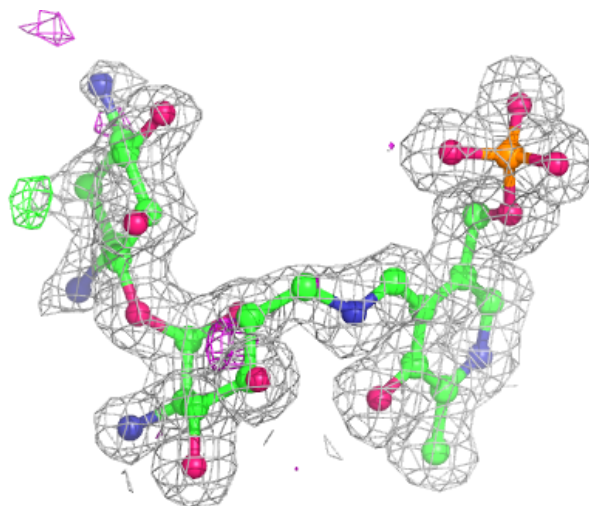
Electron density around DOW D 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
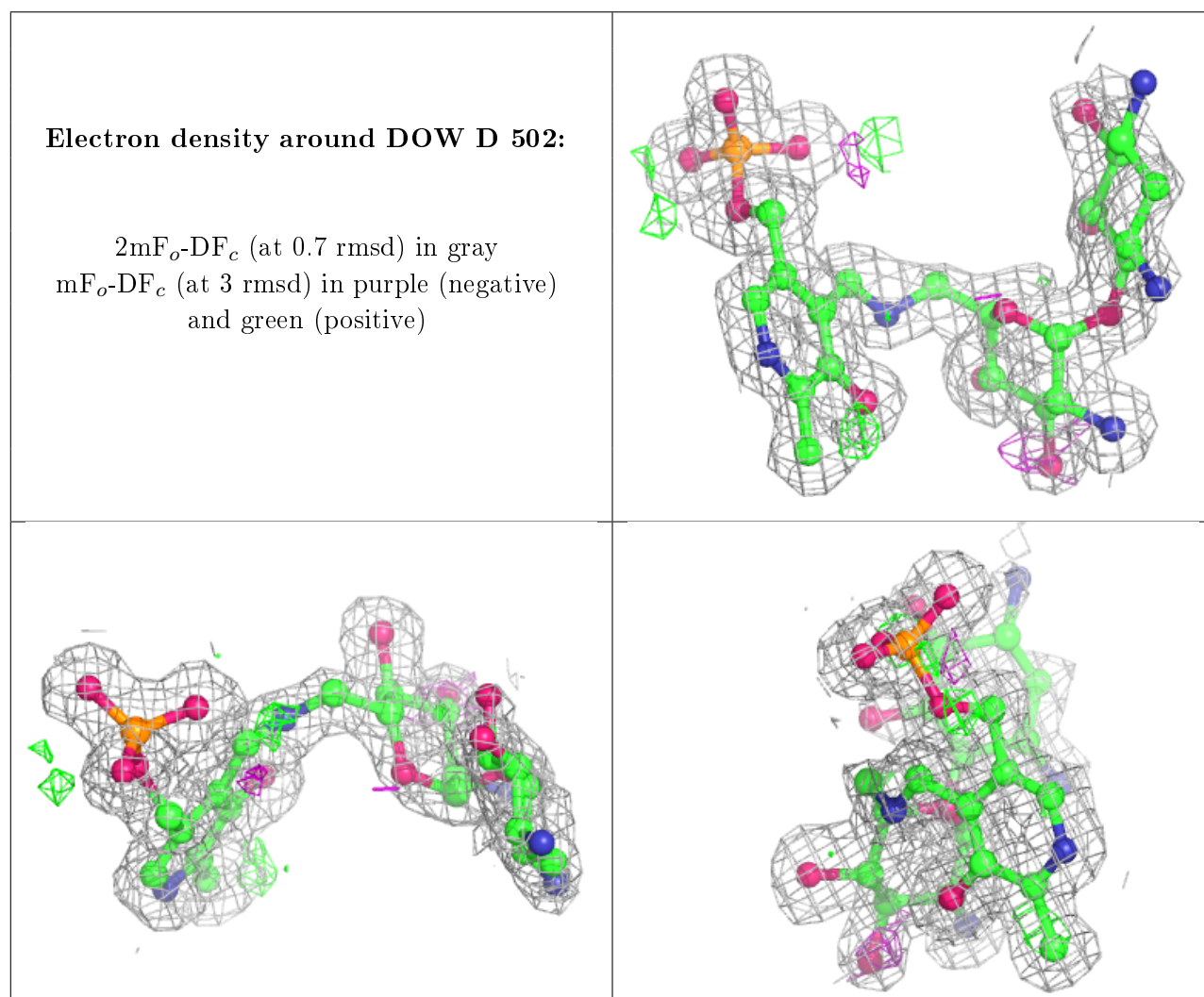
Electron density around DOW A 503:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
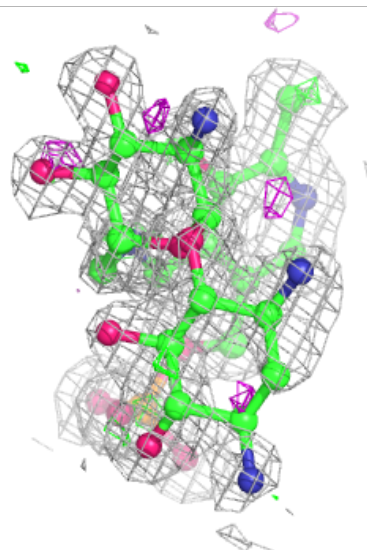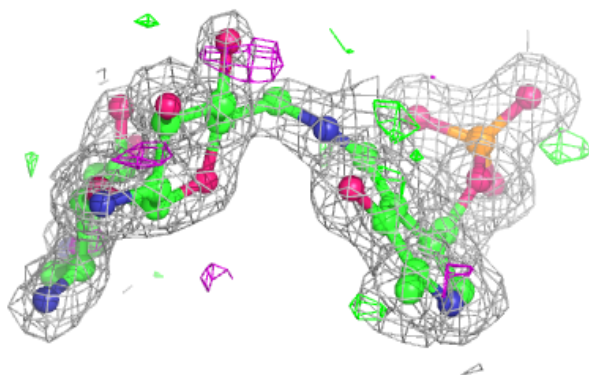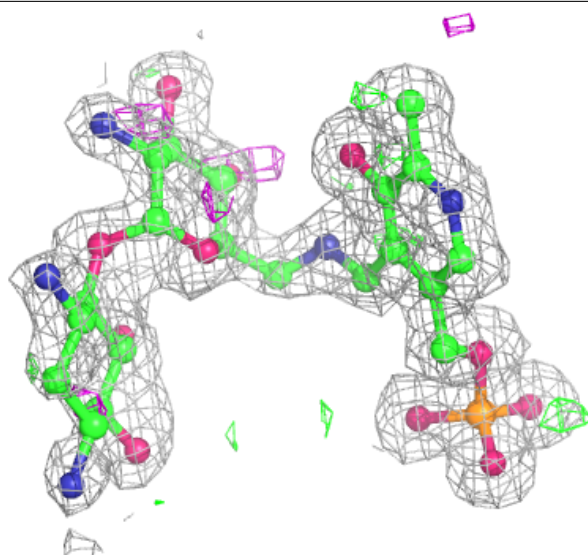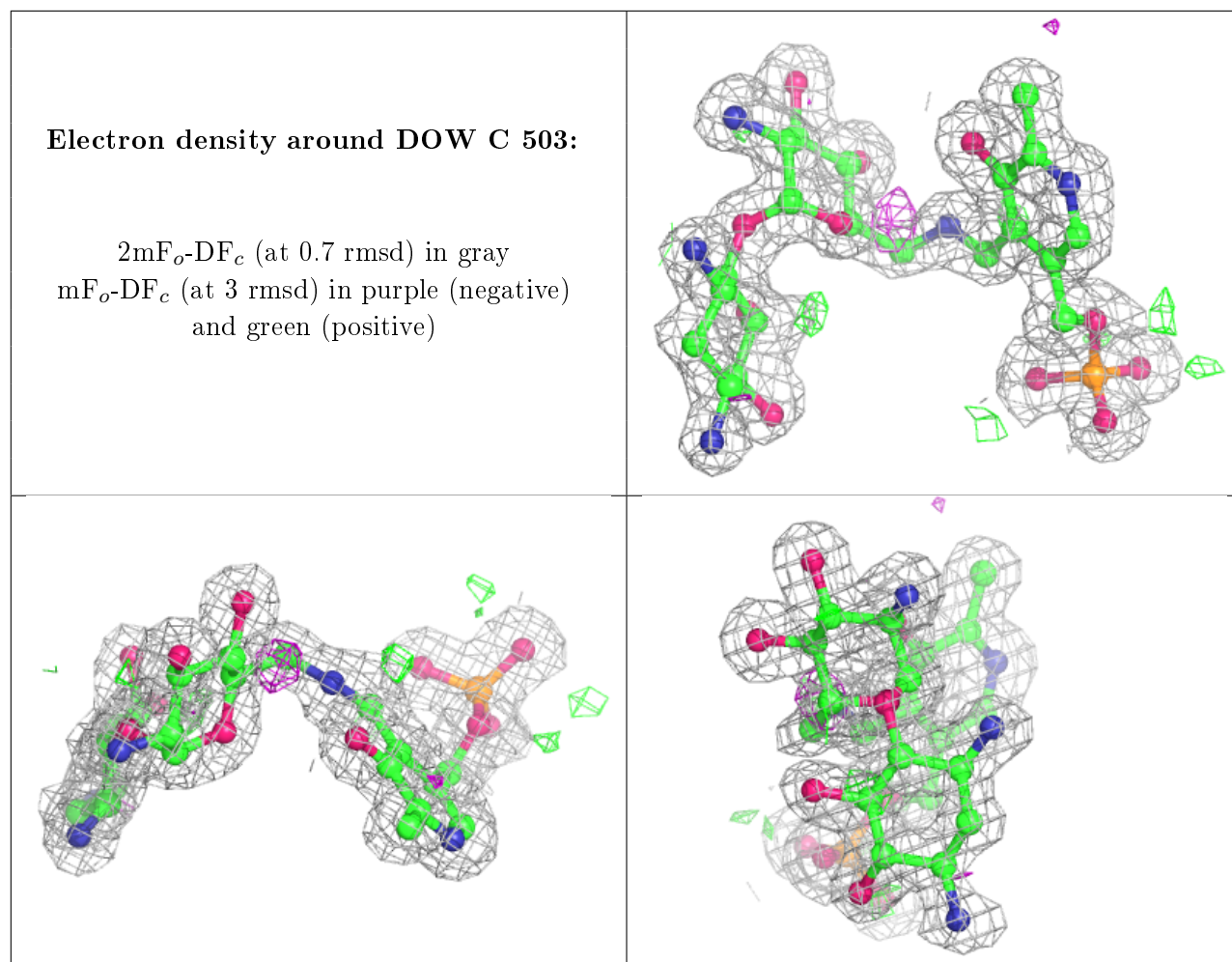
Electron density around DOW B 503:

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

Electron density around DOW C 503:

$2mF_o-DF_c$ (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.