Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 12:42 PM JST

PDB ID	:	6J27
Title	:	Crystal structure of the branched-chain polyamine synthase from Thermus thermophilus (Tth-BpsA) in complex with N4-aminopropylspermidine and 5' -methylthioadenosine
Authors	:	Mizohata, E.; Toyoda, M.; Fujita, J.; Inoue, T.
Deposited on	:	2018-12-31
Resolution	:	1.66 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:

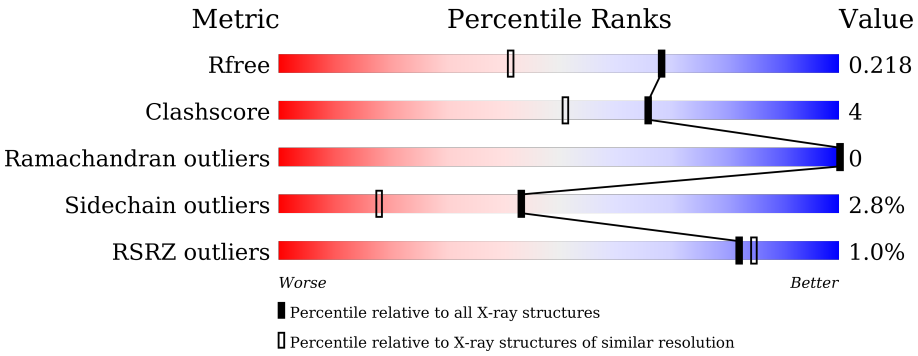
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.66 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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

Mol	Chain	Length	Quality of chain
1	A	374	79% 11% • 8%
1	B	374	82% 9% • 8%
1	C	374	83% 7% • 8%
1	D	374	79% 12% • 8%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11974 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 N(4)-bis(aminopropyl)spermidine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	6	0
			2763	1764	497	498	4			
1	B	344	Total	C	N	O	S	0	4	0
			2751	1755	497	495	4			
1	C	343	Total	C	N	O	S	0	6	0
			2760	1760	503	493	4			
1	D	344	Total	C	N	O	S	0	7	0
			2781	1773	507	497	4			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q72L89
A	-19	GLY	-	expression tag	UNP Q72L89
A	-18	SER	-	expression tag	UNP Q72L89
A	-17	SER	-	expression tag	UNP Q72L89
A	-16	HIS	-	expression tag	UNP Q72L89
A	-15	HIS	-	expression tag	UNP Q72L89
A	-14	HIS	-	expression tag	UNP Q72L89
A	-13	HIS	-	expression tag	UNP Q72L89
A	-12	HIS	-	expression tag	UNP Q72L89
A	-11	HIS	-	expression tag	UNP Q72L89
A	-10	SER	-	expression tag	UNP Q72L89
A	-9	SER	-	expression tag	UNP Q72L89
A	-8	GLY	-	expression tag	UNP Q72L89
A	-7	LEU	-	expression tag	UNP Q72L89
A	-6	VAL	-	expression tag	UNP Q72L89
A	-5	PRO	-	expression tag	UNP Q72L89
A	-4	ARG	-	expression tag	UNP Q72L89
A	-3	GLY	-	expression tag	UNP Q72L89
A	-2	SER	-	expression tag	UNP Q72L89
A	-1	HIS	-	expression tag	UNP Q72L89
A	1	VAL	-	insertion	UNP Q72L89

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	expression tag	UNP Q72L89
B	-19	GLY	-	expression tag	UNP Q72L89
B	-18	SER	-	expression tag	UNP Q72L89
B	-17	SER	-	expression tag	UNP Q72L89
B	-16	HIS	-	expression tag	UNP Q72L89
B	-15	HIS	-	expression tag	UNP Q72L89
B	-14	HIS	-	expression tag	UNP Q72L89
B	-13	HIS	-	expression tag	UNP Q72L89
B	-12	HIS	-	expression tag	UNP Q72L89
B	-11	HIS	-	expression tag	UNP Q72L89
B	-10	SER	-	expression tag	UNP Q72L89
B	-9	SER	-	expression tag	UNP Q72L89
B	-8	GLY	-	expression tag	UNP Q72L89
B	-7	LEU	-	expression tag	UNP Q72L89
B	-6	VAL	-	expression tag	UNP Q72L89
B	-5	PRO	-	expression tag	UNP Q72L89
B	-4	ARG	-	expression tag	UNP Q72L89
B	-3	GLY	-	expression tag	UNP Q72L89
B	-2	SER	-	expression tag	UNP Q72L89
B	-1	HIS	-	expression tag	UNP Q72L89
B	1	VAL	-	insertion	UNP Q72L89
C	-20	MET	-	expression tag	UNP Q72L89
C	-19	GLY	-	expression tag	UNP Q72L89
C	-18	SER	-	expression tag	UNP Q72L89
C	-17	SER	-	expression tag	UNP Q72L89
C	-16	HIS	-	expression tag	UNP Q72L89
C	-15	HIS	-	expression tag	UNP Q72L89
C	-14	HIS	-	expression tag	UNP Q72L89
C	-13	HIS	-	expression tag	UNP Q72L89
C	-12	HIS	-	expression tag	UNP Q72L89
C	-11	HIS	-	expression tag	UNP Q72L89
C	-10	SER	-	expression tag	UNP Q72L89
C	-9	SER	-	expression tag	UNP Q72L89
C	-8	GLY	-	expression tag	UNP Q72L89
C	-7	LEU	-	expression tag	UNP Q72L89
C	-6	VAL	-	expression tag	UNP Q72L89
C	-5	PRO	-	expression tag	UNP Q72L89
C	-4	ARG	-	expression tag	UNP Q72L89
C	-3	GLY	-	expression tag	UNP Q72L89
C	-2	SER	-	expression tag	UNP Q72L89
C	-1	HIS	-	expression tag	UNP Q72L89
C	1	VAL	-	insertion	UNP Q72L89

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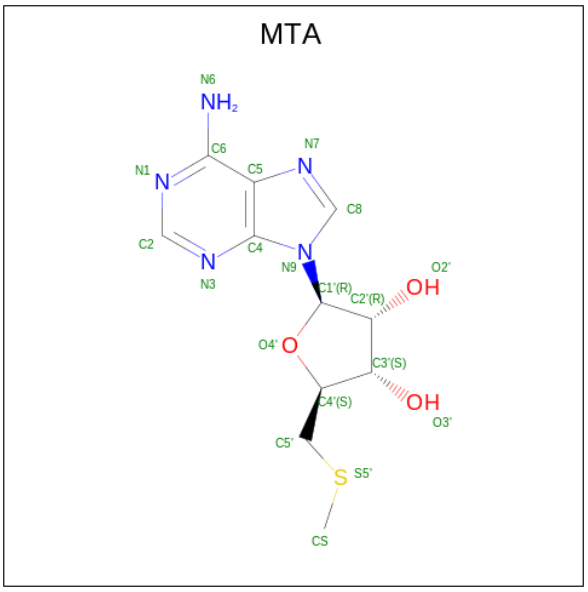
Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	expression tag	UNP Q72L89
D	-19	GLY	-	expression tag	UNP Q72L89
D	-18	SER	-	expression tag	UNP Q72L89
D	-17	SER	-	expression tag	UNP Q72L89
D	-16	HIS	-	expression tag	UNP Q72L89
D	-15	HIS	-	expression tag	UNP Q72L89
D	-14	HIS	-	expression tag	UNP Q72L89
D	-13	HIS	-	expression tag	UNP Q72L89
D	-12	HIS	-	expression tag	UNP Q72L89
D	-11	HIS	-	expression tag	UNP Q72L89
D	-10	SER	-	expression tag	UNP Q72L89
D	-9	SER	-	expression tag	UNP Q72L89
D	-8	GLY	-	expression tag	UNP Q72L89
D	-7	LEU	-	expression tag	UNP Q72L89
D	-6	VAL	-	expression tag	UNP Q72L89
D	-5	PRO	-	expression tag	UNP Q72L89
D	-4	ARG	-	expression tag	UNP Q72L89
D	-3	GLY	-	expression tag	UNP Q72L89
D	-2	SER	-	expression tag	UNP Q72L89
D	-1	HIS	-	expression tag	UNP Q72L89
D	1	VAL	-	insertion	UNP Q72L89

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

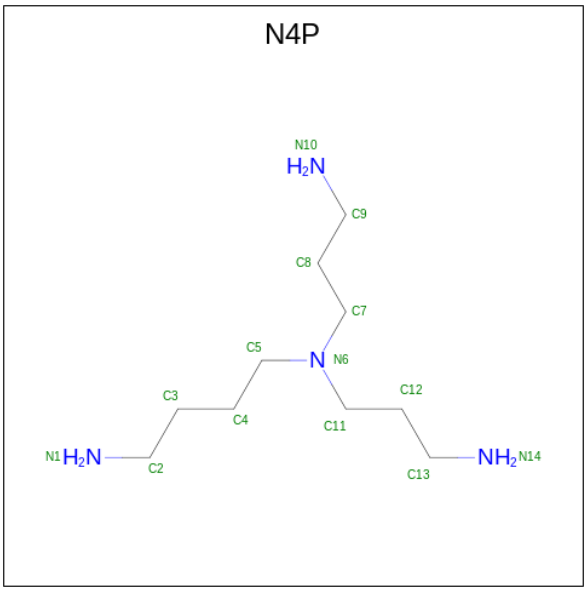
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0

- Molecule 3 is 5'-DEOXY-5'-METHYLTHIOADENOSINE (three-letter code: MTA) (formula: $C_{11}H_{15}N_5O_3S$).



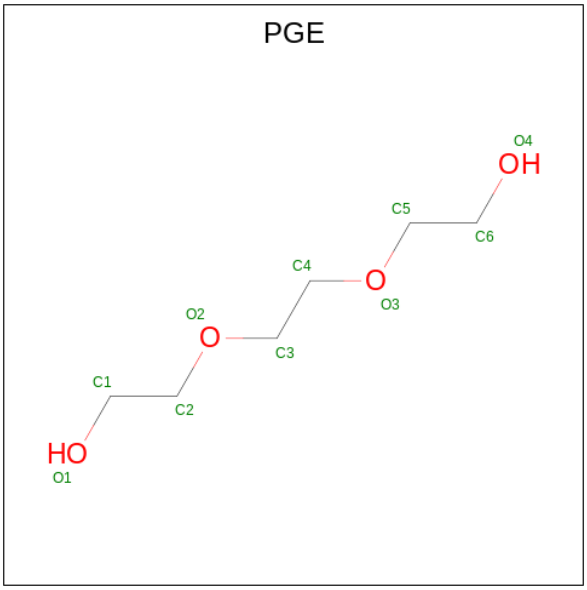
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
3	B	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
3	C	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
3	D	1	Total	C	N	O	S	0	0
			20	11	5	3	1		

- Molecule 4 is N,N-bis(3-aminopropyl)butane-1,4-diamine (three-letter code: N4P) (formula: $C_{10}H_{26}N_4$).



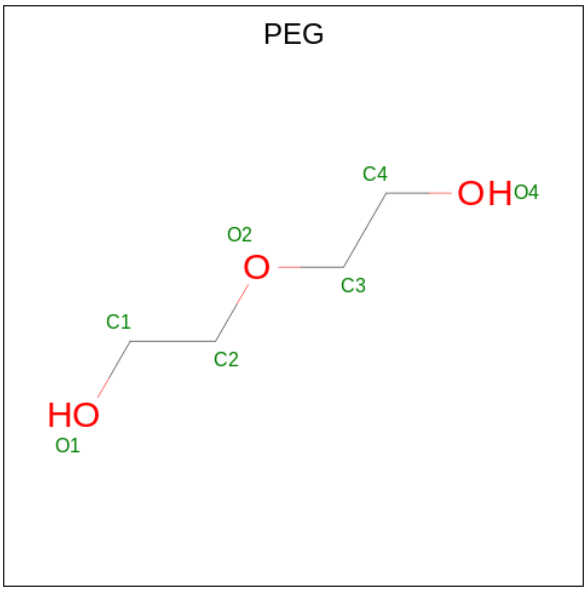
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 14 10 4	0	0
4	B	1	Total C N 14 10 4	0	0
4	C	1	Total C N 14 10 4	0	0
4	D	1	Total C N 14 10 4	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 10 6 4	0	0
5	B	1	Total C O 10 6 4	0	0
5	D	1	Total C O 10 6 4	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	D	1	Total C O 7 4 3	0	0
6	D	1	Total C O 7 4 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	173	Total O 173 173	0	0
7	B	166	Total O 166 166	0	0
7	C	180	Total O 180 180	0	0

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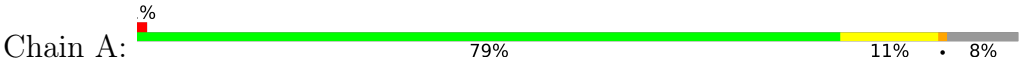
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	169	Total	O	0	0
			169	169		

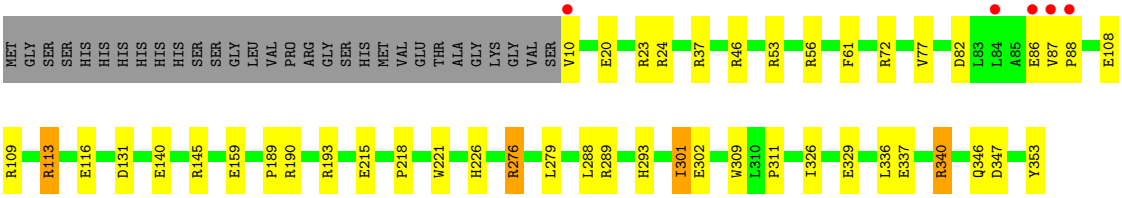
3 Residue-property plots (i)

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(4)-bis(aminopropyl)spermidine synthase

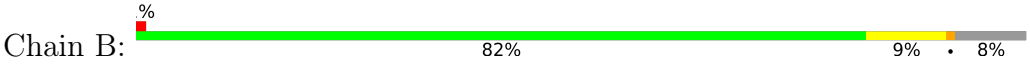
Chain A:

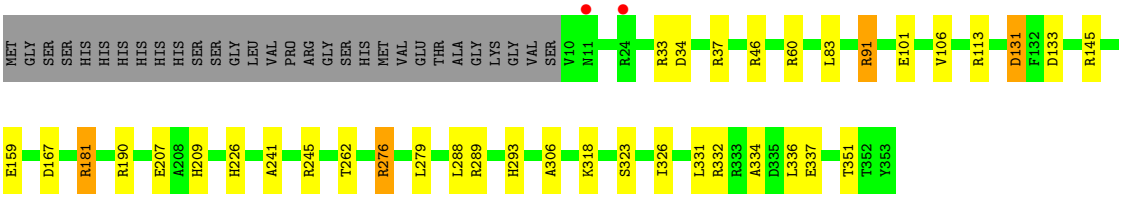




• Molecule 1: N(4)-bis(aminopropyl)spermidine synthase

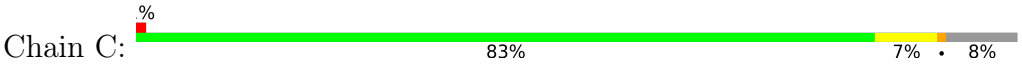
Chain B:

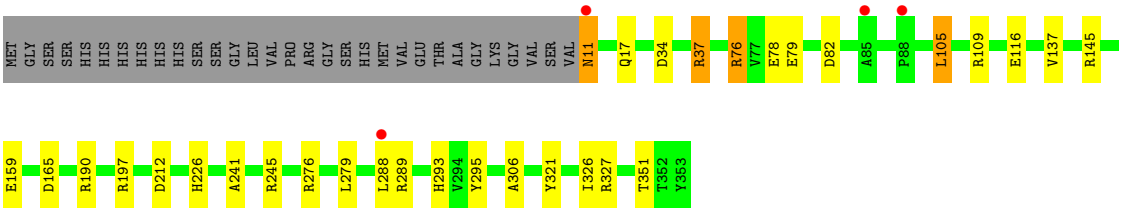




• Molecule 1: N(4)-bis(aminopropyl)spermidine synthase

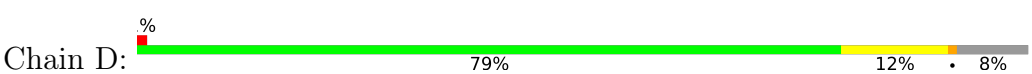
Chain C:

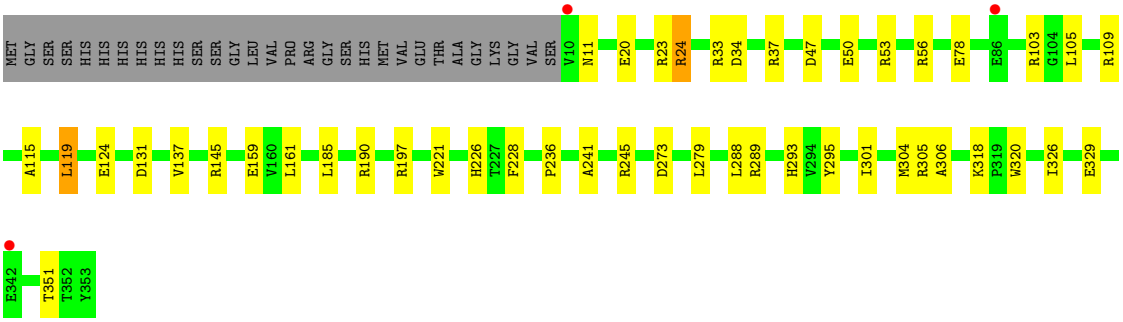




• Molecule 1: N(4)-bis(aminopropyl)spermidine synthase

Chain D:




MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET VAL GLU THR ALA GLY LYS GLY VAL SER V10 N11 E20 R23 R24 R33 D34 R37 D47 E50 R53 R56 E78 E86 R103 G104 L105 R109
A115 L119 E124 D131 V137 R145 E159 V160 L161 L185 R190 R197 W221 H226 T227 F228 P236 A241 R245 D273 L279 L288 R289 H293 V294 Y295 I301 M304 R305 A306 K318 P319 W320 I326 E329
E342 T351 T352 Y353

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.57Å 158.61Å 71.94Å 90.00° 118.95° 90.00°	Depositor
Resolution (Å)	50.00 – 1.66 39.93 – 1.66	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-1.66) 98.6 (39.93-1.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 1.66Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.167 , 0.206 0.181 , 0.218	Depositor DCC
R_{free} test set	7822 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	21.3	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.012 for l,k,-h-l 0.012 for -h-l,k,h 0.136 for h,-k,-h-l 0.025 for l,-k,h 0.027 for -h-l,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	11974	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, MTA, N4P, PEG, FE

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	0.95	1/2848 (0.0%)	1.00	10/3876 (0.3%)
1	B	0.94	0/2827	1.03	10/3847 (0.3%)
1	C	0.94	2/2842 (0.1%)	1.03	13/3865 (0.3%)
1	D	0.93	1/2863 (0.0%)	1.05	12/3894 (0.3%)
All	All	0.94	4/11380 (0.0%)	1.03	45/15482 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	309	TRP	CB-CG	-6.26	1.39	1.50
1	C	165	ASP	CB-CG	6.03	1.64	1.51
1	C	321	TYR	CG-CD2	-5.35	1.32	1.39
1	D	320	TRP	CE3-CZ3	-5.16	1.29	1.38

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	37[A]	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	D	37[B]	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	B	190	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	A	190	ARG	NE-CZ-NH2	-8.21	116.20	120.30
1	B	181	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	C	109	ARG	NE-CZ-NH1	-7.70	116.45	120.30
1	A	289	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	C	197	ARG	NE-CZ-NH1	-7.31	116.65	120.30
1	D	289	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	C	190	ARG	NE-CZ-NH2	-6.97	116.82	120.30
1	C	37[A]	ARG	NE-CZ-NH1	-6.93	116.83	120.30
1	C	37[B]	ARG	NE-CZ-NH1	-6.93	116.83	120.30
1	D	289	ARG	NE-CZ-NH2	-6.55	117.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	190	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	A	56	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	C	212	ASP	CB-CG-OD1	6.47	124.13	118.30
1	D	53[A]	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	D	53[B]	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	C	34	ASP	CB-CG-OD1	6.31	123.98	118.30
1	B	113	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	A	113	ARG	NE-CZ-NH2	6.21	123.40	120.30
1	D	56	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	D	305	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	D	190	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	276	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	289	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	D	47	ASP	CB-CG-OD2	5.65	123.39	118.30
1	C	276	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	C	105	LEU	CA-CB-CG	5.47	127.89	115.30
1	C	109	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	B	91	ARG	CG-CD-NE	-5.36	100.54	111.80
1	A	347	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	289	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	B	289	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	33	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	D	33	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	289	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	61	PHE	CB-CG-CD2	-5.18	117.18	120.80
1	C	327	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	C	289	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	D	103	ARG	NE-CZ-NH2	5.13	122.86	120.30
1	B	167	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	72	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	B	34	ASP	CB-CG-OD1	5.07	122.87	118.30
1	B	60	ARG	NE-CZ-NH2	5.01	122.81	120.30

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	2763	0	2754	33	0
1	B	2751	0	2738	22	0
1	C	2760	0	2757	12	0
1	D	2781	0	2777	30	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	20	0	15	0	0
3	B	20	0	15	0	0
3	C	20	0	15	0	0
3	D	20	0	15	0	0
4	A	14	0	0	0	0
4	B	14	0	0	1	0
4	C	14	0	0	0	0
4	D	14	0	0	0	0
5	A	10	0	14	3	0
5	B	10	0	14	0	0
5	D	10	0	14	4	0
6	A	7	0	10	0	0
6	B	28	0	40	0	0
6	C	14	0	20	0	0
6	D	14	0	20	0	0
7	A	173	0	0	2	0
7	B	166	0	0	1	0
7	C	180	0	0	0	0
7	D	169	0	0	4	0
All	All	11974	0	11218	90	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (90) 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:D:159:GLU:H	1:D:226:HIS:HD2	1.15	0.95
1:B:159:GLU:H	1:B:226:HIS:HD2	1.21	0.85
1:C:159:GLU:H	1:C:226:HIS:HD2	1.24	0.84
1:A:116[B]:GLU:OE2	1:D:318:LYS:HE3	1.79	0.82
1:A:159:GLU:H	1:A:226:HIS:HD2	1.27	0.80
1:A:113:ARG:NH1	1:A:116[A]:GLU:OE1	2.16	0.77
1:D:34:ASP:OD2	7:D:501:HOH:O	2.02	0.77
1:C:145:ARG:HE	1:C:293:HIS:CE1	2.06	0.73
1:C:241:ALA:O	1:C:245:ARG:HG3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:VAL:CG1	1:A:86:GLU:O	2.39	0.71
1:B:241:ALA:O	1:B:245:ARG:HG3	1.92	0.68
1:D:124[A]:GLU:OE2	1:D:197:ARG:NH2	2.24	0.68
1:D:145:ARG:HE	1:D:293:HIS:CE1	2.12	0.68
1:A:145:ARG:HE	1:A:293:HIS:CE1	2.12	0.67
1:C:159:GLU:H	1:C:226:HIS:CD2	2.12	0.66
1:D:159:GLU:H	1:D:226:HIS:CD2	2.06	0.66
1:C:145:ARG:HE	1:C:293:HIS:HE1	1.44	0.65
1:B:145:ARG:HE	1:B:293:HIS:CE1	2.15	0.65
1:D:11:ASN:ND2	7:D:502:HOH:O	2.30	0.65
1:D:241:ALA:O	1:D:245:ARG:HG2	1.97	0.64
1:B:336:LEU:HD12	1:B:336:LEU:H	1.63	0.64
1:A:10:VAL:HG11	1:A:86:GLU:O	1.97	0.63
1:B:159:GLU:H	1:B:226:HIS:CD2	2.11	0.63
1:D:20:GLU:HG3	1:D:23[A]:ARG:NH1	2.14	0.62
1:D:20:GLU:O	1:D:24:ARG:HG3	2.00	0.62
1:C:37[A]:ARG:NH1	1:D:329:GLU:OE1	2.29	0.61
1:A:159:GLU:H	1:A:226:HIS:CD2	2.15	0.60
1:A:116[A]:GLU:OE1	1:D:50:GLU:OE2	2.19	0.60
1:A:329:GLU:OE1	1:B:37[B]:ARG:NH1	2.32	0.60
5:D:403:PGE:H5	7:D:640:HOH:O	2.01	0.59
1:A:215:GLU:OE2	1:A:340:ARG:NE	2.37	0.58
1:A:215:GLU:OE2	1:A:340:ARG:CD	2.52	0.57
1:D:241:ALA:O	1:D:245:ARG:CG	2.52	0.57
1:B:334:ALA:HB1	1:B:336:LEU:HD11	1.87	0.55
1:B:336:LEU:HD12	1:B:336:LEU:N	2.21	0.55
1:B:91:ARG:NH1	1:D:119:LEU:HD23	2.22	0.55
1:B:288:LEU:HG	1:B:326:ILE:HG12	1.89	0.54
1:A:10:VAL:HG13	1:A:88:PRO:HD3	1.91	0.52
1:D:145:ARG:HE	1:D:293:HIS:HE1	1.58	0.51
1:B:106:VAL:HG13	7:B:639:HOH:O	2.11	0.51
1:A:215:GLU:OE2	1:A:340:ARG:HD2	2.09	0.51
1:D:159:GLU:N	1:D:226:HIS:HD2	1.97	0.50
1:D:306:ALA:HB2	1:D:351:THR:HB	1.93	0.50
1:A:215:GLU:CD	1:A:340:ARG:HE	2.15	0.50
1:B:145:ARG:HE	1:B:293:HIS:HE1	1.56	0.50
1:B:159:GLU:OE1	1:B:181:ARG:HG2	2.12	0.49
1:A:77:VAL:CG1	1:A:311:PRO:HB2	2.42	0.49
1:A:288:LEU:HG	1:A:326:ILE:HG12	1.92	0.49
1:B:207:GLU:OE2	1:B:209:HIS:HE1	1.96	0.49
1:A:279:LEU:HD12	1:B:279:LEU:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:ALA:HB2	1:B:351:THR:HB	1.95	0.48
1:C:11:ASN:N	1:C:11:ASN:OD1	2.46	0.48
1:D:301:ILE:O	1:D:304:MET:HG2	2.13	0.48
1:A:37[A]:ARG:HD3	7:A:501:HOH:O	2.12	0.47
1:A:218:PRO:HG2	1:A:221:TRP:CZ3	2.50	0.47
1:D:115:ALA:O	1:D:119:LEU:HD22	2.15	0.46
1:A:140[B]:GLU:HG3	7:A:602:HOH:O	2.14	0.46
1:A:116[B]:GLU:H	1:A:116[B]:GLU:CD	2.18	0.46
1:A:46:ARG:HG2	1:A:82:ASP:OD1	2.16	0.46
1:A:116[B]:GLU:OE2	1:D:318:LYS:CE	2.59	0.45
1:B:133:ASP:OD1	4:B:402:N4P:N1	2.49	0.45
1:D:236:PRO:HG3	5:D:403:PGE:C6	2.47	0.45
1:A:189:PRO:O	1:A:193:ARG:HG3	2.16	0.45
1:A:10:VAL:HG11	1:A:87:VAL:HA	1.99	0.44
1:A:10:VAL:HG12	1:A:86:GLU:O	2.16	0.44
1:A:346[A]:GLN:HG2	1:A:353:TYR:CD1	2.53	0.44
1:A:53:ARG:HH21	5:A:404:PGE:C4	2.31	0.44
1:C:76:ARG:HG2	1:C:82:ASP:HB2	1.99	0.44
1:C:306:ALA:HB2	1:C:351:THR:HB	2.00	0.44
1:B:131:ASP:N	1:B:131:ASP:OD1	2.51	0.44
1:D:288:LEU:HG	1:D:326:ILE:HG12	2.00	0.43
1:C:137:VAL:HA	1:C:295:TYR:HA	1.99	0.43
1:A:20:GLU:O	1:A:24:ARG:HG3	2.18	0.43
1:B:241:ALA:O	1:B:245:ARG:CG	2.62	0.43
1:D:24:ARG:NH2	7:D:507:HOH:O	2.52	0.43
1:D:137:VAL:HA	1:D:295:TYR:HA	2.00	0.43
1:A:301:ILE:HG23	1:A:302:GLU:N	2.33	0.43
1:D:236:PRO:HG3	5:D:403:PGE:H62	2.01	0.43
1:D:161:LEU:O	1:D:228:PHE:HA	2.19	0.42
1:D:273:ASP:HB3	5:D:403:PGE:H52	2.02	0.42
1:D:185:LEU:HD21	1:D:221:TRP:CZ3	2.55	0.42
1:B:262:THR:HG22	1:B:323:SER:HB3	2.02	0.42
1:C:279:LEU:CD1	1:D:279:LEU:HD12	2.50	0.41
1:C:288:LEU:HG	1:C:326:ILE:HG12	2.01	0.41
1:B:276:ARG:NH2	1:B:276:ARG:HG2	2.36	0.41
1:D:288:LEU:C	1:D:288:LEU:HD23	2.41	0.41
1:A:53:ARG:HD2	5:A:404:PGE:C6	2.51	0.40
1:B:83:LEU:HD23	1:B:83:LEU:HA	1.93	0.40
1:A:10:VAL:HG13	1:A:10:VAL:O	2.21	0.40
1:A:53:ARG:NH2	5:A:404:PGE:H62	2.36	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	348/374 (93%)	336 (97%)	12 (3%)	0	100	100
1	B	346/374 (92%)	337 (97%)	9 (3%)	0	100	100
1	C	347/374 (93%)	336 (97%)	11 (3%)	0	100	100
1	D	349/374 (93%)	339 (97%)	10 (3%)	0	100	100
All	All	1390/1496 (93%)	1348 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	278/296 (94%)	268 (96%)	10 (4%)	35	11
1	B	276/296 (93%)	268 (97%)	8 (3%)	42	16
1	C	277/296 (94%)	269 (97%)	8 (3%)	42	16
1	D	279/296 (94%)	273 (98%)	6 (2%)	52	27
All	All	1110/1184 (94%)	1078 (97%)	32 (3%)	43	16

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	108[A]	GLU

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Mol	Chain	Res	Type
1	A	108[B]	GLU
1	A	109	ARG
1	A	131	ASP
1	A	276	ARG
1	A	301	ILE
1	A	336	LEU
1	A	337	GLU
1	A	340	ARG
1	B	46	ARG
1	B	101	GLU
1	B	131	ASP
1	B	276	ARG
1	B	318	LYS
1	B	331	LEU
1	B	332	ARG
1	B	337	GLU
1	C	11	ASN
1	C	17[A]	GLN
1	C	17[B]	GLN
1	C	76	ARG
1	C	78	GLU
1	C	79	GLU
1	C	105	LEU
1	C	116	GLU
1	D	24	ARG
1	D	78	GLU
1	D	105	LEU
1	D	109	ARG
1	D	119	LEU
1	D	131	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	HIS
1	A	293	HIS
1	A	297	ASN
1	B	209	HIS
1	B	226	HIS
1	B	293	HIS
1	C	11	ASN
1	C	226	HIS

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Mol	Chain	Res	Type
1	C	293	HIS
1	C	297	ASN
1	D	226	HIS
1	D	293	HIS
1	D	297	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 for Mogul analysis.

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	$\#\|Z\| > 2$
6	PEG	B	406	-	6,6,6	0.63	0	5,5,5	0.48	0
3	MTA	B	401	-	19,22,22	1.32	2 (10%)	19,32,32	2.09	8 (42%)
4	N4P	A	403	-	13,13,13	0.58	0	13,13,13	1.30	1 (7%)
6	PEG	A	405	-	6,6,6	0.40	0	5,5,5	0.63	0
6	PEG	D	405	-	6,6,6	0.35	0	5,5,5	0.43	0
5	PGE	A	404	-	9,9,9	0.70	0	8,8,8	1.26	1 (12%)
6	PEG	C	405	-	6,6,6	0.32	0	5,5,5	0.61	0
6	PEG	B	407	-	6,6,6	0.39	0	5,5,5	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PGE	B	403	-	9,9,9	0.68	0	8,8,8	0.78	0
4	N4P	D	402	-	13,13,13	0.86	1 (7%)	13,13,13	2.10	3 (23%)
6	PEG	B	405	-	6,6,6	0.66	0	5,5,5	1.58	2 (40%)
6	PEG	D	404	-	6,6,6	0.62	0	5,5,5	0.24	0
3	MTA	C	402	-	19,22,22	1.70	4 (21%)	19,32,32	2.13	8 (42%)
3	MTA	D	401	-	19,22,22	1.14	1 (5%)	19,32,32	1.47	3 (15%)
5	PGE	D	403	-	9,9,9	0.45	0	8,8,8	0.64	0
4	N4P	B	402	-	13,13,13	0.63	0	13,13,13	2.08	4 (30%)
3	MTA	A	402	-	19,22,22	1.24	2 (10%)	19,32,32	1.61	5 (26%)
6	PEG	B	404	-	6,6,6	0.36	0	5,5,5	0.51	0
6	PEG	C	404	-	6,6,6	0.37	0	5,5,5	0.72	0
4	N4P	C	403	-	13,13,13	0.76	0	13,13,13	1.78	3 (23%)

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
6	PEG	B	406	-	-	4/4/4/4	-
3	MTA	B	401	-	-	0/3/23/23	0/3/3/3
4	N4P	A	403	-	-	1/13/13/13	-
6	PEG	A	405	-	-	2/4/4/4	-
6	PEG	D	405	-	-	3/4/4/4	-
5	PGE	A	404	-	-	3/7/7/7	-
6	PEG	C	405	-	-	0/4/4/4	-
6	PEG	B	407	-	-	2/4/4/4	-
5	PGE	B	403	-	-	1/7/7/7	-
4	N4P	D	402	-	-	1/13/13/13	-
6	PEG	B	405	-	-	3/4/4/4	-
6	PEG	D	404	-	-	0/4/4/4	-
3	MTA	C	402	-	-	0/3/23/23	0/3/3/3
3	MTA	D	401	-	-	0/3/23/23	0/3/3/3
5	PGE	D	403	-	-	4/7/7/7	-
4	N4P	B	402	-	-	3/13/13/13	-
3	MTA	A	402	-	-	0/3/23/23	0/3/3/3
6	PEG	B	404	-	-	1/4/4/4	-
6	PEG	C	404	-	-	2/4/4/4	-
4	N4P	C	403	-	-	2/13/13/13	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	MTA	O4'-C1'	4.06	1.46	1.41
3	B	401	MTA	C5'-S5'	-3.90	1.75	1.80
3	C	402	MTA	C4-N3	-3.66	1.30	1.35
3	C	402	MTA	O4'-C1'	3.60	1.46	1.41
3	C	402	MTA	C5'-S5'	-3.21	1.76	1.80
3	B	401	MTA	O4'-C1'	2.46	1.44	1.41
3	A	402	MTA	C5-C4	2.17	1.46	1.40
3	C	402	MTA	C2-N3	2.10	1.35	1.32
4	D	402	N4P	C11-N6	2.05	1.52	1.47
3	D	401	MTA	C5-C4	2.03	1.46	1.40

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	402	N4P	C7-N6-C5	-5.44	98.51	111.44
4	B	402	N4P	C7-N6-C5	-5.37	98.67	111.44
4	C	403	N4P	C11-N6-C5	-4.50	100.75	111.44
3	C	402	MTA	N3-C2-N1	-4.30	121.96	128.68
3	C	402	MTA	N6-C6-N1	4.02	126.93	118.57
3	B	401	MTA	N3-C2-N1	-3.78	122.77	128.68
3	C	402	MTA	C2-N1-C6	3.56	124.85	118.75
3	B	401	MTA	N6-C6-N1	3.41	125.66	118.57
4	B	402	N4P	C7-C8-C9	-3.28	101.23	113.85
3	B	401	MTA	C2-N1-C6	3.23	124.29	118.75
3	B	401	MTA	C3'-C2'-C1'	3.00	105.49	100.98
4	D	402	N4P	C12-C11-N6	-2.97	106.35	113.84
4	A	403	N4P	C12-C11-N6	-2.91	106.52	113.84
3	A	402	MTA	C3'-C2'-C1'	2.87	105.29	100.98
4	C	403	N4P	C7-N6-C5	2.82	118.14	111.44
3	A	402	MTA	N3-C2-N1	-2.79	124.31	128.68
3	B	401	MTA	O4'-C1'-C2'	-2.78	102.87	106.93
3	B	401	MTA	C1'-N9-C4	-2.74	121.83	126.64
3	D	401	MTA	C3'-C2'-C1'	2.72	105.07	100.98
5	A	404	PGE	O3-C4-C3	2.70	122.56	110.39
3	A	402	MTA	O2'-C2'-C3'	2.68	120.49	111.82
4	B	402	N4P	C4-C5-N6	-2.62	107.25	113.84
3	A	402	MTA	C1'-N9-C4	-2.61	122.05	126.64
4	D	402	N4P	C11-N6-C5	2.60	117.62	111.44
3	C	402	MTA	C5-C6-N1	-2.55	114.56	120.35
3	D	401	MTA	O4'-C1'-C2'	-2.55	103.21	106.93
3	A	402	MTA	O4'-C1'-C2'	-2.51	103.26	106.93
3	C	402	MTA	O4'-C1'-C2'	-2.47	103.32	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	405	PEG	O2-C2-C1	2.33	120.31	110.07
3	C	402	MTA	CS-S5'-C5'	-2.32	97.04	101.30
3	B	401	MTA	O4'-C4'-C3'	2.19	109.44	105.11
4	C	403	N4P	C12-C11-N6	-2.11	108.52	113.84
3	C	402	MTA	O4'-C4'-C3'	2.10	109.26	105.11
6	B	405	PEG	C3-O2-C2	2.08	122.30	113.29
4	B	402	N4P	C11-N6-C7	2.07	116.36	111.44
3	B	401	MTA	C5-C6-N1	-2.04	115.72	120.35
3	D	401	MTA	N3-C2-N1	-2.02	125.52	128.68
3	C	402	MTA	C1'-N9-C4	-2.00	123.13	126.64

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	404	PEG	O1-C1-C2-O2
6	A	405	PEG	C1-C2-O2-C3
5	A	404	PGE	O2-C3-C4-O3
5	A	404	PGE	C6-C5-O3-C4
4	C	403	N4P	N6-C7-C8-C9
5	D	403	PGE	O1-C1-C2-O2
6	B	406	PEG	O2-C3-C4-O4
6	B	407	PEG	O2-C3-C4-O4
4	B	402	N4P	C8-C7-N6-C11
5	D	403	PGE	O3-C5-C6-O4
6	D	405	PEG	O2-C3-C4-O4
5	D	403	PGE	O2-C3-C4-O3
4	B	402	N4P	N1-C2-C3-C4
6	B	405	PEG	O1-C1-C2-O2
6	B	406	PEG	O1-C1-C2-O2
6	A	405	PEG	O2-C3-C4-O4
6	D	405	PEG	O1-C1-C2-O2
5	A	404	PGE	C4-C3-O2-C2
5	D	403	PGE	C1-C2-O2-C3
6	B	406	PEG	C4-C3-O2-C2
6	D	405	PEG	C1-C2-O2-C3
6	C	404	PEG	C1-C2-O2-C3
4	A	403	N4P	C2-C3-C4-C5
6	B	405	PEG	O2-C3-C4-O4
5	B	403	PGE	C1-C2-O2-C3
4	C	403	N4P	C11-C12-C13-N14
6	B	405	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
6	B	404	PEG	C1-C2-O2-C3
4	D	402	N4P	C7-C8-C9-N10
6	B	406	PEG	C1-C2-O2-C3
6	B	407	PEG	O1-C1-C2-O2
4	B	402	N4P	C4-C5-N6-C11

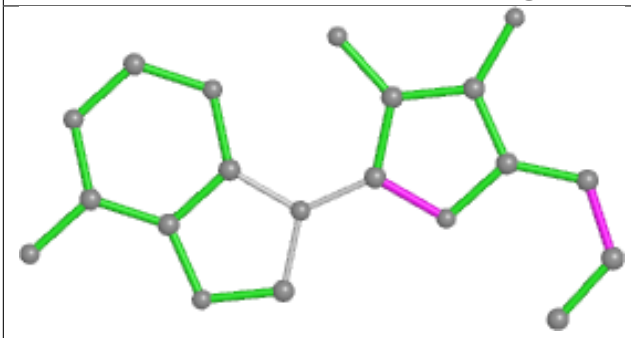
There are no ring outliers.

3 monomers are involved in 8 short contacts:

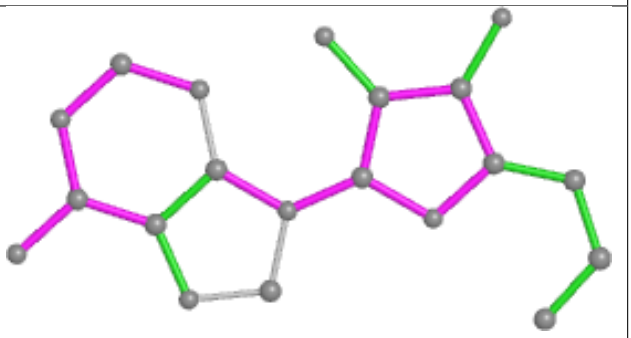
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	404	PGE	3	0
5	D	403	PGE	4	0
4	B	402	N4P	1	0

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.

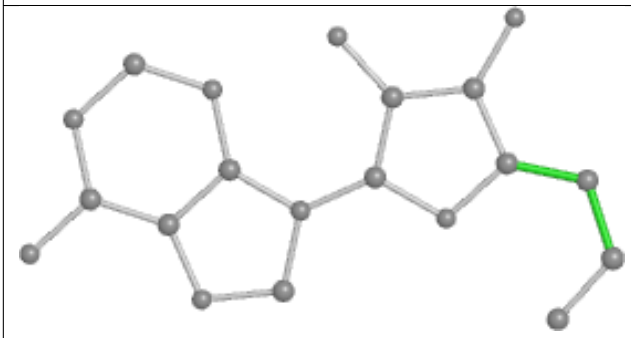
Ligand MTA B 401



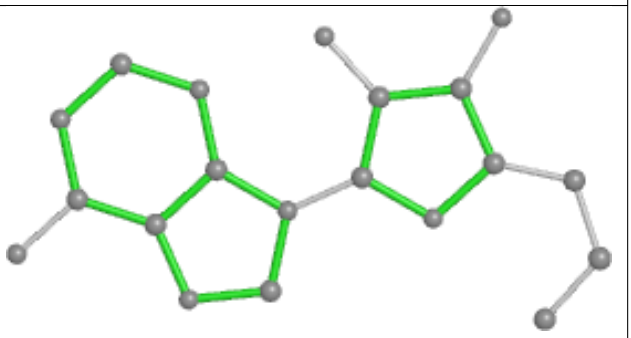
Bond lengths



Bond angles

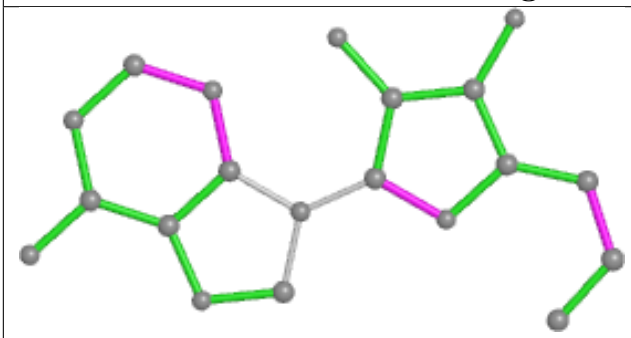


Torsions

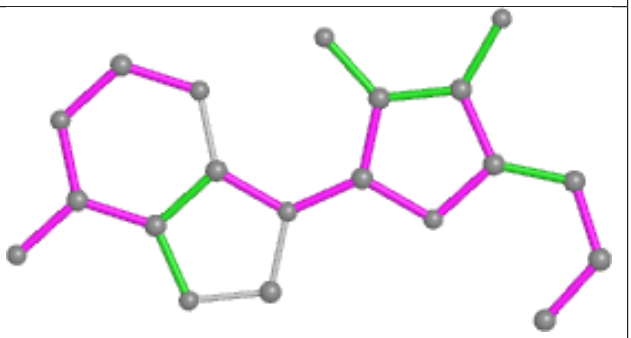


Rings

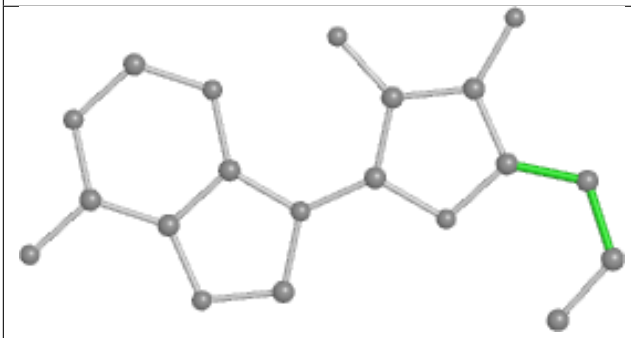
Ligand MTA C 402



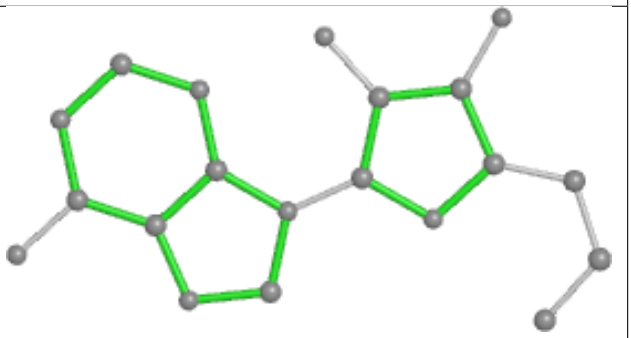
Bond lengths



Bond angles

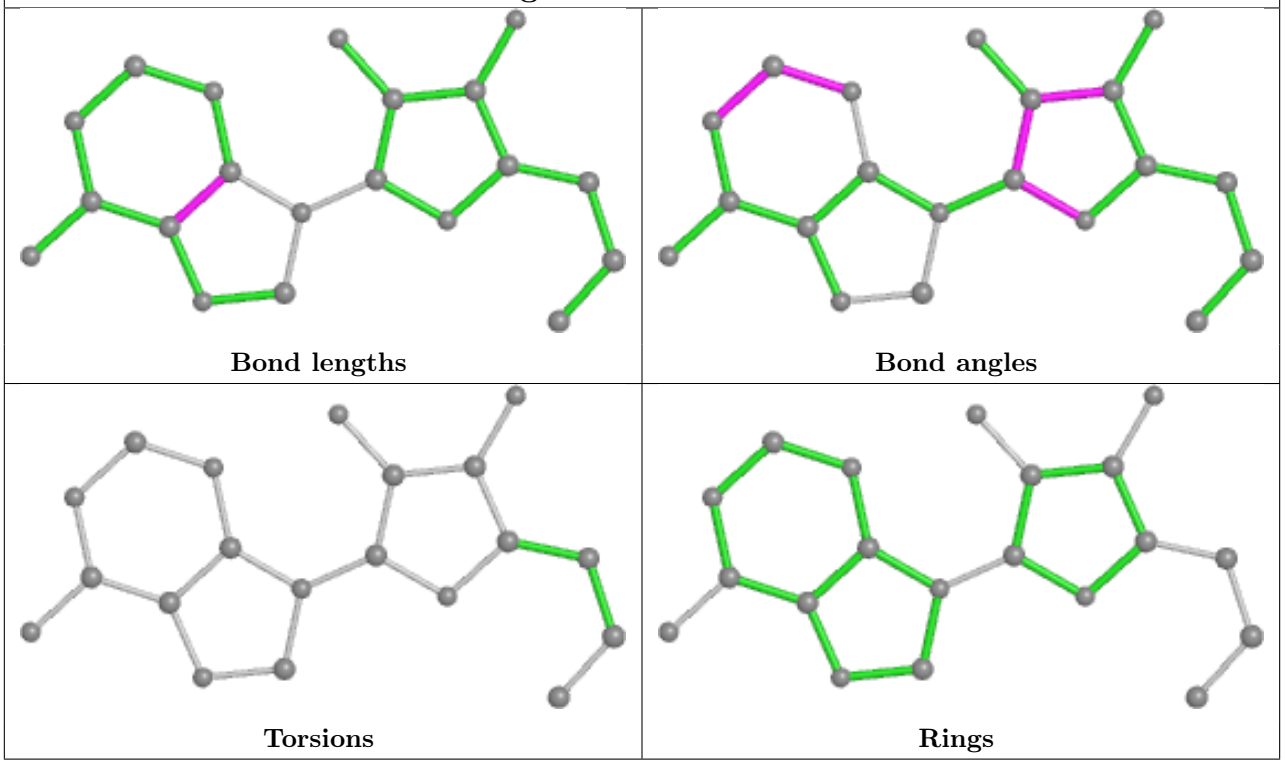


Torsions

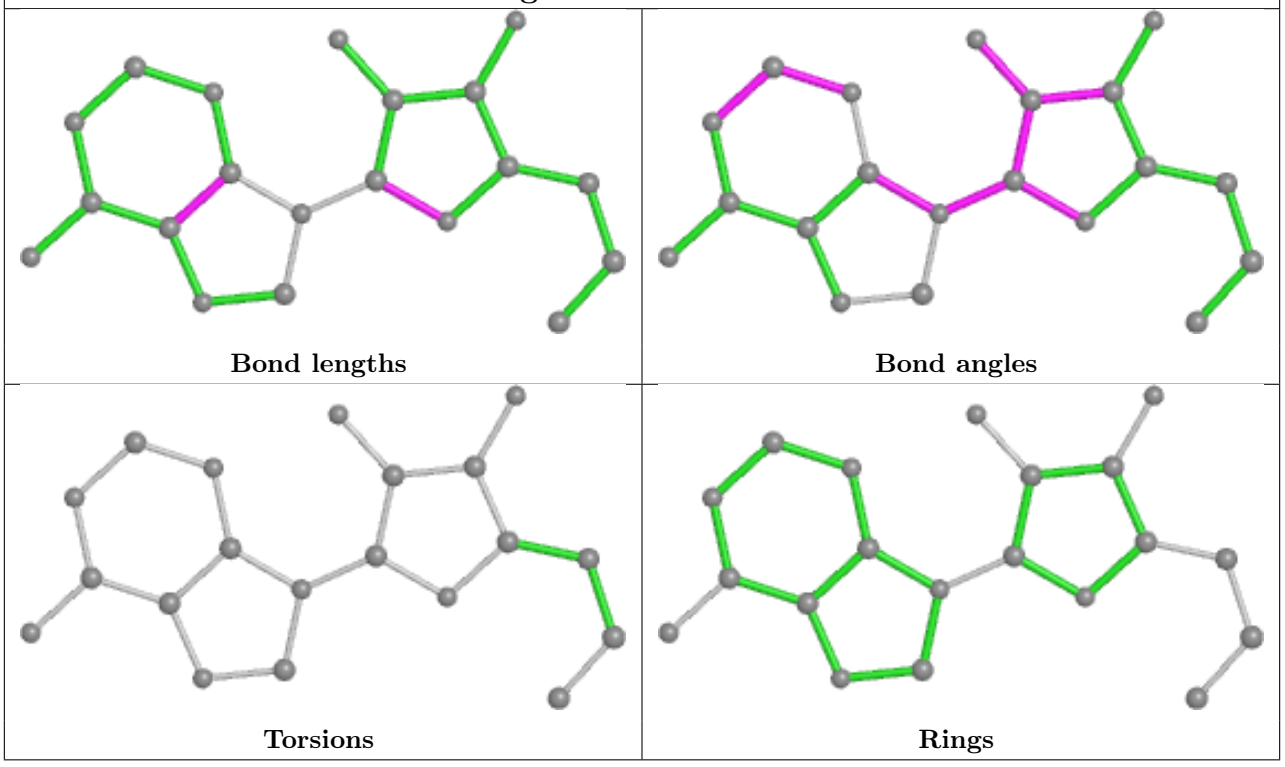


Rings

Ligand MTA D 401



Ligand MTA A 402



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, 95^{th} 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	344/374 (91%)	-0.27	5 (1%)	73	77	17, 25, 45, 60	0
1	B	344/374 (91%)	-0.29	2 (0%)	89	90	17, 25, 43, 70	0
1	C	343/374 (91%)	-0.20	4 (1%)	79	81	16, 25, 44, 70	0
1	D	344/374 (91%)	-0.30	3 (0%)	84	86	16, 24, 43, 61	0
All	All	1375/1496 (91%)	-0.26	14 (1%)	82	85	16, 25, 44, 70	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	11	ASN	4.4
1	C	88	PRO	4.3
1	B	11	ASN	3.7
1	C	85	ALA	3.2
1	A	88	PRO	3.0
1	A	86	GLU	2.9
1	A	87	VAL	2.7
1	B	24	ARG	2.6
1	A	10	VAL	2.6
1	D	10	VAL	2.5
1	D	86	GLU	2.5
1	C	288	LEU	2.3
1	A	84	LEU	2.2
1	D	342	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

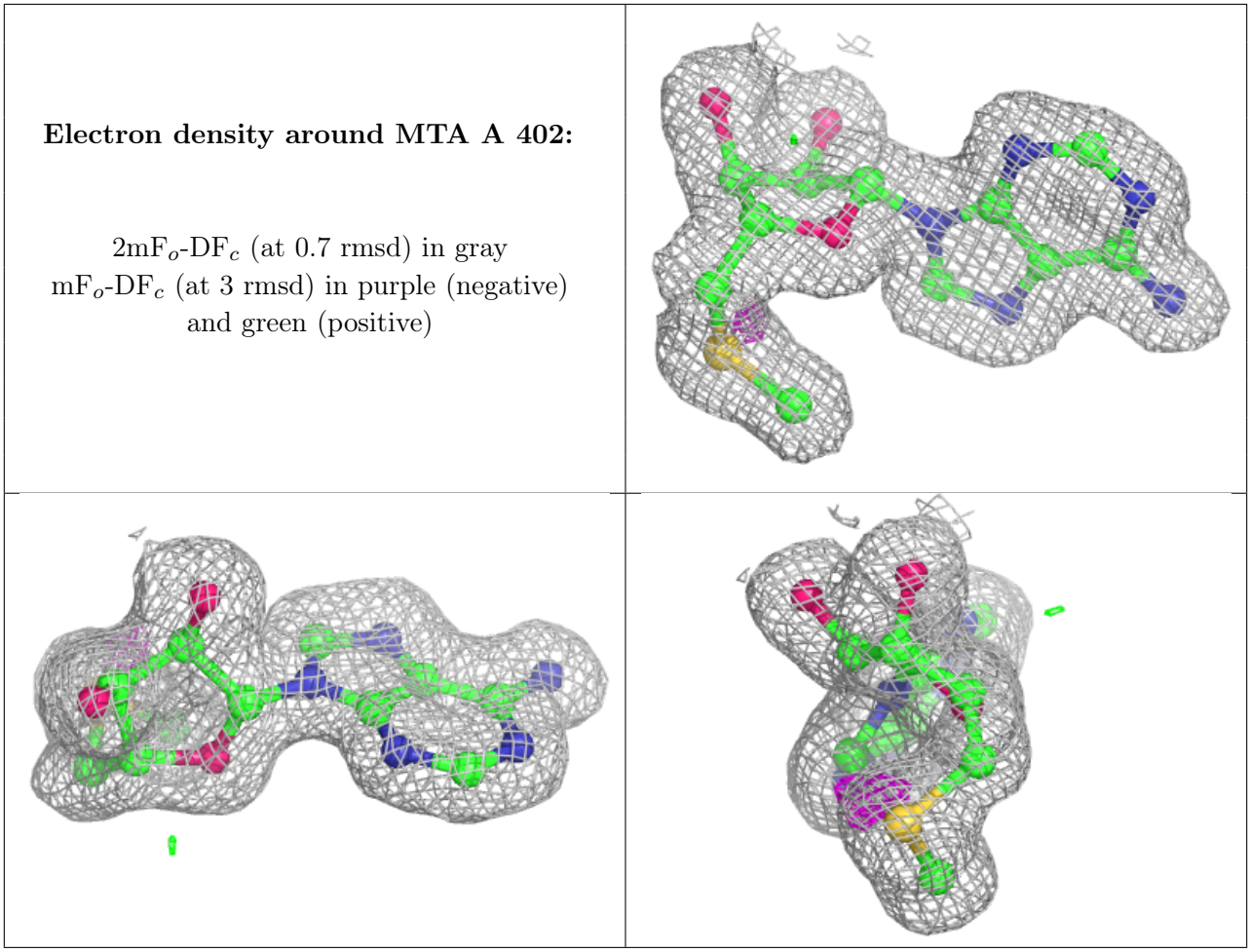
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	PEG	B	405	7/7	0.67	0.21	46,49,51,57	0
6	PEG	B	406	7/7	0.78	0.17	55,57,60,60	0
5	PGE	D	403	10/10	0.88	0.10	36,43,48,53	0
6	PEG	A	405	7/7	0.89	0.11	32,40,47,51	0
6	PEG	D	405	7/7	0.89	0.11	45,53,54,55	0
6	PEG	C	404	7/7	0.90	0.15	35,40,45,50	0
6	PEG	B	404	7/7	0.90	0.11	42,43,44,51	0
6	PEG	B	407	7/7	0.91	0.10	50,53,57,58	0
5	PGE	B	403	10/10	0.92	0.09	36,48,51,53	0
5	PGE	A	404	10/10	0.93	0.09	34,40,49,51	0
6	PEG	C	405	7/7	0.93	0.09	35,39,42,43	0
6	PEG	D	404	7/7	0.93	0.06	33,38,46,46	0
4	N4P	A	403	14/14	0.93	0.12	24,27,32,33	0
4	N4P	C	403	14/14	0.94	0.11	22,27,33,33	0
4	N4P	D	402	14/14	0.94	0.10	22,26,31,31	0
4	N4P	B	402	14/14	0.95	0.11	22,28,33,34	0
3	MTA	A	402	20/20	0.97	0.05	19,20,23,24	0
3	MTA	C	402	20/20	0.97	0.06	19,21,24,26	0
3	MTA	B	401	20/20	0.98	0.06	18,20,25,27	0
3	MTA	D	401	20/20	0.98	0.05	18,20,23,24	0
2	FE	A	401	1/1	0.99	0.03	26,26,26,26	0
2	FE	C	401	1/1	1.00	0.03	22,22,22,22	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.

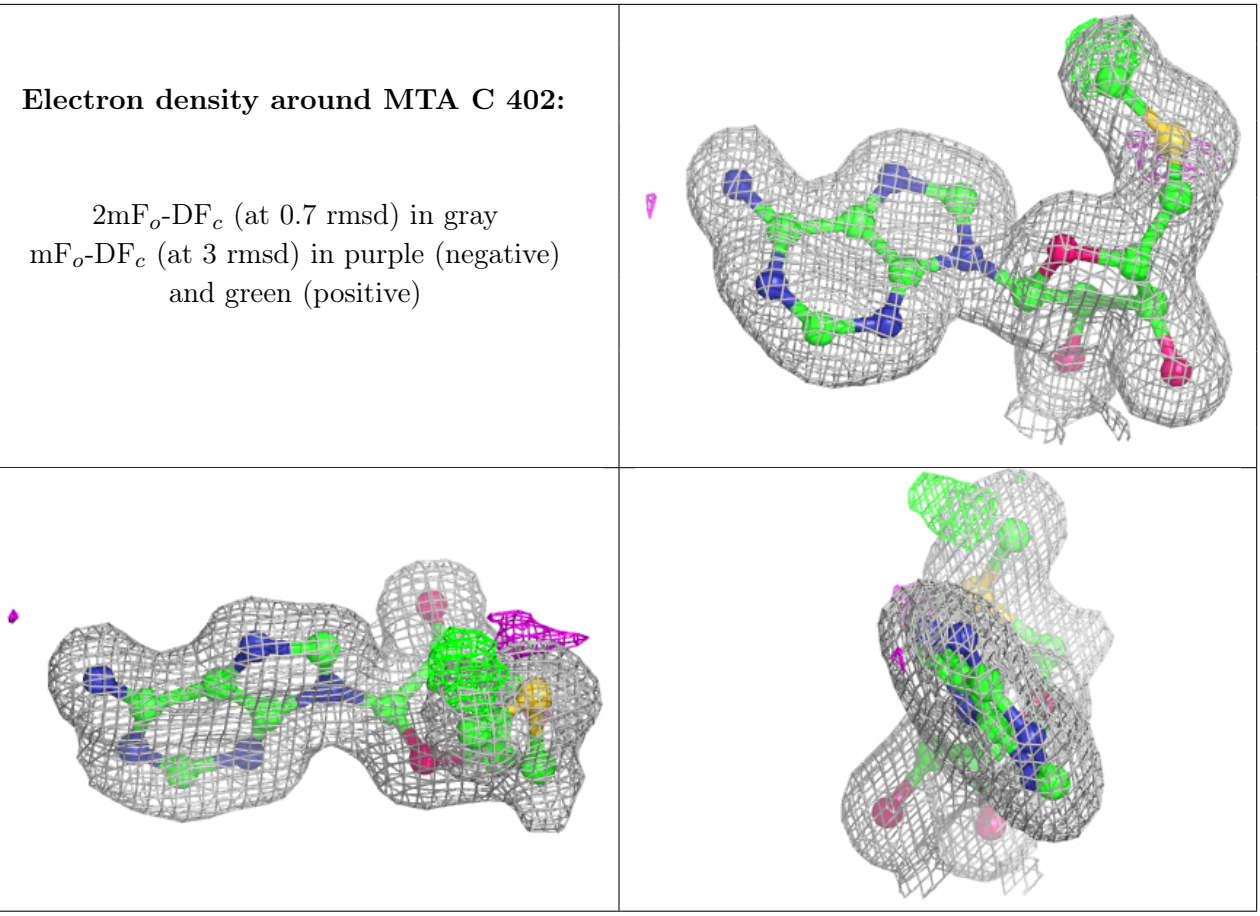
Electron density around MTA A 402:

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



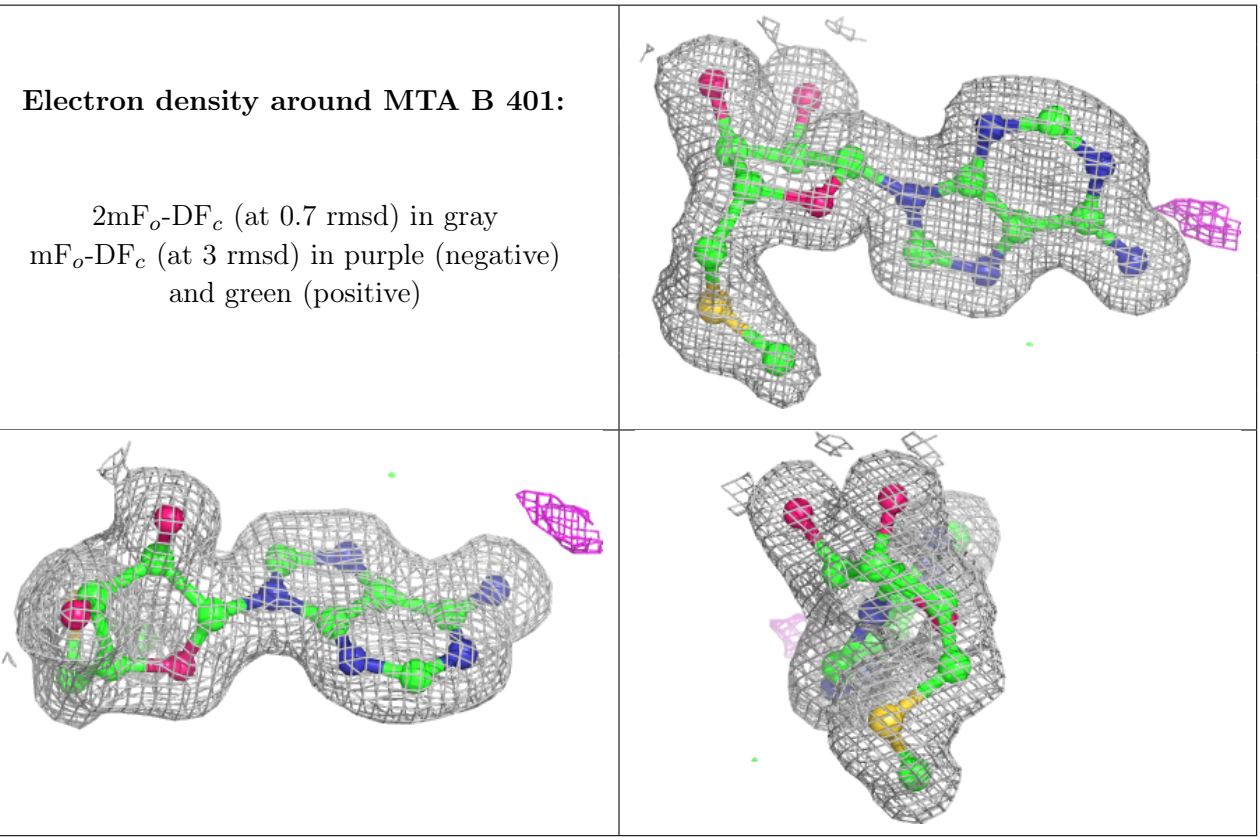
Electron density around MTA C 402:

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



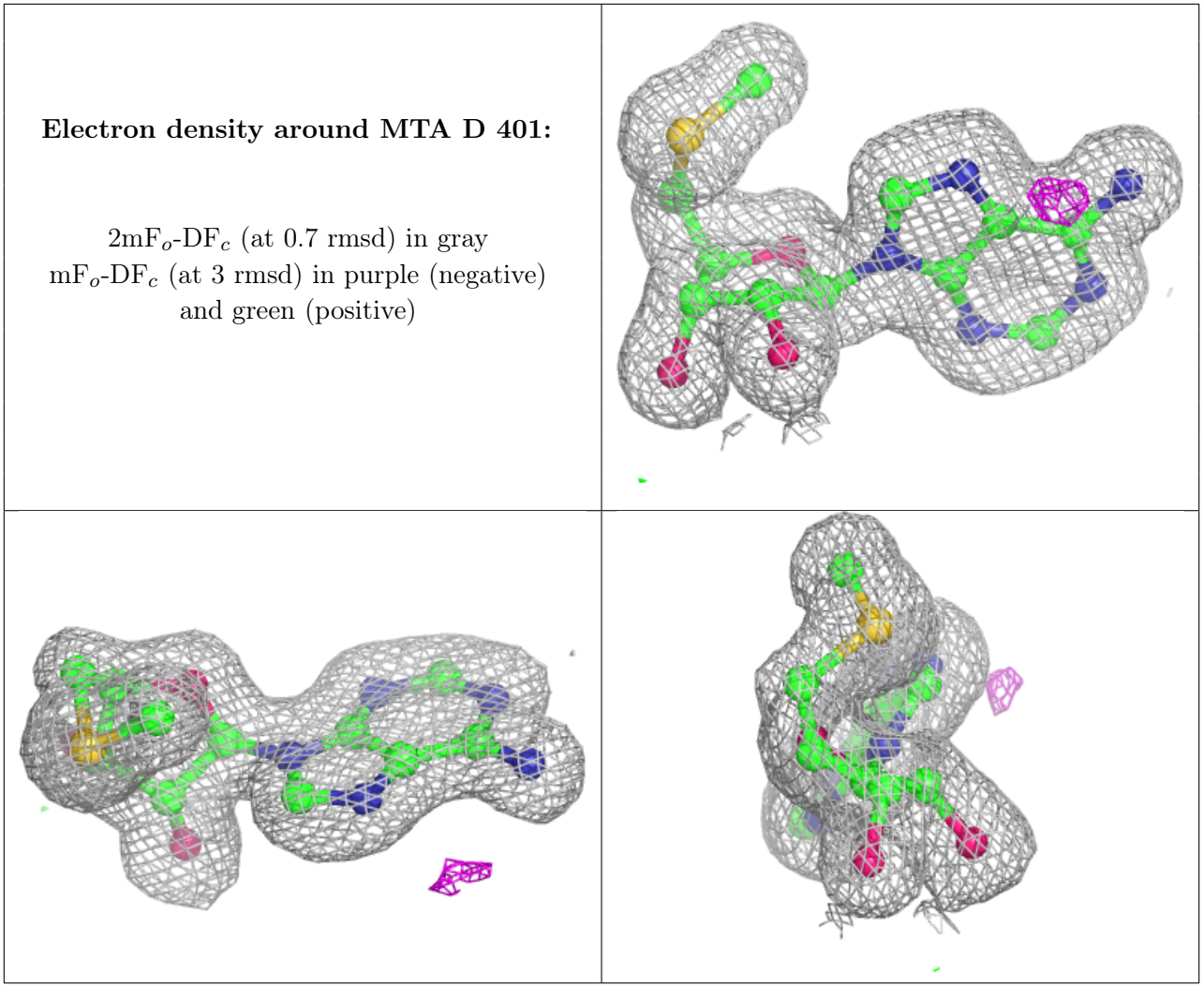
Electron density around MTA B 401:

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



Electron density around MTA D 401:

$2mF_o$-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

There are no such residues in this entry.