



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:08 PM UTC

PDB ID : 5XNC / pdb_00005xnc
Title : Crystal structure of the branched-chain polyamine synthase (BpsA) in complex with N4-aminopropylspermidine and 5-methylthioadenosine
Authors : Mizohata, E.; Tse, K.M.; Fujita, J.; Inoue, T.
Deposited on : 2017-05-22
Resolution : 1.84 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

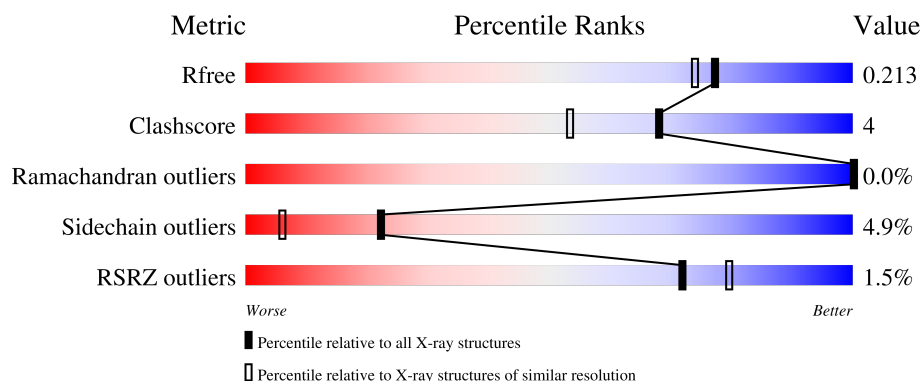
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	371	77% 16% .. 5%
1	B	371	74% 17% • 5%
1	C	371	78% 16% • 5%
1	D	371	78% 15% • 5%
1	E	371	82% 11% • 5%

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Mol	Chain	Length	Quality of chain
1	F	371	2% 77% 16% • • 5%
1	G	371	3% 81% 11% • 5%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 21380 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	353	Total	C	N	O	S	0	2	0
			2868	1831	477	553	7			
1	B	354	Total	C	N	O	S	0	0	0
			2860	1825	478	550	7			
1	C	353	Total	C	N	O	S	0	1	0
			2862	1827	477	551	7			
1	D	353	Total	C	N	O	S	0	1	0
			2857	1827	477	551	2			
1	E	353	Total	C	N	O	S	0	1	0
			2862	1827	477	551	7			
1	F	353	Total	C	N	O	S	0	0	0
			2856	1823	477	549	7			
1	G	353	Total	C	N	O	S	0	0	0
			2856	1823	477	549	7			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q5JIZ3
A	-18	GLY	-	expression tag	UNP Q5JIZ3
A	-17	SER	-	expression tag	UNP Q5JIZ3
A	-16	SER	-	expression tag	UNP Q5JIZ3
A	-15	HIS	-	expression tag	UNP Q5JIZ3
A	-14	HIS	-	expression tag	UNP Q5JIZ3
A	-13	HIS	-	expression tag	UNP Q5JIZ3
A	-12	HIS	-	expression tag	UNP Q5JIZ3
A	-11	HIS	-	expression tag	UNP Q5JIZ3
A	-10	HIS	-	expression tag	UNP Q5JIZ3
A	-9	SER	-	expression tag	UNP Q5JIZ3
A	-8	SER	-	expression tag	UNP Q5JIZ3
A	-7	GLY	-	expression tag	UNP Q5JIZ3
A	-6	LEU	-	expression tag	UNP Q5JIZ3
A	-5	VAL	-	expression tag	UNP Q5JIZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	PRO	-	expression tag	UNP Q5JIZ3
A	-3	ARG	-	expression tag	UNP Q5JIZ3
A	-2	GLY	-	expression tag	UNP Q5JIZ3
A	-1	SER	-	expression tag	UNP Q5JIZ3
A	0	HIS	-	expression tag	UNP Q5JIZ3
B	-19	MET	-	expression tag	UNP Q5JIZ3
B	-18	GLY	-	expression tag	UNP Q5JIZ3
B	-17	SER	-	expression tag	UNP Q5JIZ3
B	-16	SER	-	expression tag	UNP Q5JIZ3
B	-15	HIS	-	expression tag	UNP Q5JIZ3
B	-14	HIS	-	expression tag	UNP Q5JIZ3
B	-13	HIS	-	expression tag	UNP Q5JIZ3
B	-12	HIS	-	expression tag	UNP Q5JIZ3
B	-11	HIS	-	expression tag	UNP Q5JIZ3
B	-10	HIS	-	expression tag	UNP Q5JIZ3
B	-9	SER	-	expression tag	UNP Q5JIZ3
B	-8	SER	-	expression tag	UNP Q5JIZ3
B	-7	GLY	-	expression tag	UNP Q5JIZ3
B	-6	LEU	-	expression tag	UNP Q5JIZ3
B	-5	VAL	-	expression tag	UNP Q5JIZ3
B	-4	PRO	-	expression tag	UNP Q5JIZ3
B	-3	ARG	-	expression tag	UNP Q5JIZ3
B	-2	GLY	-	expression tag	UNP Q5JIZ3
B	-1	SER	-	expression tag	UNP Q5JIZ3
B	0	HIS	-	expression tag	UNP Q5JIZ3
C	-19	MET	-	expression tag	UNP Q5JIZ3
C	-18	GLY	-	expression tag	UNP Q5JIZ3
C	-17	SER	-	expression tag	UNP Q5JIZ3
C	-16	SER	-	expression tag	UNP Q5JIZ3
C	-15	HIS	-	expression tag	UNP Q5JIZ3
C	-14	HIS	-	expression tag	UNP Q5JIZ3
C	-13	HIS	-	expression tag	UNP Q5JIZ3
C	-12	HIS	-	expression tag	UNP Q5JIZ3
C	-11	HIS	-	expression tag	UNP Q5JIZ3
C	-10	HIS	-	expression tag	UNP Q5JIZ3
C	-9	SER	-	expression tag	UNP Q5JIZ3
C	-8	SER	-	expression tag	UNP Q5JIZ3
C	-7	GLY	-	expression tag	UNP Q5JIZ3
C	-6	LEU	-	expression tag	UNP Q5JIZ3
C	-5	VAL	-	expression tag	UNP Q5JIZ3
C	-4	PRO	-	expression tag	UNP Q5JIZ3
C	-3	ARG	-	expression tag	UNP Q5JIZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP Q5JIZ3
C	-1	SER	-	expression tag	UNP Q5JIZ3
C	0	HIS	-	expression tag	UNP Q5JIZ3
D	-19	MET	-	expression tag	UNP Q5JIZ3
D	-18	GLY	-	expression tag	UNP Q5JIZ3
D	-17	SER	-	expression tag	UNP Q5JIZ3
D	-16	SER	-	expression tag	UNP Q5JIZ3
D	-15	HIS	-	expression tag	UNP Q5JIZ3
D	-14	HIS	-	expression tag	UNP Q5JIZ3
D	-13	HIS	-	expression tag	UNP Q5JIZ3
D	-12	HIS	-	expression tag	UNP Q5JIZ3
D	-11	HIS	-	expression tag	UNP Q5JIZ3
D	-10	HIS	-	expression tag	UNP Q5JIZ3
D	-9	SER	-	expression tag	UNP Q5JIZ3
D	-8	SER	-	expression tag	UNP Q5JIZ3
D	-7	GLY	-	expression tag	UNP Q5JIZ3
D	-6	LEU	-	expression tag	UNP Q5JIZ3
D	-5	VAL	-	expression tag	UNP Q5JIZ3
D	-4	PRO	-	expression tag	UNP Q5JIZ3
D	-3	ARG	-	expression tag	UNP Q5JIZ3
D	-2	GLY	-	expression tag	UNP Q5JIZ3
D	-1	SER	-	expression tag	UNP Q5JIZ3
D	0	HIS	-	expression tag	UNP Q5JIZ3
E	-19	MET	-	expression tag	UNP Q5JIZ3
E	-18	GLY	-	expression tag	UNP Q5JIZ3
E	-17	SER	-	expression tag	UNP Q5JIZ3
E	-16	SER	-	expression tag	UNP Q5JIZ3
E	-15	HIS	-	expression tag	UNP Q5JIZ3
E	-14	HIS	-	expression tag	UNP Q5JIZ3
E	-13	HIS	-	expression tag	UNP Q5JIZ3
E	-12	HIS	-	expression tag	UNP Q5JIZ3
E	-11	HIS	-	expression tag	UNP Q5JIZ3
E	-10	HIS	-	expression tag	UNP Q5JIZ3
E	-9	SER	-	expression tag	UNP Q5JIZ3
E	-8	SER	-	expression tag	UNP Q5JIZ3
E	-7	GLY	-	expression tag	UNP Q5JIZ3
E	-6	LEU	-	expression tag	UNP Q5JIZ3
E	-5	VAL	-	expression tag	UNP Q5JIZ3
E	-4	PRO	-	expression tag	UNP Q5JIZ3
E	-3	ARG	-	expression tag	UNP Q5JIZ3
E	-2	GLY	-	expression tag	UNP Q5JIZ3
E	-1	SER	-	expression tag	UNP Q5JIZ3

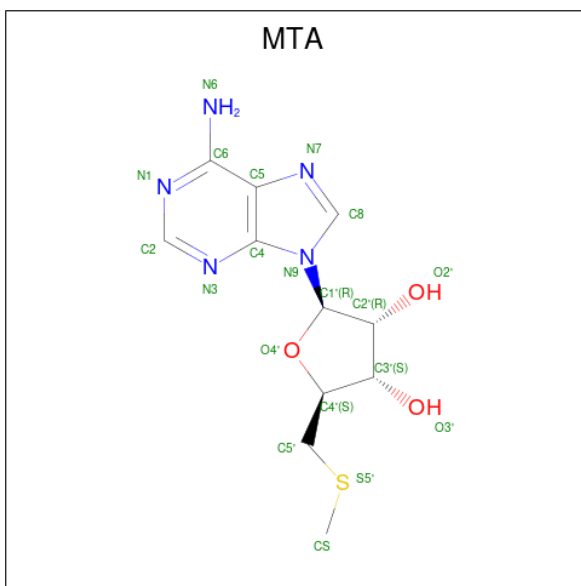
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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	HIS	-	expression tag	UNP Q5JIZ3
F	-19	MET	-	expression tag	UNP Q5JIZ3
F	-18	GLY	-	expression tag	UNP Q5JIZ3
F	-17	SER	-	expression tag	UNP Q5JIZ3
F	-16	SER	-	expression tag	UNP Q5JIZ3
F	-15	HIS	-	expression tag	UNP Q5JIZ3
F	-14	HIS	-	expression tag	UNP Q5JIZ3
F	-13	HIS	-	expression tag	UNP Q5JIZ3
F	-12	HIS	-	expression tag	UNP Q5JIZ3
F	-11	HIS	-	expression tag	UNP Q5JIZ3
F	-10	HIS	-	expression tag	UNP Q5JIZ3
F	-9	SER	-	expression tag	UNP Q5JIZ3
F	-8	SER	-	expression tag	UNP Q5JIZ3
F	-7	GLY	-	expression tag	UNP Q5JIZ3
F	-6	LEU	-	expression tag	UNP Q5JIZ3
F	-5	VAL	-	expression tag	UNP Q5JIZ3
F	-4	PRO	-	expression tag	UNP Q5JIZ3
F	-3	ARG	-	expression tag	UNP Q5JIZ3
F	-2	GLY	-	expression tag	UNP Q5JIZ3
F	-1	SER	-	expression tag	UNP Q5JIZ3
F	0	HIS	-	expression tag	UNP Q5JIZ3
G	-19	MET	-	expression tag	UNP Q5JIZ3
G	-18	GLY	-	expression tag	UNP Q5JIZ3
G	-17	SER	-	expression tag	UNP Q5JIZ3
G	-16	SER	-	expression tag	UNP Q5JIZ3
G	-15	HIS	-	expression tag	UNP Q5JIZ3
G	-14	HIS	-	expression tag	UNP Q5JIZ3
G	-13	HIS	-	expression tag	UNP Q5JIZ3
G	-12	HIS	-	expression tag	UNP Q5JIZ3
G	-11	HIS	-	expression tag	UNP Q5JIZ3
G	-10	HIS	-	expression tag	UNP Q5JIZ3
G	-9	SER	-	expression tag	UNP Q5JIZ3
G	-8	SER	-	expression tag	UNP Q5JIZ3
G	-7	GLY	-	expression tag	UNP Q5JIZ3
G	-6	LEU	-	expression tag	UNP Q5JIZ3
G	-5	VAL	-	expression tag	UNP Q5JIZ3
G	-4	PRO	-	expression tag	UNP Q5JIZ3
G	-3	ARG	-	expression tag	UNP Q5JIZ3
G	-2	GLY	-	expression tag	UNP Q5JIZ3
G	-1	SER	-	expression tag	UNP Q5JIZ3
G	0	HIS	-	expression tag	UNP Q5JIZ3

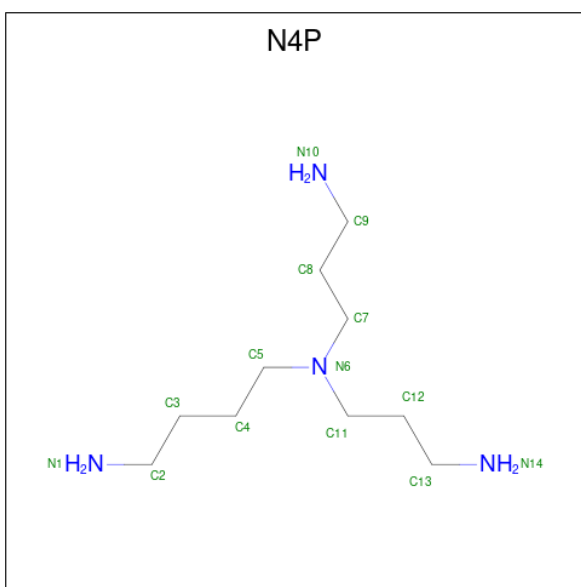
- Molecule 2 is 5'-DEOXY-5'-METHYLTHIOADENOSINE (CCD ID: MTA) (formula:

C₁₁H₁₅N₅O₃S).



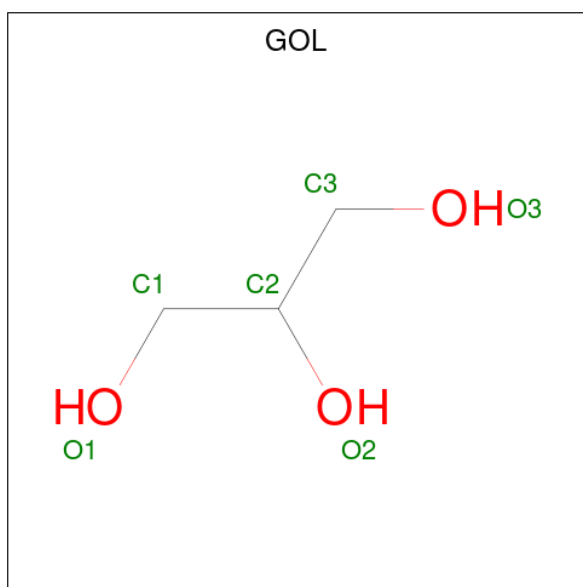
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	B	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	C	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	D	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	E	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	F	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	G	1	Total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

- Molecule 3 is N,N-bis(3-aminopropyl)butane-1,4-diamine (CCD ID: N4P) (formula: C₁₀H₂₆N₄).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

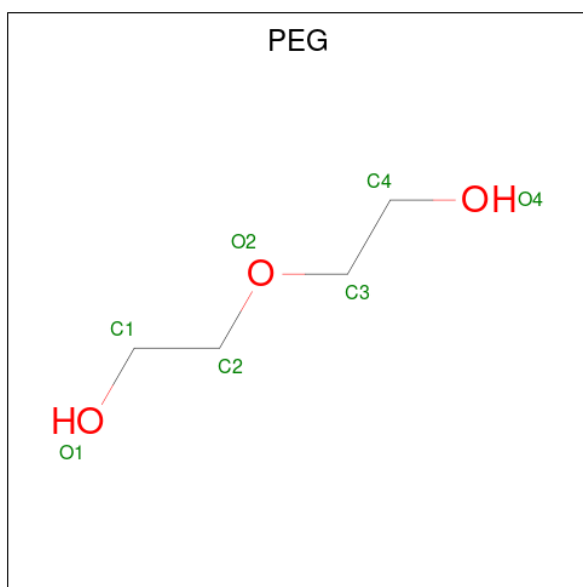


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0

- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe).

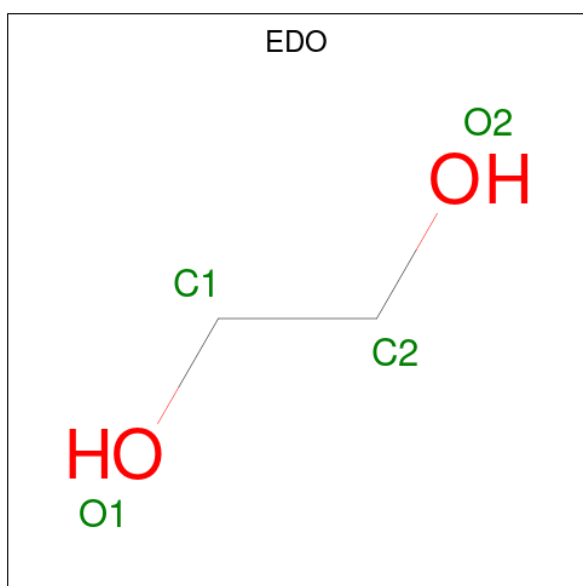
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Fe 1 1	0	0
5	C	1	Total Fe 1 1	0	0
5	E	1	Total Fe 1 1	0	0
5	G	1	Total Fe 1 1	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	C	O	0	0
			4	2	2		

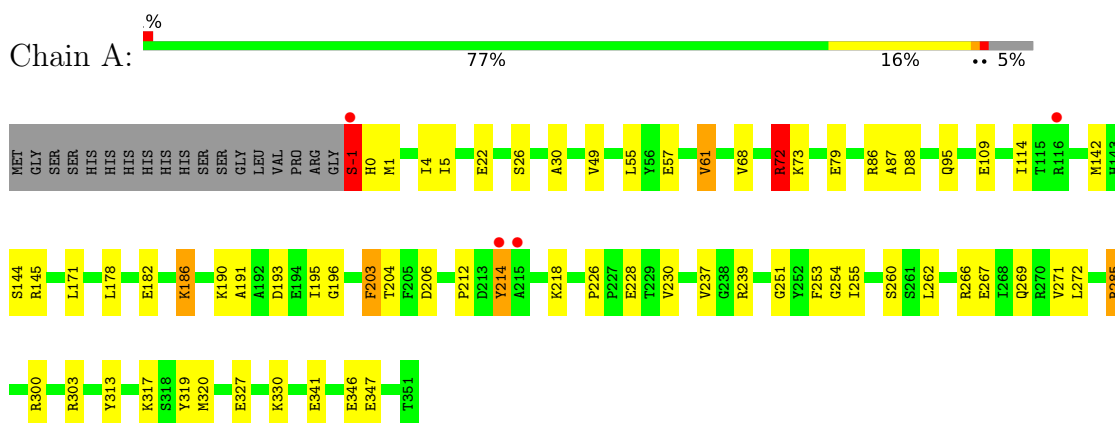
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	230	Total	O	0	0
			230	230		
8	B	233	Total	O	0	0
			233	233		
8	C	180	Total	O	0	0
			180	180		
8	D	198	Total	O	0	0
			198	198		
8	E	105	Total	O	0	0
			105	105		
8	F	68	Total	O	0	0
			68	68		
8	G	47	Total	O	0	0
			47	47		

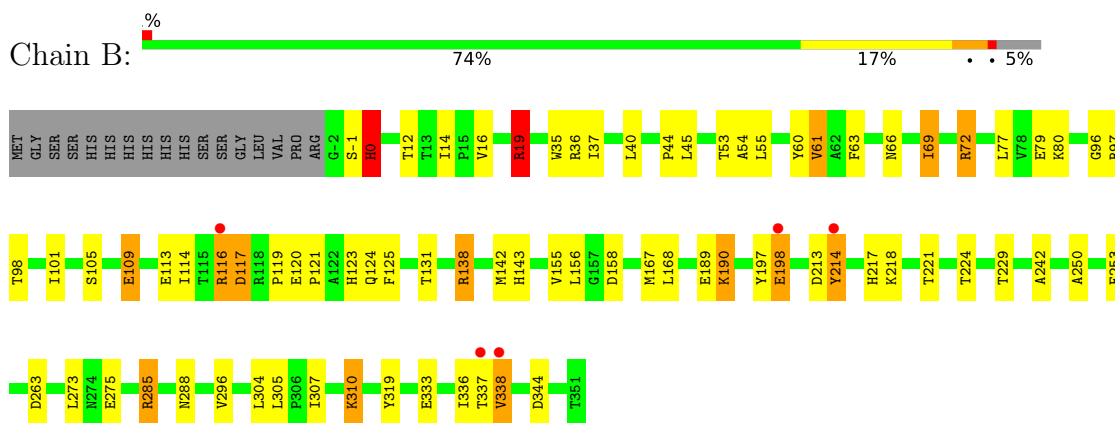
3 Residue-property plots

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

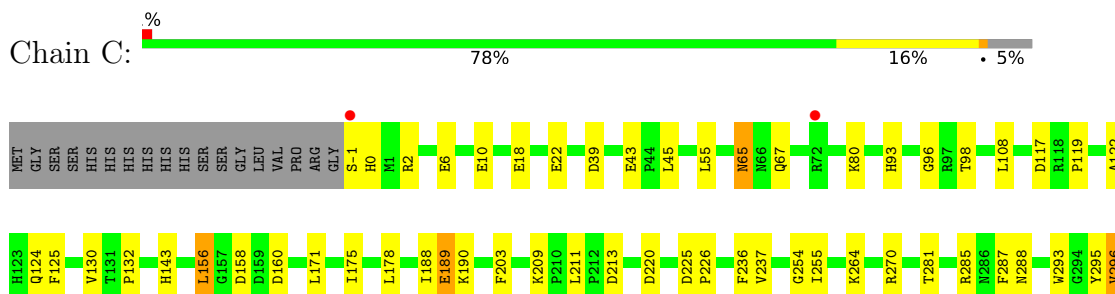
- Molecule 1: N(4)-bis(aminopropyl)spermidine synthase



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

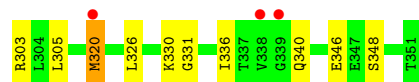
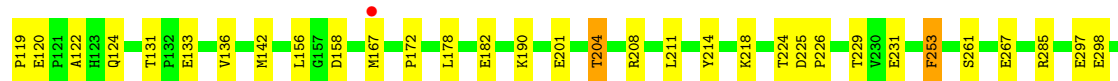
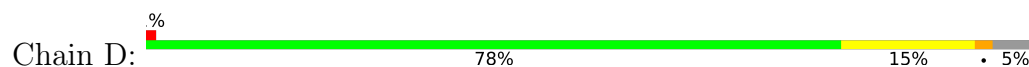


- Molecule 1: N(4)-bis(aminopropyl)spermidine synthase

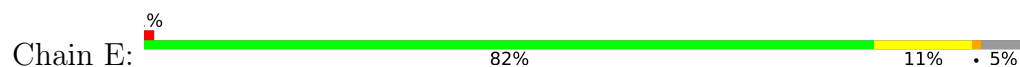




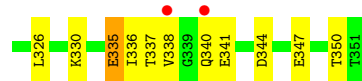
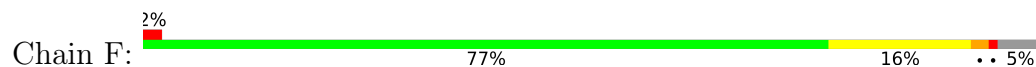
- Molecule 1: N(4)-bis(aminopropyl)spermidine synthase



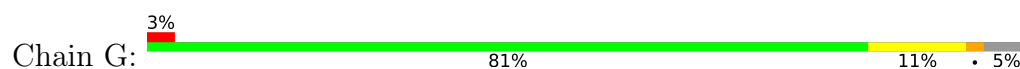
- Molecule 1: N(4)-bis(aminopropyl)spermidine synthase

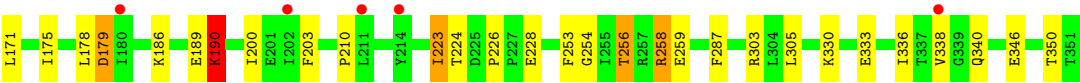


- Molecule 1: N(4)-bis(aminopropyl)spermidine synthase



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





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.53Å 50.98Å 402.43Å 90.00° 93.69° 90.00°	Depositor
Resolution (Å)	43.53 – 1.84 43.53 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.53-1.84) 99.7 (43.53-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.161 , 0.207 0.169 , 0.213	Depositor DCC
R_{free} test set	12128 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21380	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.88	42/2934 (1.4%)	1.49	21/3978 (0.5%)
1	B	1.89	40/2920 (1.4%)	1.57	26/3959 (0.7%)
1	C	1.69	32/2925 (1.1%)	1.40	16/3966 (0.4%)
1	D	1.75	37/2916 (1.3%)	1.40	18/3958 (0.5%)
1	E	1.43	10/2925 (0.3%)	1.27	10/3966 (0.3%)
1	F	1.33	10/2916 (0.3%)	1.23	12/3954 (0.3%)
1	G	1.19	3/2916 (0.1%)	1.18	12/3954 (0.3%)
All	All	1.62	174/20452 (0.9%)	1.37	115/27735 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (174) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	285	ARG	CD-NE	-13.62	1.27	1.46
1	A	285	ARG	CD-NE	-12.42	1.28	1.46
1	D	1	MET	CA-CB	10.90	1.70	1.53
1	D	1	MET	CB-CG	10.84	1.84	1.52
1	B	121	PRO	N-CA	-9.61	1.35	1.47
1	E	285	ARG	CD-NE	-9.55	1.32	1.46
1	A	271	VAL	C-O	9.12	1.34	1.24
1	A	255	ILE	CA-C	8.52	1.63	1.52
1	D	320	MET	CB-CG	8.37	1.77	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	19	ARG	CG-CD	-8.19	1.27	1.52
1	B	310	LYS	CA-C	-8.17	1.44	1.53
1	B	19	ARG	CZ-NH1	8.09	1.44	1.32
1	B	12	THR	N-CA	8.05	1.55	1.45
1	D	285	ARG	CD-NE	-7.97	1.35	1.46
1	B	337	THR	C-O	-7.69	1.14	1.23
1	C	211	LEU	CA-C	7.32	1.61	1.53
1	C	287	PHE	CA-C	7.26	1.62	1.52
1	A	327	GLU	C-O	7.26	1.32	1.23
1	B	101	ILE	CA-CB	-7.16	1.45	1.54
1	C	270	ARG	CZ-NH2	-7.12	1.24	1.33
1	A	341	GLU	CD-OE2	6.98	1.38	1.25
1	A	86	ARG	N-CA	-6.96	1.37	1.46
1	C	175	ILE	C-O	6.91	1.30	1.24
1	D	226	PRO	C-O	6.83	1.32	1.24
1	D	326	LEU	N-CA	-6.75	1.36	1.45
1	D	201	GLU	CD-OE1	6.72	1.38	1.25
1	A	330	LYS	CA-C	-6.69	1.44	1.52
1	A	-1	SER	N-CA	6.68	1.58	1.46
1	F	344	ASP	C-O	-6.68	1.16	1.24
1	D	225	ASP	C-O	6.64	1.31	1.24
1	A	239	ARG	C-O	6.60	1.31	1.24
1	C	285	ARG	CD-NE	-6.57	1.37	1.46
1	F	200	ILE	C-O	-6.55	1.17	1.24
1	B	-1	SER	CA-C	6.54	1.61	1.52
1	C	237	VAL	N-CA	6.53	1.54	1.46
1	D	218	LYS	N-CA	-6.45	1.36	1.45
1	A	260	SER	C-O	6.42	1.31	1.24
1	C	337	THR	N-CA	6.39	1.54	1.46
1	A	73	LYS	N-CA	-6.38	1.38	1.46
1	B	109	GLU	N-CA	6.35	1.53	1.46
1	B	14	ILE	N-CA	6.33	1.54	1.47
1	D	331	GLY	C-O	-6.32	1.18	1.24
1	C	122	ALA	C-O	6.31	1.31	1.24
1	B	242	ALA	CA-C	6.28	1.61	1.52
1	D	267	GLU	CA-CB	6.27	1.63	1.53
1	D	119	PRO	C-O	6.24	1.30	1.23
1	B	53	THR	C-O	6.23	1.31	1.24
1	A	145	ARG	N-CA	-6.21	1.38	1.46
1	C	255	ILE	C-O	6.20	1.30	1.24
1	D	267	GLU	CD-OE2	6.18	1.37	1.25
1	C	119	PRO	C-O	6.17	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	45	LEU	CA-CB	-6.17	1.48	1.54
1	C	293	TRP	CA-C	6.17	1.60	1.52
1	C	55	LEU	CA-C	6.16	1.60	1.52
1	D	21	ILE	C-O	6.16	1.31	1.24
1	D	42	GLU	CA-CB	6.15	1.62	1.53
1	B	156	LEU	CA-C	-6.14	1.45	1.53
1	A	313	TYR	CA-C	6.13	1.59	1.52
1	G	45	LEU	CA-C	6.09	1.59	1.52
1	A	144	SER	CA-C	-6.09	1.44	1.52
1	B	63	PHE	C-O	-6.07	1.17	1.24
1	A	346	GLU	CD-OE1	6.05	1.36	1.25
1	C	98	THR	N-CA	6.04	1.53	1.46
1	D	303	ARG	CA-C	-6.03	1.44	1.52
1	D	261	SER	N-CA	-6.03	1.37	1.45
1	B	77	LEU	CA-C	6.00	1.60	1.52
1	C	22	GLU	CA-C	-5.97	1.45	1.52
1	D	133	GLU	C-O	5.94	1.31	1.24
1	B	36	ARG	N-CA	-5.93	1.38	1.46
1	C	132	PRO	C-O	5.88	1.31	1.24
1	C	213	ASP	N-CA	5.87	1.53	1.46
1	D	118	ARG	NE-CZ	5.85	1.39	1.33
1	D	320	MET	N-CA	5.85	1.53	1.46
1	B	97	ARG	C-O	5.84	1.31	1.24
1	B	167	MET	N-CA	5.82	1.53	1.46
1	C	190	LYS	N-CA	-5.81	1.39	1.46
1	E	25	LEU	N-CA	5.80	1.53	1.46
1	B	119	PRO	N-CA	-5.80	1.40	1.47
1	A	212	PRO	C-O	5.75	1.30	1.23
1	C	125	PHE	C-O	5.74	1.31	1.24
1	A	230	VAL	C-O	5.74	1.30	1.24
1	B	35	TRP	CA-C	-5.72	1.45	1.52
1	D	253	PHE	CA-C	-5.70	1.45	1.52
1	D	336	ILE	CA-C	5.69	1.59	1.52
1	A	347	GLU	CA-CB	-5.66	1.44	1.53
1	D	78	VAL	N-CA	5.66	1.53	1.46
1	B	125	PHE	CA-C	5.65	1.60	1.52
1	A	320	MET	N-CA	5.65	1.53	1.46
1	C	143	HIS	CA-C	5.65	1.60	1.52
1	A	254	GLY	CA-C	-5.65	1.47	1.52
1	A	5	ILE	N-CA	5.64	1.53	1.46
1	A	49	VAL	C-O	5.63	1.30	1.24
1	B	288	ASN	C-O	5.63	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	119	PRO	C-O	5.61	1.29	1.23
1	A	206	ASP	C-O	5.60	1.30	1.24
1	D	267	GLU	CG-CD	5.59	1.66	1.52
1	A	253	PHE	N-CA	-5.59	1.39	1.46
1	B	138	ARG	CA-C	5.58	1.59	1.52
1	A	285	ARG	CZ-NH2	-5.58	1.26	1.33
1	A	57	GLU	CD-OE2	5.56	1.35	1.25
1	A	228	GLU	C-O	5.55	1.31	1.24
1	C	18	GLU	CA-C	5.55	1.59	1.52
1	F	292	ASN	CG-ND2	-5.53	1.21	1.33
1	B	54	ALA	C-O	5.51	1.30	1.24
1	F	274	ASN	CA-C	-5.50	1.47	1.52
1	B	40	LEU	CA-C	5.48	1.60	1.52
1	A	251	GLY	N-CA	-5.46	1.39	1.45
1	B	72	ARG	N-CA	-5.46	1.39	1.46
1	A	142	MET	SD-CE	-5.46	1.66	1.79
1	E	348	SER	C-O	-5.46	1.16	1.23
1	A	269	GLN	N-CA	-5.45	1.39	1.46
1	D	229	THR	C-O	5.44	1.30	1.23
1	E	39	ASP	N-CA	5.43	1.52	1.46
1	B	121	PRO	CA-C	5.43	1.59	1.52
1	D	156	LEU	C-O	-5.42	1.17	1.23
1	F	124	GLN	C-O	-5.42	1.16	1.24
1	F	51	VAL	C-O	5.41	1.30	1.24
1	A	193	ASP	N-CA	5.40	1.53	1.46
1	A	300	ARG	C-O	5.40	1.30	1.24
1	D	40	LEU	C-O	-5.40	1.17	1.24
1	A	313	TYR	C-O	5.36	1.30	1.23
1	C	288	ASN	N-CA	5.36	1.52	1.46
1	D	122	ALA	C-O	5.36	1.30	1.24
1	B	344	ASP	C-O	-5.36	1.17	1.24
1	A	87	ALA	CA-CB	-5.33	1.45	1.53
1	A	186	LYS	N-CA	5.33	1.52	1.46
1	F	143	HIS	C-O	5.33	1.30	1.24
1	B	96	GLY	CA-C	-5.32	1.44	1.51
1	D	346	GLU	N-CA	5.31	1.53	1.46
1	B	198	GLU	CG-CD	5.30	1.65	1.52
1	A	196	GLY	N-CA	5.30	1.52	1.45
1	C	319	TYR	C-O	5.30	1.30	1.23
1	C	2	ARG	C-O	5.29	1.30	1.24
1	C	281	THR	CB-OG1	5.28	1.52	1.43
1	C	220	ASP	N-CA	5.27	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	130	VAL	N-CA	-5.24	1.39	1.46
1	E	344	ASP	N-CA	5.23	1.52	1.46
1	D	297	GLU	CD-OE1	-5.22	1.15	1.25
1	C	160	ASP	CA-C	-5.21	1.45	1.52
1	B	155	VAL	CA-CB	5.20	1.60	1.53
1	D	172	PRO	CA-C	5.19	1.58	1.52
1	B	60	TYR	CB-CG	-5.18	1.40	1.51
1	E	245	LYS	N-CA	5.17	1.52	1.46
1	D	1	MET	N-CA	5.17	1.52	1.46
1	F	142	MET	C-O	5.17	1.30	1.24
1	D	83	ILE	CA-CB	5.17	1.59	1.53
1	C	39	ASP	C-O	-5.16	1.18	1.24
1	A	171	LEU	CA-CB	5.16	1.61	1.53
1	B	333	GLU	CA-C	5.16	1.59	1.52
1	D	26	SER	C-O	-5.16	1.18	1.24
1	A	320	MET	CG-SD	-5.16	1.67	1.80
1	E	271	VAL	N-CA	-5.15	1.40	1.46
1	E	16	VAL	CA-CB	5.14	1.61	1.54
1	B	19	ARG	CB-CG	5.13	1.67	1.52
1	B	37	ILE	CA-CB	5.12	1.61	1.54
1	E	255	ILE	C-O	5.12	1.29	1.24
1	C	299	THR	C-O	5.10	1.30	1.23
1	A	237	VAL	CA-CB	5.09	1.60	1.54
1	B	304	LEU	CA-C	-5.09	1.45	1.52
1	D	204	THR	C-O	-5.09	1.17	1.24
1	A	4	ILE	CA-C	5.09	1.59	1.52
1	F	25	LEU	N-CA	5.09	1.52	1.46
1	F	326	LEU	C-O	-5.08	1.17	1.24
1	D	131	THR	CA-C	5.07	1.58	1.53
1	C	225	ASP	CA-C	-5.07	1.46	1.52
1	B	117	ASP	CB-CG	5.06	1.64	1.52
1	C	96	GLY	C-O	5.06	1.31	1.24
1	B	44	PRO	N-CA	-5.06	1.41	1.47
1	C	117	ASP	CA-CB	5.05	1.59	1.53
1	D	83	ILE	C-O	5.04	1.29	1.23
1	G	68	VAL	N-CA	-5.04	1.40	1.46
1	B	143	HIS	N-CA	5.03	1.52	1.46
1	A	193	ASP	C-O	-5.02	1.18	1.24
1	A	255	ILE	CA-CB	-5.00	1.48	1.54

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	296	VAL	CB-CA-C	-11.02	97.77	111.88
1	B	285	ARG	NE-CZ-NH2	-9.82	110.36	119.20
1	D	158	ASP	N-CA-C	9.71	121.86	110.41
1	A	285	ARG	NE-CZ-NH2	-9.64	110.52	119.20
1	E	296	VAL	CB-CA-C	-8.54	100.86	112.04
1	F	203	PHE	CB-CA-C	-8.46	95.60	109.89
1	C	295	TYR	N-CA-C	8.33	123.06	113.15
1	A	72	ARG	N-CA-C	8.31	120.34	111.28
1	E	228	GLU	N-CA-C	8.20	123.45	112.88
1	F	296	VAL	CB-CA-C	-8.06	98.08	111.29
1	D	1	MET	N-CA-CB	7.88	121.83	110.16
1	D	225	ASP	CA-C-N	7.67	128.28	120.38
1	D	225	ASP	C-N-CA	7.67	128.28	120.38
1	B	285	ARG	NE-CZ-NH1	7.42	128.92	121.50
1	C	158	ASP	N-CA-C	7.36	119.10	110.41
1	B	158	ASP	N-CA-C	7.27	118.98	110.41
1	B	19	ARG	CA-CB-CG	-7.24	99.62	114.10
1	A	226	PRO	N-CA-C	7.12	119.38	110.70
1	B	273	LEU	CD1-CG-CD2	-7.05	95.29	110.80
1	F	158	ASP	N-CA-C	7.04	118.71	110.41
1	E	177	VAL	CB-CA-C	-6.96	100.10	110.82
1	D	320	MET	N-CA-CB	6.92	121.80	110.17
1	A	341	GLU	CG-CD-OE1	-6.88	102.59	118.40
1	B	0	HIS	CB-CA-C	-6.86	100.11	110.88
1	E	228	GLU	CA-CB-CG	-6.79	100.52	114.10
1	E	16	VAL	CB-CA-C	-6.60	100.70	110.33
1	B	-1	SER	N-CA-C	6.58	119.01	111.11
1	C	43	GLU	CA-C-N	-6.43	113.36	119.85
1	C	43	GLU	C-N-CA	-6.43	113.36	119.85
1	G	303	ARG	NE-CZ-NH1	-6.41	115.09	121.50
1	A	22	GLU	N-CA-CB	6.39	119.28	110.01
1	F	256	THR	N-CA-CB	-6.31	100.72	110.56
1	B	307	ILE	N-CA-C	-6.30	99.05	108.12
1	D	120[A]	GLU	CA-C-N	-6.29	113.03	119.83
1	D	120[A]	GLU	C-N-CA	-6.29	113.03	119.83
1	D	120[B]	GLU	CA-C-N	-6.29	113.03	119.83
1	D	120[B]	GLU	C-N-CA	-6.29	113.03	119.83
1	F	19	ARG	CG-CD-NE	6.28	125.81	112.00
1	G	226	PRO	N-CA-C	6.26	118.34	110.70
1	A	228	GLU	N-CA-C	6.18	120.45	112.41
1	C	156	LEU	CB-CG-CD1	6.10	129.01	110.70
1	A	285	ARG	CB-CG-CD	-6.08	97.31	111.30
1	F	256	THR	OG1-CB-CG2	6.03	121.36	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	THR	N-CA-C	-5.97	102.50	110.55
1	A	317	LYS	CD-CE-NZ	-5.96	92.83	111.90
1	E	40	LEU	N-CA-C	5.95	117.84	111.36
1	B	218	LYS	CA-CB-CG	-5.92	102.27	114.10
1	A	203	PHE	N-CA-C	5.91	118.27	108.99
1	A	285	ARG	NE-CZ-NH1	5.88	127.38	121.50
1	B	198	GLU	N-CA-C	5.85	121.14	113.30
1	F	228	GLU	N-CA-C	5.83	119.70	112.59
1	B	0	HIS	CA-CB-CG	5.82	119.62	113.80
1	B	69	ILE	N-CA-CB	-5.79	102.72	112.44
1	A	30	ALA	N-CA-C	-5.79	106.35	113.41
1	A	1	MET	CG-SD-CE	5.78	113.62	100.90
1	C	188	ILE	CA-C-N	-5.78	111.96	120.28
1	C	188	ILE	C-N-CA	-5.78	111.96	120.28
1	B	66	ASN	N-CA-C	5.77	119.62	112.24
1	E	237	VAL	N-CA-C	5.70	115.89	110.53
1	C	189	GLU	N-CA-C	5.64	118.20	111.71
1	A	272	LEU	N-CA-C	5.64	117.88	111.11
1	E	93	HIS	N-CA-C	5.56	118.18	111.40
1	B	105	SER	N-CA-C	5.56	117.02	111.07
1	F	43	GLU	CA-C-N	-5.55	114.24	119.85
1	F	43	GLU	C-N-CA	-5.55	114.24	119.85
1	C	0	HIS	N-CA-C	-5.55	105.13	111.07
1	B	168	LEU	N-CA-CB	5.54	118.37	110.06
1	G	190	LYS	CA-CB-CG	5.51	125.12	114.10
1	B	16	VAL	CB-CA-C	-5.44	101.31	110.71
1	G	171	LEU	CA-C-N	-5.43	114.36	119.85
1	G	171	LEU	C-N-CA	-5.43	114.36	119.85
1	C	171	LEU	N-CA-C	5.43	119.63	112.35
1	E	225	ASP	CA-C-N	-5.42	114.80	120.38
1	E	225	ASP	C-N-CA	-5.42	114.80	120.38
1	A	61	VAL	CA-CB-CG2	5.42	119.61	110.40
1	B	19	ARG	NE-CZ-NH2	-5.40	114.34	119.20
1	G	68	VAL	CB-CA-C	5.38	117.58	110.91
1	D	19	ARG	NE-CZ-NH1	-5.38	116.12	121.50
1	B	14	ILE	CB-CA-C	-5.35	105.11	110.89
1	G	303	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	A	68	VAL	CB-CA-C	-5.32	104.52	110.96
1	A	266	ARG	N-CA-C	-5.31	105.57	111.36
1	G	68	VAL	N-CA-CB	5.27	116.47	110.72
1	B	105	SER	CA-CB-OG	-5.27	100.56	111.10
1	F	310	LYS	CA-C-N	-5.25	114.55	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	310	LYS	C-N-CA	-5.25	114.55	119.85
1	D	122	ALA	N-CA-C	5.22	117.26	108.96
1	D	14	ILE	CA-C-O	5.22	124.31	119.62
1	B	98	THR	CB-CA-C	-5.20	102.57	110.06
1	A	26	SER	N-CA-C	-5.19	105.62	111.28
1	A	303	ARG	NE-CZ-NH1	-5.17	116.33	121.50
1	D	190	LYS	N-CA-C	5.17	116.92	111.28
1	D	229	THR	N-CA-C	-5.17	103.21	110.50
1	B	197	TYR	CA-C-N	-5.15	114.51	122.49
1	B	197	TYR	C-N-CA	-5.15	114.51	122.49
1	D	261	SER	N-CA-C	-5.14	103.60	110.55
1	D	208	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	B	131	THR	CA-C-N	-5.13	113.64	119.28
1	B	131	THR	C-N-CA	-5.13	113.64	119.28
1	F	204	THR	N-CA-C	-5.12	101.35	109.96
1	A	303	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	C	293	TRP	CA-C-N	5.09	126.50	120.14
1	C	293	TRP	C-N-CA	5.09	126.50	120.14
1	A	230	VAL	CB-CA-C	5.08	119.00	112.14
1	D	93	HIS	CA-C-N	-5.07	114.69	122.60
1	D	93	HIS	C-N-CA	-5.07	114.69	122.60
1	G	118	ARG	CA-C-N	-5.06	114.41	120.13
1	G	118	ARG	C-N-CA	-5.06	114.41	120.13
1	C	65	ASN	CB-CA-C	5.05	119.87	112.09
1	A	61	VAL	CG1-CB-CG2	5.05	121.91	110.80
1	G	258	ARG	N-CA-C	5.05	117.68	111.82
1	C	189	GLU	N-CA-CB	5.04	117.98	110.22
1	C	296	VAL	N-CA-CB	5.04	116.10	110.51
1	B	123	HIS	N-CA-C	-5.02	105.80	111.28
1	G	16	VAL	CB-CA-C	-5.01	103.01	110.33

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-1	SER	Peptide
1	B	0	HIS	Sidechain
1	B	19	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2868	0	2837	17	0
1	B	2860	0	2828	18	0
1	C	2862	0	2831	13	0
1	D	2857	0	2808	24	0
1	E	2862	0	2831	13	0
1	F	2856	0	2825	35	0
1	G	2856	0	2825	26	0
2	A	20	0	15	0	0
2	B	20	0	15	0	0
2	C	20	0	15	0	0
2	D	20	0	15	0	0
2	E	20	0	15	0	0
2	F	20	0	15	0	0
2	G	20	0	15	1	0
3	A	14	0	0	0	0
3	B	14	0	0	0	0
3	C	14	0	0	0	0
3	D	14	0	0	0	0
3	E	14	0	0	0	0
3	F	14	0	0	1	0
3	G	14	0	0	2	0
4	A	18	0	24	1	0
4	B	6	0	8	0	0
4	D	6	0	8	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
6	A	7	0	10	0	0
6	E	7	0	10	0	0
7	D	8	0	12	0	0
7	E	4	0	6	0	0
8	A	230	0	0	2	0
8	B	233	0	0	5	0
8	C	180	0	0	4	0
8	D	198	0	0	4	0
8	E	105	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	68	0	0	1	0
8	G	47	0	0	1	0
All	All	21380	0	19968	143	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 (143) 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:320:MET:CB	1:D:320:MET:CG	1.77	1.58
1:D:1:MET:CB	1:D:1:MET:CG	1.85	1.55
1:D:142:MET:CE	1:D:142:MET:CG	1.86	1.53
1:D:1:MET:CG	1:D:1:MET:CE	1.86	1.53
1:F:209:LYS:NZ	1:F:335:GLU:OE2	1.68	1.27
1:D:320:MET:CG	1:D:320:MET:CE	2.19	1.20
1:F:228:GLU:OE1	1:F:256:THR:HG22	1.81	0.81
1:F:185:THR:HG23	1:F:202:ILE:HG22	1.68	0.75
1:F:113:GLU:OE1	1:F:116:ARG:NH1	2.20	0.75
1:D:113:GLU:OE1	1:D:116:ARG:NH1	2.21	0.74
1:B:217:HIS:CE1	8:B:615:HOH:O	2.41	0.72
1:B:275:GLU:OE1	8:B:501:HOH:O	2.06	0.72
1:G:113:GLU:OE1	1:G:116:ARG:NH2	2.24	0.71
1:B:117:ASP:HB3	8:B:697:HOH:O	1.90	0.70
1:B:213:ASP:HB2	8:B:654:HOH:O	1.90	0.70
1:A:72:ARG:HH11	1:A:72:ARG:HG3	1.57	0.69
1:F:1:MET:HE1	1:F:21:ILE:HG13	1.75	0.68
1:B:336:ILE:HG22	1:B:338:VAL:HG22	1.76	0.66
1:G:186:LYS:O	1:G:190:LYS:HD2	1.98	0.64
4:A:404:GOL:H11	1:B:19:ARG:HG3	1.81	0.63
1:G:13:THR:OG1	1:G:346:GLU:OE1	2.15	0.63
1:F:209:LYS:CE	1:F:335:GLU:OE2	2.46	0.63
1:B:113:GLU:OE2	1:B:116:ARG:NH1	2.33	0.62
1:A:214:TYR:O	1:A:218:LYS:HE2	2.01	0.61
1:A:72:ARG:HG3	1:A:72:ARG:NH1	2.15	0.60
1:G:228:GLU:OE2	1:G:256:THR:HG22	2.02	0.59
1:F:256:THR:HG23	1:F:259:GLU:H	1.68	0.58
1:F:285:ARG:HG3	1:F:319:TYR:CZ	2.38	0.58
1:G:256:THR:CG2	1:G:259:GLU:H	2.17	0.58
1:F:1:MET:HE1	1:F:21:ILE:CB	2.34	0.58
1:A:191:ALA:O	1:A:195:ILE:HG12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ARG:HH11	1:A:72:ARG:CG	2.16	0.58
1:D:167:MET:CE	1:D:167:MET:CG	2.82	0.58
1:B:55:LEU:HB3	1:B:61:VAL:HG13	1.86	0.57
1:G:178:LEU:C	1:G:178:LEU:HD12	2.28	0.57
1:D:320:MET:CG	1:D:320:MET:CA	2.76	0.57
1:G:224:THR:O	1:G:253:PHE:HA	2.05	0.57
1:A:214:TYR:C	1:A:214:TYR:CD1	2.84	0.56
1:C:209:LYS:NZ	8:C:505:HOH:O	2.37	0.56
1:F:1:MET:HE1	1:F:21:ILE:CG1	2.36	0.56
1:D:348:SER:HB3	8:D:580:HOH:O	2.07	0.55
1:C:346[B]:GLU:OE1	8:C:501:HOH:O	2.18	0.55
1:F:256:THR:CG2	1:F:259:GLU:H	2.19	0.55
1:C:346[A]:GLU:HG3	8:C:530:HOH:O	2.06	0.54
1:G:55:LEU:HB3	1:G:61:VAL:HG13	1.90	0.54
1:G:178:LEU:O	1:G:179:ASP:HB2	2.06	0.54
1:E:285:ARG:HG3	1:E:319:TYR:CZ	2.43	0.54
1:D:182:GLU:HG2	1:D:204:THR:HG21	1.90	0.54
1:G:254:GLY:O	3:G:402:N4P:N14	2.42	0.53
1:E:124:GLN:NE2	8:E:503:HOH:O	2.40	0.53
1:B:45:LEU:C	1:B:45:LEU:HD23	2.34	0.53
1:F:256:THR:HG23	1:F:258:ARG:H	1.74	0.52
1:G:256:THR:HG23	1:G:259:GLU:H	1.73	0.52
1:D:124:GLN:HG2	8:D:636:HOH:O	2.10	0.52
1:F:256:THR:HG23	1:F:258:ARG:N	2.25	0.51
1:D:142:MET:CE	1:D:142:MET:CB	2.83	0.51
1:F:210:PRO:HD3	1:F:335:GLU:HG2	1.92	0.51
1:A:285:ARG:HA	1:A:319:TYR:CD2	2.47	0.50
1:F:20:THR:HG21	1:F:47:LEU:HD21	1.94	0.50
1:E:179:ASP:O	1:E:204:THR:HA	2.12	0.50
1:C:10:GLU:OE1	1:E:56:TYR:OH	2.27	0.49
1:A:178:LEU:C	1:A:178:LEU:HD12	2.38	0.49
1:F:338:VAL:HB	1:F:341:GLU:HB2	1.94	0.48
1:D:-1:SER:HA	8:D:627:HOH:O	2.13	0.48
1:F:110:GLN:HE21	1:F:168:LEU:HD22	1.79	0.48
1:F:117:ASP:N	1:F:117:ASP:OD1	2.44	0.48
1:A:285:ARG:HG3	1:A:319:TYR:CZ	2.49	0.48
1:G:340:GLN:NE2	1:G:340:GLN:HA	2.29	0.48
1:D:1:MET:CG	1:D:1:MET:CA	2.89	0.47
1:A:182:GLU:HG2	1:A:204:THR:HG21	1.96	0.47
1:D:178:LEU:C	1:D:178:LEU:HD12	2.39	0.47
1:D:55:LEU:HB3	1:D:61:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:GLN:HB3	8:F:532:HOH:O	2.13	0.47
1:F:203:PHE:CE1	1:F:214:TYR:HE2	2.33	0.47
1:G:210:PRO:HB3	1:G:333:GLU:O	2.14	0.47
1:F:142:MET:HG2	1:F:252:TYR:CZ	2.50	0.47
1:F:235:ALA:HB2	1:F:336:ILE:CD1	2.44	0.47
1:G:0:HIS:HB3	1:G:60:TYR:OH	2.15	0.47
1:G:259:GLU:OE1	1:G:350:THR:OG1	2.31	0.47
1:G:340:GLN:HA	1:G:340:GLN:HE21	1.79	0.47
1:A:214:TYR:HE1	8:A:613:HOH:O	1.97	0.46
1:B:190:LYS:HE2	1:B:190:LYS:HB3	1.72	0.46
1:D:231:GLU:HA	1:D:231:GLU:OE1	2.15	0.46
1:C:264:LYS:HE3	1:C:347:GLU:OE1	2.16	0.46
1:A:88:ASP:OD2	8:A:501:HOH:O	2.21	0.45
1:A:72:ARG:NH1	1:A:72:ARG:CG	2.77	0.45
1:F:1:MET:CE	1:F:21:ILE:HG13	2.43	0.45
1:C:124:GLN:HG2	8:C:621:HOH:O	2.16	0.45
1:E:178:LEU:C	1:E:178:LEU:HD23	2.41	0.45
1:B:124:GLN:NE2	8:B:502:HOH:O	2.22	0.45
1:D:107:LEU:HD13	1:D:136:VAL:HG22	1.98	0.45
1:G:175:ILE:O	1:G:200:ILE:HA	2.17	0.45
1:E:100:GLU:OE1	1:F:92:SER:N	2.40	0.45
1:F:228:GLU:OE1	1:F:256:THR:CG2	2.60	0.45
1:D:2:ARG:O	1:D:6:GLU:HG2	2.17	0.44
1:A:55:LEU:HB3	1:A:61:VAL:HG13	1.99	0.44
1:F:254:GLY:HA2	1:F:319:TYR:O	2.17	0.44
1:G:97:ARG:HD3	1:G:287:PHE:O	2.17	0.44
1:E:214:TYR:CD2	1:E:214:TYR:N	2.78	0.44
1:A:178:LEU:HA	1:A:203:PHE:O	2.18	0.44
1:B:214:TYR:C	1:B:214:TYR:CD1	2.96	0.44
1:C:93:HIS:CG	1:D:93:HIS:CD2	3.06	0.44
1:G:223:ILE:HG13	1:G:224:THR:N	2.33	0.43
1:E:235:ALA:HB2	1:E:336:ILE:HD12	2.01	0.43
1:G:2:ARG:NH2	8:G:502:HOH:O	2.48	0.43
1:C:346[A]:GLU:HG2	1:C:347:GLU:HG3	2.00	0.43
1:F:14:ILE:HG12	1:F:347:GLU:HG2	2.00	0.43
1:B:285:ARG:HA	1:B:319:TYR:CD2	2.54	0.43
1:E:113:GLU:CD	1:E:116:ARG:HH21	2.26	0.43
1:F:350:THR:OG1	3:F:402:N4P:N1	2.52	0.43
1:B:224:THR:O	1:B:253:PHE:HA	2.19	0.42
1:G:178:LEU:HA	1:G:203:PHE:O	2.18	0.42
1:D:224:THR:O	1:D:253:PHE:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:228:GLU:OE1	3:G:402:N4P:N14	2.52	0.42
1:D:34:VAL:HG21	1:D:305:LEU:HD22	2.01	0.42
1:G:256:THR:HG23	1:G:258:ARG:N	2.35	0.42
1:F:142:MET:HG2	1:F:252:TYR:CE1	2.55	0.42
1:A:114:ILE:CD1	1:A:195:ILE:HD11	2.50	0.41
1:F:285:ARG:HG3	1:F:319:TYR:OH	2.19	0.41
1:F:1:MET:HE1	1:F:21:ILE:HG21	2.02	0.41
1:F:285:ARG:HA	1:F:319:TYR:CD2	2.55	0.41
1:B:138:ARG:O	1:B:142:MET:HG3	2.19	0.41
1:C:178:LEU:C	1:C:178:LEU:HD12	2.45	0.41
1:E:47:LEU:O	1:E:51:VAL:HG23	2.20	0.41
1:D:214:TYR:CD1	1:D:214:TYR:C	2.99	0.41
1:F:154:PHE:O	1:F:222:PHE:HA	2.19	0.41
1:G:0:HIS:H	1:G:0:HIS:CD2	2.38	0.41
1:G:125:PHE:O	2:G:401:MTA:H8	2.20	0.41
1:B:296:VAL:HG11	1:B:310:LYS:HD2	2.03	0.41
1:C:254:GLY:HA2	1:C:319:TYR:O	2.21	0.41
1:C:45:LEU:HD23	1:C:45:LEU:C	2.45	0.41
1:C:178:LEU:HA	1:C:203:PHE:O	2.20	0.41
1:F:1:MET:HE1	1:F:21:ILE:HB	2.01	0.41
1:E:254:GLY:HA2	1:E:319:TYR:O	2.21	0.41
1:A:262:LEU:HA	1:A:262:LEU:HD23	1.84	0.40
1:E:33:ASP:OD1	1:E:33:ASP:C	2.63	0.40
1:B:0:HIS:CE1	1:B:80:LYS:HE2	2.56	0.40
1:B:221:THR:HA	1:B:250:ALA:O	2.21	0.40
1:D:80:LYS:NZ	8:D:511:HOH:O	2.54	0.40
1:E:222:PHE:CD1	1:E:222:PHE:C	2.99	0.40
1:F:19:ARG:HA	1:F:19:ARG:HD3	1.98	0.40
1:C:226:PRO:HB3	1:C:236:PHE:CB	2.52	0.40
1:G:0:HIS:CD2	1:G:0:HIS:N	2.90	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	353/371 (95%)	343 (97%)	10 (3%)	0	100	100
1	B	352/371 (95%)	343 (97%)	9 (3%)	0	100	100
1	C	352/371 (95%)	343 (97%)	9 (3%)	0	100	100
1	D	352/371 (95%)	340 (97%)	12 (3%)	0	100	100
1	E	352/371 (95%)	341 (97%)	11 (3%)	0	100	100
1	F	351/371 (95%)	336 (96%)	15 (4%)	0	100	100
1	G	351/371 (95%)	339 (97%)	11 (3%)	1 (0%)	36	25
All	All	2463/2597 (95%)	2385 (97%)	77 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	179	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	313/326 (96%)	302 (96%)	11 (4%)	32	14
1	B	311/326 (95%)	295 (95%)	16 (5%)	21	5
1	C	312/326 (96%)	300 (96%)	12 (4%)	29	12
1	D	307/326 (94%)	300 (98%)	7 (2%)	44	27
1	E	312/326 (96%)	295 (95%)	17 (5%)	20	4
1	F	311/326 (95%)	285 (92%)	26 (8%)	10	1
1	G	311/326 (95%)	292 (94%)	19 (6%)	17	3
All	All	2177/2282 (95%)	2069 (95%)	108 (5%)	22	6

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	A	0	HIS
1	A	72	ARG
1	A	79	GLU
1	A	95	GLN
1	A	109	GLU
1	A	186	LYS
1	A	190	LYS
1	A	214	TYR
1	A	267[A]	GLU
1	A	267[B]	GLU
1	B	19	ARG
1	B	61	VAL
1	B	69	ILE
1	B	72	ARG
1	B	79	GLU
1	B	109	GLU
1	B	114	ILE
1	B	116	ARG
1	B	120	GLU
1	B	189	GLU
1	B	190	LYS
1	B	198	GLU
1	B	214	TYR
1	B	263	ASP
1	B	305	LEU
1	B	338	VAL
1	C	-1	SER
1	C	6	GLU
1	C	65	ASN
1	C	67	GLN
1	C	80	LYS
1	C	108	LEU
1	C	156	LEU
1	C	189	GLU
1	C	296	VAL
1	C	305	LEU
1	C	327	GLU
1	C	330	LYS
1	D	61	VAL
1	D	102	ASP
1	D	107	LEU
1	D	211	LEU

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Mol	Chain	Res	Type
1	D	298	GLU
1	D	330	LYS
1	D	340	GLN
1	E	26	SER
1	E	29	GLN
1	E	72	ARG
1	E	75	LYS
1	E	86	ARG
1	E	99	VAL
1	E	102	ASP
1	E	114	ILE
1	E	177	VAL
1	E	178	LEU
1	E	186	LYS
1	E	214	TYR
1	E	296	VAL
1	E	305	LEU
1	E	323	ILE
1	E	327	GLU
1	E	338	VAL
1	F	2	ARG
1	F	19	ARG
1	F	22	GLU
1	F	67	GLN
1	F	72	ARG
1	F	73	LYS
1	F	79	GLU
1	F	106	GLU
1	F	112	LYS
1	F	114	ILE
1	F	124	GLN
1	F	174	ARG
1	F	198	GLU
1	F	199	ASN
1	F	203	PHE
1	F	214	TYR
1	F	216	LEU
1	F	231	GLU
1	F	256	THR
1	F	296	VAL
1	F	305	LEU
1	F	310	LYS

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Mol	Chain	Res	Type
1	F	330	LYS
1	F	335	GLU
1	F	337	THR
1	F	340	GLN
1	G	0	HIS
1	G	7	ARG
1	G	61	VAL
1	G	65	ASN
1	G	68	VAL
1	G	72	ARG
1	G	75	LYS
1	G	80	LYS
1	G	95	GLN
1	G	113	GLU
1	G	124	GLN
1	G	189	GLU
1	G	190	LYS
1	G	223	ILE
1	G	256	THR
1	G	305	LEU
1	G	330	LYS
1	G	336	ILE
1	G	338	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	93	HIS
1	A	150	ASN
1	B	0	HIS
1	B	65	ASN
1	B	66	ASN
1	B	110	GLN
1	B	217	HIS
1	C	0	HIS
1	C	67	GLN
1	C	124	GLN
1	C	150	ASN
1	C	217	HIS
1	C	340	GLN
1	D	93	HIS

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Mol	Chain	Res	Type
1	D	124	GLN
1	D	292	ASN
1	E	67	GLN
1	E	93	HIS
1	E	124	GLN
1	E	217	HIS
1	E	274	ASN
1	E	292	ASN
1	F	0	HIS
1	F	65	ASN
1	F	93	HIS
1	F	110	GLN
1	F	199	ASN
1	F	217	HIS
1	F	274	ASN
1	F	292	ASN
1	F	314	ASN
1	G	0	HIS
1	G	67	GLN
1	G	124	GLN
1	G	274	ASN
1	G	340	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 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
2	MTA	D	401	-	22,22,22	1.59	4 (18%)	32,32,32	2.10	10 (31%)
4	GOL	A	403	-	5,5,5	0.43	0	5,5,5	0.57	0
7	EDO	D	405	-	3,3,3	0.82	0	2,2,2	0.16	0
3	N4P	A	402	-	13,13,13	0.91	1 (7%)	13,13,13	1.43	2 (15%)
4	GOL	B	403	-	5,5,5	0.93	0	5,5,5	1.01	0
2	MTA	B	401	-	22,22,22	1.26	3 (13%)	32,32,32	1.80	8 (25%)
3	N4P	C	402	-	13,13,13	1.15	2 (15%)	13,13,13	1.10	1 (7%)
6	PEG	E	405	-	6,6,6	0.68	0	5,5,5	0.26	0
2	MTA	E	401	-	22,22,22	1.71	5 (22%)	32,32,32	2.08	10 (31%)
7	EDO	E	404	-	3,3,3	0.47	0	2,2,2	0.42	0
3	N4P	D	402	-	13,13,13	1.35	2 (15%)	13,13,13	1.24	3 (23%)
3	N4P	B	402	-	13,13,13	0.68	0	13,13,13	1.36	2 (15%)
3	N4P	F	402	-	13,13,13	0.85	0	13,13,13	1.28	2 (15%)
7	EDO	D	404	-	3,3,3	0.73	0	2,2,2	0.42	0
4	GOL	A	404	-	5,5,5	0.23	0	5,5,5	0.95	0
4	GOL	D	403	-	5,5,5	0.19	0	5,5,5	0.51	0
6	PEG	A	407	-	6,6,6	0.76	0	5,5,5	1.39	1 (20%)
3	N4P	G	402	-	13,13,13	0.68	0	13,13,13	1.14	1 (7%)
4	GOL	A	405	-	5,5,5	0.90	0	5,5,5	1.31	2 (40%)
2	MTA	G	401	-	22,22,22	1.65	5 (22%)	32,32,32	2.27	10 (31%)
2	MTA	A	401	-	22,22,22	1.55	3 (13%)	32,32,32	1.67	7 (21%)
2	MTA	F	401	-	22,22,22	1.71	5 (22%)	32,32,32	2.06	11 (34%)
3	N4P	E	402	-	13,13,13	1.07	1 (7%)	13,13,13	1.00	0
2	MTA	C	401	-	22,22,22	1.60	3 (13%)	32,32,32	2.50	13 (40%)

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
2	MTA	D	401	-	-	1/7/23/23	0/3/3/3
4	GOL	A	403	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	D	405	-	-	0/1/1/1	-
3	N4P	A	402	-	-	3/13/13/13	-
4	GOL	B	403	-	-	2/4/4/4	-
2	MTA	B	401	-	-	1/7/23/23	0/3/3/3
3	N4P	C	402	-	-	2/13/13/13	-
6	PEG	E	405	-	-	2/4/4/4	-
2	MTA	E	401	-	-	0/7/23/23	0/3/3/3
7	EDO	E	404	-	-	1/1/1/1	-
3	N4P	D	402	-	-	4/13/13/13	-
3	N4P	B	402	-	-	2/13/13/13	-
3	N4P	F	402	-	-	4/13/13/13	-
7	EDO	D	404	-	-	0/1/1/1	-
4	GOL	A	404	-	-	2/4/4/4	-
4	GOL	D	403	-	-	1/4/4/4	-
6	PEG	A	407	-	-	2/4/4/4	-
3	N4P	G	402	-	-	5/13/13/13	-
4	GOL	A	405	-	-	2/4/4/4	-
2	MTA	G	401	-	-	2/7/23/23	0/3/3/3
2	MTA	A	401	-	-	1/7/23/23	0/3/3/3
2	MTA	F	401	-	-	0/7/23/23	0/3/3/3
3	N4P	E	402	-	-	3/13/13/13	-
2	MTA	C	401	-	-	1/7/23/23	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	MTA	C5-C4	4.77	1.47	1.39
2	G	401	MTA	C5-C4	4.52	1.47	1.39
2	E	401	MTA	C4-N9	-4.33	1.28	1.37
2	C	401	MTA	C5-C4	4.22	1.46	1.39
2	E	401	MTA	C5-C4	3.67	1.45	1.39
2	D	401	MTA	C8-N9	-3.53	1.31	1.37
2	A	401	MTA	C5-C4	3.43	1.45	1.39
2	C	401	MTA	C8-N7	3.39	1.38	1.31
2	E	401	MTA	C5-N7	-3.35	1.33	1.39
3	D	402	N4P	C11-N6	3.20	1.54	1.47
2	G	401	MTA	C5-N7	-3.07	1.33	1.39
2	A	401	MTA	C5'-S5'	-3.02	1.73	1.81
2	D	401	MTA	C5-C6	2.96	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	MTA	C5-N7	-2.90	1.33	1.39
3	C	402	N4P	C11-N6	2.85	1.53	1.47
3	D	402	N4P	C7-N6	2.81	1.53	1.47
3	E	402	N4P	C5-N6	2.80	1.53	1.47
2	F	401	MTA	C4-N9	-2.78	1.31	1.37
2	D	401	MTA	C5-N7	-2.77	1.34	1.39
2	B	401	MTA	C4-N9	-2.76	1.32	1.37
2	F	401	MTA	O4'-C1'	2.48	1.47	1.42
2	B	401	MTA	C5-C6	2.42	1.47	1.41
2	F	401	MTA	C8-N7	2.41	1.36	1.31
3	C	402	N4P	C12-C13	2.39	1.62	1.51
2	G	401	MTA	C5-C6	2.36	1.47	1.41
3	A	402	N4P	C11-N6	2.33	1.52	1.47
2	A	401	MTA	C5-N7	-2.30	1.34	1.39
2	F	401	MTA	C3'-C4'	2.27	1.58	1.53
2	E	401	MTA	C5-C6	2.26	1.47	1.41
2	D	401	MTA	C4-N3	2.25	1.38	1.34
2	C	401	MTA	C5-N7	-2.22	1.35	1.39
2	G	401	MTA	C5'-S5'	-2.22	1.75	1.81
2	G	401	MTA	C8-N9	-2.12	1.33	1.37
2	E	401	MTA	C8-N7	2.04	1.35	1.31

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	MTA	N3-C4-N9	5.71	136.88	127.17
2	C	401	MTA	C4-N9-C8	5.33	111.34	105.74
2	D	401	MTA	C5-C4-N3	-5.25	119.48	126.72
2	C	401	MTA	C5-C4-N3	-5.24	119.50	126.72
2	G	401	MTA	C5-C4-N3	-5.16	119.62	126.72
2	G	401	MTA	N3-C2-N1	-4.96	121.07	128.58
2	E	401	MTA	C5-C4-N3	-4.82	120.08	126.72
2	C	401	MTA	N3-C2-N1	-4.78	121.34	128.58
2	E	401	MTA	C4-N9-C8	4.50	110.47	105.74
2	D	401	MTA	N3-C2-N1	-4.44	121.86	128.58
2	E	401	MTA	N3-C4-N9	4.33	134.53	127.17
2	F	401	MTA	N3-C2-N1	-4.13	122.32	128.58
2	F	401	MTA	C5-C4-N3	-4.13	121.03	126.72
2	G	401	MTA	N3-C4-N9	4.06	134.06	127.17
2	D	401	MTA	N3-C4-N9	4.05	134.05	127.17
2	G	401	MTA	C2-N3-C4	4.04	121.70	111.83
2	D	401	MTA	C2-N3-C4	4.01	121.62	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	MTA	O4'-C1'-C2'	-3.98	98.10	106.62
2	G	401	MTA	C4-C5-N7	-3.97	106.05	110.58
2	F	401	MTA	C4-N9-C8	3.95	109.89	105.74
2	B	401	MTA	N9-C8-N7	-3.85	108.47	113.94
2	F	401	MTA	N3-C4-N9	3.75	133.55	127.17
2	E	401	MTA	N9-C8-N7	-3.74	108.63	113.94
2	C	401	MTA	C2-N3-C4	3.66	120.78	111.83
3	A	402	N4P	C7-N6-C5	3.66	120.16	111.44
2	A	401	MTA	C4-N9-C8	3.65	109.57	105.74
2	G	401	MTA	O4'-C4'-C5'	3.56	118.01	108.83
2	F	401	MTA	C2-N3-C4	3.47	120.31	111.83
2	B	401	MTA	C4-N9-C8	3.33	109.24	105.74
2	C	401	MTA	N9-C8-N7	-3.31	109.25	113.94
2	E	401	MTA	C2-N3-C4	3.26	119.79	111.83
2	E	401	MTA	N3-C2-N1	-3.13	123.84	128.58
2	G	401	MTA	C5-N7-C8	3.07	108.28	103.45
3	C	402	N4P	C7-N6-C5	3.00	118.59	111.44
3	B	402	N4P	C11-N6-C7	-2.98	104.34	111.44
2	G	401	MTA	C6-C5-N7	2.96	137.80	132.09
2	A	401	MTA	C4-N9-C1'	-2.88	119.89	126.63
2	D	401	MTA	C4-N9-C1'	-2.85	119.97	126.63
2	B	401	MTA	N6-C6-N1	2.78	124.57	118.38
2	B	401	MTA	N3-C2-N1	-2.76	124.41	128.58
3	F	402	N4P	C8-C7-N6	2.73	121.60	113.93
2	F	401	MTA	N6-C6-N1	2.70	124.40	118.38
2	E	401	MTA	O2'-C2'-C3'	2.68	120.42	111.82
2	C	401	MTA	C4'-O4'-C1'	-2.68	103.55	109.47
2	C	401	MTA	C2-N1-C6	2.68	123.13	118.73
2	A	401	MTA	N3-C4-N9	2.68	131.72	127.17
2	F	401	MTA	C4-N9-C1'	-2.63	120.47	126.63
2	A	401	MTA	C5-C4-N3	-2.63	123.09	126.72
3	F	402	N4P	C7-C8-C9	2.55	123.13	113.72
3	B	402	N4P	C8-C7-N6	2.55	121.10	113.93
2	B	401	MTA	C5-C4-N3	-2.53	123.23	126.72
2	E	401	MTA	O4'-C4'-C5'	2.50	115.28	108.83
2	G	401	MTA	C2-N1-C6	2.50	122.84	118.73
2	F	401	MTA	O4'-C4'-C5'	2.50	115.26	108.83
2	A	401	MTA	N9-C8-N7	-2.48	110.42	113.94
3	D	402	N4P	C11-N6-C7	-2.47	105.55	111.44
2	D	401	MTA	C5-C6-N6	-2.38	117.39	123.29
2	C	401	MTA	C5-C6-N6	-2.38	117.39	123.29
2	D	401	MTA	C4-N9-C8	2.36	108.22	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	MTA	C5-C6-N6	-2.36	117.45	123.29
2	C	401	MTA	O3'-C3'-C2'	2.30	119.20	111.82
6	A	407	PEG	O2-C3-C4	2.30	120.24	110.11
3	D	402	N4P	C12-C11-N6	-2.29	107.49	113.93
2	C	401	MTA	N6-C6-N1	2.27	123.43	118.38
2	B	401	MTA	C2-N1-C6	2.26	122.45	118.73
2	F	401	MTA	N9-C8-N7	-2.26	110.73	113.94
2	F	401	MTA	C2-N1-C6	2.23	122.39	118.73
2	E	401	MTA	C5-N7-C8	2.23	106.95	103.45
2	B	401	MTA	C3'-C2'-C1'	2.22	105.66	101.46
3	G	402	N4P	C11-N6-C7	-2.19	106.22	111.44
2	G	401	MTA	C4-N9-C8	2.17	108.02	105.74
2	C	401	MTA	C5-N7-C8	2.14	106.82	103.45
2	A	401	MTA	N6-C6-N1	2.14	123.14	118.38
2	F	401	MTA	C5-C6-N6	-2.10	118.08	123.29
3	D	402	N4P	C7-N6-C5	2.09	116.42	111.44
2	D	401	MTA	N9-C8-N7	-2.07	110.99	113.94
3	A	402	N4P	C11-C12-C13	-2.07	106.09	113.72
2	D	401	MTA	C1'-N9-C8	2.05	131.63	127.09
4	A	405	GOL	O1-C1-C2	2.03	119.54	110.38
4	A	405	GOL	C3-C2-C1	2.02	119.19	111.80
2	E	401	MTA	C4-N9-C1'	-2.02	121.92	126.63
2	C	401	MTA	C5-C4-N9	-2.01	103.62	105.81
2	D	401	MTA	C4-C5-N7	-2.00	108.29	110.58

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	GOL	C1-C2-C3-O3
4	A	404	GOL	C1-C2-C3-O3
4	A	405	GOL	O1-C1-C2-C3
3	F	402	N4P	C8-C7-N6-C11
4	A	403	GOL	O2-C2-C3-O3
3	C	402	N4P	N6-C7-C8-C9
3	C	402	N4P	C4-C5-N6-C7
3	G	402	N4P	N6-C7-C8-C9
6	A	407	PEG	O1-C1-C2-O2
4	B	403	GOL	C1-C2-C3-O3
6	E	405	PEG	O1-C1-C2-O2
4	A	405	GOL	O1-C1-C2-O2
3	D	402	N4P	N6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	B	402	N4P	N6-C7-C8-C9
4	A	404	GOL	O2-C2-C3-O3
3	G	402	N4P	C3-C4-C5-N6
7	E	404	EDO	O1-C1-C2-O2
3	E	402	N4P	N6-C7-C8-C9
3	F	402	N4P	C12-C11-N6-C5
3	A	402	N4P	N6-C7-C8-C9
3	F	402	N4P	C4-C5-N6-C7
3	F	402	N4P	C8-C7-N6-C5
3	A	402	N4P	C11-C12-C13-N14
3	D	402	N4P	C11-C12-C13-N14
3	G	402	N4P	C11-C12-C13-N14
6	A	407	PEG	O2-C3-C4-O4
3	G	402	N4P	C2-C3-C4-C5
4	D	403	GOL	O2-C2-C3-O3
3	A	402	N4P	C4-C5-N6-C7
3	B	402	N4P	C8-C7-N6-C5
6	E	405	PEG	C1-C2-O2-C3
3	G	402	N4P	N1-C2-C3-C4
4	B	403	GOL	O2-C2-C3-O3
3	D	402	N4P	C4-C5-N6-C7
2	B	401	MTA	C2'-C1'-N9-C8
2	G	401	MTA	C2'-C1'-N9-C8
3	D	402	N4P	C8-C7-N6-C5
2	A	401	MTA	C2'-C1'-N9-C8
2	C	401	MTA	C2'-C1'-N9-C8
3	E	402	N4P	C8-C7-N6-C5
3	E	402	N4P	C11-C12-C13-N14
2	G	401	MTA	O4'-C1'-N9-C8
2	D	401	MTA	C2'-C1'-N9-C8

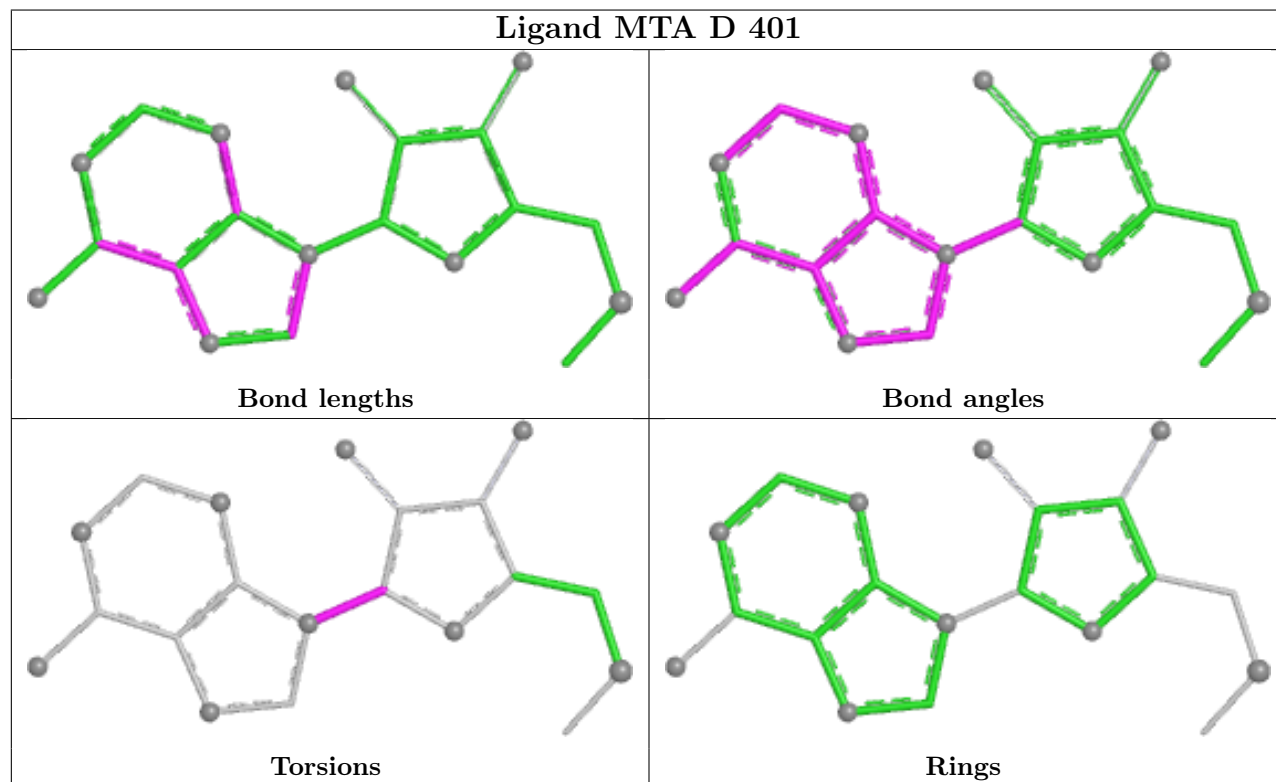
There are no ring outliers.

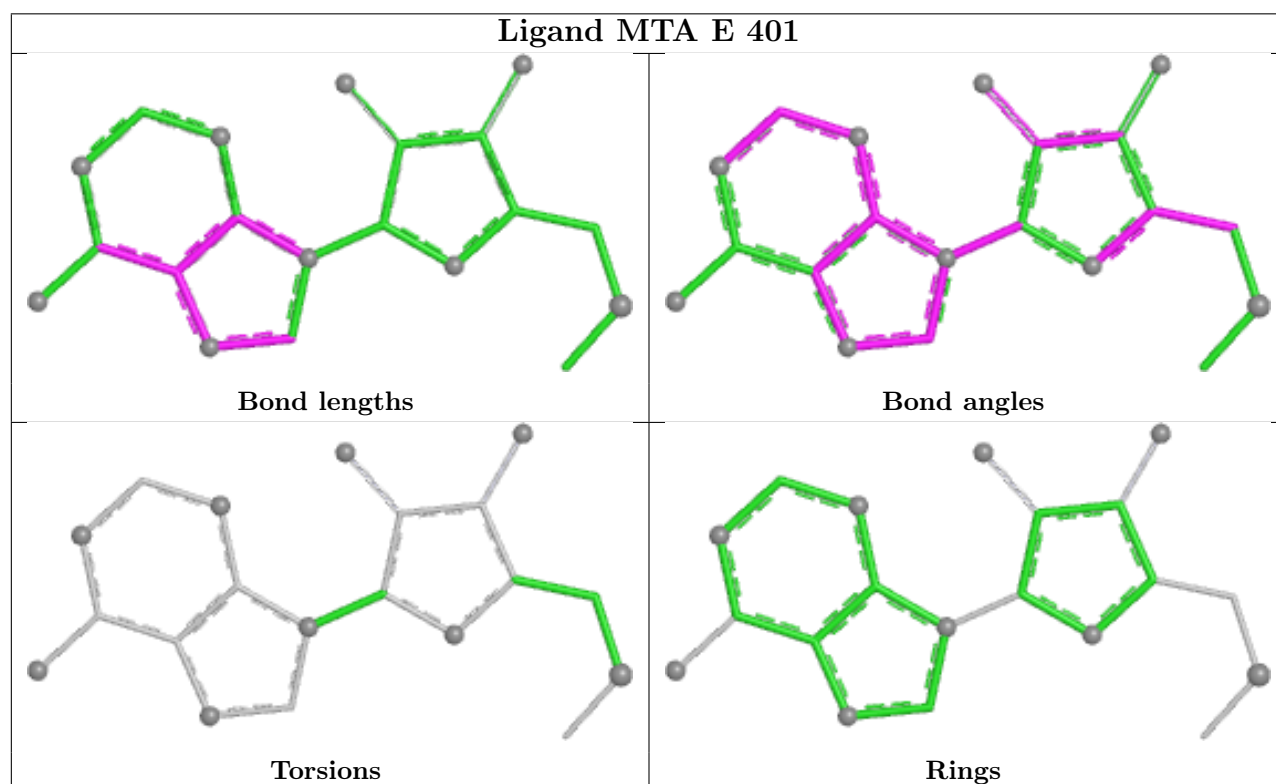
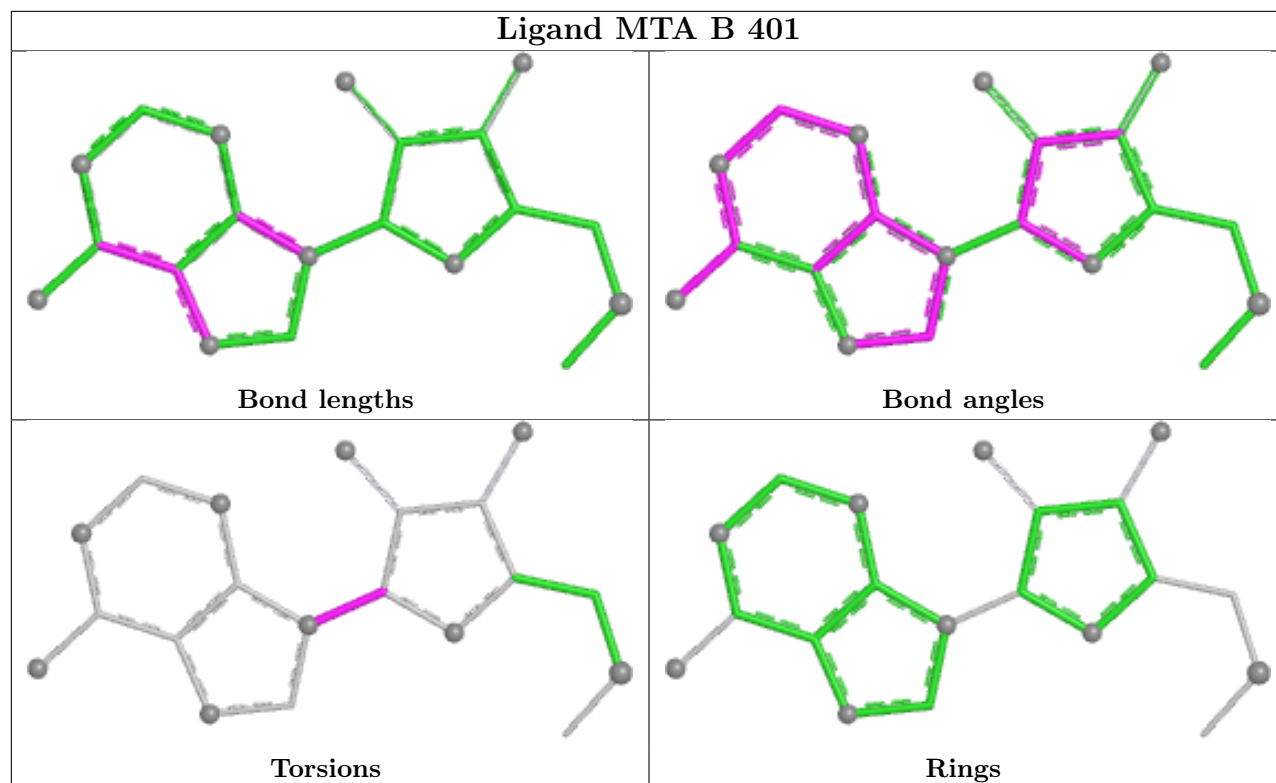
4 monomers are involved in 5 short contacts:

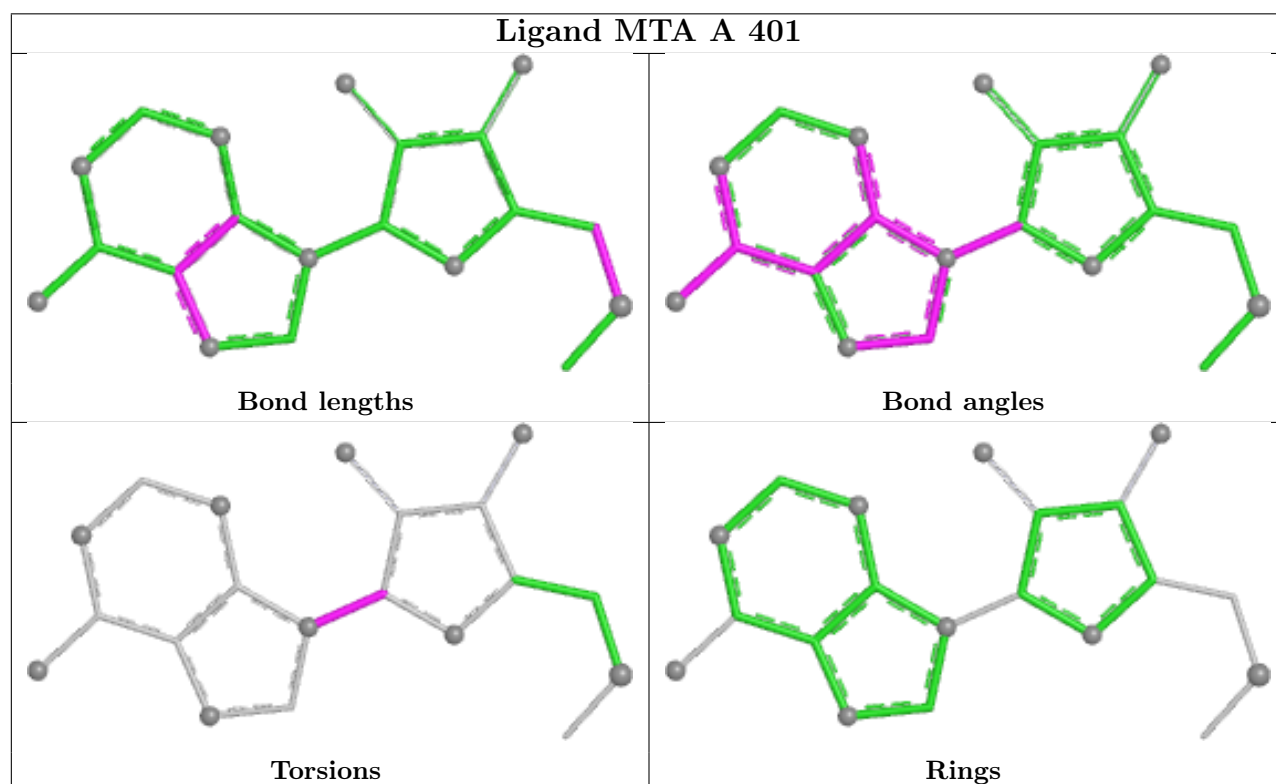
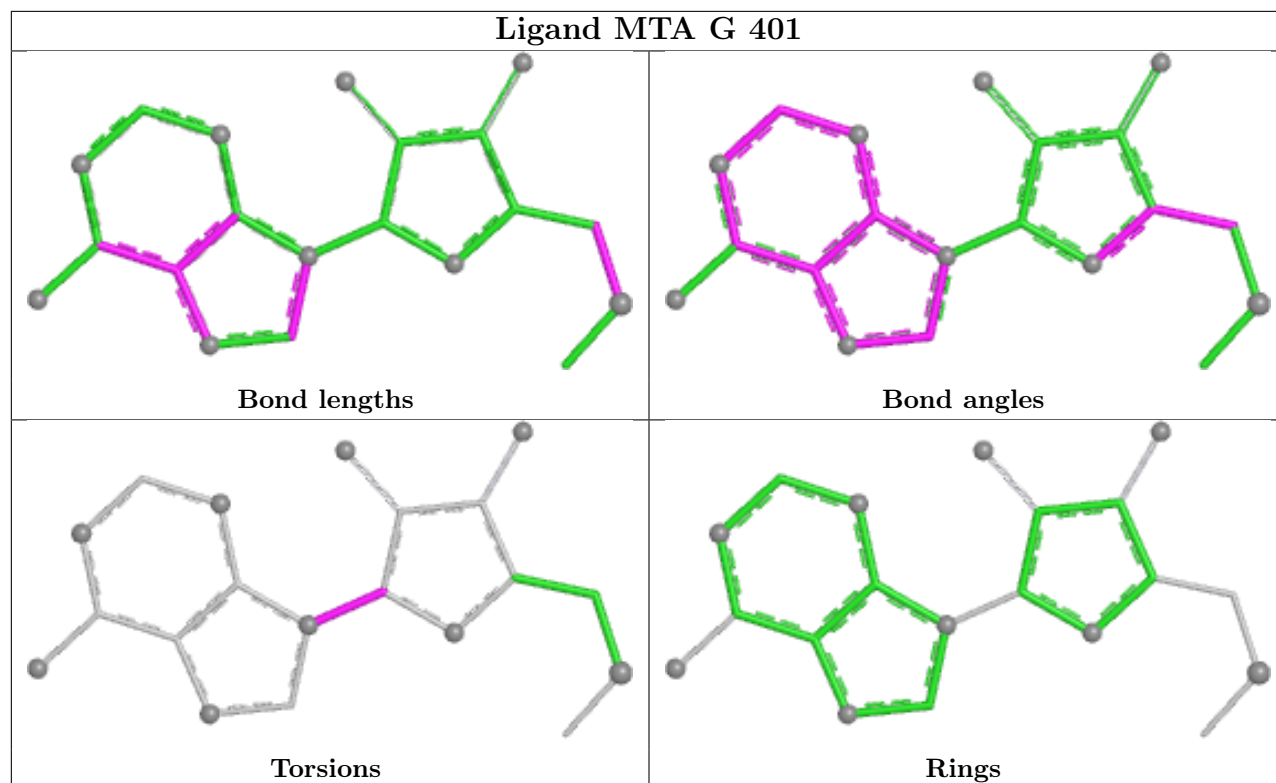
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	402	N4P	1	0
4	A	404	GOL	1	0
3	G	402	N4P	2	0
2	G	401	MTA	1	0

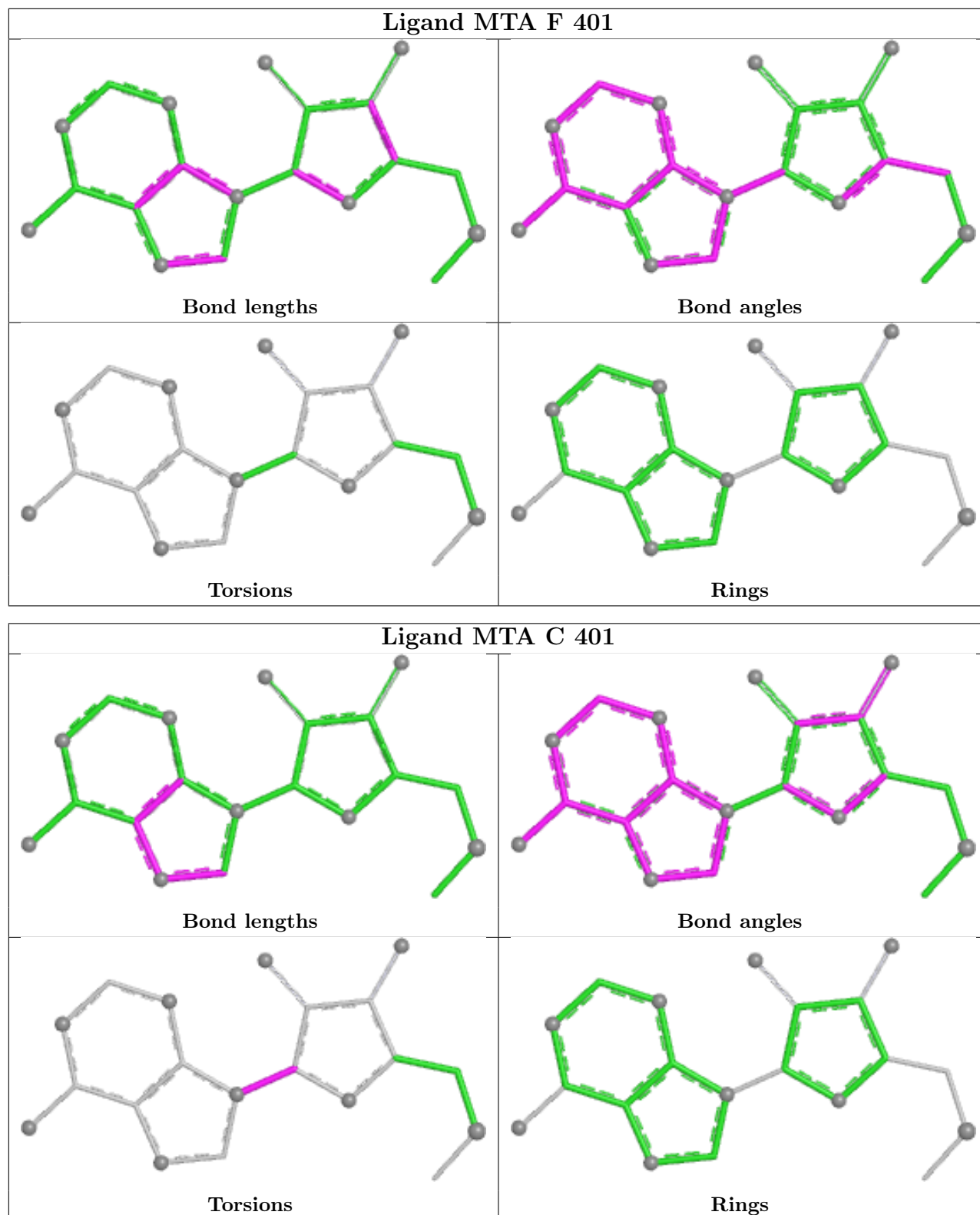
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	353/371 (95%)	-0.36	4 (1%) 78 84	16, 30, 51, 87	2 (0%)
1	B	354/371 (95%)	-0.36	5 (1%) 73 81	19, 31, 54, 100	0
1	C	353/371 (95%)	-0.21	3 (0%) 82 88	25, 38, 62, 78	2 (0%)
1	D	353/371 (95%)	-0.26	5 (1%) 73 81	25, 36, 60, 79	1 (0%)
1	E	353/371 (95%)	0.04	4 (1%) 78 84	22, 47, 75, 99	2 (0%)
1	F	353/371 (95%)	0.25	6 (1%) 69 77	32, 55, 86, 105	0
1	G	353/371 (95%)	0.38	10 (2%) 55 60	32, 58, 90, 129	3 (0%)
All	All	2472/2597 (95%)	-0.07	37 (1%) 72 79	16, 42, 75, 129	10 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	214	TYR	4.8
1	G	72	ARG	4.3
1	G	113	GLU	4.1
1	A	214	TYR	4.1
1	E	72	ARG	3.8
1	C	338	VAL	3.5
1	F	214	TYR	3.4
1	G	214	TYR	3.4
1	A	215	ALA	3.1
1	F	338	VAL	3.1
1	F	-1	SER	2.9
1	G	338	VAL	2.9
1	G	119	PRO	2.9
1	D	338	VAL	2.8
1	E	214	TYR	2.8
1	B	198	GLU	2.7
1	C	72	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	-1	SER	2.5
1	G	-1	SER	2.4
1	E	203	PHE	2.4
1	B	337	THR	2.4
1	A	-1	SER	2.4
1	D	339	GLY	2.3
1	B	116	ARG	2.3
1	G	125	PHE	2.3
1	F	195	ILE	2.2
1	G	180	ILE	2.2
1	F	340	GLN	2.2
1	F	231	GLU	2.1
1	D	320	MET	2.1
1	B	338	VAL	2.1
1	D	1	MET	2.1
1	G	211	LEU	2.1
1	A	116	ARG	2.1
1	E	-1	SER	2.0
1	D	167	MET	2.0
1	G	202	ILE	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(Å ²)	Q<0.9
6	PEG	E	405	7/7	0.73	0.16	63,64,67,68	0
4	GOL	A	405	6/6	0.84	0.16	34,53,65,65	0
4	GOL	A	403	6/6	0.84	0.15	53,57,62,62	0

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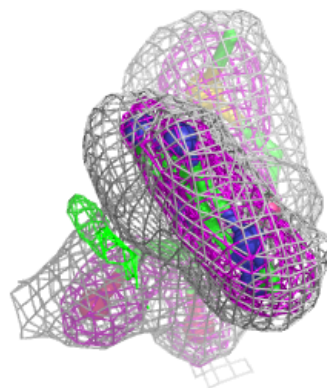
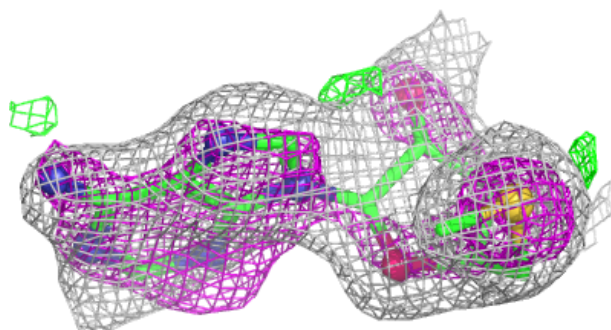
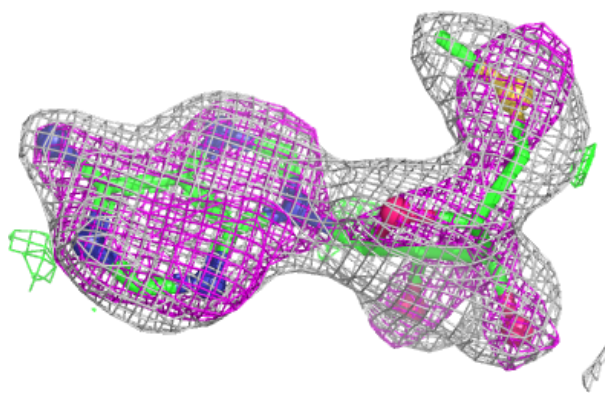
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PEG	A	407	7/7	0.86	0.15	52,56,66,72	0
3	N4P	F	402	14/14	0.87	0.12	24,27,34,35	0
2	MTA	G	401	20/20	0.87	0.12	35,37,40,41	0
4	GOL	A	404	6/6	0.87	0.12	42,60,63,64	0
7	EDO	D	404	4/4	0.87	0.14	44,54,55,59	0
7	EDO	E	404	4/4	0.87	0.12	69,69,72,73	0
7	EDO	D	405	4/4	0.88	0.15	56,57,60,61	0
4	GOL	B	403	6/6	0.88	0.14	36,48,56,56	0
2	MTA	F	401	20/20	0.89	0.11	26,28,30,31	0
3	N4P	G	402	14/14	0.90	0.12	32,39,41,41	0
3	N4P	C	402	14/14	0.91	0.10	13,16,18,18	0
4	GOL	D	403	6/6	0.92	0.11	49,57,64,70	0
2	MTA	C	401	20/20	0.92	0.09	12,13,15,17	0
2	MTA	D	401	20/20	0.93	0.09	13,14,16,17	0
2	MTA	B	401	20/20	0.93	0.09	11,13,14,14	0
3	N4P	D	402	14/14	0.93	0.09	14,16,18,18	0
3	N4P	B	402	14/14	0.94	0.07	10,12,13,15	0
2	MTA	A	401	20/20	0.94	0.09	11,12,15,15	0
2	MTA	E	401	20/20	0.94	0.08	21,24,26,26	0
3	N4P	A	402	14/14	0.95	0.07	11,13,13,14	0
3	N4P	E	402	14/14	0.95	0.08	24,25,28,28	0
5	FE	A	406	1/1	0.98	0.11	30,30,30,30	1
5	FE	G	403	1/1	0.99	0.11	46,46,46,46	1
5	FE	C	403	1/1	0.99	0.11	43,43,43,43	1
5	FE	E	403	1/1	0.99	0.10	50,50,50,50	1

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.

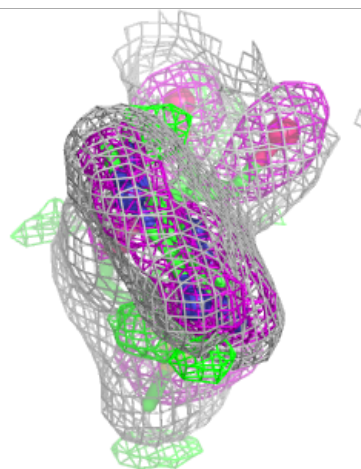
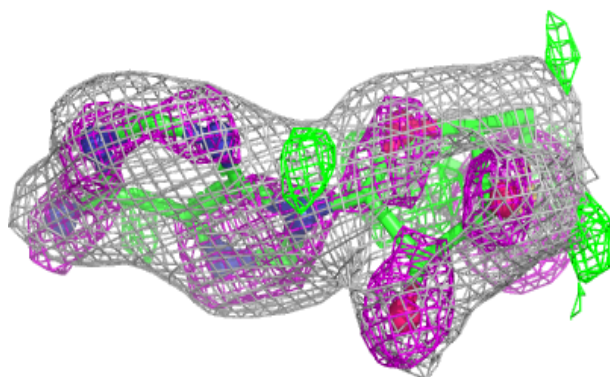
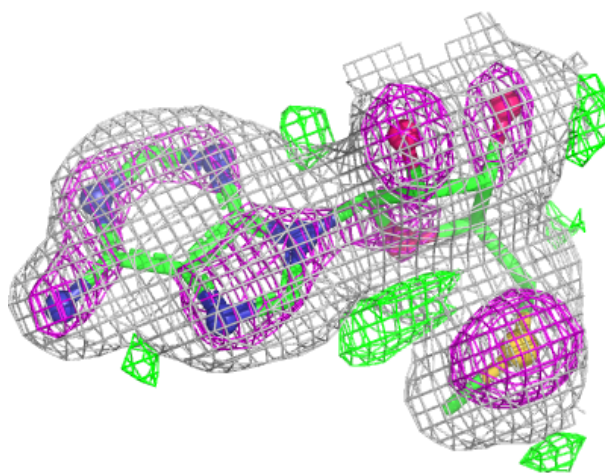
Electron density around MTA G 401:

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and green (positive)



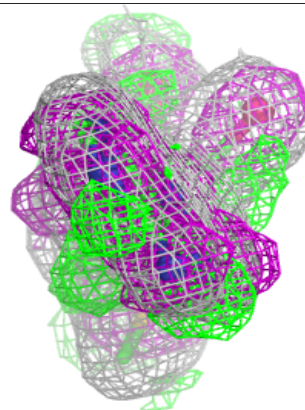
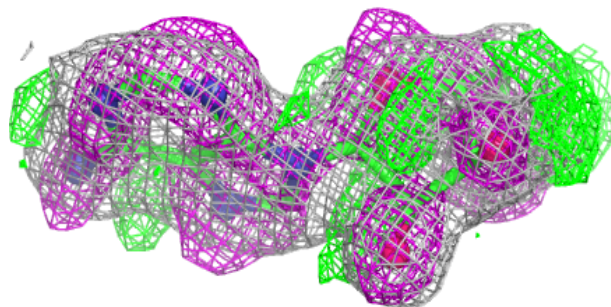
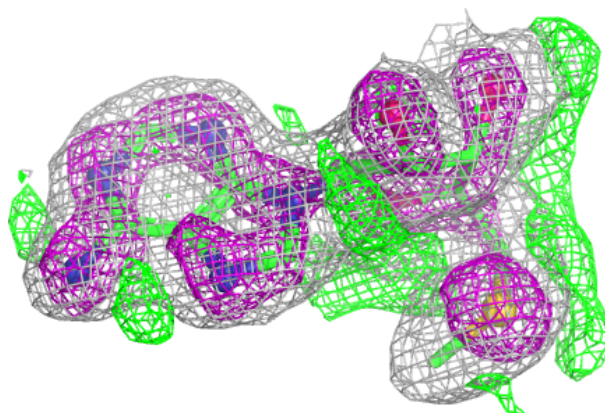
Electron density around MTA F 401:

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



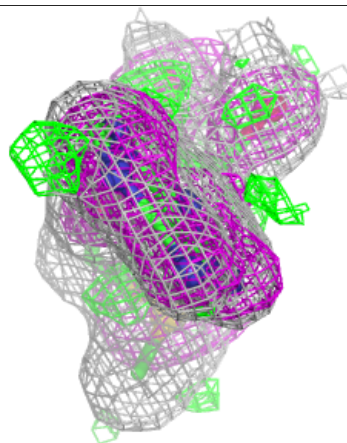
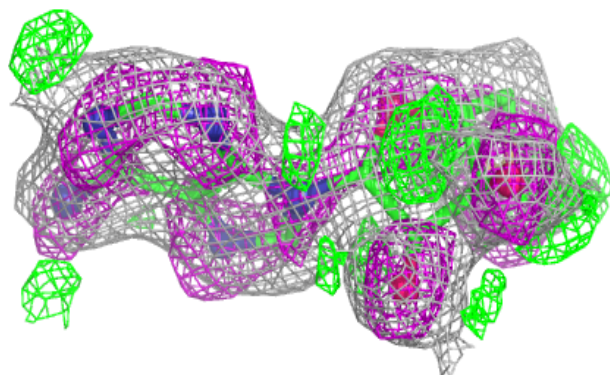
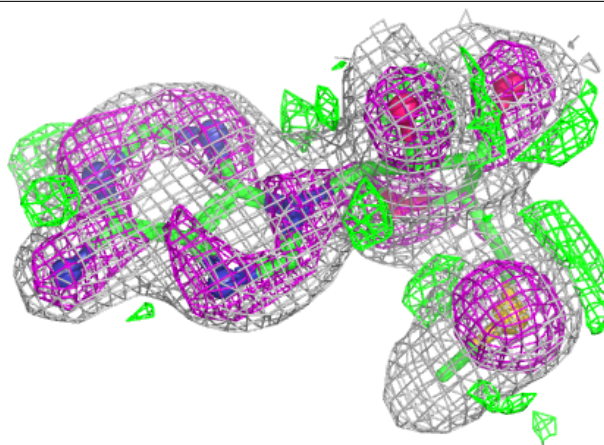
Electron density around MTA C 401:

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and green (positive)

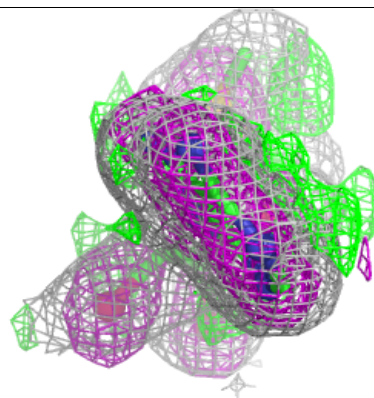
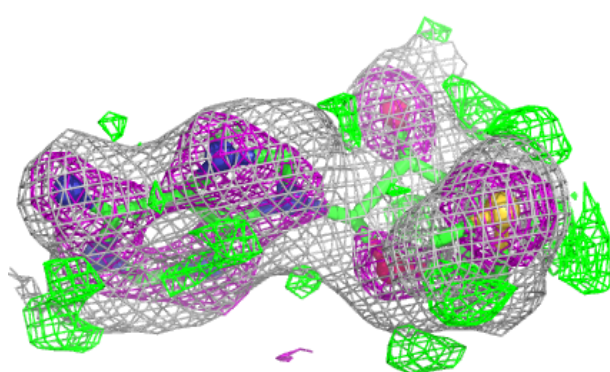
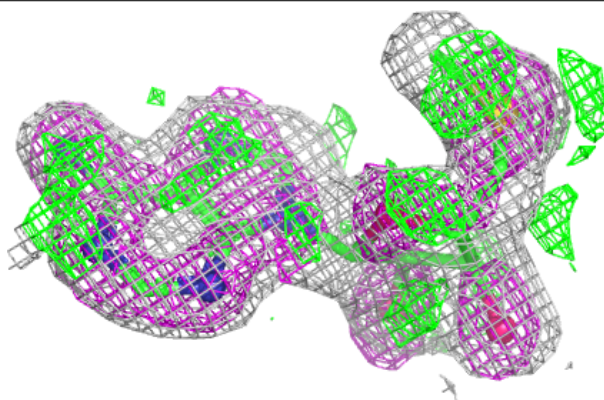


Electron density around MTA D 401:

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

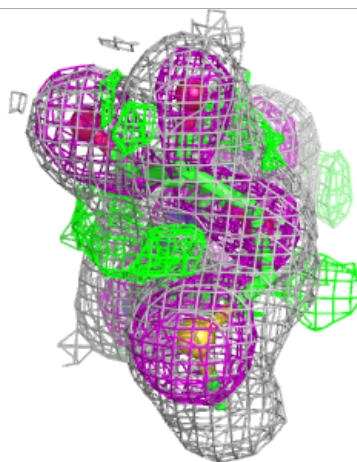
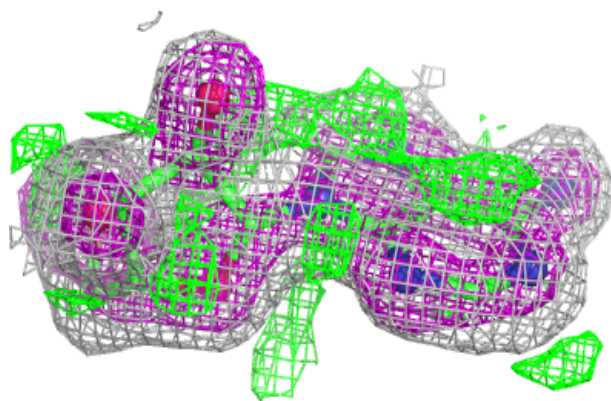
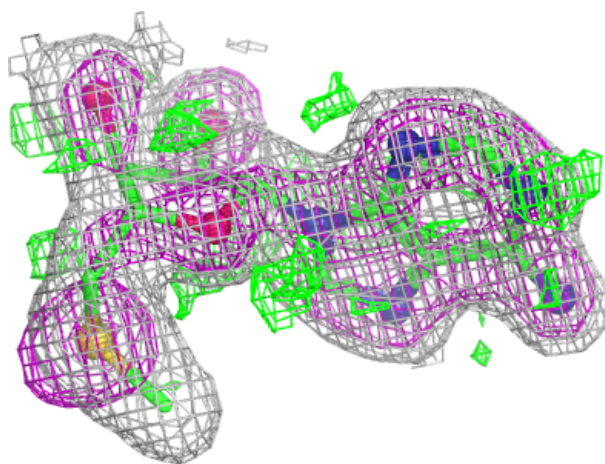
**Electron density around MTA B 401:**

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and green (positive)



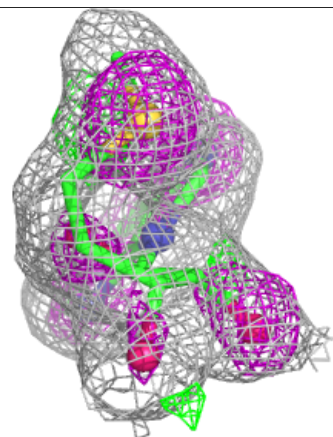
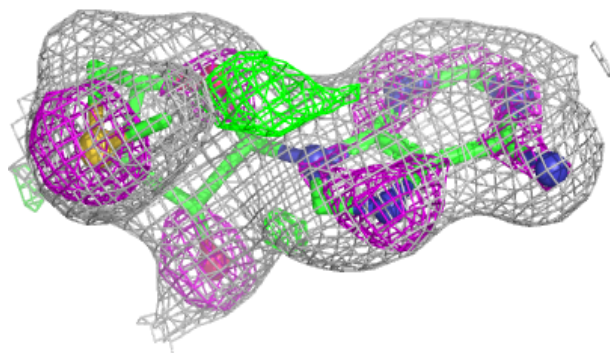
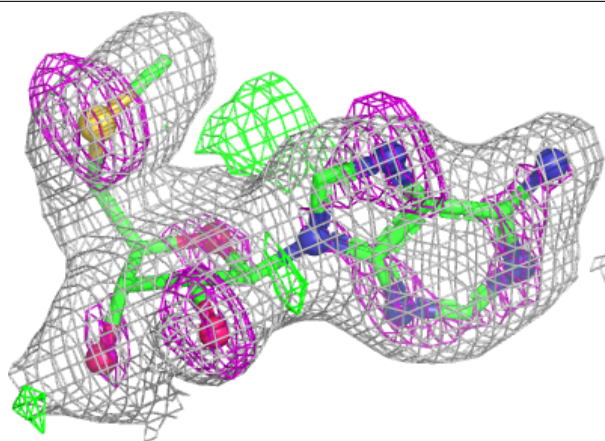
Electron density around MTA A 401:

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



Electron density around MTA E 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 [i](#)

There are no such residues in this entry.