



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 1, 2022 – 06:27 pm BST

PDB ID : 7P9Y
Title : N-acetylglucosamine kinase from Plesiomonas shigelloides complexed with alpha-N-acetylglucosamine
Authors : Roy, S.; Isupov, M.N.; Harmer, N.J.; Ames, J.R.
Deposited on : 2021-07-28
Resolution : 1.94 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.29
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

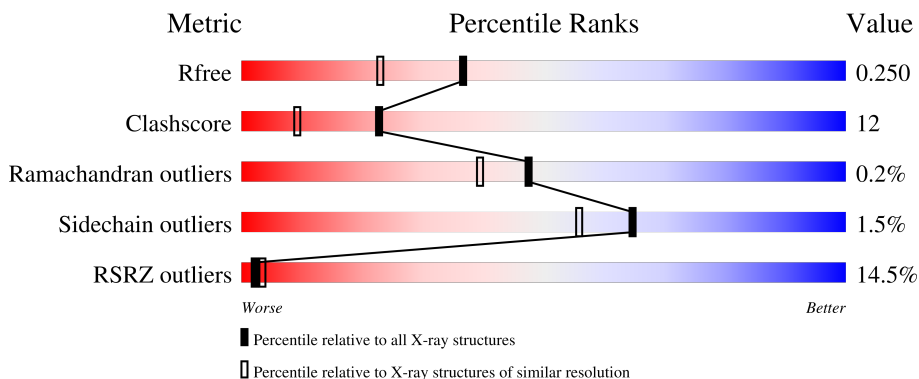
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	AAA	417	
1	BBB	417	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MPD	AAA	601	-	-	X	-
3	EDO	AAA	602	-	-	X	-
3	EDO	BBB	504	-	-	X	-
9	PEG	BBB	501	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 5095 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 Ubiquitin-like protein SMT3,N-acetyl-D-glucosamine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	304	2335	1491	405	429	10	0	3	0
1	BBB	304	2344	1498	405	431	10	0	6	0

There are 40 discrepancies between the modelled and reference sequences:

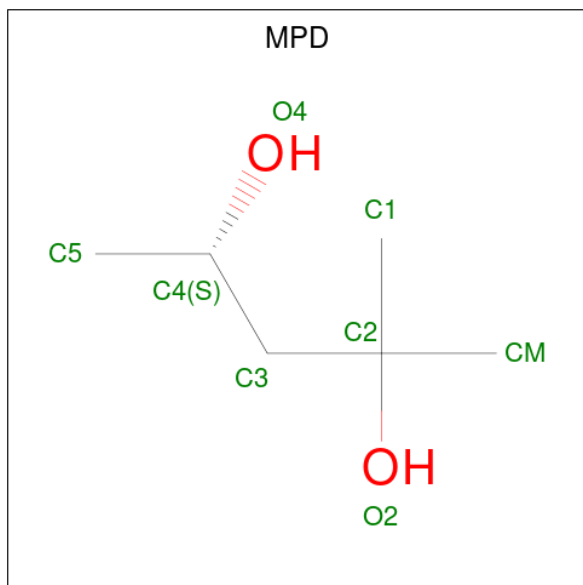
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-114	MET	-	initiating methionine	UNP Q12306
AAA	-113	ALA	-	expression tag	UNP Q12306
AAA	-112	HIS	-	expression tag	UNP Q12306
AAA	-111	HIS	-	expression tag	UNP Q12306
AAA	-110	HIS	-	expression tag	UNP Q12306
AAA	-109	HIS	-	expression tag	UNP Q12306
AAA	-108	HIS	-	expression tag	UNP Q12306
AAA	-107	HIS	-	expression tag	UNP Q12306
AAA	-106	GLY	-	expression tag	UNP Q12306
AAA	-10	SER	-	linker	UNP Q12306
AAA	-9	SER	-	linker	UNP Q12306
AAA	-8	GLY	-	linker	UNP Q12306
AAA	-7	LEU	-	linker	UNP Q12306
AAA	-6	GLU	-	linker	UNP Q12306
AAA	-5	VAL	-	linker	UNP Q12306
AAA	-4	LEU	-	linker	UNP Q12306
AAA	-3	PHE	-	linker	UNP Q12306
AAA	-2	GLN	-	linker	UNP Q12306
AAA	-1	GLY	-	linker	UNP Q12306
AAA	0	THR	-	linker	UNP Q12306
BBB	-114	MET	-	initiating methionine	UNP Q12306
BBB	-113	ALA	-	expression tag	UNP Q12306
BBB	-112	HIS	-	expression tag	UNP Q12306
BBB	-111	HIS	-	expression tag	UNP Q12306
BBB	-110	HIS	-	expression tag	UNP Q12306

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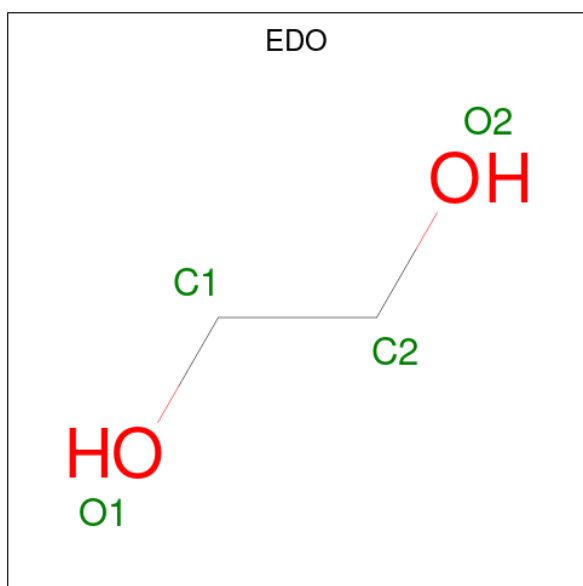
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-109	HIS	-	expression tag	UNP Q12306
BBB	-108	HIS	-	expression tag	UNP Q12306
BBB	-107	HIS	-	expression tag	UNP Q12306
BBB	-106	GLY	-	expression tag	UNP Q12306
BBB	-10	SER	-	linker	UNP Q12306
BBB	-9	SER	-	linker	UNP Q12306
BBB	-8	GLY	-	linker	UNP Q12306
BBB	-7	LEU	-	linker	UNP Q12306
BBB	-6	GLU	-	linker	UNP Q12306
BBB	-5	VAL	-	linker	UNP Q12306
BBB	-4	LEU	-	linker	UNP Q12306
BBB	-3	PHE	-	linker	UNP Q12306
BBB	-2	GLN	-	linker	UNP Q12306
BBB	-1	GLY	-	linker	UNP Q12306
BBB	0	THR	-	linker	UNP Q12306

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



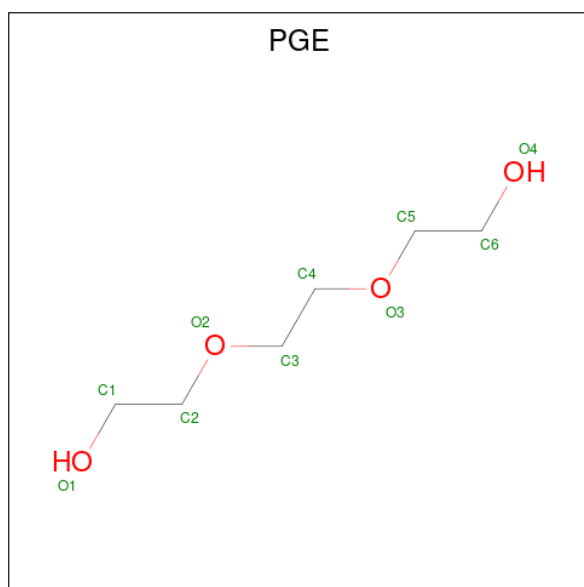
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0

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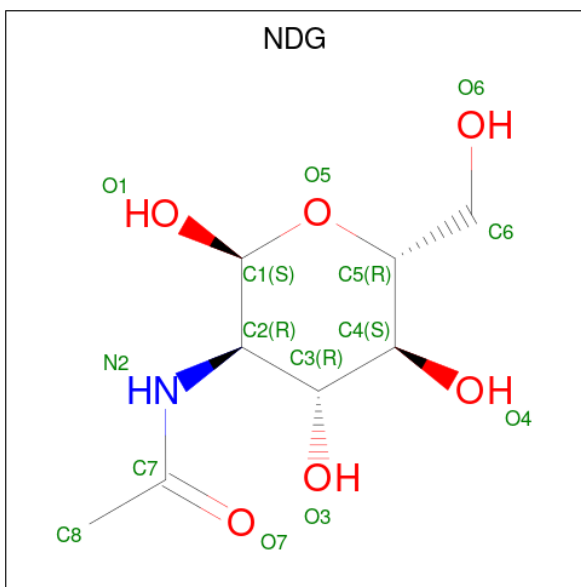
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	BBB	1	Total	C	O	0	0
			4	2	2		
3	BBB	1	Total	C	O	0	0
			4	2	2		
3	BBB	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (three-letter code: NDG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	AAA	1	15	8	1	6	0	0
5	BBB	1	15	8	1	6	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
6	AAA	2	2	2	0	0
6	BBB	2	2	2	0	0

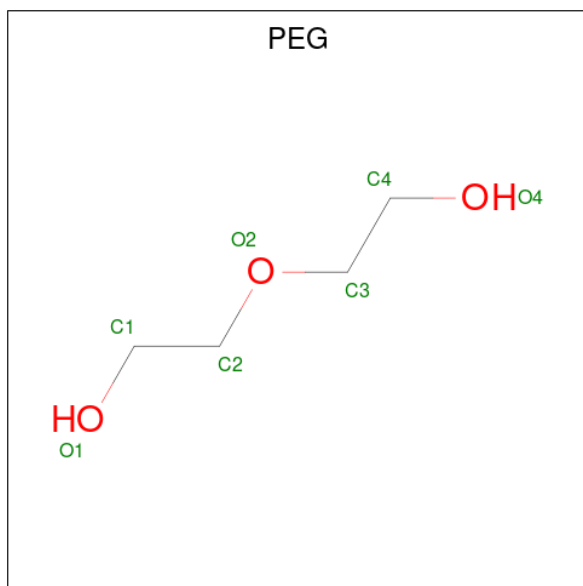
- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
7	AAA	1	1	1	0	0
7	BBB	1	1	1	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
8	AAA	2	2	2	0	0

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	BBB	1	Total	C O	0	0
			7	4 3		

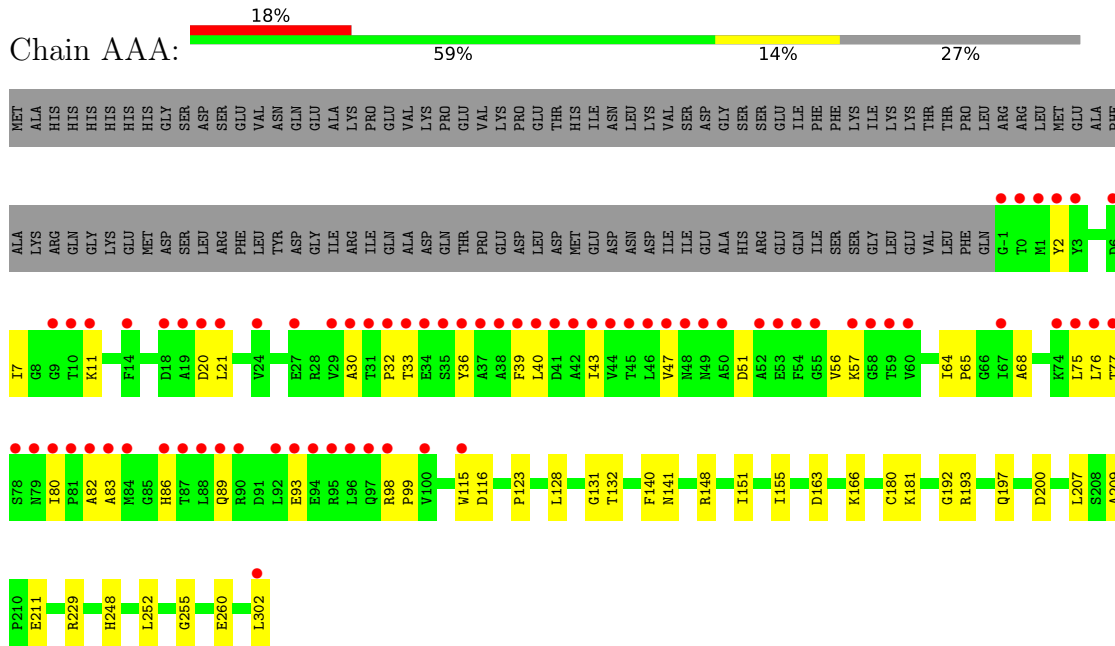
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	AAA	141	Total	O	0	0
			141	141		
10	BBB	132	Total	O	0	0
			132	132		

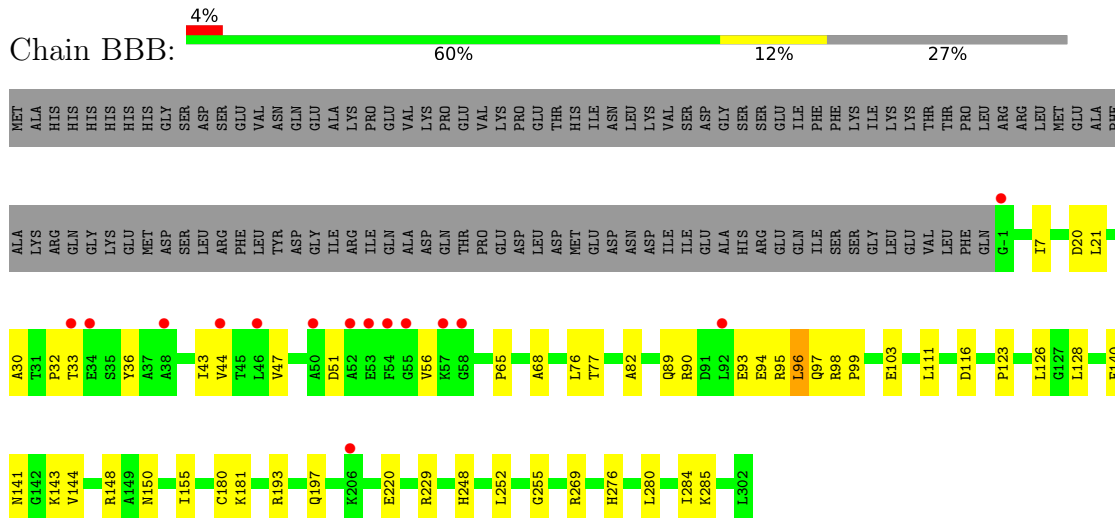
3 Residue-property plots

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: Ubiquitin-like protein SMT3,N-acetyl-D-glucosamine kinase



- Molecule 1: Ubiquitin-like protein SMT3,N-acetyl-D-glucosamine kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	115.48Å 115.48Å 119.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.14 – 1.94 52.00 – 1.94	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.14-1.94) 100.0 (52.00-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 1.94Å)	Xtrriage
Refinement program	REFMAC 5.8.0267, BUSTER	Depositor
R, R_{free}	0.209 , 0.250 0.209 , 0.250	Depositor DCC
R_{free} test set	3517 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtrriage
Anisotropy	0.118	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5095	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NDG, MPD, PGE, PEG, EDO, CL, K, ZN

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	AAA	0.43	0/2393	0.79	2/3240 (0.1%)
1	BBB	0.43	0/2406	0.77	2/3257 (0.1%)
All	All	0.43	0/4799	0.78	4/6497 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	229	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	AAA	229	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	BBB	229	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	BBB	269	ARG	NE-CZ-NH1	-5.83	117.39	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	AAA	2335	0	2334	60	0
1	BBB	2344	0	2359	50	0
2	AAA	16	0	28	8	0
2	BBB	8	0	14	2	0
3	AAA	36	0	54	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BBB	28	0	42	13	0
4	AAA	10	0	14	2	0
5	AAA	15	0	12	0	0
5	BBB	15	0	12	0	0
6	AAA	2	0	0	0	0
6	BBB	2	0	0	0	0
7	AAA	1	0	0	0	0
7	BBB	1	0	0	0	0
8	AAA	2	0	0	0	0
9	BBB	7	0	10	10	0
10	AAA	141	0	0	2	0
10	BBB	132	0	0	1	0
All	All	5095	0	4879	112	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 12.

All (112) 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:BBB:276:HIS:H	3:BBB:504:EDO:H11	1.08	1.16
1:BBB:141:ASN:HD22	9:BBB:501:PEG:H41	1.20	1.04
1:BBB:140:PHE:HB2	9:BBB:501:PEG:H12	1.41	1.00
1:AAA:141:ASN:OD1	9:BBB:501:PEG:H22	1.66	0.95
1:BBB:280:LEU:H	3:BBB:505:EDO:H11	1.31	0.94
1:AAA:255:GLY:HA3	2:AAA:601:MPD:H52	1.48	0.93
1:AAA:57:LYS:HB2	1:AAA:98:ARG:HH22	1.36	0.91
1:AAA:39:PHE:HE2	1:AAA:80:ILE:HG21	1.34	0.90
1:AAA:57:LYS:HB2	1:AAA:98:ARG:NH2	1.88	0.89
1:AAA:68:ALA:HB3	3:AAA:602:EDO:H21	1.63	0.80
1:BBB:143:LYS:HB3	9:BBB:501:PEG:H21	1.64	0.79
1:BBB:276:HIS:N	3:BBB:504:EDO:H11	1.93	0.79
1:BBB:111[B]:LEU:HD11	1:BBB:144[B]:VAL:HG21	1.63	0.79
1:AAA:57:LYS:CB	1:AAA:98:ARG:HH22	2.03	0.72
1:AAA:260:GLU:H	4:AAA:605:PGE:H42	1.57	0.70
1:BBB:111[B]:LEU:CD1	1:BBB:144[B]:VAL:HG21	2.22	0.70
1:BBB:68:ALA:HB3	3:BBB:502:EDO:H22	1.73	0.69
1:BBB:285:LYS:H	3:BBB:509:EDO:H12	1.58	0.68
1:BBB:141:ASN:HD22	9:BBB:501:PEG:C4	2.02	0.67
1:AAA:30:ALA:O	1:AAA:32:PRO:HD3	1.94	0.67
1:BBB:30:ALA:O	1:BBB:32:PRO:HD3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:103:GLU:HA	3:BBB:502:EDO:H11	1.78	0.66
1:AAA:33:THR:HA	1:AAA:82:ALA:HB2	1.79	0.63
1:AAA:40:LEU:HD23	10:AAA:816:HOH:O	1.97	0.63
1:BBB:111[B]:LEU:HG	1:BBB:144[B]:VAL:CG2	2.30	0.62
1:BBB:255:GLY:HA3	2:BBB:503:MPD:H4	1.80	0.62
1:AAA:39:PHE:CE2	1:AAA:80:ILE:HG21	2.26	0.62
2:AAA:601:MPD:H53	2:AAA:601:MPD:H11	1.81	0.60
1:AAA:43:ILE:O	1:AAA:47:VAL:HG23	2.01	0.60
1:AAA:255:GLY:CA	2:AAA:601:MPD:H52	2.27	0.60
1:BBB:111[B]:LEU:HD11	1:BBB:144[B]:VAL:CG2	2.30	0.59
1:BBB:36:TYR:HB2	1:BBB:82:ALA:O	2.02	0.59
1:BBB:280:LEU:N	3:BBB:505:EDO:H11	2.10	0.59
1:AAA:39:PHE:CE2	1:AAA:83:ALA:HB2	2.38	0.58
1:BBB:141:ASN:ND2	9:BBB:501:PEG:H41	2.05	0.58
1:AAA:51:ASP:HA	1:AAA:56:VAL:O	2.05	0.57
1:BBB:98:ARG:HB2	1:BBB:99:PRO:HD2	1.86	0.57
1:BBB:43:ILE:O	1:BBB:47:VAL:HG23	2.04	0.57
1:AAA:36:TYR:HB2	1:AAA:82:ALA:O	2.04	0.56
1:AAA:89:GLN:O	1:AAA:93:GLU:HG3	2.06	0.56
1:BBB:89:GLN:O	1:BBB:93:GLU:HG3	2.05	0.55
1:BBB:140:PHE:HB2	9:BBB:501:PEG:C1	2.25	0.55
1:AAA:255:GLY:HA3	2:AAA:601:MPD:C5	2.31	0.54
1:AAA:57:LYS:CB	1:AAA:98:ARG:NH2	2.64	0.54
1:BBB:33:THR:HA	1:BBB:82:ALA:HB2	1.88	0.54
1:BBB:128[A]:LEU:CD1	1:BBB:155:ILE:HD11	2.37	0.54
1:AAA:115[A]:TRP:HA	1:AAA:115[A]:TRP:CE3	2.43	0.54
1:AAA:86:HIS:HB3	10:AAA:719:HOH:O	2.08	0.53
1:AAA:128:LEU:CD1	1:AAA:155:ILE:HD11	2.38	0.53
1:BBB:128[A]:LEU:HD23	1:BBB:252:LEU:HD22	1.90	0.53
1:BBB:111[B]:LEU:CG	1:BBB:144[B]:VAL:CG2	2.87	0.53
1:AAA:140:PHE:HB2	9:BBB:501:PEG:H32	1.91	0.52
1:AAA:57:LYS:C	1:AAA:98:ARG:HH22	2.13	0.52
1:AAA:68:ALA:CB	3:AAA:602:EDO:H21	2.38	0.52
1:BBB:111[B]:LEU:CD1	1:BBB:144[B]:VAL:CG2	2.87	0.52
1:AAA:75:LEU:HG	1:AAA:77:THR:HG22	1.92	0.52
1:AAA:98:ARG:HB2	1:AAA:99:PRO:HD2	1.91	0.51
1:AAA:39:PHE:HE2	1:AAA:80:ILE:CG2	2.16	0.50
2:AAA:601:MPD:H53	2:AAA:601:MPD:C1	2.40	0.50
1:BBB:280:LEU:H	3:BBB:505:EDO:C1	2.13	0.50
1:AAA:180:CYS:O	1:AAA:181:LYS:HB2	2.12	0.50
1:AAA:193:ARG:HH11	1:AAA:197:GLN:HE22	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:57:LYS:CA	1:AAA:98:ARG:HH22	2.24	0.49
1:AAA:140:PHE:CB	9:BBB:501:PEG:H32	2.42	0.49
1:AAA:248:HIS:HA	1:BBB:148:ARG:HB2	1.95	0.49
1:AAA:2:TYR:CE2	1:AAA:302:LEU:HD12	2.47	0.49
1:AAA:68:ALA:H	3:AAA:602:EDO:C2	2.26	0.49
1:AAA:128:LEU:HD23	1:AAA:252:LEU:HD22	1.94	0.49
1:BBB:150:ASN:ND2	3:BBB:502:EDO:H21	2.28	0.48
1:BBB:284:ILE:HG22	3:BBB:509:EDO:H22	1.95	0.48
1:AAA:57:LYS:HB2	1:AAA:98:ARG:CZ	2.43	0.48
1:BBB:111[B]:LEU:HG	1:BBB:144[B]:VAL:HG22	1.94	0.48
1:AAA:68:ALA:H	3:AAA:602:EDO:H21	1.79	0.48
1:AAA:77:THR:HG23	1:AAA:77:THR:O	2.14	0.48
1:AAA:57:LYS:C	1:AAA:98:ARG:NH2	2.68	0.47
1:AAA:132:THR:H	3:AAA:604:EDO:H12	1.80	0.47
1:AAA:211:GLU:OE2	3:AAA:609:EDO:H11	2.15	0.47
1:BBB:276:HIS:HB3	3:BBB:504:EDO:H22	1.97	0.46
1:AAA:131:GLY:HA2	2:AAA:601:MPD:H4	1.97	0.46
1:BBB:51:ASP:HA	1:BBB:56:VAL:O	2.16	0.46
1:BBB:180:CYS:O	1:BBB:181:LYS:HB2	2.16	0.45
1:AAA:128:LEU:HD23	1:AAA:252:LEU:CD2	2.47	0.45
1:BBB:193:ARG:HH11	1:BBB:197:GLN:HE22	1.65	0.45
1:AAA:11:LYS:HG2	1:AAA:30:ALA:HA	2.00	0.44
1:AAA:7:ILE:O	1:AAA:65:PRO:HD3	2.18	0.43
1:BBB:20:ASP:O	1:BBB:21:LEU:HB2	2.18	0.43
1:AAA:180:CYS:HB2	3:BBB:504:EDO:H12	2.00	0.43
1:BBB:94:GLU:C	1:BBB:96:LEU:H	2.21	0.43
1:BBB:111[B]:LEU:HD21	1:BBB:144[B]:VAL:HG23	2.00	0.43
1:BBB:123:PRO:HB2	1:BBB:248:HIS:CE1	2.54	0.43
1:BBB:220:GLU:HG3	3:BBB:507:EDO:H22	2.00	0.43
1:AAA:192:GLY:HA3	2:AAA:601:MPD:H31	2.01	0.43
1:AAA:20:ASP:O	1:AAA:21:LEU:HB2	2.19	0.42
1:BBB:7:ILE:O	1:BBB:65:PRO:HD3	2.19	0.42
2:BBB:503:MPD:H53	10:BBB:701:HOH:O	2.19	0.42
1:AAA:123:PRO:HB2	1:AAA:248:HIS:CE1	2.54	0.42
1:AAA:200:ASP:O	3:AAA:608:EDO:H11	2.20	0.42
4:AAA:605:PGE:H1	4:AAA:605:PGE:H52	2.01	0.42
1:AAA:21:LEU:HD12	1:AAA:115[B]:TRP:CZ3	2.55	0.42
1:AAA:207:LEU:CD2	3:AAA:609:EDO:H22	2.50	0.42
1:BBB:77:THR:HG23	1:BBB:77:THR:O	2.20	0.42
1:BBB:44:VAL:HG11	1:BBB:95:ARG:NH2	2.35	0.42
1:BBB:90:ARG:HD3	1:BBB:90:ARG:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:140:PHE:HB3	9:BBB:501:PEG:H11	2.01	0.41
1:AAA:151:ILE:O	1:AAA:151:ILE:CG2	2.68	0.41
1:AAA:209:ALA:HB3	2:AAA:601:MPD:CM	2.50	0.41
1:BBB:128[A]:LEU:HD23	1:BBB:252:LEU:CD2	2.49	0.41
1:AAA:75:LEU:HD23	1:AAA:83:ALA:HB1	2.03	0.41
1:AAA:148:ARG:HB2	1:BBB:248:HIS:HA	2.03	0.41
1:BBB:126:LEU:HG	1:BBB:128[B]:LEU:HG	2.03	0.40
1:AAA:47:VAL:O	1:AAA:51:ASP:CG	2.59	0.40
1:BBB:97:GLN:HG3	1:BBB:97:GLN:O	2.21	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	AAA	305/417 (73%)	291 (95%)	14 (5%)	0	100	100
1	BBB	308/417 (74%)	292 (95%)	15 (5%)	1 (0%)	41	32
All	All	613/834 (74%)	583 (95%)	29 (5%)	1 (0%)	47	39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	96	LEU

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	AAA	241/340 (71%)	236 (98%)	5 (2%)	53	41
1	BBB	244/340 (72%)	242 (99%)	2 (1%)	81	78
All	All	485/680 (71%)	478 (99%)	7 (1%)	65	58

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	64	ILE
1	AAA	76	LEU
1	AAA	116	ASP
1	AAA	163	ASP
1	AAA	166	LYS
1	BBB	76	LEU
1	BBB	116	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 8 are monoatomic - leaving 23 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
3	EDO	BBB	506	-	3,3,3	0.11	0	2,2,2	0.21	0
3	EDO	AAA	610	-	3,3,3	0.30	0	2,2,2	0.67	0
4	PGE	AAA	605	-	9,9,9	0.35	0	8,8,8	0.27	0
3	EDO	BBB	508	-	3,3,3	0.16	0	2,2,2	0.14	0
3	EDO	AAA	603	-	3,3,3	0.09	0	2,2,2	0.66	0
2	MPD	AAA	601	-	7,7,7	0.41	0	9,10,10	1.15	0
3	EDO	AAA	607	-	3,3,3	0.16	0	2,2,2	0.37	0
3	EDO	AAA	609	-	3,3,3	0.24	0	2,2,2	0.72	0
9	PEG	BBB	501	-	6,6,6	0.56	0	5,5,5	0.27	0
3	EDO	AAA	606	-	3,3,3	0.06	0	2,2,2	0.20	0
2	MPD	BBB	503	-	7,7,7	0.43	0	9,10,10	1.23	1 (11%)
5	NDG	BBB	510	-	15,15,15	0.38	0	21,21,21	1.82	2 (9%)
5	NDG	AAA	612	-	15,15,15	0.37	0	21,21,21	2.37	2 (9%)
3	EDO	AAA	604	-	3,3,3	0.32	0	2,2,2	0.67	0
3	EDO	BBB	507	-	3,3,3	0.15	0	2,2,2	0.30	0
3	EDO	BBB	509	-	3,3,3	0.18	0	2,2,2	0.47	0
2	MPD	AAA	611	-	7,7,7	0.13	0	9,10,10	0.50	0
3	EDO	AAA	616	-	3,3,3	0.38	0	2,2,2	0.13	0
3	EDO	BBB	502	-	3,3,3	0.44	0	2,2,2	0.25	0
3	EDO	AAA	602	-	3,3,3	0.09	0	2,2,2	0.53	0
3	EDO	BBB	504	-	3,3,3	0.28	0	2,2,2	0.14	0
3	EDO	AAA	608	-	3,3,3	0.13	0	2,2,2	0.58	0
3	EDO	BBB	505	-	3,3,3	0.19	0	2,2,2	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	BBB	506	-	-	1/1/1/1	-
3	EDO	AAA	610	-	-	0/1/1/1	-
4	PGE	AAA	605	-	-	2/7/7/7	-
3	EDO	BBB	508	-	-	1/1/1/1	-
3	EDO	AAA	603	-	-	1/1/1/1	-
2	MPD	AAA	601	-	-	1/5/5/5	-
3	EDO	AAA	607	-	-	1/1/1/1	-
3	EDO	AAA	609	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PEG	BBB	501	-	-	3/4/4/4	-
3	EDO	AAA	606	-	-	0/1/1/1	-
2	MPD	BBB	503	-	-	4/5/5/5	-
5	NDG	BBB	510	-	-	2/6/26/26	0/1/1/1
5	NDG	AAA	612	-	-	1/6/26/26	0/1/1/1
3	EDO	AAA	604	-	-	1/1/1/1	-
3	EDO	BBB	507	-	-	1/1/1/1	-
3	EDO	BBB	509	-	-	0/1/1/1	-
2	MPD	AAA	611	-	-	0/5/5/5	-
3	EDO	AAA	616	-	-	1/1/1/1	-
3	EDO	BBB	502	-	-	0/1/1/1	-
3	EDO	AAA	602	-	-	0/1/1/1	-
3	EDO	BBB	504	-	-	1/1/1/1	-
3	EDO	AAA	608	-	-	0/1/1/1	-
3	EDO	BBB	505	-	-	0/1/1/1	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AAA	612	NDG	C1-C2-N2	7.87	119.84	110.73
5	AAA	612	NDG	O5-C1-C2	6.98	116.53	109.52
5	BBB	510	NDG	C1-C2-N2	6.27	117.99	110.73
5	BBB	510	NDG	O5-C1-C2	4.26	113.80	109.52
2	BBB	503	MPD	C5-C4-C3	3.23	126.90	111.69

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BBB	503	MPD	C1-C2-C3-C4
2	BBB	503	MPD	O2-C2-C3-C4
2	BBB	503	MPD	C2-C3-C4-O4
5	BBB	510	NDG	C8-C7-N2-C2
5	BBB	510	NDG	O7-C7-N2-C2
3	AAA	604	EDO	O1-C1-C2-O2
3	AAA	607	EDO	O1-C1-C2-O2
3	BBB	507	EDO	O1-C1-C2-O2
3	BBB	508	EDO	O1-C1-C2-O2
9	BBB	501	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
3	BBB	506	EDO	O1-C1-C2-O2
4	AAA	605	PGE	C4-C3-O2-C2
2	AAA	601	MPD	C2-C3-C4-C5
3	AAA	616	EDO	O1-C1-C2-O2
2	BBB	503	MPD	CM-C2-C3-C4
9	BBB	501	PEG	O1-C1-C2-O2
3	AAA	603	EDO	O1-C1-C2-O2
4	AAA	605	PGE	O2-C3-C4-O3
3	AAA	609	EDO	O1-C1-C2-O2
3	BBB	504	EDO	O1-C1-C2-O2
5	AAA	612	NDG	O7-C7-N2-C2
9	BBB	501	PEG	C1-C2-O2-C3

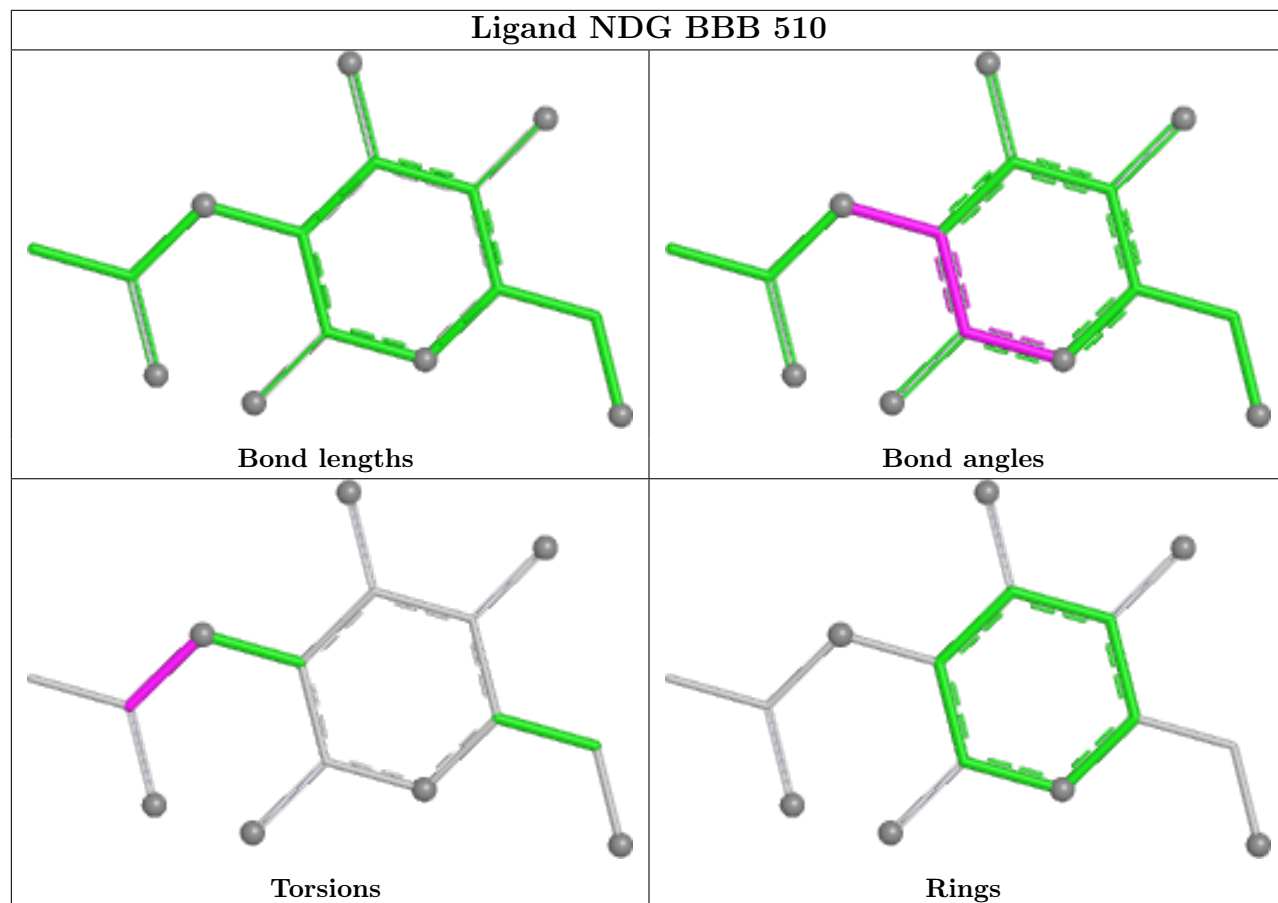
There are no ring outliers.

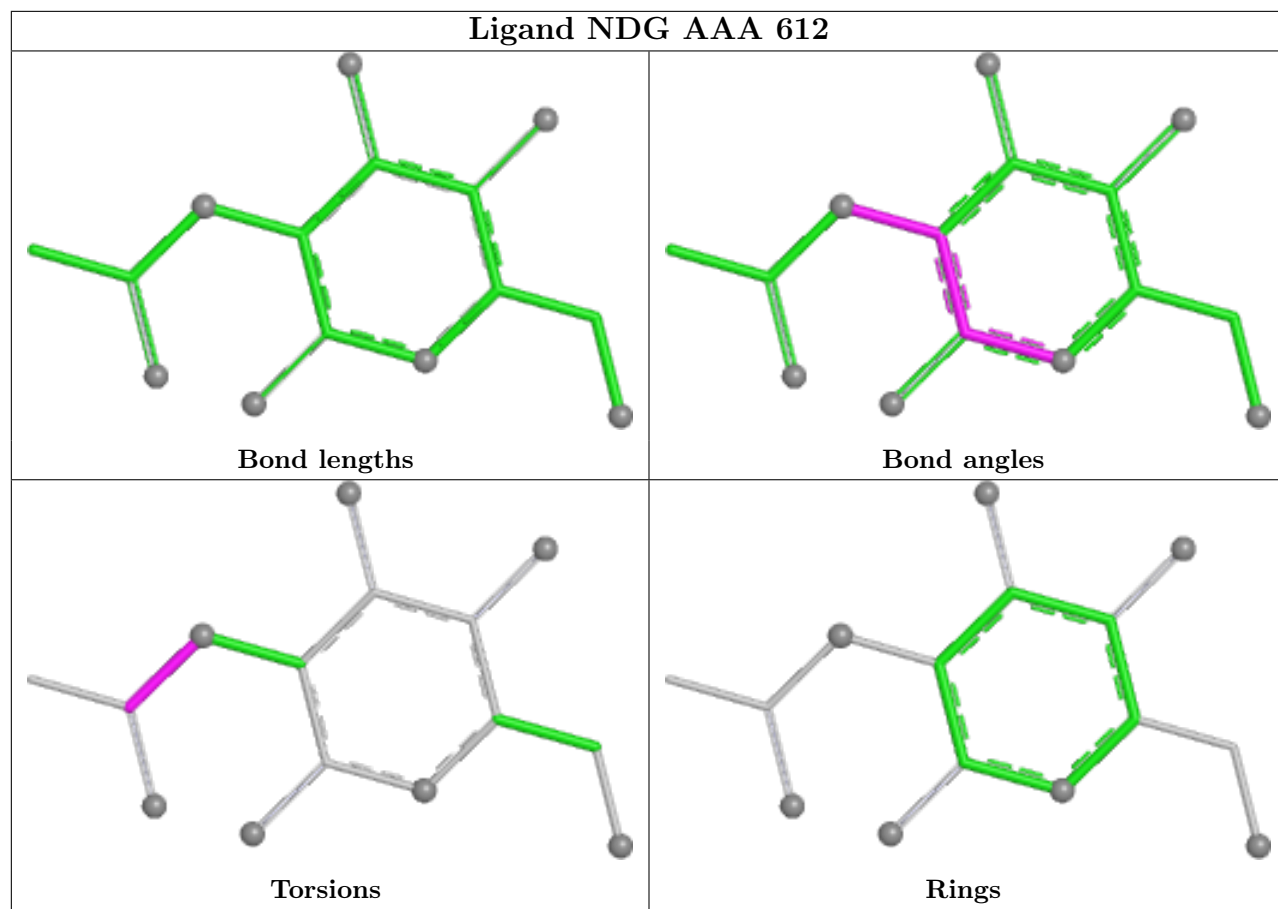
13 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	605	PGE	2	0
2	AAA	601	MPD	8	0
3	AAA	609	EDO	2	0
9	BBB	501	PEG	10	0
2	BBB	503	MPD	2	0
3	AAA	604	EDO	1	0
3	BBB	507	EDO	1	0
3	BBB	509	EDO	2	0
3	BBB	502	EDO	3	0
3	AAA	602	EDO	4	0
3	BBB	504	EDO	4	0
3	AAA	608	EDO	1	0
3	BBB	505	EDO	3	0

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

equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	304/417 (72%)	1.18	73 (24%) 0 0	27, 45, 114, 150	0
1	BBB	304/417 (72%)	0.37	15 (4%) 29 37	29, 44, 93, 140	0
All	All	608/834 (72%)	0.78	88 (14%) 2 3	27, 45, 106, 150	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	43	ILE	12.2
1	AAA	39	PHE	10.2
1	AAA	92	LEU	9.4
1	AAA	88	LEU	9.1
1	AAA	96	LEU	8.7
1	AAA	94	GLU	7.7
1	AAA	58	GLY	7.6
1	AAA	34	GLU	7.5
1	AAA	33	THR	7.3
1	AAA	302	LEU	7.1
1	AAA	40	LEU	6.3
1	AAA	1	MET	5.9
1	AAA	45	THR	5.8
1	BBB	52	ALA	5.7
1	AAA	29	VAL	5.6
1	AAA	41	ASP	5.4
1	AAA	42	ALA	5.3
1	AAA	36	TYR	5.1
1	AAA	50	ALA	5.1
1	AAA	54	PHE	4.9
1	AAA	78	SER	4.9
1	AAA	83	ALA	4.8
1	AAA	24	VAL	4.8
1	AAA	90	ARG	4.8

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Mol	Chain	Res	Type	RSRZ
1	AAA	60	VAL	4.7
1	AAA	52	ALA	4.5
1	AAA	81	PRO	4.4
1	AAA	46	LEU	4.4
1	AAA	115[A]	TRP	4.3
1	AAA	0	THR	4.3
1	AAA	19	ALA	4.3
1	AAA	55	GLY	4.2
1	BBB	33	THR	4.2
1	AAA	30	ALA	4.1
1	AAA	21	LEU	4.1
1	AAA	84	MET	4.0
1	AAA	3	TYR	4.0
1	AAA	32	PRO	4.0
1	AAA	79	ASN	3.9
1	BBB	54	PHE	3.9
1	AAA	100	VAL	3.8
1	AAA	37	ALA	3.8
1	AAA	87	THR	3.8
1	AAA	53	GLU	3.8
1	AAA	97	GLN	3.8
1	AAA	57	LYS	3.7
1	BBB	34	GLU	3.7
1	AAA	49	ASN	3.7
1	AAA	-1	GLY	3.6
1	AAA	74	LYS	3.6
1	AAA	82	ALA	3.5
1	AAA	59	THR	3.5
1	AAA	47	VAL	3.5
1	BBB	55	GLY	3.4
1	AAA	75	LEU	3.4
1	AAA	20	ASP	3.3
1	AAA	95	ARG	3.3
1	AAA	98	ARG	3.2
1	AAA	38	ALA	3.0
1	BBB	57	LYS	3.0
1	AAA	48	ASN	2.9
1	AAA	10	THR	2.8
1	AAA	67	ILE	2.8
1	AAA	44	VAL	2.8
1	BBB	44	VAL	2.8
1	AAA	11	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	AAA	35	SER	2.7
1	AAA	77	THR	2.7
1	AAA	9	GLY	2.7
1	BBB	92	LEU	2.7
1	BBB	38	ALA	2.5
1	AAA	76	LEU	2.5
1	AAA	89	GLN	2.5
1	AAA	31	THR	2.5
1	AAA	80	ILE	2.4
1	AAA	86	HIS	2.3
1	BBB	53	GLU	2.2
1	BBB	50	ALA	2.2
1	AAA	6	ASP	2.2
1	AAA	27	GLU	2.2
1	BBB	58	GLY	2.1
1	AAA	93	GLU	2.1
1	AAA	18	ASP	2.1
1	BBB	-1	GLY	2.1
1	BBB	46	LEU	2.0
1	AAA	2	TYR	2.0
1	AAA	14	PHE	2.0
1	BBB	206	LYS	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 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, 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
3	EDO	AAA	608	4/4	0.70	0.27	64,76,78,86	0

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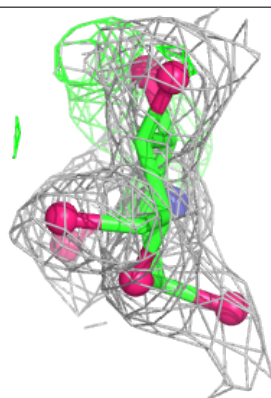
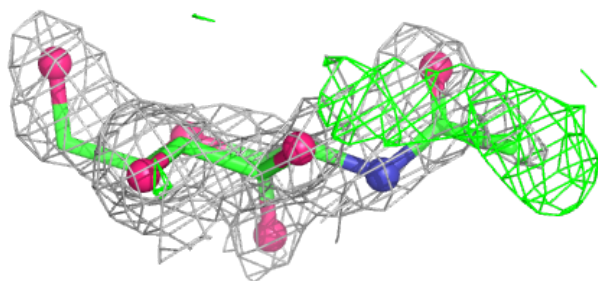
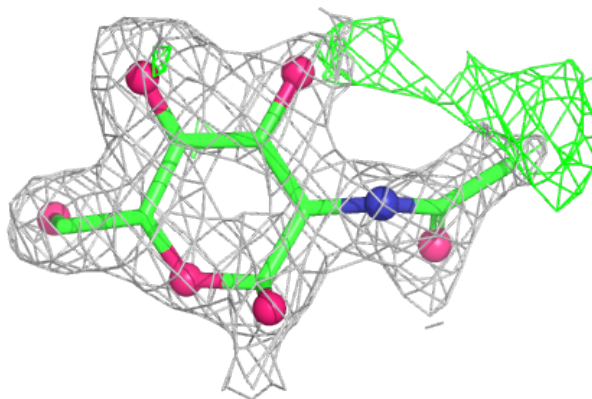
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NDG	BBB	510	15/15	0.73	0.28	49,63,71,86	15
5	NDG	AAA	612	15/15	0.76	0.21	57,75,100,107	15
3	EDO	BBB	506	4/4	0.76	0.24	68,83,89,91	0
2	MPD	AAA	611	8/8	0.77	0.14	67,76,93,96	8
3	EDO	AAA	610	4/4	0.78	0.22	63,63,65,78	0
7	K	AAA	615	1/1	0.78	0.15	70,70,70,70	0
3	EDO	BBB	508	4/4	0.79	0.20	75,96,97,102	0
3	EDO	AAA	606	4/4	0.79	0.18	68,69,77,83	0
4	PGE	AAA	605	10/10	0.80	0.21	39,65,81,89	10
3	EDO	BBB	509	4/4	0.81	0.24	48,70,70,80	0
3	EDO	AAA	607	4/4	0.84	0.20	58,70,89,100	0
3	EDO	BBB	507	4/4	0.84	0.47	59,62,63,85	4
9	PEG	BBB	501	7/7	0.84	0.38	32,43,51,57	7
3	EDO	AAA	604	4/4	0.88	0.11	56,64,69,81	0
3	EDO	AAA	603	4/4	0.88	0.40	56,70,77,87	0
2	MPD	AAA	601	8/8	0.90	0.21	37,64,73,78	0
3	EDO	AAA	602	4/4	0.91	0.50	56,60,62,77	0
3	EDO	AAA	609	4/4	0.92	0.18	44,53,62,82	0
2	MPD	BBB	503	8/8	0.93	0.21	36,71,83,88	0
3	EDO	BBB	504	4/4	0.93	0.25	56,58,65,79	0
3	EDO	BBB	505	4/4	0.93	0.20	42,54,62,65	0
3	EDO	AAA	616	4/4	0.94	0.23	42,51,58,63	0
7	K	BBB	513	1/1	0.95	0.12	60,60,60,60	0
8	CL	AAA	617	1/1	0.96	0.11	72,72,72,72	0
3	EDO	BBB	502	4/4	0.97	0.15	43,51,53,53	0
6	ZN	BBB	512	1/1	0.98	0.04	56,56,56,56	0
6	ZN	AAA	614	1/1	0.99	0.09	44,44,44,44	0
8	CL	AAA	618	1/1	0.99	0.15	41,41,41,41	0
6	ZN	AAA	613	1/1	0.99	0.07	44,44,44,44	0
6	ZN	BBB	511	1/1	1.00	0.15	38,38,38,38	0

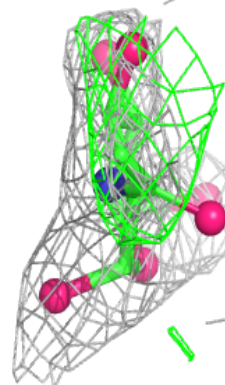
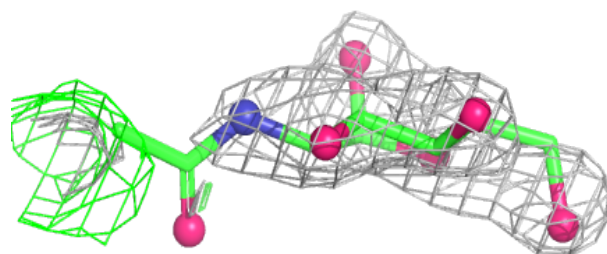
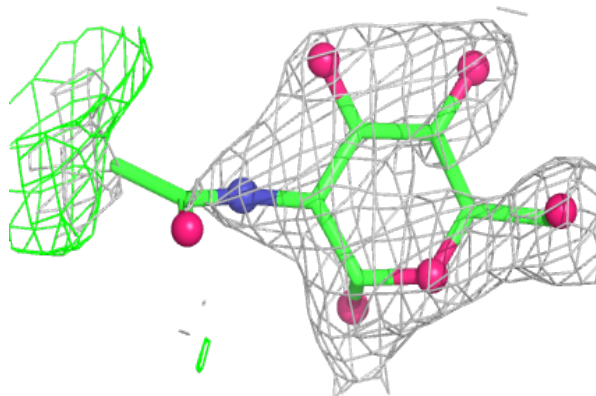
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NDG BBB 510:

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

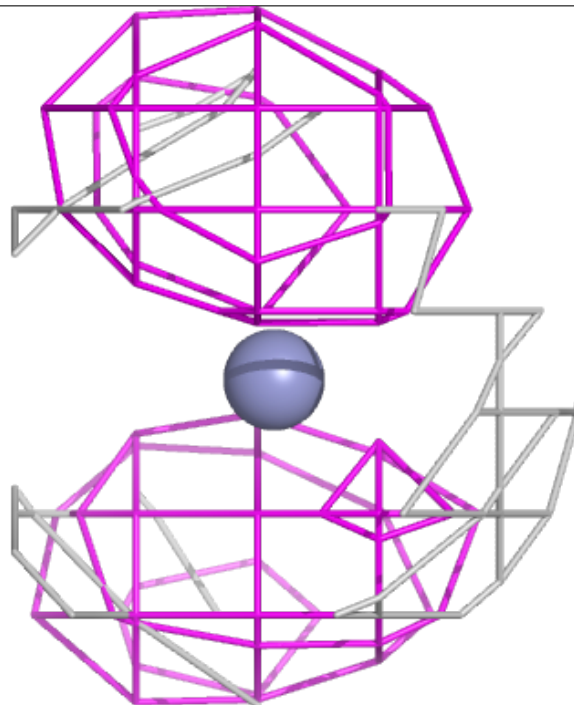
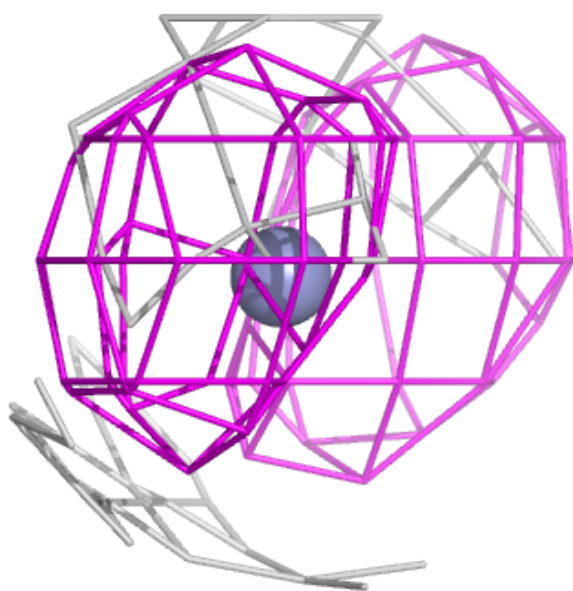
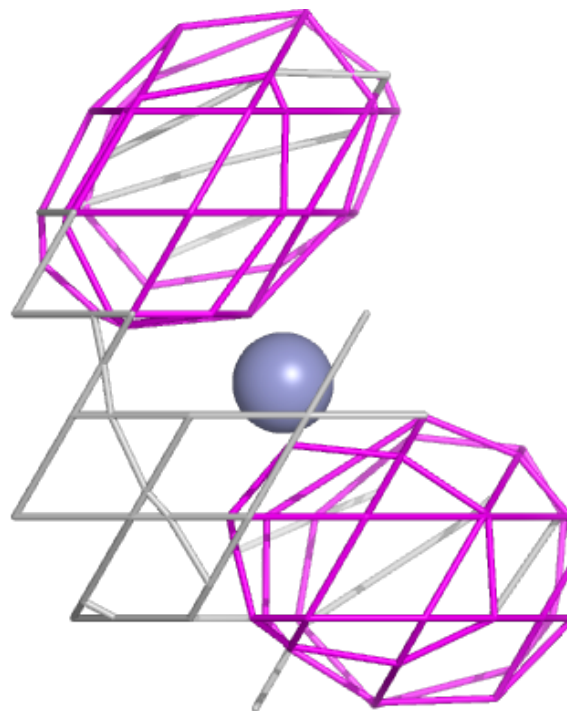
**Electron density around NDG AAA 612:**

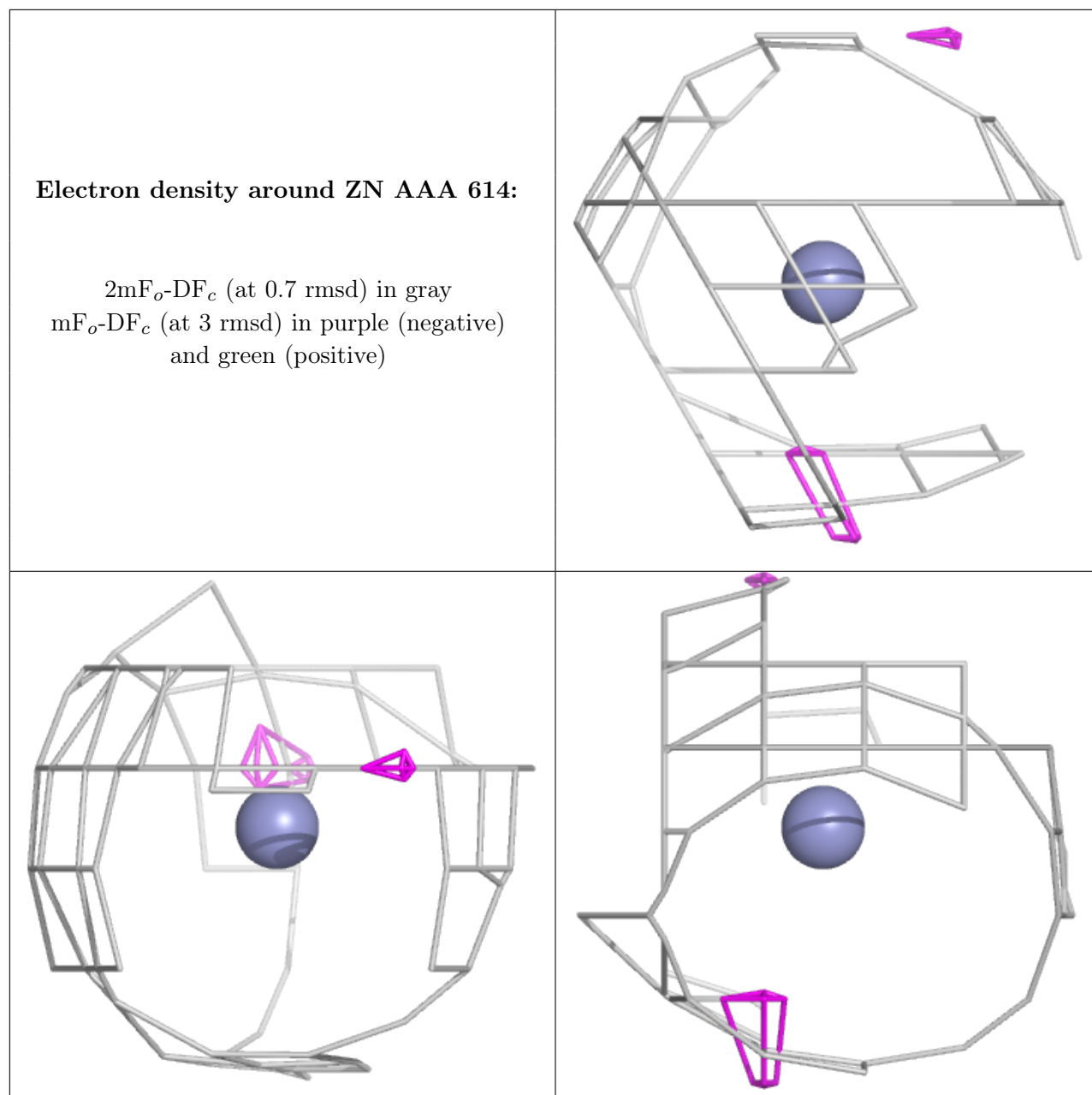
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

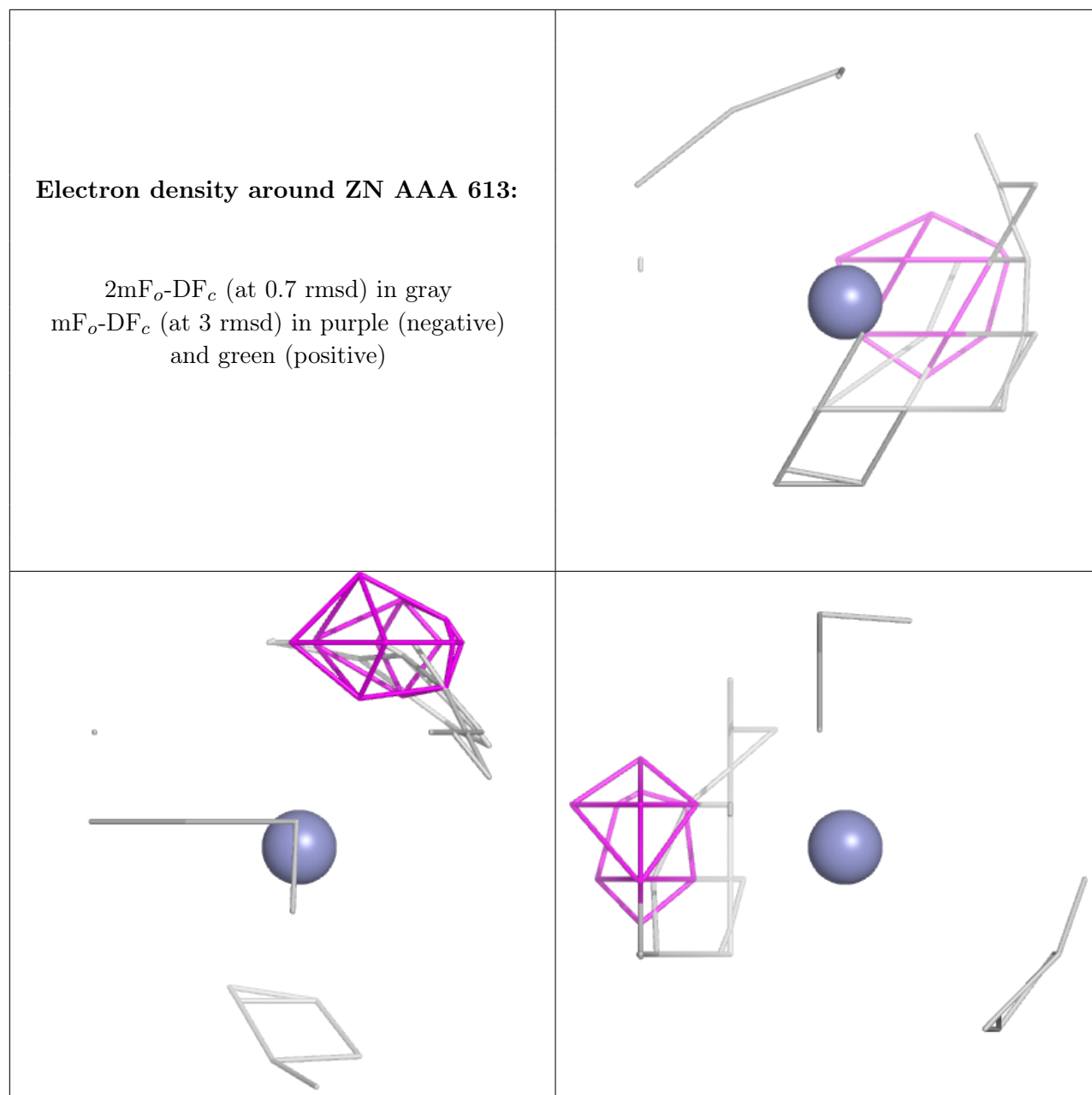


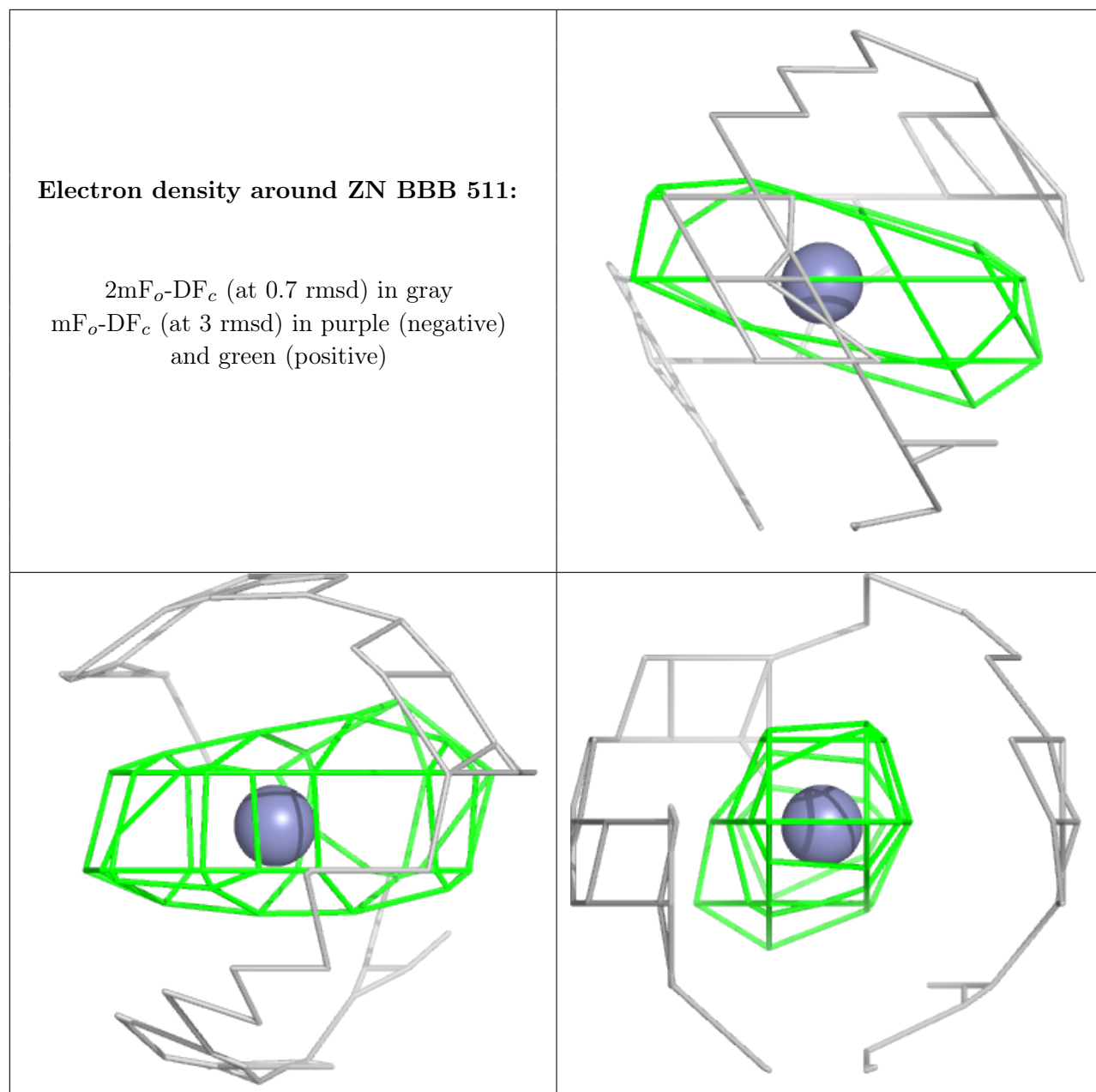
Electron density around ZN BBB 512:

$2mF_o-DF_c$ (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.