



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:07 AM UTC

PDB ID : 7P9L / pdb_00007p9l
Title : N-acetylglucosamine kinase from Plesiomonas shigelloides complexed with alp
ha-N-acetylglucosamine-6-phosphate
Authors : Roy, S.; Isupov, M.N.; Harmer, N.J.; Ames, J.R.
Deposited on : 2021-07-27
Resolution : 1.75 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

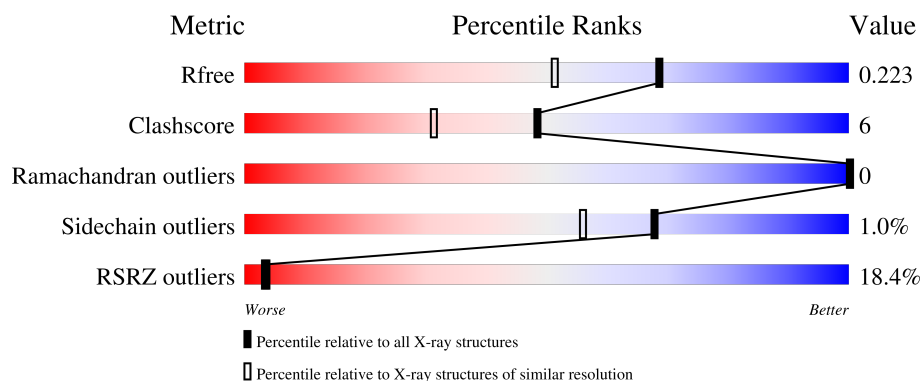
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	14% 63% 10% 27%
1	BBB	417	12% 63% 9% 27%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5453 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
1	AAA	303	Total	C	N	O	S	0	23	0
			2443	1573	424	436	10			
1	BBB	306	Total	C	N	O	S	0	20	0
			2457	1582	426	439	10			

There are 40 discrepancies between the modelled and reference sequences:

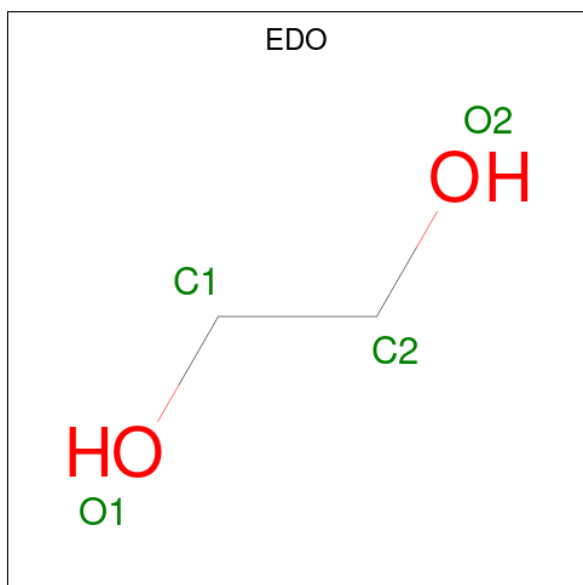
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-114	MET	-	initiating methionine	UNP Q12306
AAA	-113	ALA	-	expression tag	UNP Q12306
AAA	-112	HIS	-	expression tag	UNP Q12306
AAA	-111	HIS	-	expression tag	UNP Q12306
AAA	-110	HIS	-	expression tag	UNP Q12306
AAA	-109	HIS	-	expression tag	UNP Q12306
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

Continued on next page...

Continued from previous page...

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



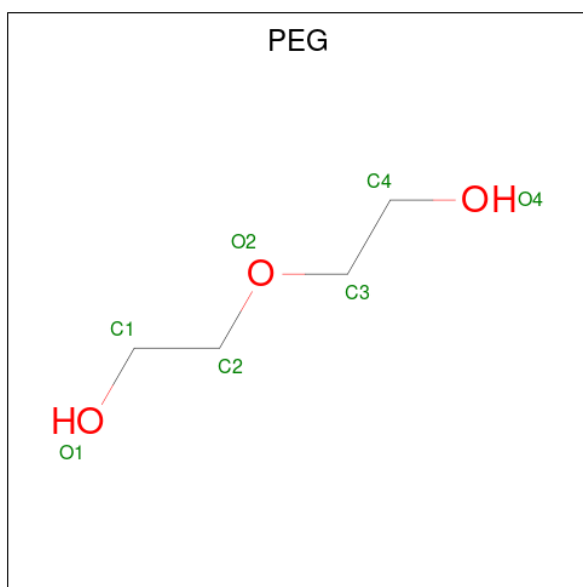
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	C	O	0	0
			4	2	2		
2	AAA	1	Total	C	O	0	0
			4	2	2		
2	AAA	1	Total	C	O	0	0
			4	2	2		
2	AAA	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

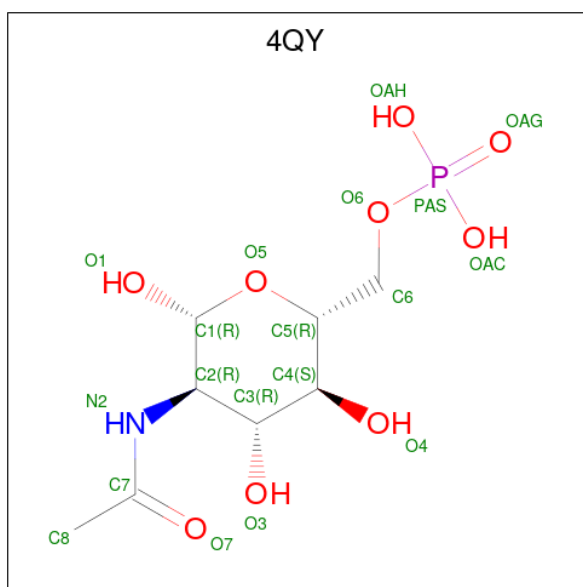
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	C	O	0	0
			4	2	2		
2	AAA	1	Total	C	O	0	0
			4	2	2		
2	AAA	1	Total	C	O	0	0
			4	2	2		
2	AAA	1	Total	C	O	0	0
			4	2	2		
2	AAA	1	Total	C	O	0	0
			4	2	2		
2	AAA	1	Total	C	O	0	0
			4	2	2		
2	AAA	1	Total	C	O	0	0
			4	2	2		
2	AAA	1	Total	C	O	0	0
			4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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 4 is 2-acetamido-2-deoxy-6-O-phosphono-beta-D-glucopyranose (CCD ID: 4QY) (formula: C₈H₁₆NO₉P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	AAA	1	Total	C	N	O	P	0	0
			19	8	1	9	1		
4	BBB	1	Total	C	N	O	P	0	0
			19	8	1	9	1		

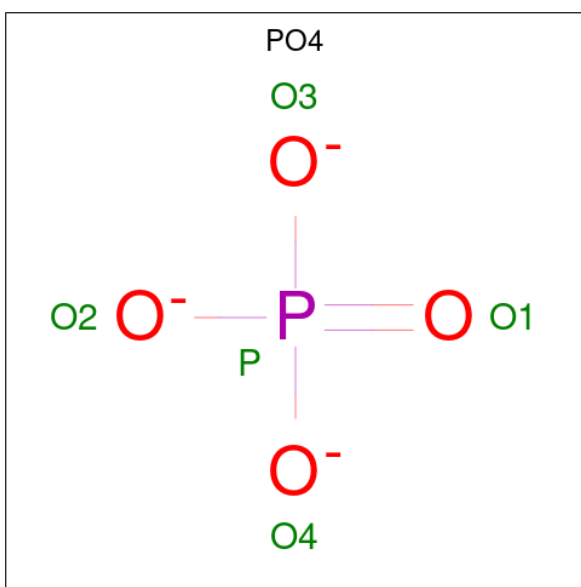
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

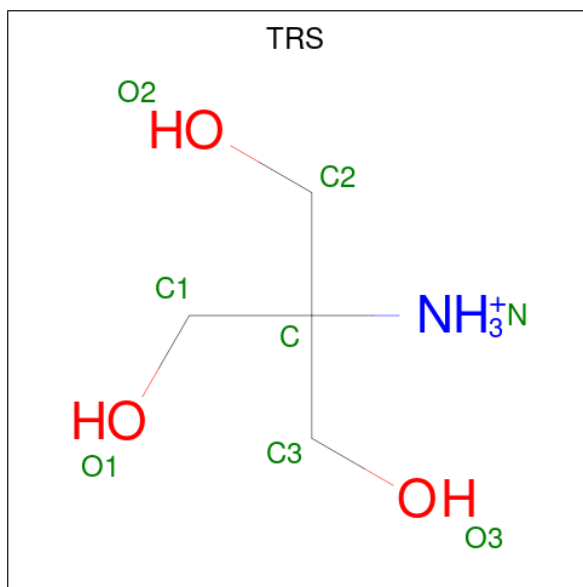


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	AAA	1	Total	O	P	0	0
			5	4	1		
7	BBB	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	1	Total	Cl	0	0
			1	1		

- Molecule 9 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	BBB	1	Total	C	N	O	0	0
			8	4	1	3		

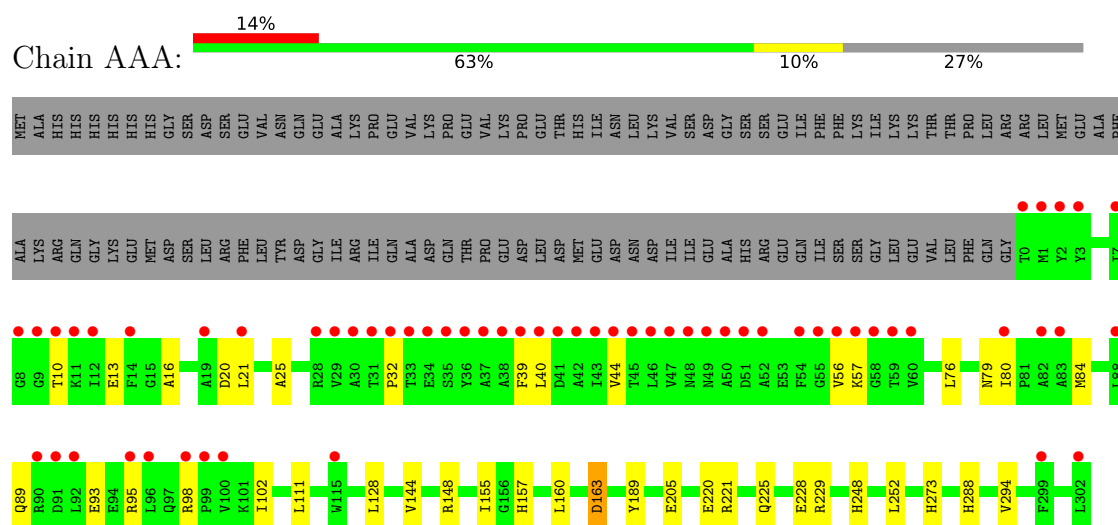
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	AAA	185	Total	O	0	0
			185	185		
10	BBB	168	Total	O	0	0
			168	168		

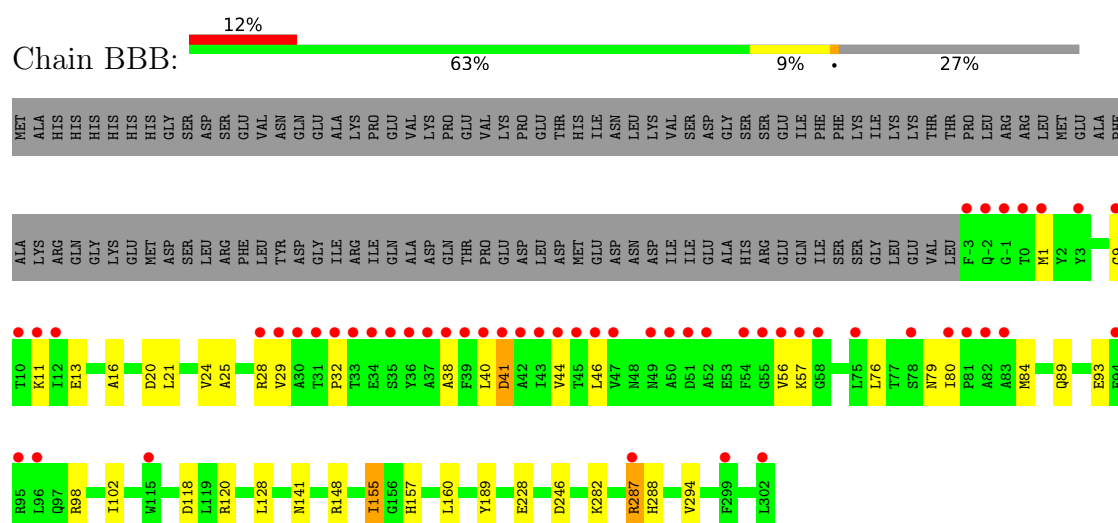
3 Residue-property plots [i](#)

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

- Molecule 1: 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	114.51Å 114.51Å 119.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	76.25 – 1.75 76.25 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.0 (76.25-1.75) 99.0 (76.25-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.193 , 0.223 0.193 , 0.223	Depositor DCC
R_{free} test set	4568 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5453	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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: ZN, EDO, CL, PO4, PEG, 4QY, K, TRS

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	0.67	1/2561 (0.0%)	1.05	5/3463 (0.1%)
1	BBB	0.70	0/2567	1.09	5/3471 (0.1%)
All	All	0.69	1/5128 (0.0%)	1.07	10/6934 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	273	HIS	CE1-NE2	5.29	1.37	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	157	HIS	CA-CB-CG	-7.86	105.94	113.80
1	AAA	288	HIS	CA-CB-CG	-7.31	106.49	113.80
1	AAA	157	HIS	CA-CB-CG	-7.01	106.79	113.80
1	BBB	246	ASP	O-C-N	-6.79	118.41	121.53
1	BBB	288	HIS	CA-CB-CG	-6.71	107.09	113.80
1	AAA	163	ASP	CA-CB-CG	6.31	118.91	112.60
1	AAA	205	GLU	CB-CG-CD	5.45	121.86	112.60
1	BBB	141	ASN	CA-CB-CG	-5.38	107.22	112.60
1	AAA	10	THR	CB-CA-C	5.34	119.16	110.24
1	BBB	120	ARG	CB-CG-CD	-5.05	99.68	111.30

There are no chirality outliers.

There are no planarity outliers.

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	AAA	2443	0	2527	26	0
1	BBB	2457	0	2526	28	0
2	AAA	56	0	84	4	0
2	BBB	32	0	48	0	0
3	AAA	7	0	10	0	0
3	BBB	42	0	60	5	0
4	AAA	19	0	0	0	0
4	BBB	19	0	0	0	0
5	AAA	2	0	0	0	0
5	BBB	2	0	0	0	0
6	AAA	1	0	0	0	0
6	BBB	1	0	0	0	0
7	AAA	5	0	0	0	0
7	BBB	5	0	0	0	0
8	AAA	1	0	0	0	0
9	BBB	8	0	12	0	0
10	AAA	185	0	0	3	0
10	BBB	168	0	0	1	0
All	All	5453	0	5267	57	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 6.

All (57) 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:128[B]:LEU:CD1	1:BBB:155[B]:ILE:HD11	1.81	1.09
1:BBB:128[B]:LEU:HD11	1:BBB:155[B]:ILE:HD11	1.29	1.05
1:BBB:9:GLY:HA2	1:BBB:80[A]:ILE:HD11	1.62	0.81
1:BBB:56:VAL:HG12	1:BBB:57:LYS:H	1.48	0.77
3:BBB:1402:PEG:H42	10:BBB:1650:HOH:O	1.85	0.75
1:AAA:79:ASN:O	1:AAA:80[B]:ILE:HD13	1.88	0.74
1:BBB:228[A]:GLU:OE2	3:BBB:1409:PEG:H11	1.87	0.73
1:BBB:79:ASN:O	1:BBB:80[A]:ILE:HD13	1.88	0.73
1:BBB:40:LEU:O	1:BBB:44:VAL:HG23	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:1:MET:HE1	1:BBB:24:VAL:CG2	2.26	0.66
1:BBB:56:VAL:HG12	1:BBB:57:LYS:N	2.11	0.66
1:AAA:40:LEU:O	1:AAA:44:VAL:HG23	1.97	0.64
1:BBB:128[B]:LEU:CD1	1:BBB:155[B]:ILE:CD1	2.68	0.64
1:AAA:95[A]:ARG:HH11	1:AAA:95[A]:ARG:HG3	1.64	0.63
1:AAA:32:PRO:HG2	1:AAA:39:PHE:HA	1.80	0.63
1:BBB:32:PRO:HG2	1:BBB:38:ALA:O	1.99	0.63
1:AAA:225[B]:GLN:HG3	10:AAA:887:HOH:O	2.00	0.62
1:BBB:128[B]:LEU:HD11	1:BBB:155[B]:ILE:CD1	2.19	0.61
1:BBB:1:MET:HE1	1:BBB:24:VAL:HG21	1.85	0.59
1:AAA:128[A]:LEU:CD1	1:AAA:155[A]:ILE:HD11	2.33	0.58
1:AAA:111:LEU:HD13	1:AAA:144[B]:VAL:HG23	1.86	0.57
1:AAA:95[A]:ARG:HG3	1:AAA:95[A]:ARG:NH1	2.20	0.55
1:BBB:38:ALA:HA	1:BBB:41:ASP:HB2	1.88	0.55
1:BBB:16:ALA:HB3	1:BBB:25:ALA:HB3	1.93	0.51
1:AAA:128[A]:LEU:HD23	1:AAA:252:LEU:HD22	1.91	0.51
1:AAA:16:ALA:HB3	1:AAA:25:ALA:HB3	1.91	0.51
1:AAA:225[B]:GLN:CG	10:AAA:887:HOH:O	2.58	0.51
1:AAA:229:ARG:HA	2:AAA:714:EDO:H21	1.94	0.50
1:BBB:13:GLU:HG2	1:BBB:294:VAL:HG21	1.95	0.49
1:AAA:128[A]:LEU:HD11	1:AAA:155[A]:ILE:HD11	1.94	0.49
1:BBB:13:GLU:CG	1:BBB:294:VAL:HG21	2.43	0.48
1:AAA:13:GLU:CG	1:AAA:294:VAL:HG21	2.43	0.48
1:BBB:93:GLU:HG2	1:BBB:98:ARG:O	2.14	0.47
1:AAA:220:GLU:HG3	2:AAA:710:EDO:H21	1.97	0.47
1:BBB:282:LYS:HD2	3:BBB:1405:PEG:H21	1.97	0.46
1:AAA:13:GLU:HG3	1:AAA:294:VAL:HG21	1.98	0.46
1:AAA:221:ARG:O	1:AAA:225[B]:GLN:HG3	2.16	0.46
1:BBB:89:GLN:HB2	1:BBB:102:ILE:HG13	1.97	0.46
1:BBB:56:VAL:CG1	1:BBB:57:LYS:H	2.24	0.46
1:BBB:29:VAL:HG22	1:BBB:46:LEU:HD11	1.97	0.46
1:AAA:56:VAL:HG22	1:AAA:57:LYS:N	2.31	0.46
1:BBB:118[A]:ASP:HB2	1:BBB:287[A]:ARG:HH12	1.81	0.45
1:AAA:89:GLN:HB2	1:AAA:102:ILE:HG13	1.99	0.45
3:BBB:1401:PEG:H42	3:BBB:1401:PEG:H21	1.34	0.45
1:AAA:228:GLU:HG3	2:AAA:714:EDO:H22	1.99	0.44
1:AAA:160:LEU:HD11	1:AAA:189:TYR:CZ	2.53	0.43
1:AAA:20:ASP:O	1:AAA:21:LEU:HB2	2.18	0.43
1:BBB:11:LYS:HD2	1:BBB:28[B]:ARG:CZ	2.49	0.42
1:AAA:56:VAL:HG22	1:AAA:57:LYS:H	1.84	0.42
2:AAA:717:EDO:H21	10:AAA:896:HOH:O	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:93:GLU:HG2	1:AAA:98:ARG:O	2.18	0.42
1:AAA:248:HIS:HA	1:BBB:148[B]:ARG:HB2	2.00	0.42
3:BBB:1414:PEG:H11	3:BBB:1414:PEG:H31	1.60	0.42
1:AAA:76:LEU:HD12	1:AAA:84:MET:SD	2.60	0.42
1:BBB:160:LEU:HD11	1:BBB:189:TYR:CZ	2.55	0.42
1:BBB:20:ASP:O	1:BBB:21:LEU:HB2	2.20	0.42
1:BBB:76[A]:LEU:HD12	1:BBB:84:MET:SD	2.61	0.41

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	324/417 (78%)	317 (98%)	7 (2%)	0	100	100
1	BBB	324/417 (78%)	316 (98%)	8 (2%)	0	100	100
All	All	648/834 (78%)	633 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	261/340 (77%)	258 (99%)	3 (1%)	65	52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BBB	260/340 (76%)	255 (98%)	5 (2%)	50	31
All	All	521/680 (77%)	513 (98%)	8 (2%)	68	41

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	148[A]	ARG
1	AAA	148[B]	ARG
1	AAA	163	ASP
1	BBB	41	ASP
1	BBB	155[A]	ILE
1	BBB	155[B]	ILE
1	BBB	287[A]	ARG
1	BBB	287[B]	ARG

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 41 ligands modelled in this entry, 7 are monoatomic - leaving 34 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	EDO	BBB	1403	-	3,3,3	0.03	0	2,2,2	0.06	0
2	EDO	AAA	709	-	3,3,3	0.17	0	2,2,2	0.37	0
2	EDO	AAA	719	-	3,3,3	0.11	0	2,2,2	0.26	0
9	TRS	BBB	1407	-	7,7,7	0.32	0	9,9,9	0.34	0
7	PO4	BBB	1420	-	4,4,4	0.89	0	6,6,6	0.57	0
2	EDO	BBB	1408	-	3,3,3	0.10	0	2,2,2	0.15	0
2	EDO	BBB	1413	-	3,3,3	0.23	0	2,2,2	0.39	0
2	EDO	AAA	713	-	3,3,3	0.15	0	2,2,2	0.23	0
2	EDO	AAA	705	-	3,3,3	0.12	0	2,2,2	0.41	0
3	PEG	BBB	1401	-	6,6,6	0.22	0	5,5,5	0.20	0
2	EDO	AAA	702	-	3,3,3	0.13	0	2,2,2	0.30	0
3	PEG	BBB	1405	-	6,6,6	0.19	0	5,5,5	0.17	0
2	EDO	AAA	712	-	3,3,3	0.16	0	2,2,2	0.26	0
3	PEG	BBB	1415	-	6,6,6	0.18	0	5,5,5	0.13	0
2	EDO	AAA	714	-	3,3,3	0.18	0	2,2,2	0.04	0
2	EDO	AAA	711	-	3,3,3	0.09	0	2,2,2	0.14	0
4	4QY	AAA	704	-	19,19,19	1.12	2 (10%)	27,28,28	1.80	8 (29%)
2	EDO	BBB	1411	-	3,3,3	0.29	0	2,2,2	0.17	0
3	PEG	AAA	703	-	6,6,6	0.19	0	5,5,5	0.15	0
2	EDO	BBB	1404	-	3,3,3	0.11	0	2,2,2	0.04	0
3	PEG	BBB	1409	-	6,6,6	0.23	0	5,5,5	0.17	0
2	EDO	BBB	1412	-	3,3,3	0.10	0	2,2,2	0.18	0
4	4QY	BBB	1406	-	19,19,19	1.05	1 (5%)	27,28,28	1.96	5 (18%)
2	EDO	AAA	708	-	3,3,3	0.17	0	2,2,2	0.48	0
3	PEG	BBB	1414	-	6,6,6	0.17	0	5,5,5	0.09	0
2	EDO	AAA	706	-	3,3,3	0.40	0	2,2,2	0.29	0
2	EDO	BBB	1410	-	3,3,3	0.14	0	2,2,2	0.13	0
2	EDO	BBB	1416	-	3,3,3	0.20	0	2,2,2	0.27	0
2	EDO	AAA	717	-	3,3,3	0.06	0	2,2,2	0.08	0
3	PEG	BBB	1402	-	6,6,6	0.27	0	5,5,5	0.11	0
2	EDO	AAA	707	-	3,3,3	0.10	0	2,2,2	0.06	0
2	EDO	AAA	710	-	3,3,3	0.17	0	2,2,2	0.13	0
2	EDO	AAA	701	-	3,3,3	0.27	0	2,2,2	0.41	0
7	PO4	AAA	720	-	4,4,4	0.76	0	6,6,6	0.53	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
2	EDO	BBB	1403	-	-	1/1/1/1	-
2	EDO	AAA	709	-	-	1/1/1/1	-
2	EDO	AAA	719	-	-	1/1/1/1	-
9	TRS	BBB	1407	-	-	3/9/9/9	-
2	EDO	BBB	1408	-	-	1/1/1/1	-
2	EDO	BBB	1413	-	-	1/1/1/1	-
2	EDO	AAA	713	-	-	1/1/1/1	-
2	EDO	AAA	705	-	-	1/1/1/1	-
3	PEG	BBB	1401	-	-	4/4/4/4	-
2	EDO	AAA	702	-	-	1/1/1/1	-
3	PEG	BBB	1405	-	-	1/4/4/4	-
2	EDO	AAA	712	-	-	0/1/1/1	-
3	PEG	BBB	1415	-	-	3/4/4/4	-
2	EDO	AAA	714	-	-	0/1/1/1	-
2	EDO	AAA	711	-	-	1/1/1/1	-
4	4QY	AAA	704	-	-	3/10/30/30	0/1/1/1
2	EDO	BBB	1411	-	-	0/1/1/1	-
3	PEG	AAA	703	-	-	3/4/4/4	-
2	EDO	BBB	1404	-	-	0/1/1/1	-
3	PEG	BBB	1409	-	-	1/4/4/4	-
2	EDO	BBB	1412	-	-	1/1/1/1	-
4	4QY	BBB	1406	-	-	3/10/30/30	0/1/1/1
2	EDO	AAA	708	-	-	1/1/1/1	-
3	PEG	BBB	1414	-	-	2/4/4/4	-
2	EDO	AAA	706	-	-	1/1/1/1	-
2	EDO	BBB	1410	-	-	1/1/1/1	-
2	EDO	BBB	1416	-	-	1/1/1/1	-
2	EDO	AAA	717	-	-	0/1/1/1	-
3	PEG	BBB	1402	-	-	2/4/4/4	-
2	EDO	AAA	707	-	-	1/1/1/1	-
2	EDO	AAA	710	-	-	1/1/1/1	-
2	EDO	AAA	701	-	-	1/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BBB	1406	4QY	PAS-O6	2.71	1.68	1.60
4	AAA	704	4QY	C1-C2	2.40	1.55	1.52
4	AAA	704	4QY	PAS-O6	2.39	1.67	1.60

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BBB	1406	4QY	OAC-PAS-O6	5.14	120.07	106.67
4	BBB	1406	4QY	C1-C2-C3	-4.80	104.00	110.54
4	AAA	704	4QY	C1-C2-C3	-4.20	104.81	110.54
4	BBB	1406	4QY	O7-C7-C8	-4.06	114.83	122.05
4	AAA	704	4QY	O7-C7-C8	-4.01	114.91	122.05
4	AAA	704	4QY	O6-PAS-OAG	3.33	115.44	106.44
4	AAA	704	4QY	O5-C5-C6	2.83	112.31	106.69
4	BBB	1406	4QY	O7-C7-N2	2.57	126.53	121.98
4	AAA	704	4QY	OAC-PAS-O6	2.49	113.17	106.67
4	AAA	704	4QY	C8-C7-N2	2.49	120.25	116.12
4	AAA	704	4QY	O1-C1-O5	-2.28	103.65	110.41
4	AAA	704	4QY	OAC-PAS-OAG	-2.25	102.06	110.83
4	BBB	1406	4QY	C3-C2-N2	-2.09	106.77	110.62

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	704	4QY	C6-O6-PAS-OAH
4	BBB	1406	4QY	C6-O6-PAS-OAH
4	BBB	1406	4QY	C6-O6-PAS-OAC
3	BBB	1401	PEG	C4-C3-O2-C2
3	BBB	1414	PEG	C1-C2-O2-C3
3	BBB	1401	PEG	O1-C1-C2-O2
3	BBB	1405	PEG	O1-C1-C2-O2
3	BBB	1409	PEG	O2-C3-C4-O4
2	AAA	702	EDO	O1-C1-C2-O2
2	AAA	706	EDO	O1-C1-C2-O2
2	AAA	710	EDO	O1-C1-C2-O2
2	BBB	1416	EDO	O1-C1-C2-O2
3	BBB	1415	PEG	O2-C3-C4-O4
3	BBB	1414	PEG	O1-C1-C2-O2
3	BBB	1415	PEG	O1-C1-C2-O2
2	AAA	701	EDO	O1-C1-C2-O2
2	AAA	713	EDO	O1-C1-C2-O2
2	BBB	1410	EDO	O1-C1-C2-O2
2	BBB	1412	EDO	O1-C1-C2-O2
4	AAA	704	4QY	C6-O6-PAS-OAG
4	BBB	1406	4QY	C6-O6-PAS-OAG
3	BBB	1401	PEG	O2-C3-C4-O4
2	AAA	705	EDO	O1-C1-C2-O2
2	AAA	708	EDO	O1-C1-C2-O2
4	AAA	704	4QY	C6-O6-PAS-OAC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	BBB	1402	PEG	C1-C2-O2-C3
2	BBB	1403	EDO	O1-C1-C2-O2
3	BBB	1402	PEG	C4-C3-O2-C2
2	AAA	707	EDO	O1-C1-C2-O2
2	BBB	1408	EDO	O1-C1-C2-O2
2	BBB	1413	EDO	O1-C1-C2-O2
3	BBB	1401	PEG	C1-C2-O2-C3
2	AAA	711	EDO	O1-C1-C2-O2
3	AAA	703	PEG	C1-C2-O2-C3
9	BBB	1407	TRS	C3-C-C1-O1
9	BBB	1407	TRS	C1-C-C2-O2
3	AAA	703	PEG	O1-C1-C2-O2
2	AAA	709	EDO	O1-C1-C2-O2
3	AAA	703	PEG	C4-C3-O2-C2
2	AAA	719	EDO	O1-C1-C2-O2
3	BBB	1415	PEG	C1-C2-O2-C3
9	BBB	1407	TRS	N-C-C2-O2

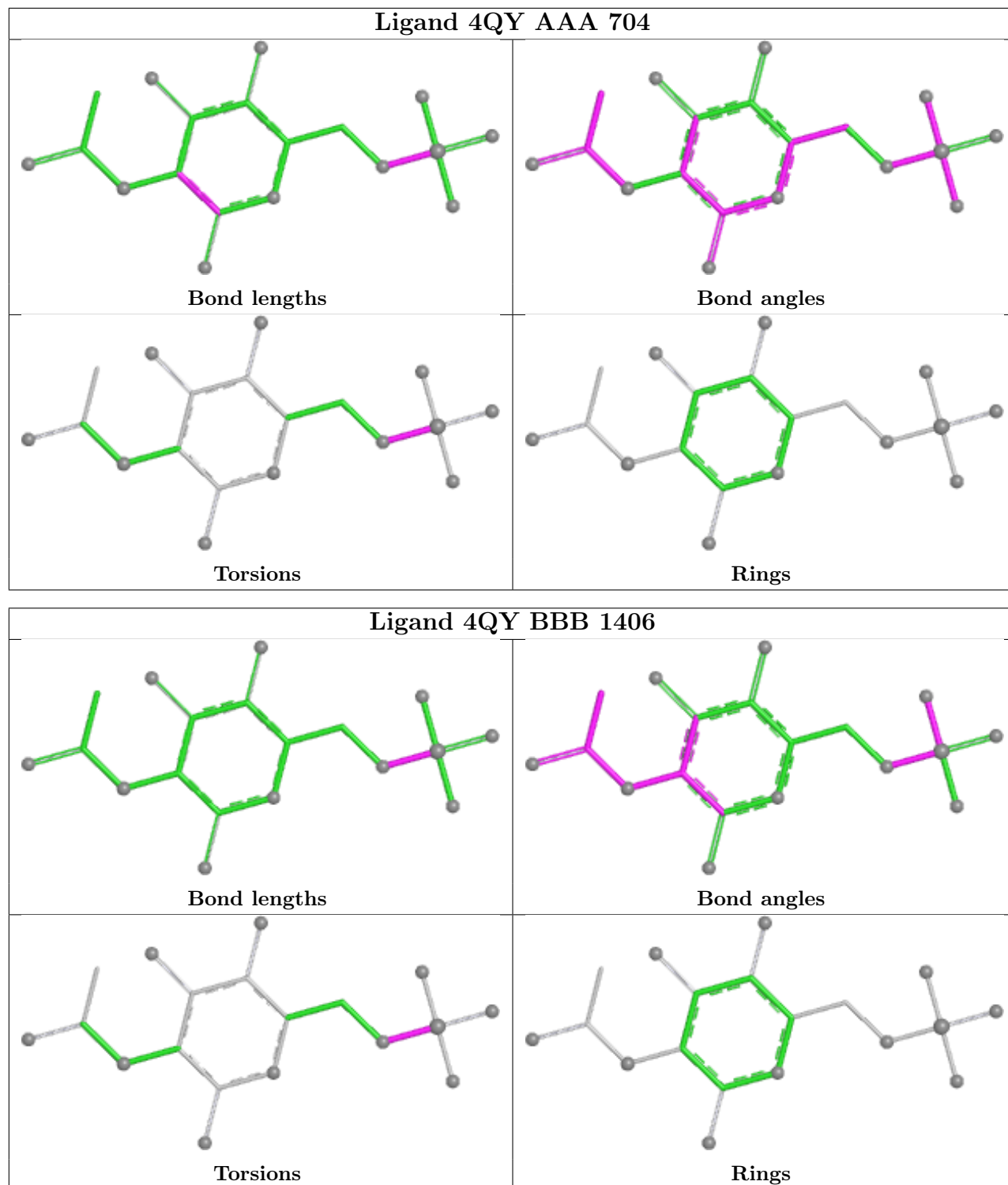
There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BBB	1401	PEG	1	0
3	BBB	1405	PEG	1	0
2	AAA	714	EDO	2	0
3	BBB	1409	PEG	1	0
3	BBB	1414	PEG	1	0
2	AAA	717	EDO	1	0
3	BBB	1402	PEG	1	0
2	AAA	710	EDO	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 ⓘ

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	AAA	303/417 (72%)	0.81	60 (19%) 3 3	12, 27, 71, 121	23 (7%)
1	BBB	306/417 (73%)	0.56	52 (16%) 4 4	13, 27, 59, 113	20 (6%)
All	All	609/834 (73%)	0.69	112 (18%) 3 3	12, 27, 66, 121	43 (7%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	29	VAL	8.4
1	BBB	115[A]	TRP	7.9
1	AAA	33	THR	7.8
1	AAA	30	ALA	7.8
1	AAA	39	PHE	7.3
1	AAA	42	ALA	6.8
1	AAA	9	GLY	6.0
1	AAA	96	LEU	5.9
1	AAA	0	THR	5.8
1	AAA	90[A]	ARG	5.6
1	AAA	56	VAL	5.6
1	AAA	38	ALA	5.5
1	BBB	82	ALA	5.5
1	BBB	56	VAL	5.4
1	AAA	115[A]	TRP	5.4
1	AAA	54	PHE	5.3
1	AAA	92	LEU	5.0
1	BBB	33	THR	5.0
1	AAA	44	VAL	5.0
1	BBB	81	PRO	4.9
1	BBB	42	ALA	4.9
1	AAA	31	THR	4.8
1	BBB	39	PHE	4.8
1	BBB	80[A]	ILE	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	BBB	30	ALA	4.5
1	AAA	43	ILE	4.5
1	BBB	40	LEU	4.4
1	AAA	46	LEU	4.3
1	AAA	59	THR	4.3
1	AAA	36	TYR	4.3
1	AAA	40	LEU	4.3
1	AAA	52	ALA	4.2
1	AAA	3	TYR	4.2
1	AAA	41	ASP	4.1
1	BBB	-3	PHE	4.1
1	BBB	29	VAL	4.1
1	BBB	45	THR	4.0
1	BBB	36	TYR	4.0
1	AAA	58	GLY	3.9
1	BBB	-2	GLN	3.8
1	BBB	302	LEU	3.8
1	AAA	55	GLY	3.8
1	AAA	32	PRO	3.8
1	AAA	1	MET	3.8
1	AAA	299	PHE	3.7
1	BBB	54	PHE	3.6
1	BBB	9	GLY	3.6
1	AAA	12	ILE	3.5
1	BBB	38	ALA	3.5
1	AAA	302	LEU	3.5
1	AAA	82	ALA	3.5
1	BBB	28[A]	ARG	3.5
1	BBB	55	GLY	3.5
1	AAA	48	ASN	3.4
1	BBB	37	ALA	3.4
1	BBB	32	PRO	3.4
1	AAA	37	ALA	3.3
1	AAA	8	GLY	3.3
1	AAA	10	THR	3.2
1	AAA	47	VAL	3.2
1	AAA	7	ILE	3.2
1	AAA	11	LYS	3.2
1	BBB	96	LEU	3.2
1	BBB	12	ILE	3.1
1	AAA	45	THR	3.1
1	AAA	28	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	AAA	99	PRO	3.0
1	BBB	83	ALA	3.0
1	BBB	46	LEU	3.0
1	AAA	95[A]	ARG	3.0
1	BBB	-1	GLY	3.0
1	BBB	0	THR	2.9
1	AAA	98	ARG	2.9
1	AAA	80[A]	ILE	2.9
1	AAA	60	VAL	2.8
1	AAA	57	LYS	2.8
1	AAA	2	TYR	2.8
1	BBB	1	MET	2.8
1	AAA	21	LEU	2.8
1	AAA	34	GLU	2.7
1	AAA	88	LEU	2.7
1	AAA	83	ALA	2.7
1	BBB	44	VAL	2.6
1	AAA	14	PHE	2.6
1	BBB	10	THR	2.6
1	BBB	43	ILE	2.6
1	BBB	50	ALA	2.6
1	AAA	100	VAL	2.5
1	AAA	35	SER	2.5
1	BBB	35	SER	2.5
1	BBB	52	ALA	2.5
1	BBB	94	GLU	2.5
1	BBB	299	PHE	2.4
1	AAA	51	ASP	2.4
1	BBB	41	ASP	2.4
1	BBB	57	LYS	2.4
1	BBB	34	GLU	2.4
1	AAA	19	ALA	2.3
1	BBB	75	LEU	2.3
1	BBB	58	GLY	2.3
1	AAA	49	ASN	2.3
1	BBB	51	ASP	2.2
1	BBB	287[A]	ARG	2.2
1	BBB	11	LYS	2.2
1	BBB	95[A]	ARG	2.1
1	BBB	47	VAL	2.1
1	AAA	91	ASP	2.1
1	BBB	31	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	AAA	50	ALA	2.0
1	BBB	78	SER	2.0
1	BBB	49	ASN	2.0
1	BBB	3	TYR	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
2	EDO	BBB	1416	4/4	0.59	0.23	52,55,67,76	0
2	EDO	AAA	706	4/4	0.69	0.23	51,53,57,59	0
2	EDO	AAA	712	4/4	0.70	0.25	72,76,77,86	0
2	EDO	BBB	1411	4/4	0.74	0.23	64,64,66,81	0
2	EDO	AAA	707	4/4	0.75	0.20	58,59,70,71	0
2	EDO	AAA	710	4/4	0.78	0.26	53,63,64,74	0
2	EDO	AAA	708	4/4	0.80	0.22	46,60,65,71	0
3	PEG	BBB	1401	7/7	0.80	0.18	68,71,85,86	0
2	EDO	AAA	719	4/4	0.83	0.17	57,62,66,68	0
2	EDO	AAA	711	4/4	0.83	0.17	60,69,69,73	0
7	PO4	BBB	1420	5/5	0.83	0.15	46,47,64,64	5
2	EDO	AAA	717	4/4	0.84	0.18	63,67,81,87	0
3	PEG	BBB	1409	7/7	0.85	0.16	55,69,72,76	0
2	EDO	AAA	713	4/4	0.85	0.15	69,69,70,76	0
2	EDO	AAA	702	4/4	0.86	0.20	60,63,78,80	0
3	PEG	BBB	1414	7/7	0.86	0.16	50,63,81,81	0
3	PEG	BBB	1415	7/7	0.86	0.15	48,55,70,71	0
2	EDO	BBB	1412	4/4	0.86	0.18	63,69,72,74	0
3	PEG	BBB	1402	7/7	0.87	0.17	40,59,73,88	0

Continued on next page...

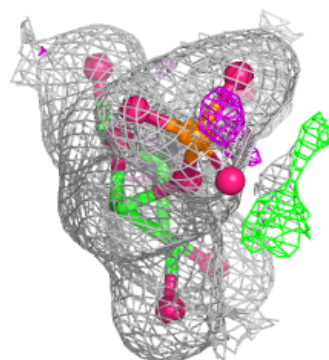
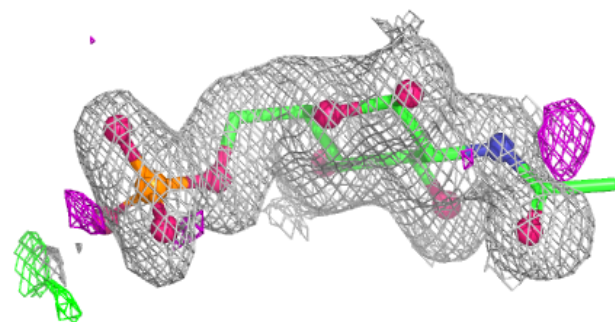
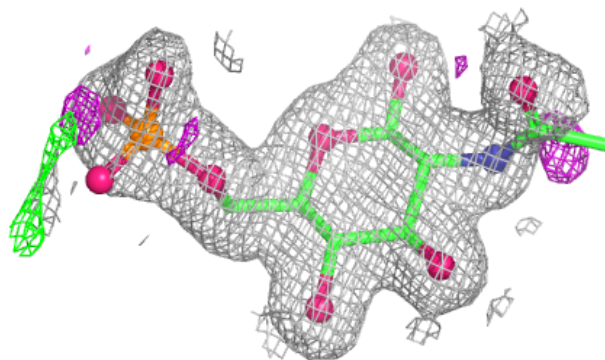
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	TRS	BBB	1407	8/8	0.87	0.13	42,51,61,72	0
2	EDO	BBB	1413	4/4	0.88	0.15	60,63,65,70	0
3	PEG	BBB	1405	7/7	0.90	0.14	39,54,61,61	0
2	EDO	AAA	705	4/4	0.90	0.15	49,51,56,62	0
2	EDO	AAA	701	4/4	0.90	0.14	47,54,55,62	0
2	EDO	BBB	1403	4/4	0.90	0.13	55,56,58,69	0
2	EDO	BBB	1408	4/4	0.90	0.20	26,31,31,34	4
2	EDO	AAA	714	4/4	0.90	0.14	40,48,49,70	0
7	PO4	AAA	720	5/5	0.91	0.23	53,56,62,71	5
2	EDO	AAA	709	4/4	0.92	0.12	58,60,66,68	0
2	EDO	BBB	1410	4/4	0.92	0.12	46,52,59,62	0
3	PEG	AAA	703	7/7	0.92	0.13	39,46,52,69	0
2	EDO	BBB	1404	4/4	0.94	0.11	46,57,59,60	0
4	4QY	BBB	1406	19/19	0.95	0.13	24,29,74,81	4
5	ZN	AAA	716	1/1	0.95	0.10	42,42,42,42	1
8	CL	AAA	721	1/1	0.95	0.17	67,67,67,67	0
5	ZN	BBB	1418	1/1	0.95	0.11	44,44,44,44	1
4	4QY	AAA	704	19/19	0.96	0.12	27,35,61,62	4
6	K	AAA	718	1/1	0.98	0.14	40,40,40,40	0
6	K	BBB	1419	1/1	0.98	0.16	39,39,39,39	0
5	ZN	BBB	1417	1/1	0.99	0.03	23,23,23,23	0
5	ZN	AAA	715	1/1	0.99	0.02	26,26,26,26	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.

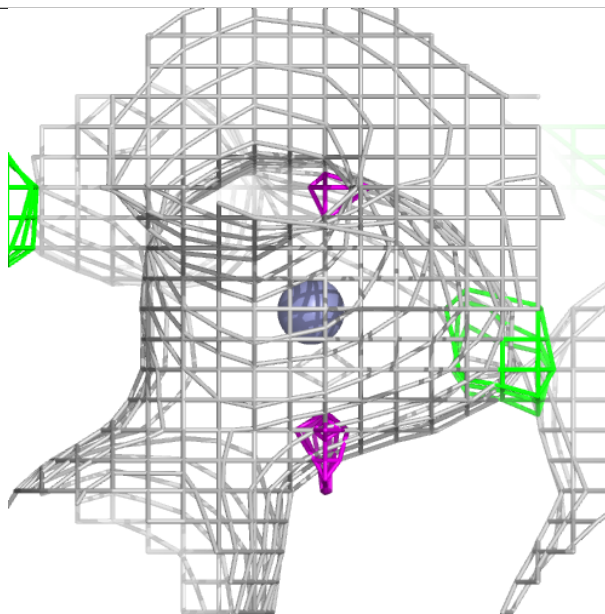
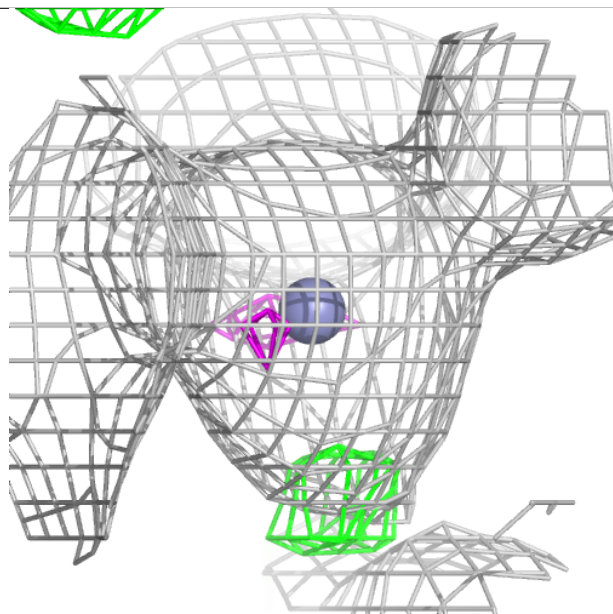
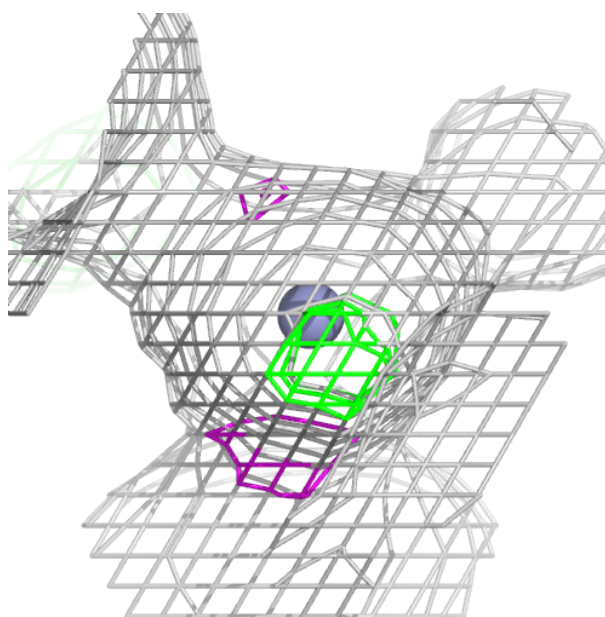
Electron density around 4QY BBB 1406:

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



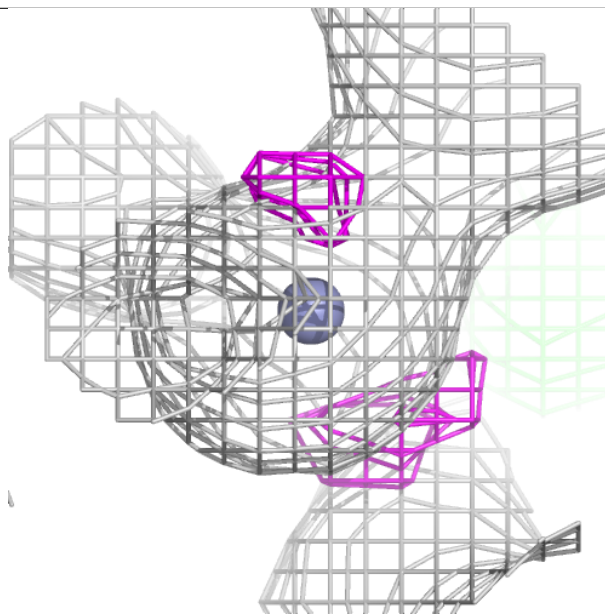
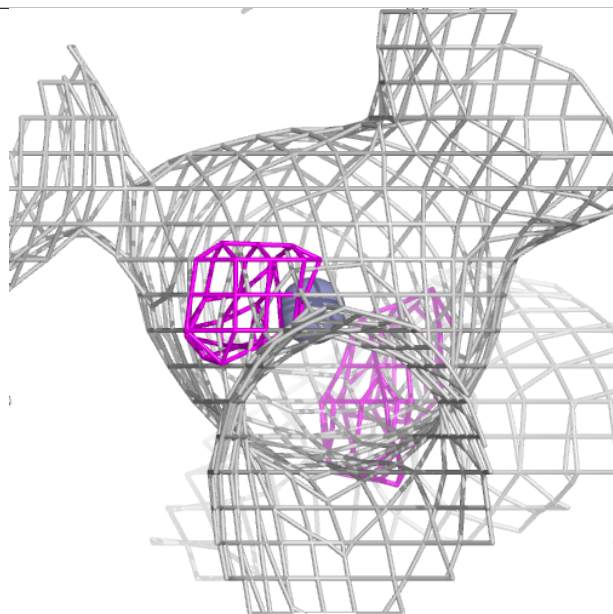
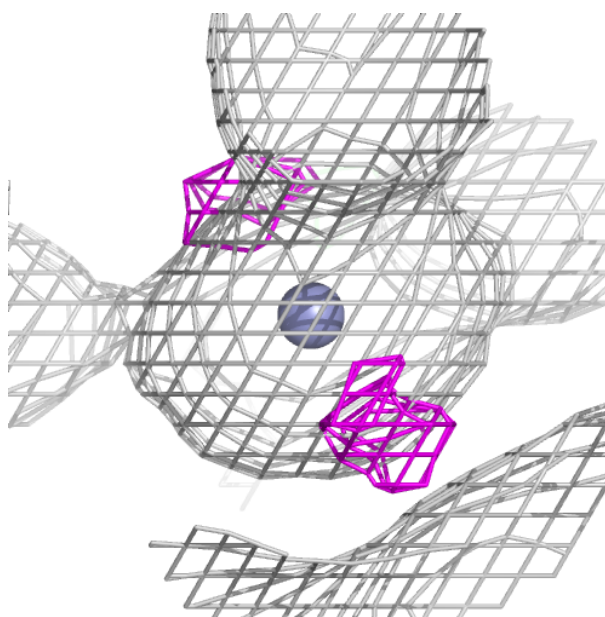
Electron density around ZN AAA 716:

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



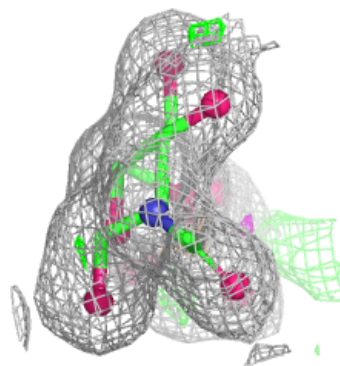
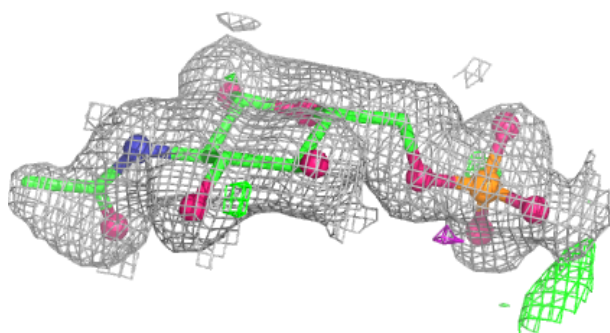
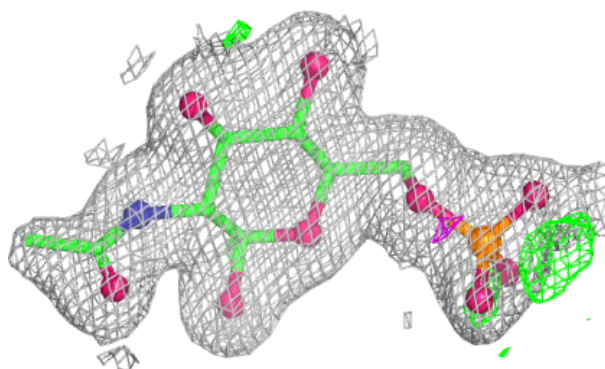
Electron density around ZN BBB 1418:

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



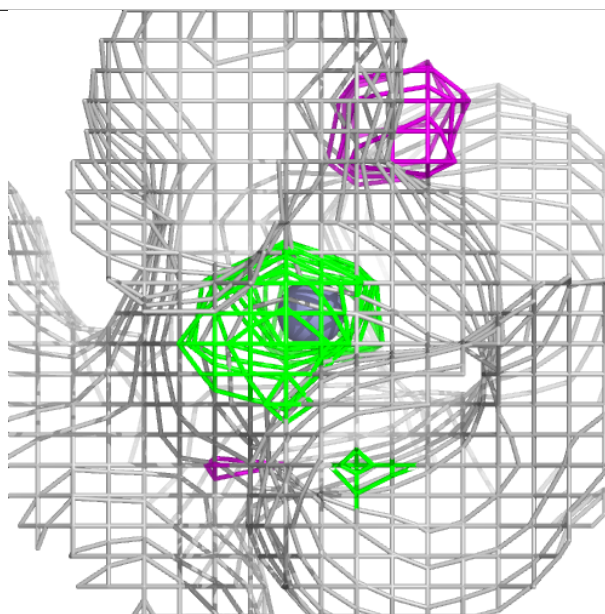
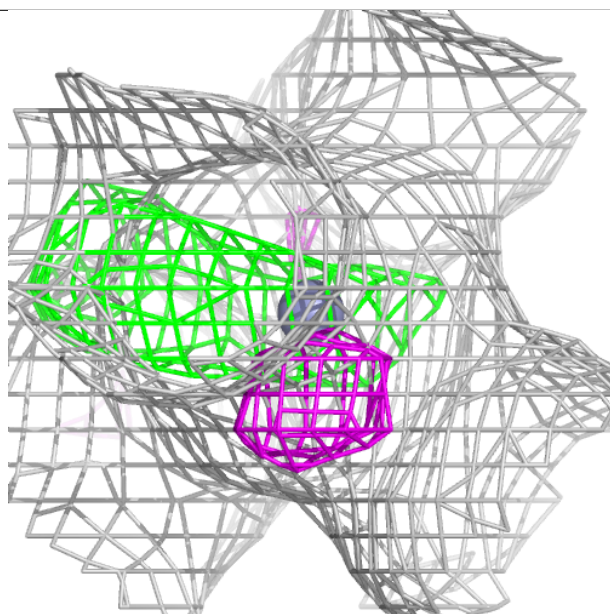
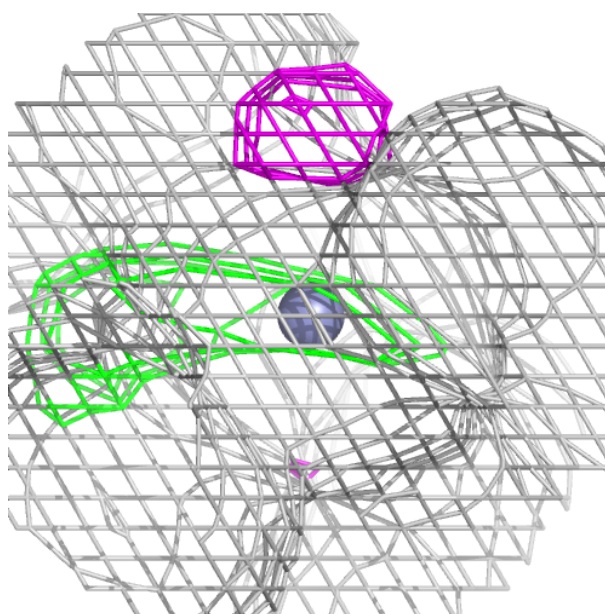
Electron density around 4QY AAA 704:

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



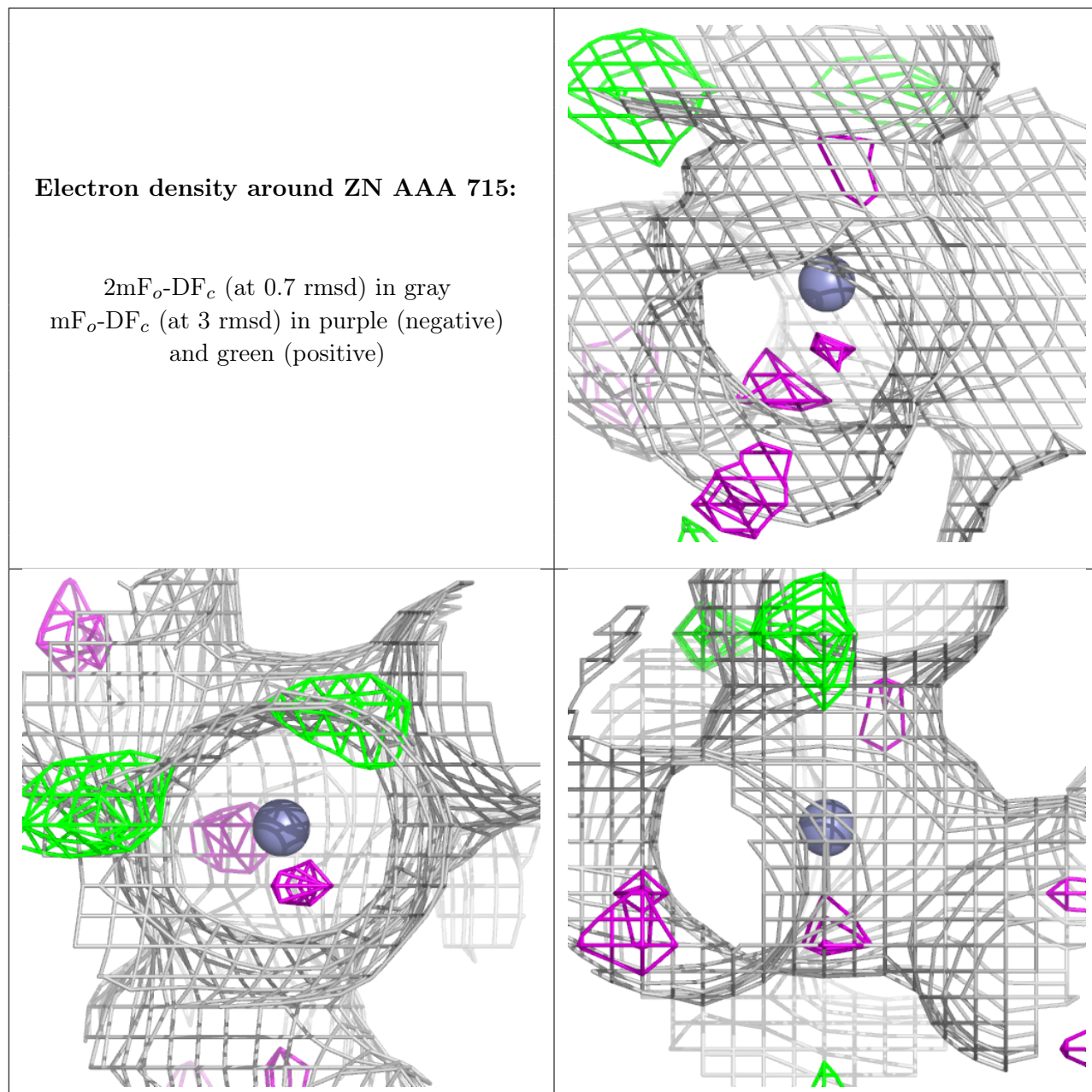
Electron density around ZN BBB 1417:

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



Electron density around ZN AAA 715:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.