wwPDB X-ray Structure Validation Summary Report (i)

Aug 1, 2022 – 05:55 pm BST

PDB ID	:	7P9L
Title	:	N-acetylglucosamine kinase from Plesiomonas shigelloides compexed with alpha-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 wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

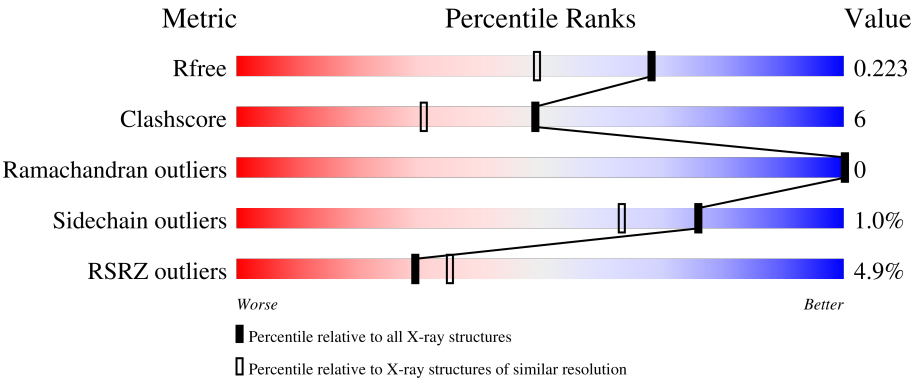
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

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}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (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 <=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	5% 64% 9% 27%
1	BBB	417	2% 65% 8% 27%

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	EDO	BBB	1408	-	-	X	-

2 Entry composition (i)

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

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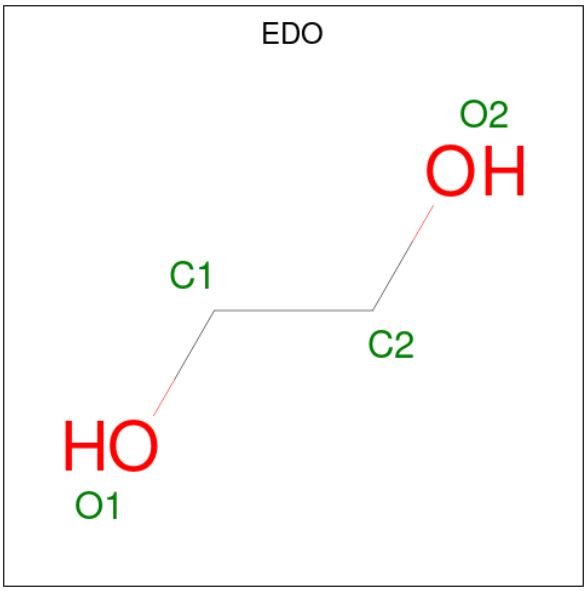
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-109	HIS	-	expression tag	UNP Q12306
BBB	-108	HIS	-	expression tag	UNP Q12306
BBB	-107	HIS	-	expression tag	UNP Q12306
BBB	-106	GLY	-	expression tag	UNP Q12306
BBB	-10	SER	-	linker	UNP Q12306
BBB	-9	SER	-	linker	UNP Q12306
BBB	-8	GLY	-	linker	UNP Q12306
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 1,2-ETHANEDIOL (three-letter code: 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		

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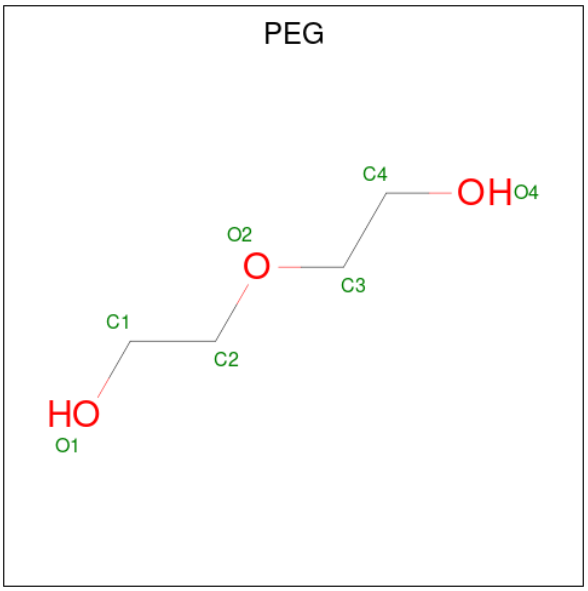
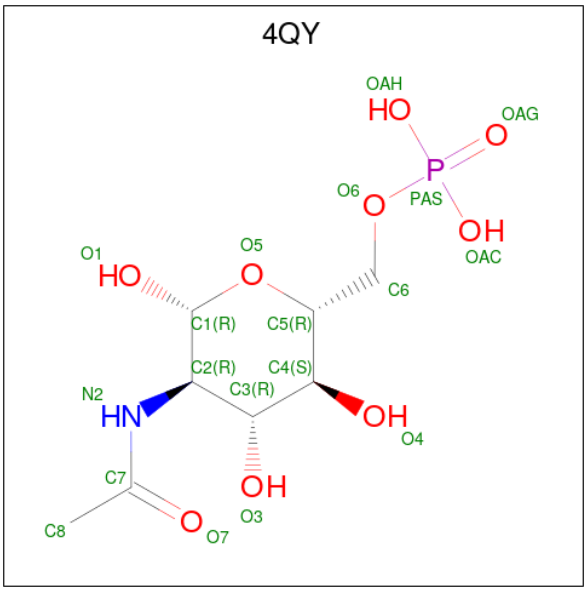
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 4 is 2-acetamido-2-deoxy-6-O-phosphono-beta-D-glucopyranose (three-letter code: 4QY) (formula: $C_8H_{16}NO_9P$) (labeled as "Ligand of Interest" by depositor).



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

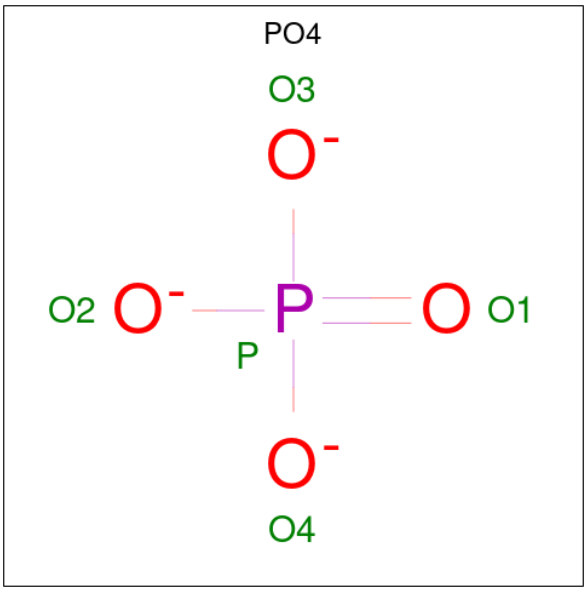
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

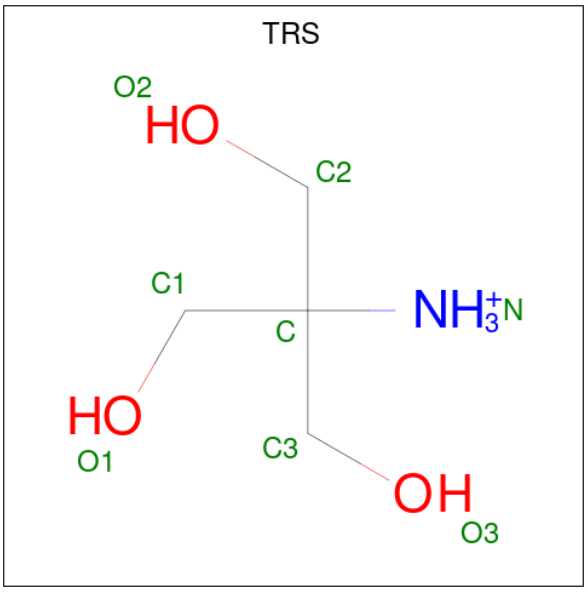


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	1	Total O P 5 4 1	0	0
7	BBB	1	Total O P 5 4 1	0	0

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

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

- Molecule 9 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



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

- Molecule 10 is water.

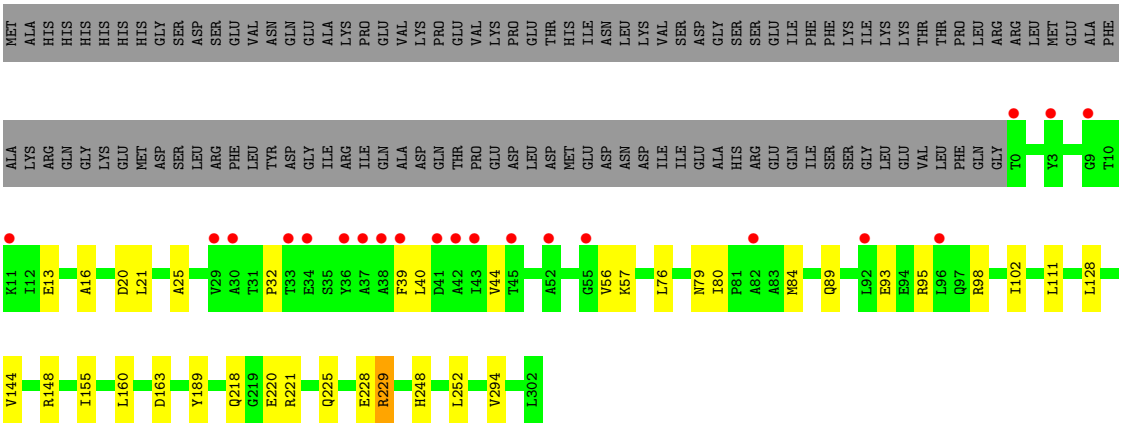
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	AAA	185	Total O 185 185	0	0
10	BBB	168	Total O 168 168	0	0

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.

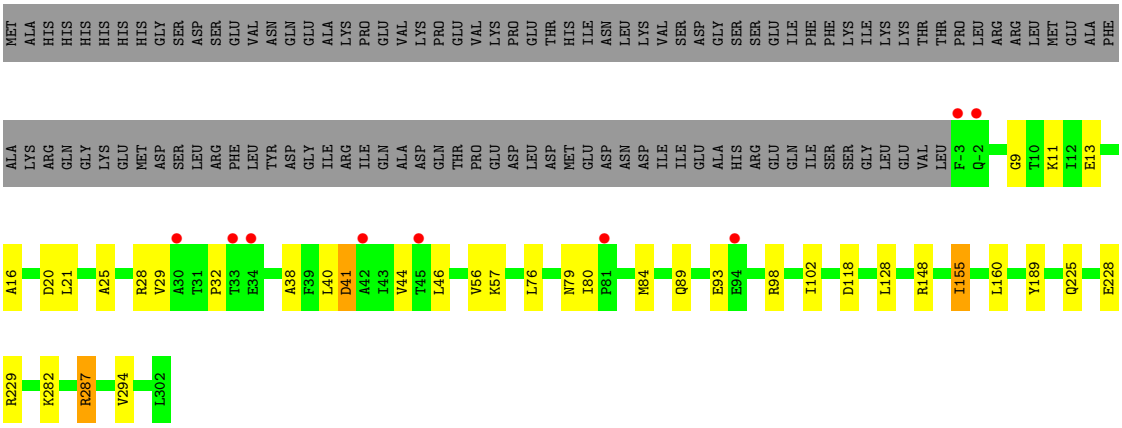
• Molecule 1: Ubiquitin-like protein SMT3,N-acetyl-D-glucosamine kinase

Chain AAA:



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

Chain BBB:



4 Data and refinement statistics (i)

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 99.17 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.0 (76.25-1.75) 99.0 (99.17-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.06%)	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)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	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.*

[1]Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, TRS, PEG, EDO, ZN, CL, K, 4QY

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	0.49	0/2561	0.81	1/3463 (0.0%)
1	BBB	0.51	0/2567	0.83	1/3471 (0.0%)
All	All	0.50	0/5128	0.82	2/6934 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	229	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	BBB	229	ARG	NE-CZ-NH2	-5.31	117.64	120.30

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	27	0
1	BBB	2457	0	2526	31	0
2	AAA	56	0	84	4	0
2	BBB	32	0	48	5	0
3	AAA	7	0	10	0	0
3	BBB	42	0	60	5	0
4	AAA	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	4	0
10	BBB	168	0	0	1	0
All	All	5453	0	5267	61	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.

The worst 5 of 61 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:225[A]:GLN:NE2	2:BBB:1408:EDO:O1	1.75	1.16
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:225[A]:GLN:HE22	2:BBB:1408:EDO:H11	1.32	0.94
1:BBB:225[A]:GLN:NE2	2:BBB:1408:EDO:C1	2.34	0.90

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	73	60
1	BBB	260/340 (76%)	255 (98%)	5 (2%)	57	37
All	All	521/680 (77%)	513 (98%)	8 (2%)	76	49

5 of 8 residues with a non-rotameric sidechain are listed below:

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

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 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	AAA	712	-	3,3,3	0.16	0	2,2,2	0.33	0
7	PO4	AAA	720	-	4,4,4	0.71	0	6,6,6	0.50	0
2	EDO	AAA	702	-	3,3,3	0.13	0	2,2,2	0.25	0
2	EDO	AAA	707	-	3,3,3	0.10	0	2,2,2	0.03	0
2	EDO	AAA	710	-	3,3,3	0.18	0	2,2,2	0.12	0
2	EDO	AAA	719	-	3,3,3	0.11	0	2,2,2	0.23	0
2	EDO	AAA	705	-	3,3,3	0.12	0	2,2,2	0.48	0
2	EDO	AAA	706	-	3,3,3	0.41	0	2,2,2	0.35	0
3	PEG	AAA	703	-	6,6,6	0.19	0	5,5,5	0.14	0
2	EDO	BBB	1410	-	3,3,3	0.15	0	2,2,2	0.11	0
2	EDO	AAA	709	-	3,3,3	0.18	0	2,2,2	0.46	0
2	EDO	AAA	701	-	3,3,3	0.28	0	2,2,2	0.39	0
2	EDO	AAA	714	-	3,3,3	0.19	0	2,2,2	0.04	0
2	EDO	AAA	717	-	3,3,3	0.06	0	2,2,2	0.11	0
3	PEG	BBB	1409	-	6,6,6	0.23	0	5,5,5	0.18	0
3	PEG	BBB	1414	-	6,6,6	0.18	0	5,5,5	0.10	0
2	EDO	AAA	711	-	3,3,3	0.09	0	2,2,2	0.17	0
4	4QY	BBB	1406	-	19,19,19	1.04	1 (5%)	28,28,28	1.90	5 (17%)
2	EDO	AAA	708	-	3,3,3	0.18	0	2,2,2	0.52	0
3	PEG	BBB	1405	-	6,6,6	0.20	0	5,5,5	0.18	0
3	PEG	BBB	1401	-	6,6,6	0.22	0	5,5,5	0.20	0
3	PEG	BBB	1402	-	6,6,6	0.27	0	5,5,5	0.10	0
9	TRS	BBB	1407	-	7,7,7	0.29	0	9,9,9	0.28	0
2	EDO	BBB	1408	-	3,3,3	0.10	0	2,2,2	0.21	0
2	EDO	AAA	713	-	3,3,3	0.15	0	2,2,2	0.18	0
2	EDO	BBB	1413	-	3,3,3	0.23	0	2,2,2	0.34	0
7	PO4	BBB	1420	-	4,4,4	0.84	0	6,6,6	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	EDO	BBB	1403	-	3,3,3	0.04	0	2,2,2	0.03	0
3	PEG	BBB	1415	-	6,6,6	0.18	0	5,5,5	0.13	0
2	EDO	BBB	1416	-	3,3,3	0.21	0	2,2,2	0.29	0
2	EDO	BBB	1412	-	3,3,3	0.10	0	2,2,2	0.20	0
4	4QY	AAA	704	-	19,19,19	1.10	2 (10%)	28,28,28	1.77	8 (28%)
2	EDO	BBB	1404	-	3,3,3	0.11	0	2,2,2	0.10	0
2	EDO	BBB	1411	-	3,3,3	0.30	0	2,2,2	0.25	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	AAA	712	-	-	0/1/1/1	-
2	EDO	AAA	702	-	-	1/1/1/1	-
2	EDO	AAA	707	-	-	1/1/1/1	-
2	EDO	AAA	710	-	-	1/1/1/1	-
2	EDO	AAA	719	-	-	0/1/1/1	-
2	EDO	AAA	705	-	-	1/1/1/1	-
2	EDO	AAA	706	-	-	1/1/1/1	-
3	PEG	AAA	703	-	-	3/4/4/4	-
2	EDO	BBB	1410	-	-	1/1/1/1	-
2	EDO	AAA	709	-	-	1/1/1/1	-
2	EDO	AAA	701	-	-	1/1/1/1	-
2	EDO	AAA	714	-	-	0/1/1/1	-
2	EDO	AAA	717	-	-	0/1/1/1	-
3	PEG	BBB	1409	-	-	1/4/4/4	-
3	PEG	BBB	1414	-	-	2/4/4/4	-
2	EDO	AAA	711	-	-	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	1405	-	-	1/4/4/4	-
3	PEG	BBB	1401	-	-	4/4/4/4	-
3	PEG	BBB	1402	-	-	2/4/4/4	-
9	TRS	BBB	1407	-	-	0/9/9/9	-
2	EDO	BBB	1408	-	-	1/1/1/1	-
2	EDO	AAA	713	-	-	1/1/1/1	-
2	EDO	BBB	1413	-	-	1/1/1/1	-
2	EDO	BBB	1403	-	-	1/1/1/1	-
3	PEG	BBB	1415	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	BBB	1416	-	-	1/1/1/1	-
2	EDO	BBB	1412	-	-	1/1/1/1	-
4	4QY	AAA	704	-	-	3/10/30/30	0/1/1/1
2	EDO	BBB	1404	-	-	0/1/1/1	-
2	EDO	BBB	1411	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BBB	1406	4QY	PAS-O6	2.69	1.68	1.60
4	AAA	704	4QY	C1-C2	2.40	1.55	1.52
4	AAA	704	4QY	PAS-O6	2.37	1.67	1.60

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	BBB	1406	4QY	OAC-PAS-O6	5.01	120.07	106.73
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	-3.89	114.83	122.06
4	AAA	704	4QY	O7-C7-C8	-3.85	114.91	122.06

There are no chirality outliers.

5 of 38 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

There are no ring outliers.

9 monomers are involved in 14 short contacts:

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

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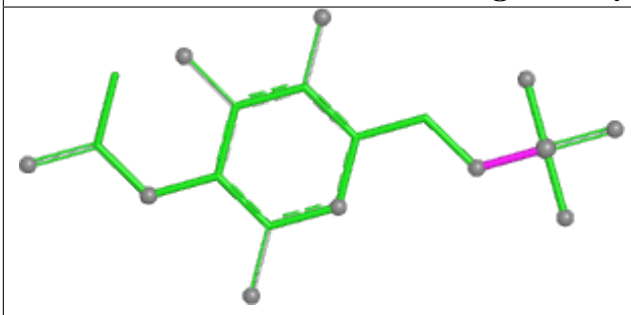
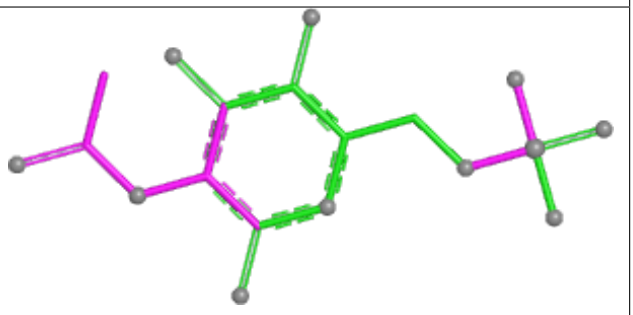
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BBB	1405	PEG	1	0
3	BBB	1401	PEG	1	0
3	BBB	1402	PEG	1	0
2	BBB	1408	EDO	5	0

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

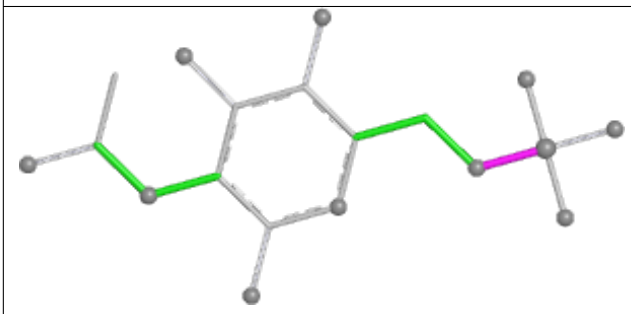
Ligand 4QY BBB 1406



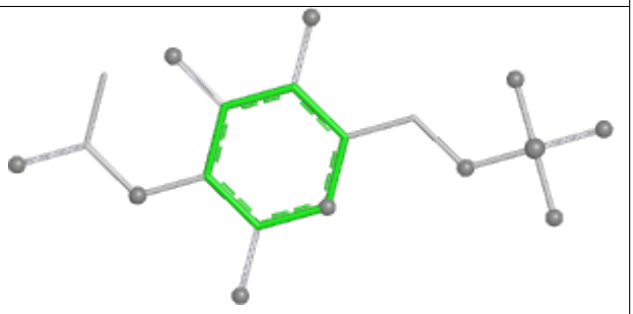
Bond lengths



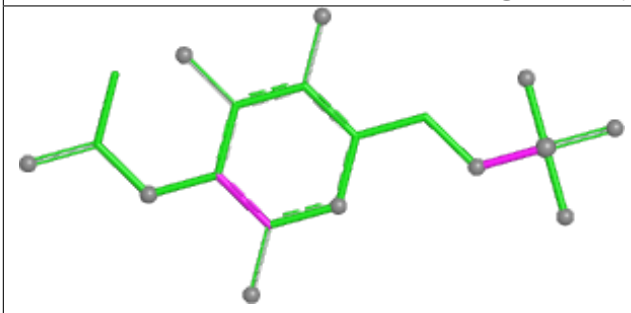
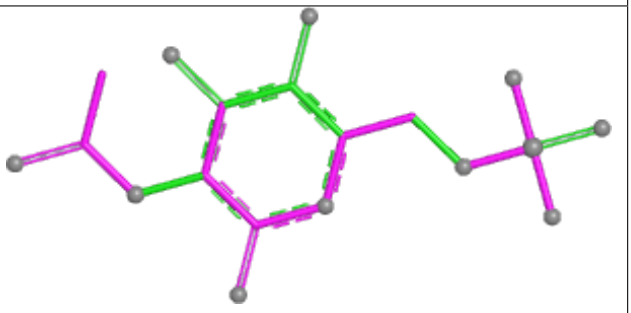
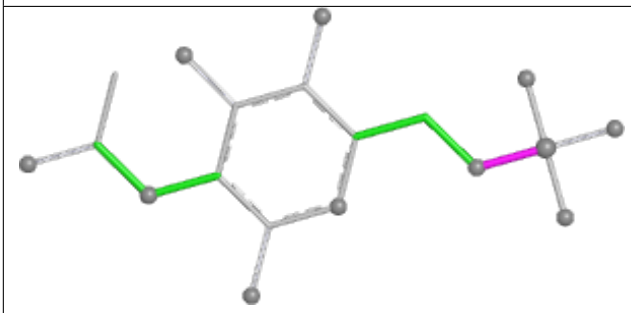
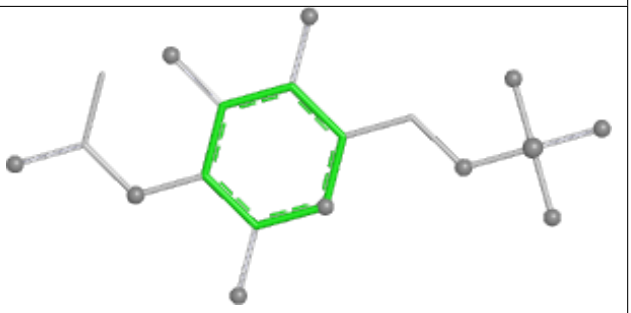
Bond angles



Torsions



Rings

Ligand 4QY AAA 704	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AAA	303/417 (72%)	0.21	21 (6%) 16 22	17, 28, 71, 121	0
1	BBB	306/417 (73%)	0.00	9 (2%) 51 57	17, 28, 59, 113	0
All	All	609/834 (73%)	0.10	30 (4%) 29 35	17, 28, 66, 121	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	39	PHE	8.0
1	AAA	34	GLU	7.1
1	AAA	33	THR	6.1
1	AAA	42	ALA	4.8
1	AAA	52	ALA	4.4

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

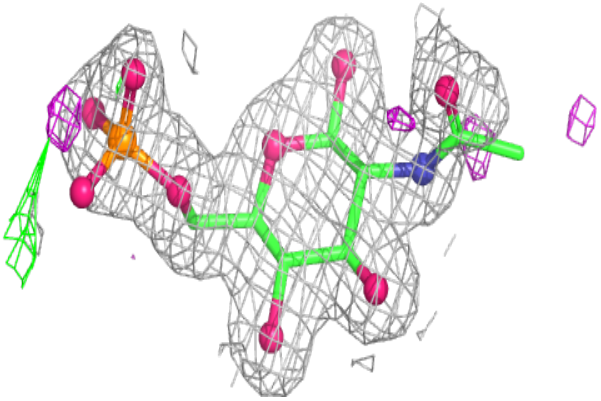
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	AAA	712	4/4	0.61	0.23	72,76,77,86	0
2	EDO	AAA	708	4/4	0.71	0.12	46,60,65,71	0
2	EDO	BBB	1411	4/4	0.73	0.18	64,64,66,81	0
2	EDO	BBB	1412	4/4	0.73	0.14	63,69,72,74	0
3	PEG	BBB	1401	7/7	0.74	0.15	68,71,85,86	0
2	EDO	AAA	709	4/4	0.75	0.12	58,60,66,68	0
2	EDO	AAA	711	4/4	0.77	0.14	60,69,69,73	0
2	EDO	BBB	1416	4/4	0.78	0.18	52,55,67,76	0
2	EDO	AAA	719	4/4	0.78	0.12	57,62,66,68	0
2	EDO	AAA	713	4/4	0.79	0.11	69,69,70,76	0
2	EDO	AAA	706	4/4	0.80	0.10	51,53,57,59	0
3	PEG	BBB	1409	7/7	0.81	0.24	55,69,72,76	0
2	EDO	AAA	707	4/4	0.84	0.20	58,59,70,71	0
3	PEG	BBB	1402	7/7	0.86	0.16	40,59,73,88	0
2	EDO	AAA	705	4/4	0.86	0.16	49,51,56,62	0
2	EDO	AAA	710	4/4	0.87	0.13	53,63,64,74	0
2	EDO	BBB	1403	4/4	0.88	0.09	55,56,58,69	0
3	PEG	BBB	1415	7/7	0.88	0.12	48,55,70,71	0
3	PEG	BBB	1405	7/7	0.89	0.10	39,54,61,61	0
3	PEG	BBB	1414	7/7	0.90	0.13	50,63,81,81	0
2	EDO	AAA	714	4/4	0.90	0.13	40,48,49,70	0
2	EDO	BBB	1413	4/4	0.91	0.08	60,63,65,70	0
9	TRS	BBB	1407	8/8	0.91	0.15	42,51,61,72	0
2	EDO	BBB	1404	4/4	0.92	0.08	46,57,59,60	0
2	EDO	AAA	702	4/4	0.92	0.09	60,63,78,80	0
2	EDO	AAA	717	4/4	0.92	0.09	63,67,81,87	0
7	PO4	AAA	720	5/5	0.94	0.16	53,56,62,71	5
8	CL	AAA	721	1/1	0.94	0.09	67,67,67,67	0
2	EDO	BBB	1408	4/4	0.94	0.21	26,31,31,34	4
2	EDO	BBB	1410	4/4	0.95	0.20	46,52,59,62	0
2	EDO	AAA	701	4/4	0.95	0.07	47,54,55,62	0
3	PEG	AAA	703	7/7	0.96	0.10	39,46,52,69	0
4	4QY	BBB	1406	19/19	0.96	0.12	24,29,74,81	4
5	ZN	AAA	716	1/1	0.96	0.06	42,42,42,42	1
4	4QY	AAA	704	19/19	0.97	0.12	27,35,61,62	4
7	PO4	BBB	1420	5/5	0.97	0.11	46,47,64,64	5
5	ZN	BBB	1418	1/1	0.98	0.06	44,44,44,44	1
6	K	AAA	718	1/1	0.99	0.06	40,40,40,40	0
6	K	BBB	1419	1/1	0.99	0.04	39,39,39,39	0
5	ZN	AAA	715	1/1	0.99	0.11	26,26,26,26	0
5	ZN	BBB	1417	1/1	1.00	0.15	23,23,23,23	0

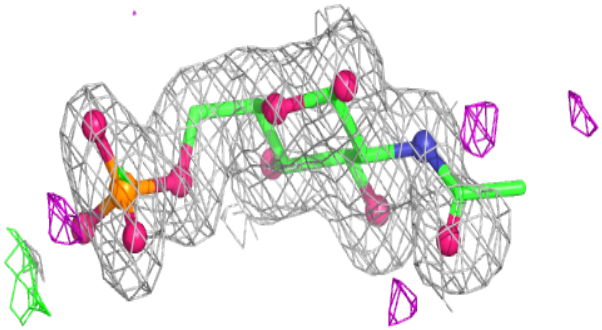
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

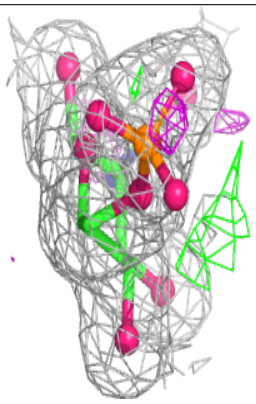
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

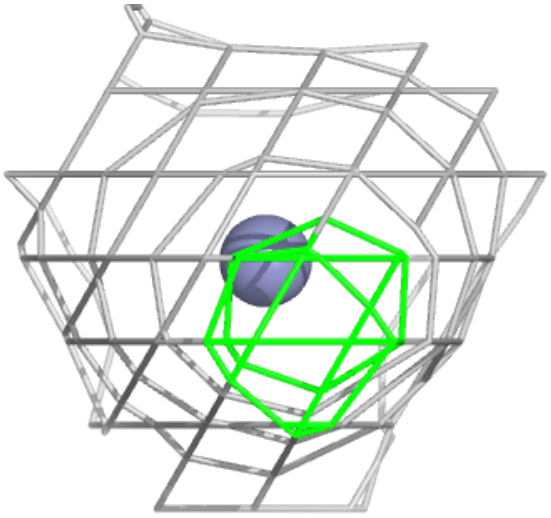


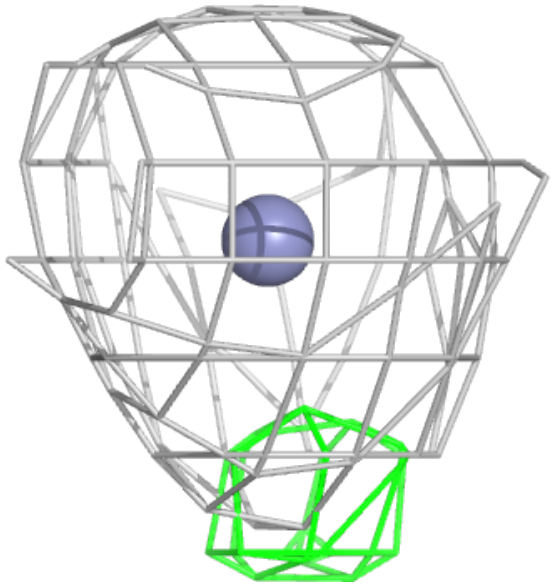


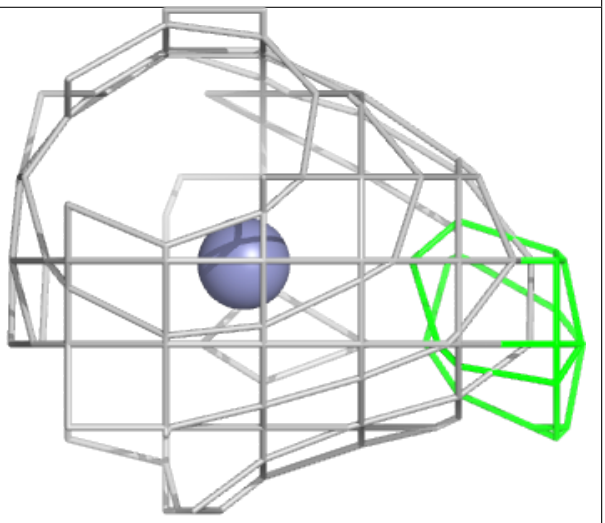


Electron density around ZN AAA 716:

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

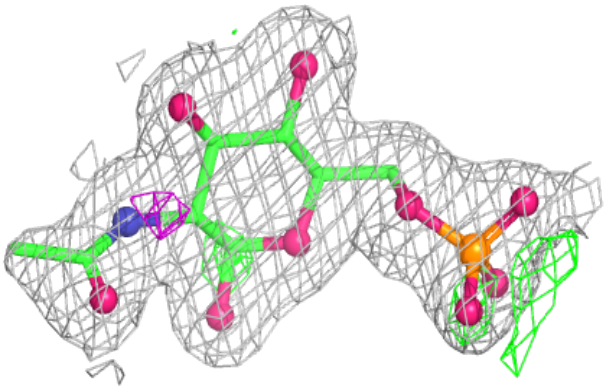


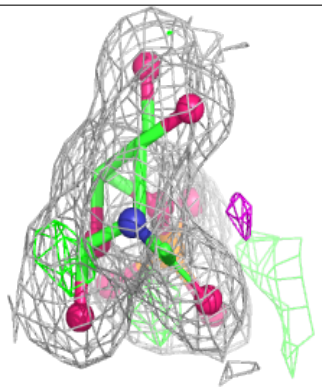




Electron density around 4QY AAA 704:

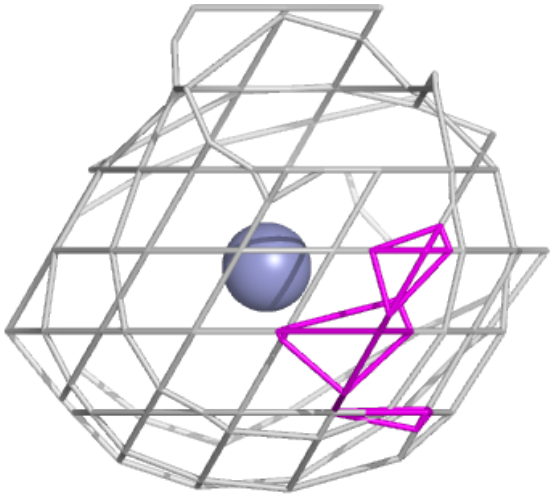
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

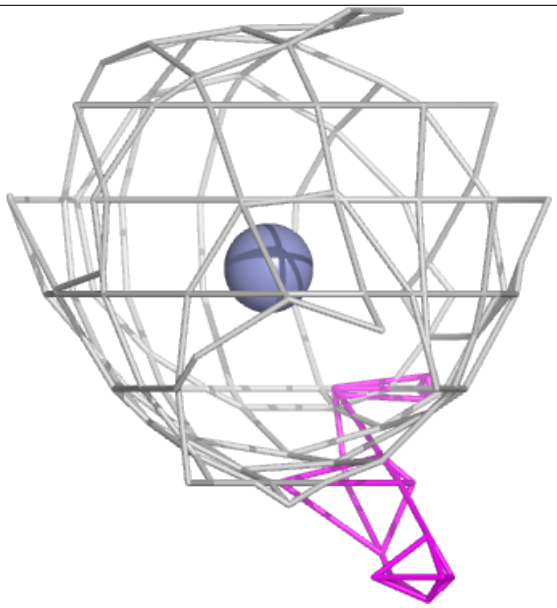


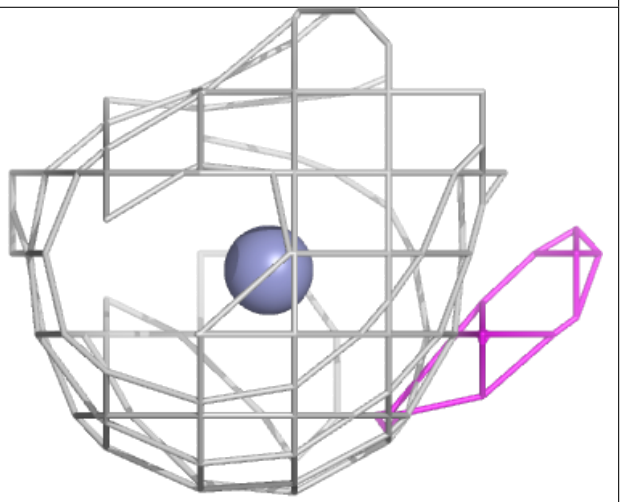


Electron density around ZN BBB 1418:

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







Electron density around ZN AAA 715:

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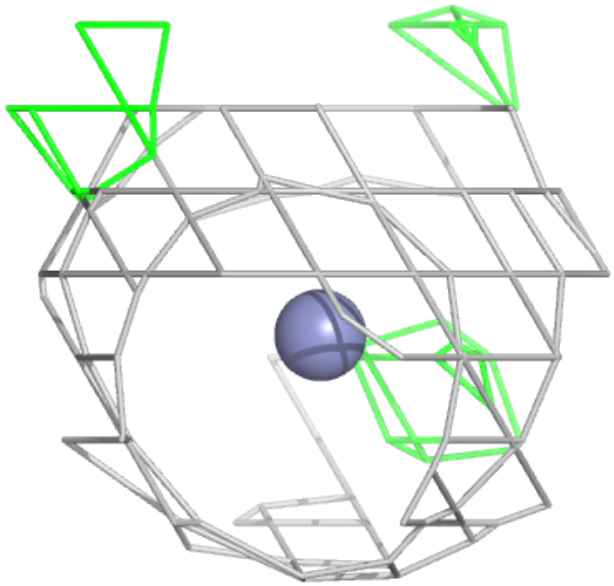
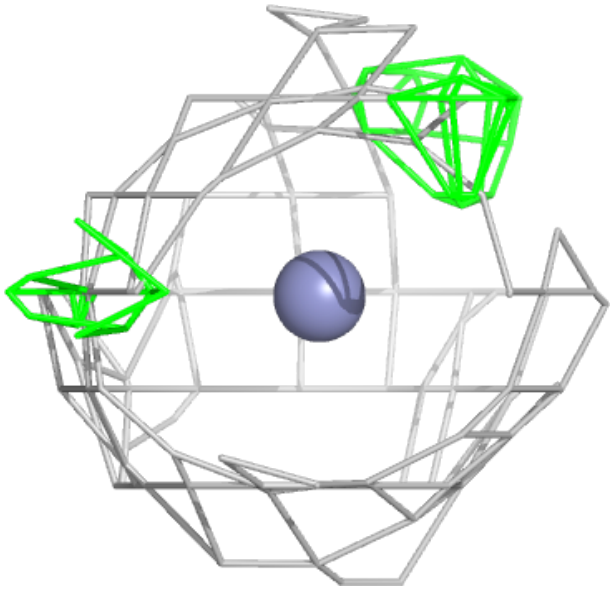
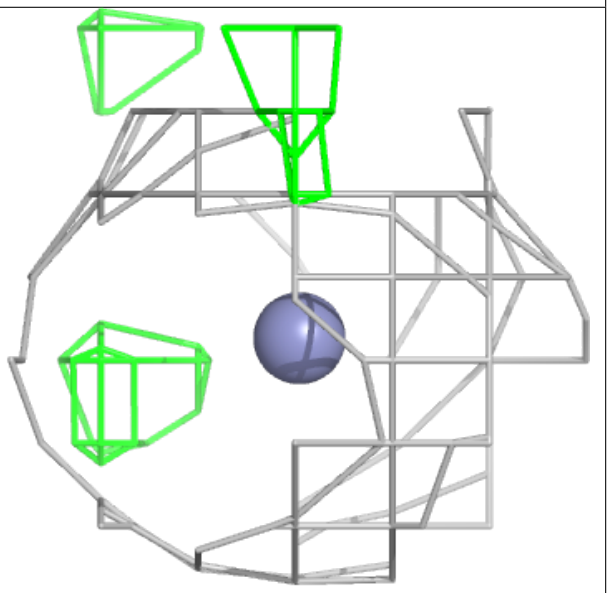
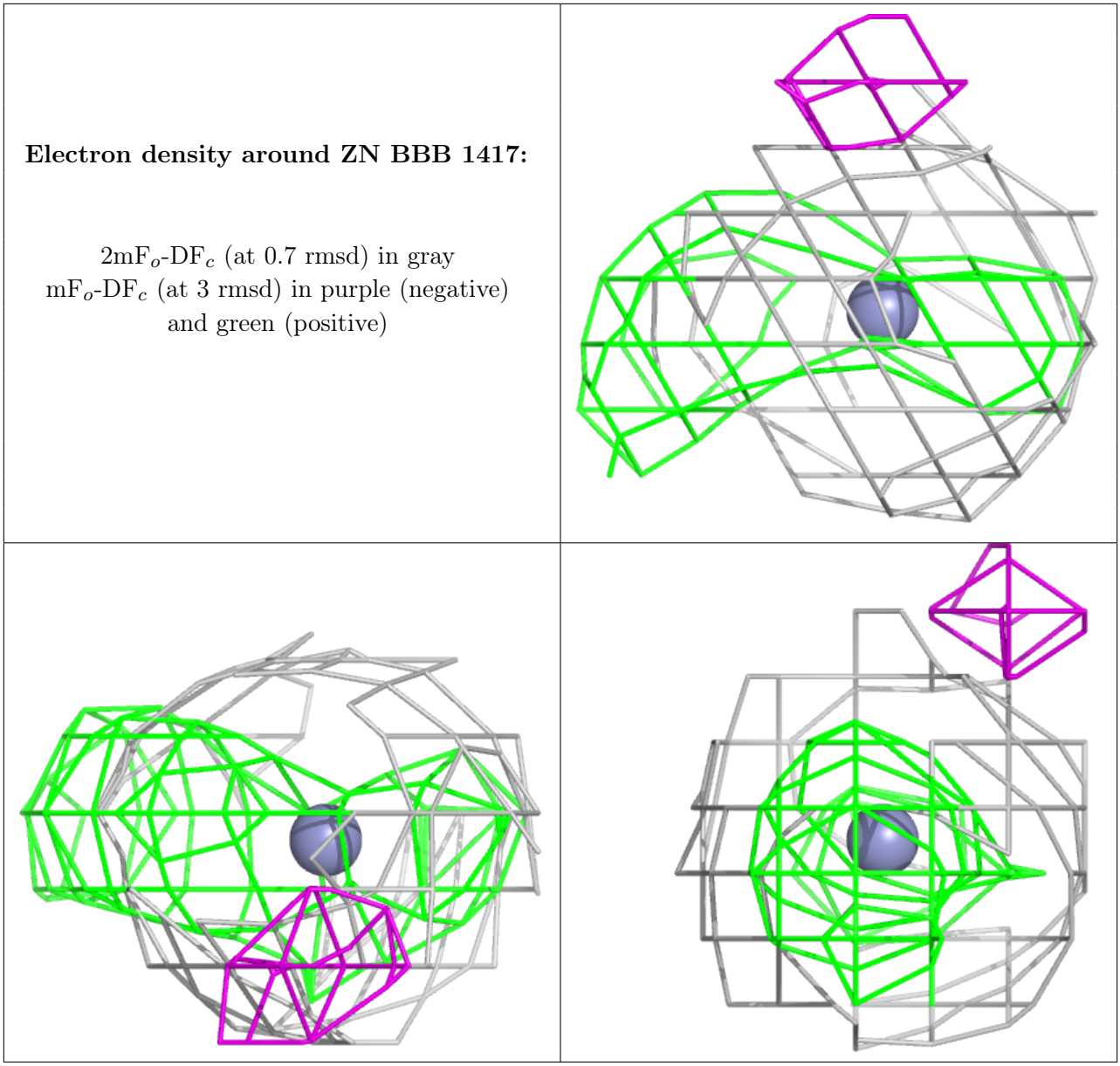






Electron density around ZN BBB 1417:

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



6.5 Other polymers (i)

There are no such residues in this entry.