



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 07:43 AM EDT

PDB ID : 7L7X  
Title : X-ray structure of the Pcryo\_0638 aminotransferase from *Psychrobacter cryohalolentis*  
Authors : Linehan, M.P.; Thoden, J.B.; Holden, H.M.  
Deposited on : 2020-12-30  
Resolution : 1.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

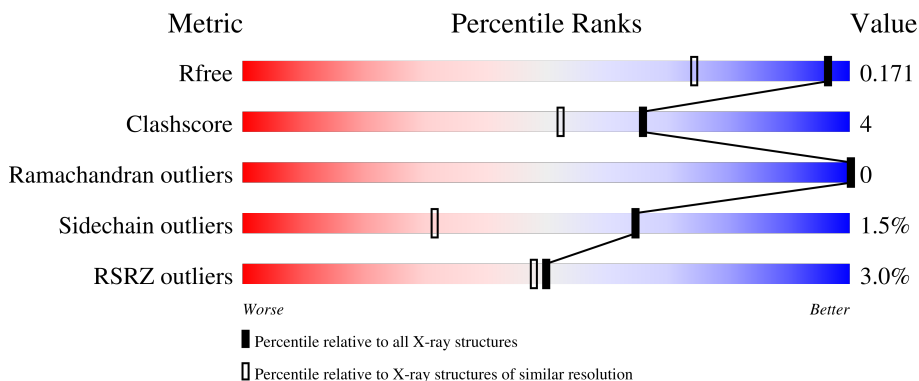
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

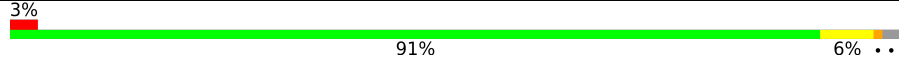
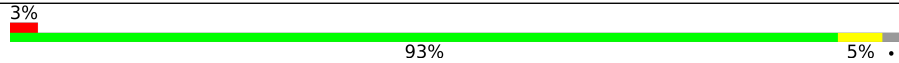
The reported resolution of this entry is 1.30 Å.

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	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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  $\geq 3$ , 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	404	 3% 91% 6% ..
1	BBB	404	 3% 93% 5% .

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7834 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.

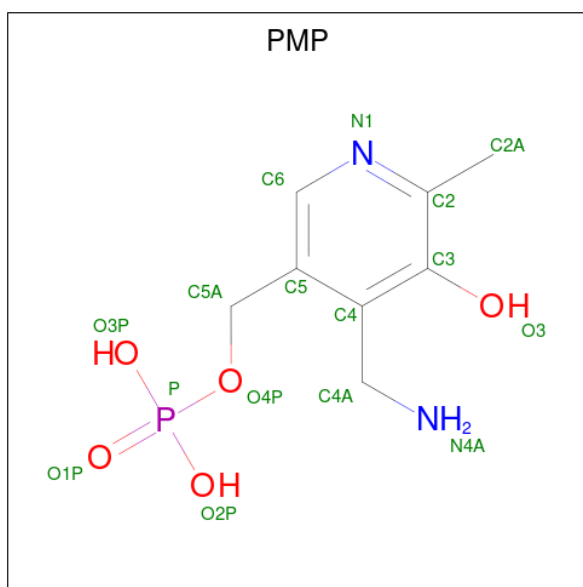
- Molecule 1 is a protein called DegT/DnrJ/EryC1/StrS aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	395	3189	2026	538	608	17	0	19	0
1	BBB	395	3165	2005	533	610	17	0	14	0

There are 8 discrepancies between the modelled and reference sequences:

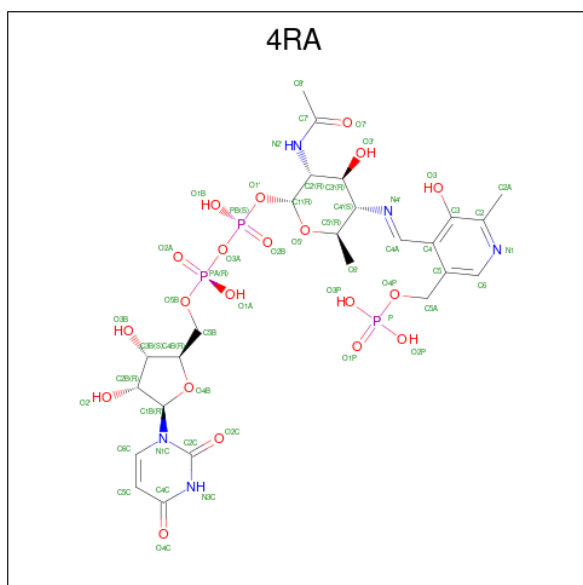
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-3	GLY	-	expression tag	UNP Q1QD32
AAA	-2	GLY	-	expression tag	UNP Q1QD32
AAA	-1	GLY	-	expression tag	UNP Q1QD32
AAA	0	HIS	-	expression tag	UNP Q1QD32
BBB	-3	GLY	-	expression tag	UNP Q1QD32
BBB	-2	GLY	-	expression tag	UNP Q1QD32
BBB	-1	GLY	-	expression tag	UNP Q1QD32
BBB	0	HIS	-	expression tag	UNP Q1QD32

- Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: C<sub>8</sub>H<sub>13</sub>N<sub>2</sub>O<sub>5</sub>P).



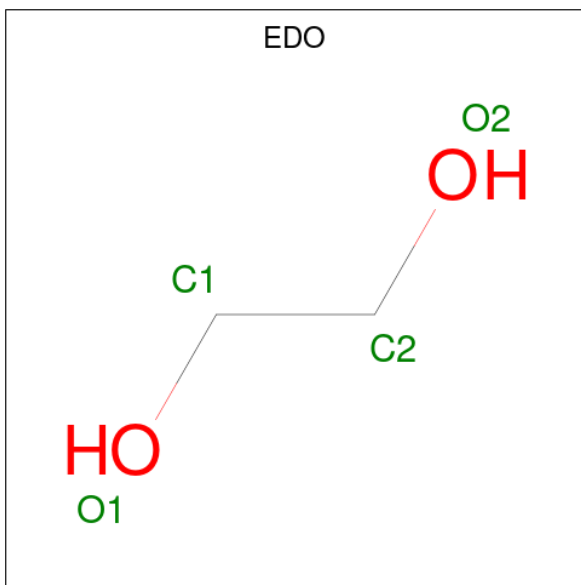
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	AAA	1	16	8	2	5	1	0	1
2	BBB	1	16	8	2	5	1	0	1

- Molecule 3 is [(2R,3R,4R,5S,6R)-3-acetamido-6-methyl-5-[(E)-[2-methyl-3-oxidanyl-5-(phosphonoxymethyl)pyridin-4-yl]methylideneamino]-4-oxidanyl-oxan-2-yl] [[[2R,3S,4R,5R)-5-[2,4-bis(oxidanylidene)pyrimidin-1-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] hydrogen phosphate (three-letter code: 4RA) (formula: C<sub>25</sub>H<sub>36</sub>N<sub>5</sub>O<sub>20</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



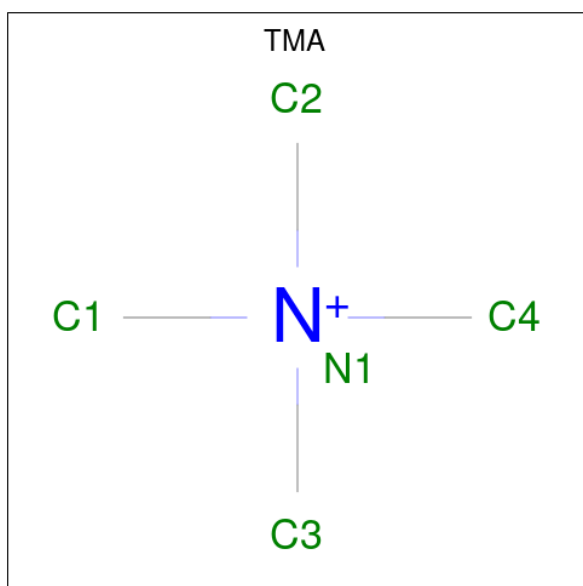
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
3	AAA	1	53	25	5	20	3	0	1
3	BBB	1	53	25	5	20	3	0	1

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 5 is TETRAMETHYLAMMONIUM ION (three-letter code: TMA) (formula:  $C_4H_{12}N$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total C N 5 4 1	0	0
5	BBB	1	Total C N 5 4 1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	2	Total Na 2 2	0	0

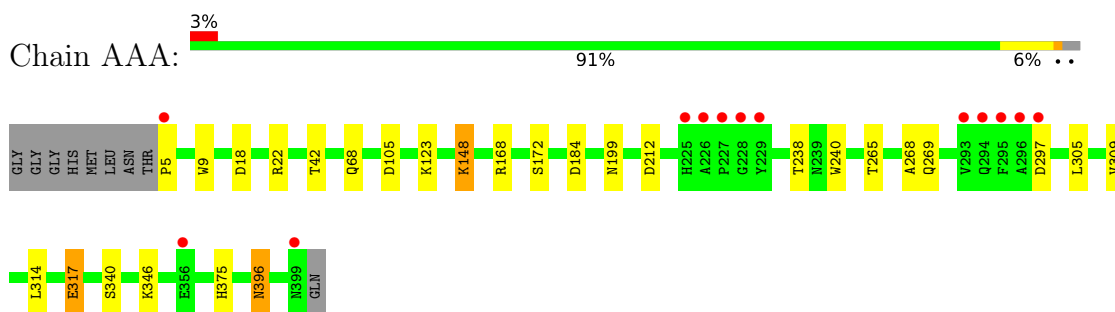
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	659	Total O 665 665	0	6
7	BBB	621	Total O 625 625	0	4

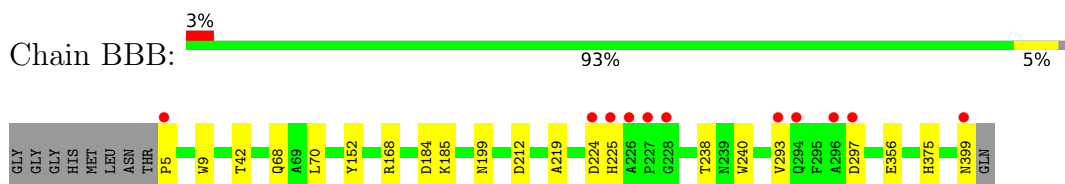
### 3 Residue-property plots [i](#)

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: DegT/DnrJ/EryC1/StrS aminotransferase



- Molecule 1: DegT/DnrJ/EryC1/StrS aminotransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.53Å 63.14Å 69.85Å 81.75° 78.59° 66.82°	Depositor
Resolution (Å)	29.96 – 1.30 29.94 – 1.30	Depositor EDS
% Data completeness (in resolution range)	92.9 (29.96-1.30) 92.9 (29.94-1.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 1.30Å)	Xtrriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.150 , 0.169 0.151 , 0.171	Depositor DCC
$R_{free}$ test set	10084 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	9.2	Xtrriage
Anisotropy	0.114	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7834	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 4RA, EDO, NA, TMA, PMP

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	0.64	0/3318	0.72	1/4509 (0.0%)
1	BBB	0.64	0/3267	0.71	1/4443 (0.0%)
All	All	0.64	0/6585	0.71	2/8952 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	5	PRO	N-CA-CB	6.14	110.66	103.30
1	BBB	5	PRO	N-CA-CB	5.72	110.16	103.30

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	3189	0	3129	26	0
1	BBB	3165	0	3070	18	0
2	AAA	16	0	10	0	0
2	BBB	16	0	10	4	0
3	AAA	53	0	31	1	0
3	BBB	53	0	31	2	0
4	AAA	20	0	29	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	BBB	20	0	29	1	0
5	AAA	5	0	12	2	0
5	BBB	5	0	12	1	0
6	AAA	2	0	0	0	0
7	AAA	665	0	0	18	0
7	BBB	625	0	0	13	0
All	All	7834	0	6363	51	0

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

All (51) 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)
3:BBB:502[A]:4RA:H26	7:BBB:842:HOH:O	1.49	1.09
3:AAA:502[A]:4RA:H26	7:AAA:898:HOH:O	1.52	1.08
1:AAA:42[A]:THR:HG22	7:AAA:922:HOH:O	1.57	1.04
1:AAA:42[A]:THR:CG2	7:AAA:922:HOH:O	2.10	0.97
1:AAA:68[A]:GLN:OE1	7:AAA:601:HOH:O	1.85	0.92
1:BBB:356:GLU:OE1	7:BBB:603:HOH:O	1.95	0.85
1:BBB:185[B]:LYS:CE	2:BBB:501[B]:PMP:N4A	2.41	0.83
1:AAA:297:ASP:O	7:AAA:602:HOH:O	1.98	0.80
1:AAA:317[B]:GLU:HG3	7:AAA:967:HOH:O	1.82	0.79
1:BBB:185[B]:LYS:HE2	2:BBB:501[B]:PMP:N4A	1.98	0.78
1:AAA:309[A]:VAL:HG11	1:AAA:314:LEU:HD11	1.64	0.78
1:BBB:297:ASP:O	7:BBB:604:HOH:O	2.03	0.76
4:BBB:507:EDO:O2	7:BBB:602:HOH:O	1.84	0.74
1:BBB:68[A]:GLN:HG3	7:BBB:601:HOH:O	1.93	0.68
1:BBB:224:ASP:OD2	7:BBB:605:HOH:O	2.11	0.68
1:BBB:185[B]:LYS:HE3	2:BBB:501[B]:PMP:HNA1	1.59	0.67
1:AAA:105[A]:ASP:OD1	7:AAA:604:HOH:O	2.14	0.64
1:AAA:68[A]:GLN:HG3	7:AAA:601:HOH:O	1.96	0.64
1:AAA:168:ARG:NH1	7:AAA:603:HOH:O	2.12	0.60
1:AAA:309[A]:VAL:CG1	1:AAA:314:LEU:HD11	2.32	0.59
1:AAA:199:ASN:ND2	7:AAA:612:HOH:O	2.37	0.58
1:BBB:185[B]:LYS:HE2	2:BBB:501[B]:PMP:HNA2	1.66	0.58
1:BBB:68[A]:GLN:CG	7:BBB:601:HOH:O	2.51	0.57
1:AAA:42[A]:THR:HG21	7:AAA:922:HOH:O	1.90	0.57
1:AAA:68[A]:GLN:CG	7:AAA:601:HOH:O	2.51	0.56
1:BBB:68[A]:GLN:NE2	7:BBB:601:HOH:O	1.78	0.52
1:BBB:42[B]:THR:CG2	7:BBB:935:HOH:O	2.57	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:18:ASP:O	1:AAA:22[B]:ARG:HG3	2.11	0.50
1:AAA:123:LYS:HD3	7:AAA:941:HOH:O	2.14	0.47
1:AAA:309[A]:VAL:HG11	1:AAA:314:LEU:CD1	2.42	0.47
3:BBB:502[A]:4RA:O3	3:BBB:502[A]:4RA:N4'	2.48	0.47
1:BBB:70:LEU:HD22	1:BBB:152[B]:TYR:CD2	2.50	0.46
1:AAA:268:ALA:HB1	1:AAA:305[B]:LEU:HD13	1.97	0.46
1:AAA:238:THR:HG21	1:AAA:240:TRP:CE2	2.51	0.46
1:BBB:42[B]:THR:HG22	7:BBB:935:HOH:O	2.15	0.46
5:AAA:508:TMA:C1	7:AAA:647:HOH:O	2.63	0.46
1:AAA:346:LYS:HE3	7:AAA:622:HOH:O	2.17	0.45
1:AAA:268:ALA:HA	1:AAA:305[B]:LEU:HD22	1.99	0.44
5:AAA:508:TMA:H12	7:AAA:647:HOH:O	2.17	0.44
1:BBB:238:THR:HG21	1:BBB:240:TRP:CE2	2.53	0.44
1:AAA:148:LYS:HB3	1:AAA:148:LYS:HE2	1.82	0.44
1:AAA:148:LYS:HD3	7:AAA:1133:HOH:O	2.17	0.43
5:BBB:508:TMA:C3	7:BBB:636:HOH:O	2.65	0.43
1:AAA:396[A]:ASN:ND2	7:AAA:626:HOH:O	2.49	0.43
1:BBB:293:VAL:HG23	7:BBB:679:HOH:O	2.17	0.43
1:BBB:9:TRP:HB2	1:BBB:375:HIS:CD2	2.52	0.43
1:AAA:265:THR:O	1:AAA:269[A]:GLN:HG2	2.18	0.42
1:AAA:9:TRP:HB2	1:AAA:375:HIS:CD2	2.54	0.42
1:BBB:219:ALA:O	1:BBB:225:HIS:NE2	2.51	0.42
1:BBB:199:ASN:ND2	7:BBB:630:HOH:O	2.54	0.41
1:AAA:168:ARG:HH11	1:AAA:172:SER:CB	2.35	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	412/404 (102%)	405 (98%)	7 (2%)	0	<b>100</b> <b>100</b>

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BBB	407/404 (101%)	398 (98%)	9 (2%)	0	100	100
All	All	819/808 (101%)	803 (98%)	16 (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	344/332 (104%)	336 (98%)	8 (2%)	50	13
1	BBB	339/332 (102%)	335 (99%)	4 (1%)	71	40
All	All	683/664 (103%)	671 (98%)	12 (2%)	65	24

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	148	LYS
1	AAA	184	ASP
1	AAA	212	ASP
1	AAA	317[A]	GLU
1	AAA	317[B]	GLU
1	AAA	340	SER
1	AAA	396[A]	ASN
1	AAA	396[B]	ASN
1	BBB	168	ARG
1	BBB	184	ASP
1	BBB	212	ASP
1	BBB	399	ASN

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 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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
4	EDO	AAA	503	6	3,3,3	0.17	0	2,2,2	0.23	0
2	PMP	BBB	501[B]	-	16,16,16	0.32	0	21,23,23	0.73	0
4	EDO	BBB	505	-	3,3,3	0.08	0	2,2,2	0.06	0
4	EDO	BBB	507	-	3,3,3	0.12	0	2,2,2	0.04	0
4	EDO	BBB	503	-	3,3,3	0.27	0	2,2,2	0.22	0
4	EDO	AAA	505	-	3,3,3	0.02	0	2,2,2	0.18	0
4	EDO	AAA	507	-	3,3,3	0.09	0	2,2,2	0.14	0
2	PMP	AAA	501[B]	-	16,16,16	0.54	0	21,23,23	0.70	1 (4%)
4	EDO	AAA	506	-	3,3,3	0.11	0	2,2,2	0.19	0
4	EDO	AAA	504	-	3,3,3	0.13	0	2,2,2	0.12	0
4	EDO	BBB	506	-	3,3,3	1.86	1 (33%)	2,2,2	1.09	0
4	EDO	BBB	504	-	3,3,3	0.70	0	2,2,2	0.57	0
3	4RA	AAA	502[A]	-	53,56,56	0.50	0	74,85,85	0.90	2 (2%)
5	TMA	AAA	508	-	4,4,4	0.17	0	6,6,6	0.09	0
3	4RA	BBB	502[A]	-	53,56,56	0.48	0	74,85,85	0.80	2 (2%)
5	TMA	BBB	508	-	4,4,4	0.25	0	6,6,6	0.05	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
4	EDO	AAA	503	6	-	0/1/1/1	-
2	PMP	BBB	501[B]	-	-	0/8/8/8	0/1/1/1
4	EDO	BBB	505	-	-	0/1/1/1	-
4	EDO	BBB	507	-	-	0/1/1/1	-
4	EDO	BBB	503	-	-	0/1/1/1	-
4	EDO	AAA	505	-	-	1/1/1/1	-
4	EDO	AAA	507	-	-	0/1/1/1	-
2	PMP	AAA	501[B]	-	-	0/8/8/8	0/1/1/1
4	EDO	AAA	506	-	-	1/1/1/1	-
4	EDO	AAA	504	-	-	0/1/1/1	-
4	EDO	BBB	506	-	-	1/1/1/1	-
4	EDO	BBB	504	-	-	0/1/1/1	-
3	4RA	AAA	502[A]	-	-	7/35/72/72	0/4/4/4
3	4RA	BBB	502[A]	-	-	4/35/72/72	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BBB	506	EDO	O2-C2	-3.15	1.25	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	502[A]	4RA	C4'-N4'-C4A	4.54	126.05	117.99
3	BBB	502[A]	4RA	C4'-N4'-C4A	4.08	125.22	117.99
3	AAA	502[A]	4RA	C4-C4A-N4'	-2.32	117.85	123.01
3	BBB	502[A]	4RA	C4-C4A-N4'	-2.18	118.16	123.01
2	AAA	501[B]	PMP	O2P-P-O4P	-2.00	101.41	106.73

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	502[A]	4RA	PB-O3A-PA-O5B
3	AAA	502[A]	4RA	C3'-C4'-N4'-C4A
3	BBB	502[A]	4RA	C3'-C4'-N4'-C4A
3	AAA	502[A]	4RA	C1'-O1'-PB-O3A

*Continued on next page...*

*Continued from previous page...*

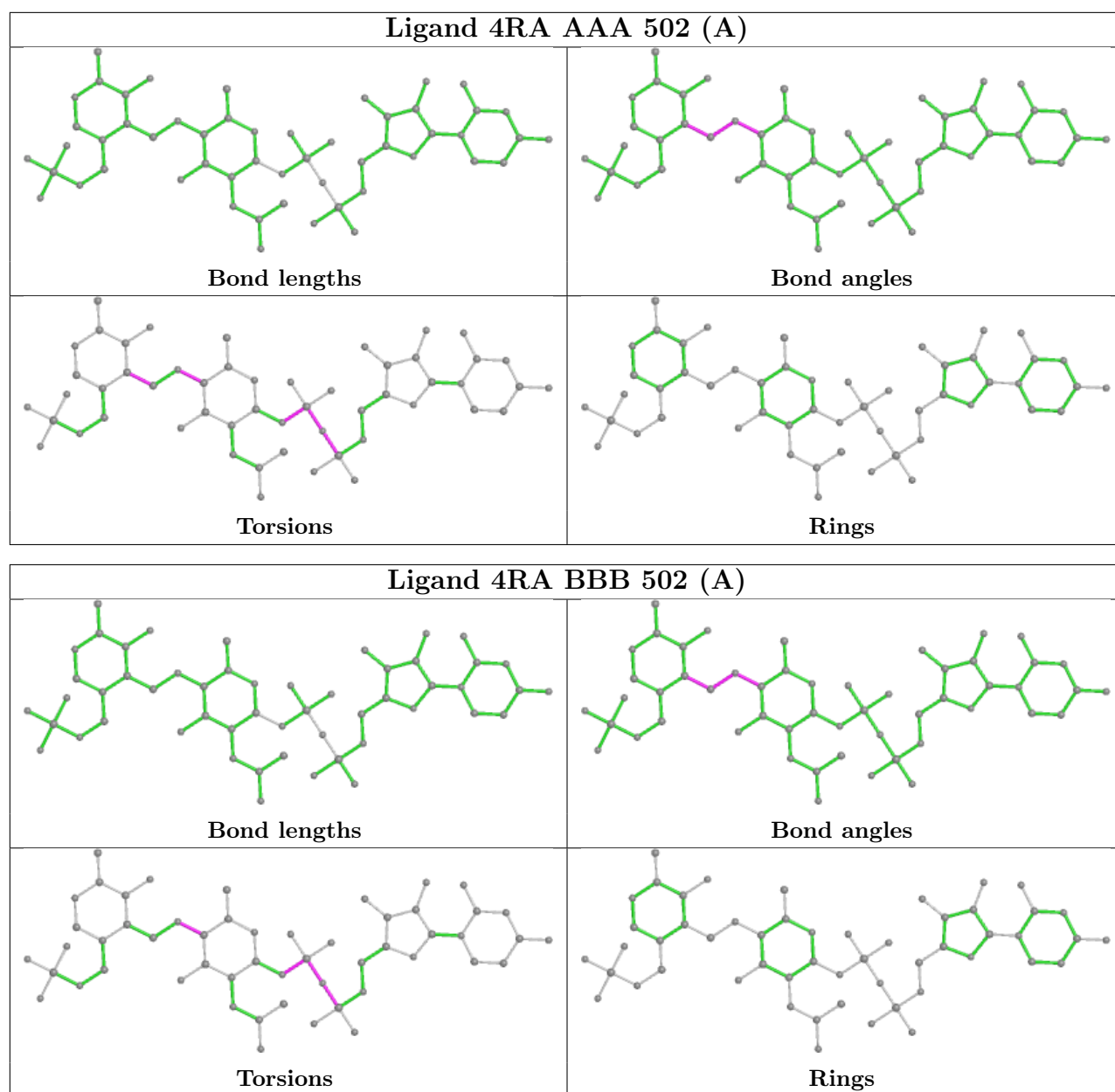
Mol	Chain	Res	Type	Atoms
3	BBB	502[A]	4RA	C1'-O1'-PB-O3A
4	AAA	505	EDO	O1-C1-C2-O2
4	AAA	506	EDO	O1-C1-C2-O2
4	BBB	506	EDO	O1-C1-C2-O2
3	BBB	502[A]	4RA	PB-O3A-PA-O5B
3	AAA	502[A]	4RA	C3-C4-C4A-N4'
3	AAA	502[A]	4RA	C5'-C4'-N4'-C4A
3	AAA	502[A]	4RA	PA-O3A-PB-O2B
3	AAA	502[A]	4RA	PA-O3A-PB-O1B
3	BBB	502[A]	4RA	PA-O3A-PB-O1B

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	501[B]	PMP	4	0
4	BBB	507	EDO	1	0
3	AAA	502[A]	4RA	1	0
5	AAA	508	TMA	2	0
3	BBB	502[A]	4RA	2	0
5	BBB	508	TMA	1	0

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AAA	395/404 (97%)	-0.12	13 (3%) 46 44	6, 10, 22, 53	0
1	BBB	395/404 (97%)	-0.11	11 (2%) 53 50	6, 11, 24, 62	0
All	All	790/808 (97%)	-0.12	24 (3%) 50 48	6, 10, 24, 62	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	226	ALA	8.4
1	AAA	226	ALA	6.6
1	BBB	227	PRO	5.7
1	AAA	227	PRO	5.4
1	AAA	296	ALA	4.8
1	AAA	293	VAL	4.7
1	BBB	5	PRO	4.6
1	BBB	296	ALA	4.0
1	AAA	5	PRO	4.0
1	BBB	297	ASP	3.1
1	AAA	295	PHE	3.0
1	BBB	228	GLY	2.9
1	AAA	297	ASP	2.9
1	AAA	294	GLN	2.7
1	AAA	356	GLU	2.6
1	AAA	225	HIS	2.5
1	BBB	225	HIS	2.4
1	AAA	399	ASN	2.3
1	BBB	224	ASP	2.3
1	AAA	228	GLY	2.3
1	AAA	229	TYR	2.2
1	BBB	399	ASN	2.2
1	BBB	294	GLN	2.1
1	BBB	293	VAL	2.1

## 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](#)

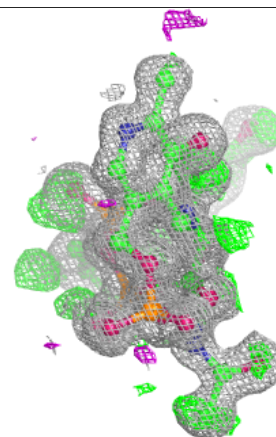
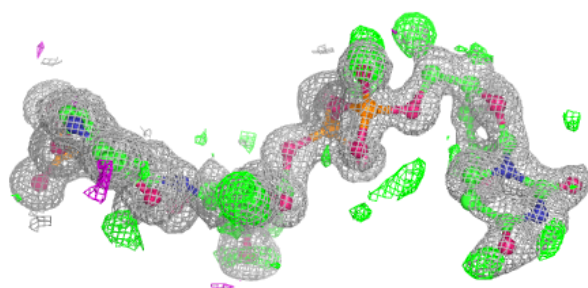
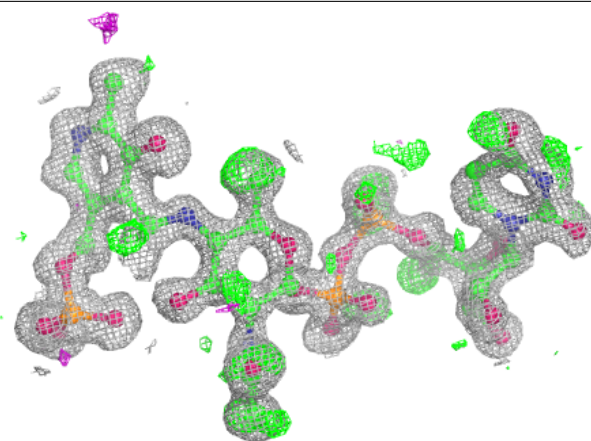
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	BBB	505	4/4	0.76	0.12	37,40,41,43	0
5	TMA	BBB	508	5/5	0.76	0.15	26,31,33,34	0
4	EDO	BBB	507	4/4	0.77	0.18	31,36,37,38	0
4	EDO	AAA	504	4/4	0.81	0.12	25,28,30,33	0
4	EDO	AAA	506	4/4	0.83	0.11	40,47,48,49	0
4	EDO	AAA	505	4/4	0.85	0.20	39,41,44,45	0
5	TMA	AAA	508	5/5	0.88	0.11	22,27,28,28	0
4	EDO	AAA	507	4/4	0.89	0.24	30,30,33,35	0
4	EDO	BBB	506	4/4	0.93	0.20	5,9,17,20	0
4	EDO	BBB	504	4/4	0.94	0.12	9,18,19,27	0
4	EDO	AAA	503	4/4	0.94	0.22	16,29,32,33	0
4	EDO	BBB	503	4/4	0.94	0.08	14,15,17,19	0
3	4RA	AAA	502[A]	53/53	0.97	0.13	7,9,17,19	53
3	4RA	BBB	502[A]	53/53	0.97	0.12	7,10,19,20	53
6	NA	AAA	510	1/1	0.97	0.28	26,26,26,26	0
2	PMP	BBB	501[B]	16/16	0.99	0.08	5,6,9,10	16
6	NA	AAA	509	1/1	0.99	0.10	16,16,16,16	0
2	PMP	AAA	501[B]	16/16	0.99	0.07	5,5,8,9	16

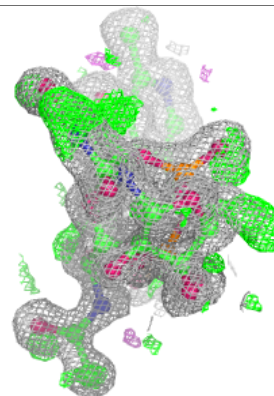
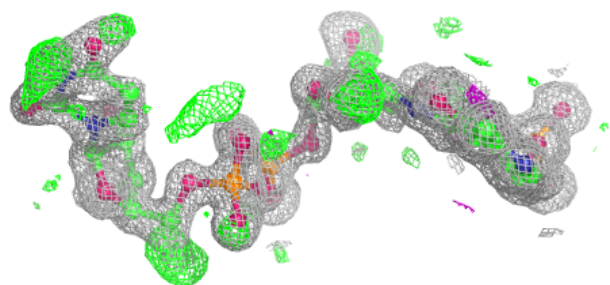
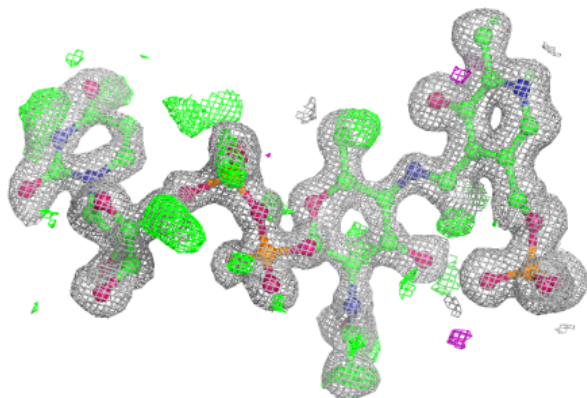
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 4RA AAA 502 (A):**

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

**Electron density around 4RA BBB 502 (A):**

$2mF_o-DF_c$  (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.