



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 24, 2020 – 11:06 AM BST

PDB ID : 6Z5H
Title : Crystal structure of Aeromonas exotoxin A
Authors : Masuyer, G.
Deposited on : 2020-05-26
Resolution : 2.30 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 ⓘ symbol.

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 : 2.14.6
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) : 2.14.6

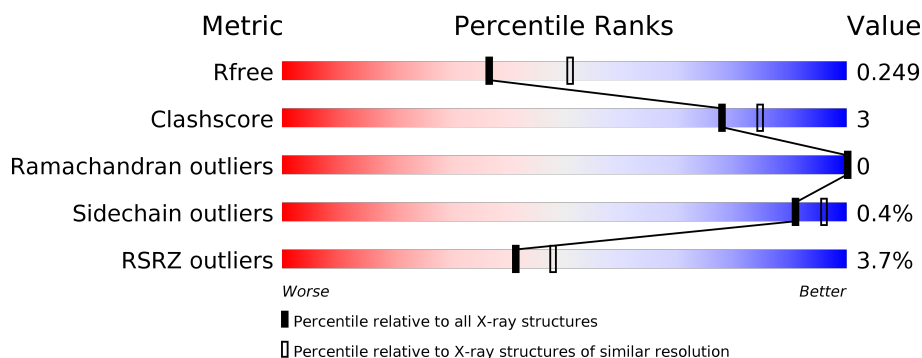
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	628	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div></div> </div> </div>
1	BBB	628	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div></div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9568 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 Exotoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	605	Total	C	N	O	S	0	3	0
			4632	2892	834	895	11			
1	BBB	602	Total	C	N	O	S	0	1	0
			4593	2869	824	889	11			

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-1	MET	-	initiating methionine	UNP A0A347A7N6
AAA	0	HIS	-	expression tag	UNP A0A347A7N6
AAA	1	HIS	-	expression tag	UNP A0A347A7N6
AAA	2	HIS	-	expression tag	UNP A0A347A7N6
AAA	3	HIS	-	expression tag	UNP A0A347A7N6
AAA	4	HIS	-	expression tag	UNP A0A347A7N6
AAA	5	HIS	-	expression tag	UNP A0A347A7N6
AAA	6	GLU	-	expression tag	UNP A0A347A7N6
AAA	7	ASN	-	expression tag	UNP A0A347A7N6
AAA	8	LEU	-	expression tag	UNP A0A347A7N6
AAA	9	TYR	-	expression tag	UNP A0A347A7N6
AAA	10	PHE	-	expression tag	UNP A0A347A7N6
AAA	11	GLN	-	expression tag	UNP A0A347A7N6
AAA	12	GLY	-	expression tag	UNP A0A347A7N6
AAA	44	SER	GLY	conflict	UNP A0A347A7N6
AAA	106	ARG	HIS	conflict	UNP A0A347A7N6
AAA	156	THR	SER	conflict	UNP A0A347A7N6
AAA	172	GLU	GLN	conflict	UNP A0A347A7N6
AAA	204	THR	SER	conflict	UNP A0A347A7N6
AAA	243	THR	ALA	conflict	UNP A0A347A7N6
AAA	307	VAL	ILE	conflict	UNP A0A347A7N6
AAA	528	ARG	HIS	conflict	UNP A0A347A7N6
AAA	530	PHE	TYR	conflict	UNP A0A347A7N6
AAA	538	ALA	ASP	conflict	UNP A0A347A7N6
AAA	545	ILE	VAL	conflict	UNP A0A347A7N6

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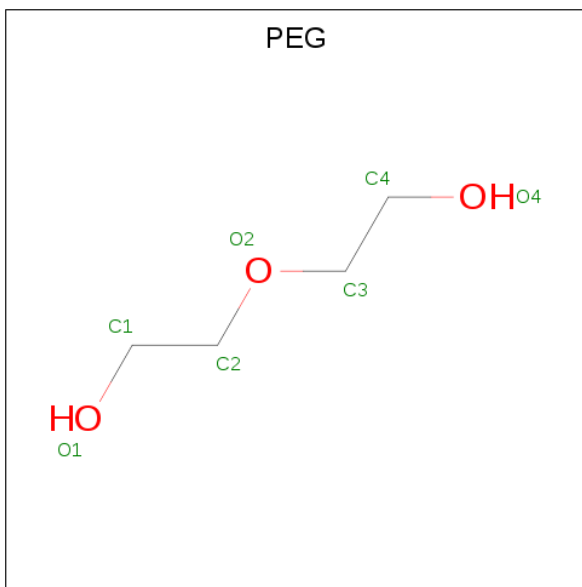
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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	571	ALA	GLU	engineered mutation	UNP A0A347A7N6
AAA	602	PRO	LEU	conflict	UNP A0A347A7N6
AAA	611	ALA	SER	conflict	UNP A0A347A7N6
AAA	614	THR	ALA	conflict	UNP A0A347A7N6
AAA	624	ASP	GLU	conflict	UNP A0A347A7N6
AAA	625	GLU	ASP	conflict	UNP A0A347A7N6
BBB	-1	MET	-	initiating methionine	UNP A0A347A7N6
BBB	0	HIS	-	expression tag	UNP A0A347A7N6
BBB	1	HIS	-	expression tag	UNP A0A347A7N6
BBB	2	HIS	-	expression tag	UNP A0A347A7N6
BBB	3	HIS	-	expression tag	UNP A0A347A7N6
BBB	4	HIS	-	expression tag	UNP A0A347A7N6
BBB	5	HIS	-	expression tag	UNP A0A347A7N6
BBB	6	GLU	-	expression tag	UNP A0A347A7N6
BBB	7	ASN	-	expression tag	UNP A0A347A7N6
BBB	8	LEU	-	expression tag	UNP A0A347A7N6
BBB	9	TYR	-	expression tag	UNP A0A347A7N6
BBB	10	PHE	-	expression tag	UNP A0A347A7N6
BBB	11	GLN	-	expression tag	UNP A0A347A7N6
BBB	12	GLY	-	expression tag	UNP A0A347A7N6
BBB	44	SER	GLY	conflict	UNP A0A347A7N6
BBB	106	ARG	HIS	conflict	UNP A0A347A7N6
BBB	156	THR	SER	conflict	UNP A0A347A7N6
BBB	172	GLU	GLN	conflict	UNP A0A347A7N6
BBB	204	THR	SER	conflict	UNP A0A347A7N6
BBB	243	THR	ALA	conflict	UNP A0A347A7N6
BBB	307	VAL	ILE	conflict	UNP A0A347A7N6
BBB	528	ARG	HIS	conflict	UNP A0A347A7N6
BBB	530	PHE	TYR	conflict	UNP A0A347A7N6
BBB	538	ALA	ASP	conflict	UNP A0A347A7N6
BBB	545	ILE	VAL	conflict	UNP A0A347A7N6
BBB	571	ALA	GLU	engineered mutation	UNP A0A347A7N6
BBB	602	PRO	LEU	conflict	UNP A0A347A7N6
BBB	611	ALA	SER	conflict	UNP A0A347A7N6
BBB	614	THR	ALA	conflict	UNP A0A347A7N6
BBB	624	ASP	GLU	conflict	UNP A0A347A7N6
BBB	625	GLU	ASP	conflict	UNP A0A347A7N6

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by author).

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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: 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		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

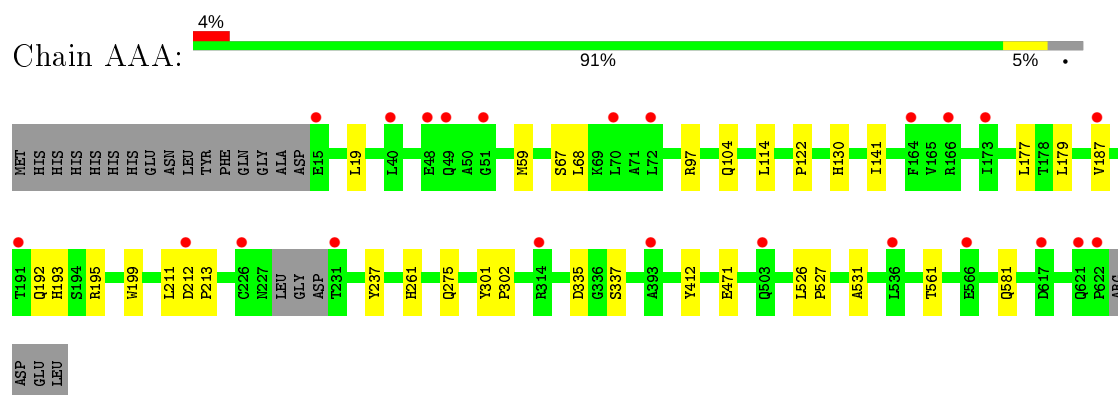
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	178	Total	O	0	0
			178	178		
5	BBB	145	Total	O	0	0
			145	145		

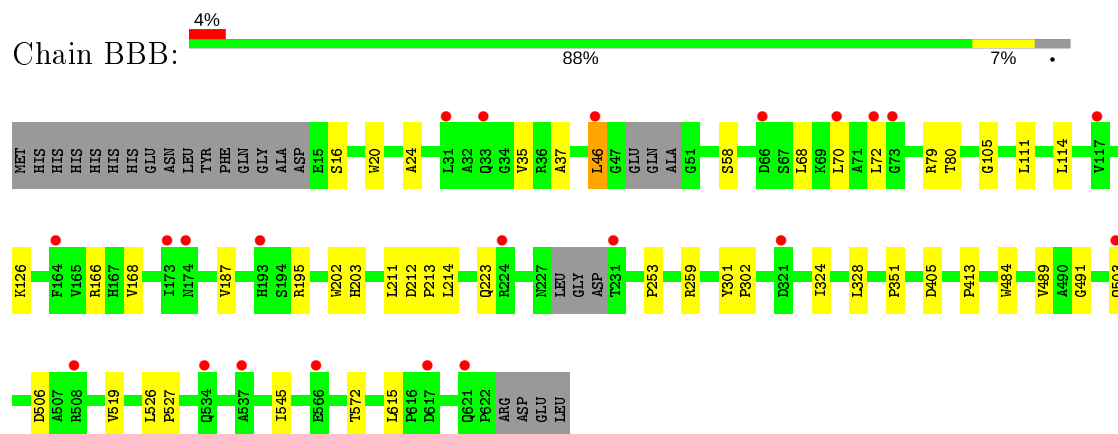
3 Residue-property plots [i](#)

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: Exotoxin



- Molecule 1: Exotoxin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.37Å 140.22Å 96.82Å 90.00° 101.79° 90.00°	Depositor
Resolution (Å)	49.58 – 2.30 49.53 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.58-2.30) 98.9 (49.53-2.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.204 , 0.247 0.208 , 0.249	Depositor DCC
R_{free} test set	2999 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9568	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8592e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NA, PEG, ACT

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	0/4744	0.76	0/6476
1	BBB	0.64	0/4698	0.76	0/6414
All	All	0.64	0/9442	0.76	0/12890

There are no bond length outliers.

There are no bond angle outliers.

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	4632	0	4507	20	0
1	BBB	4593	0	4461	33	0
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
3	AAA	7	0	10	0	0
3	BBB	7	0	10	0	0
4	AAA	4	0	3	0	0
5	AAA	178	0	0	0	0
5	BBB	145	0	0	4	0
All	All	9568	0	8991	52	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 3.

The worst 5 of 52 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:AAA:68:LEU:HD21	1:AAA:177:LEU:HD22	1.76	0.68
1:BBB:351:PRO:HG2	1:BBB:506:ASP:HA	1.82	0.62
1:BBB:223:GLN:NE2	1:BBB:253:PRO:HG3	2.18	0.59
1:AAA:212:ASP:N	1:AAA:213:PRO:HD2	2.19	0.57
1:BBB:503:GLN:NE2	5:BBB:803:HOH:O	2.37	0.56

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	604/628 (96%)	581 (96%)	23 (4%)	0	100	100
1	BBB	597/628 (95%)	578 (97%)	19 (3%)	0	100	100
All	All	1201/1256 (96%)	1159 (96%)	42 (4%)	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	488/505 (97%)	486 (100%)	2 (0%)	91	96
1	BBB	484/505 (96%)	482 (100%)	2 (0%)	91	96
All	All	972/1010 (96%)	968 (100%)	4 (0%)	91	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	67	SER
1	AAA	195	ARG
1	BBB	46	LEU
1	BBB	195	ARG

Some 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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	ACT	AAA	702	-	1,3,3	4.08	1 (100%)	0,3,3	0.00	-
3	PEG	AAA	701	-	6,6,6	0.22	0	5,5,5	0.14	0
3	PEG	BBB	701	-	6,6,6	0.17	0	5,5,5	0.07	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	AAA	701	-	-	3/4/4/4	-
3	PEG	BBB	701	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	AAA	702	ACT	CH3-C	4.08	1.53	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	701	PEG	O1-C1-C2-O2
3	BBB	701	PEG	O2-C3-C4-O4
3	AAA	701	PEG	O2-C3-C4-O4
3	BBB	701	PEG	O1-C1-C2-O2
3	AAA	701	PEG	C4-C3-O2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	605/628 (96%)	0.28	23 (3%) 40 47	17, 37, 66, 108	0
1	BBB	602/628 (95%)	0.29	22 (3%) 41 48	18, 40, 71, 102	0
All	All	1207/1256 (96%)	0.29	45 (3%) 41 48	17, 38, 71, 108	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	72	LEU	9.2
1	AAA	49	GLN	5.2
1	BBB	72	LEU	5.1
1	AAA	48	GLU	4.9
1	AAA	231	THR	4.8

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

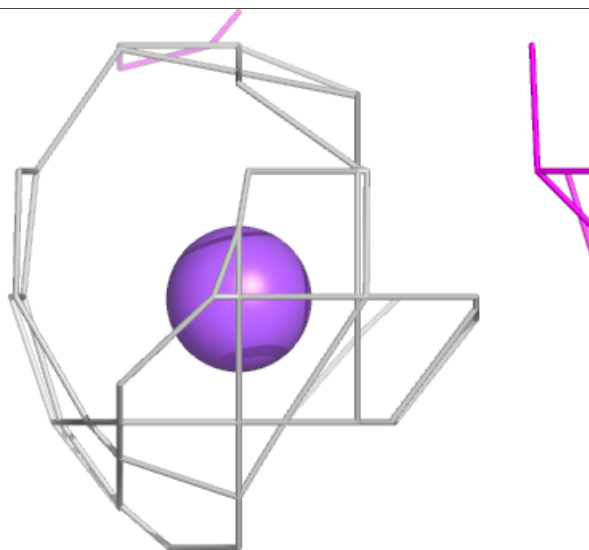
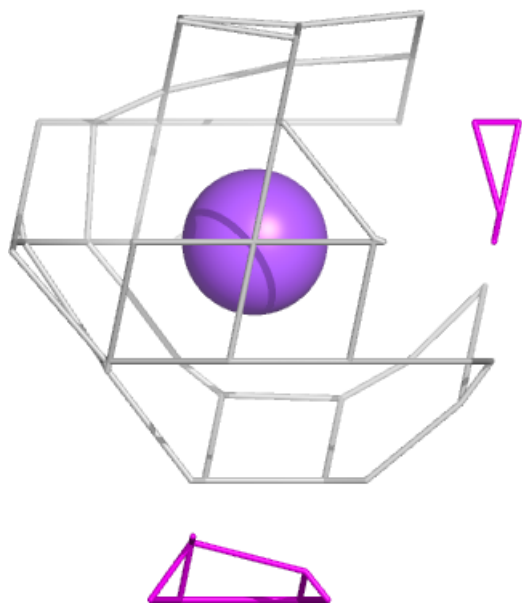
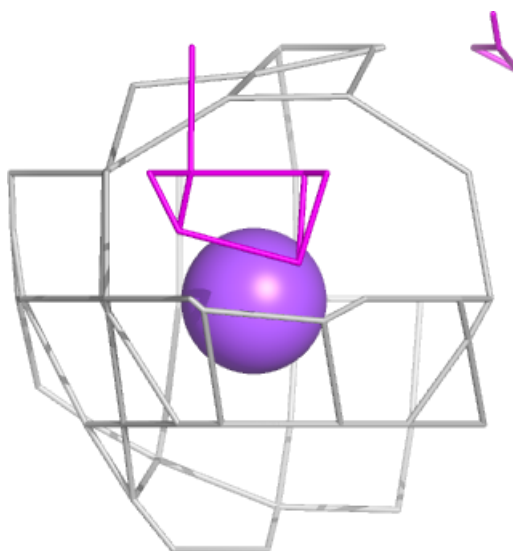
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PEG	BBB	701	7/7	0.80	0.18	57,60,62,62	0
3	PEG	AAA	701	7/7	0.84	0.14	63,68,70,70	0
4	ACT	AAA	702	4/4	0.92	0.17	38,40,41,42	0
2	NA	AAA	700	1/1	0.98	0.09	29,29,29,29	0
2	NA	BBB	700	1/1	0.98	0.09	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.

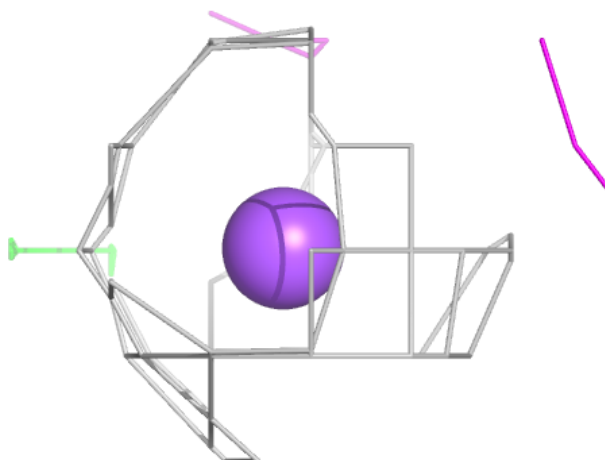
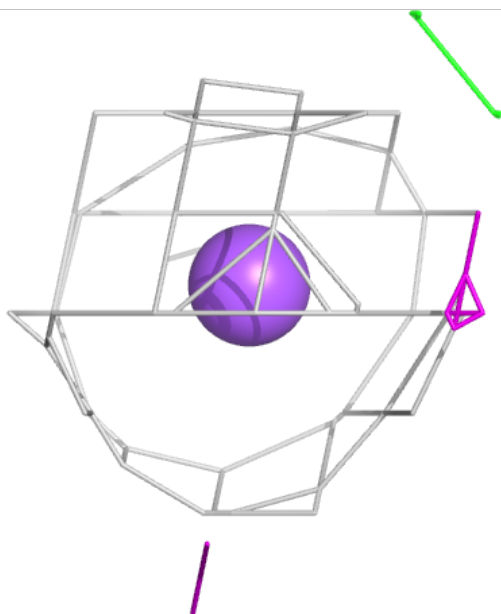
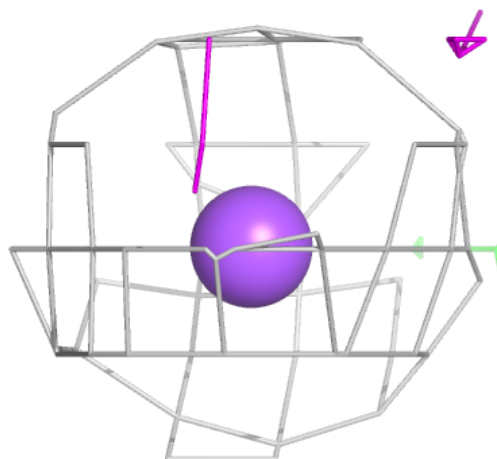
Electron density around NA AAA 700:

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



Electron density around NA BBB 700:

$2mF_o-DF_c$ (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.