



wwPDB EM Validation Summary Report ⓘ

Jul 21, 2024 – 12:08 AM JST

PDB ID : 8J5S
EMDB ID : EMD-35992
Title : Cryo-EM structure of Mycobacterium tuberculosis OppABCD in the pre-catalytic intermediate state
Authors : Yang, X.; Hu, T.; Zhang, B.; Rao, Z.
Deposited on : 2023-04-24
Resolution : 3.00 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis	: FAILED
Mogul	: 1.8.5 (274361), CSD as541be (2020)
MolProbity	: 4.02b-467
buster-report	: 1.1.7 (2018)
Percentile statistics	: 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	: FAILED
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.37.1

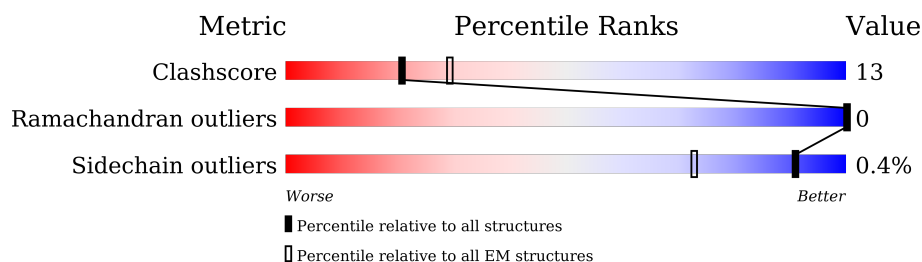
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	599	63% 25% 12%
2	B	325	78% 22%
3	C	291	75% 22% .
4	D	612	69% 30% .
5	E	8	88% 12%

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
8	SF4	D	705	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13275 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Uncharacterized protein Rv1280c.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	527	Total	C	N	O	S	0	0
			4003	2517	712	768	6		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	MET	conflict	UNP P9WGU5
A	592	ASP	-	expression tag	UNP P9WGU5
A	593	TYR	-	expression tag	UNP P9WGU5
A	594	LYS	-	expression tag	UNP P9WGU5
A	595	ASP	-	expression tag	UNP P9WGU5
A	596	ASP	-	expression tag	UNP P9WGU5
A	597	ASP	-	expression tag	UNP P9WGU5
A	598	ASP	-	expression tag	UNP P9WGU5
A	599	LYS	-	expression tag	UNP P9WGU5

- Molecule 2 is a protein called Putative peptide transport permease protein Rv1283c.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	325	Total	C	N	O	S	0	0
			2475	1598	444	425	8		

- Molecule 3 is a protein called Putative peptide transport permease protein Rv1282c.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	282	Total	C	N	O	S	0	0
			2130	1387	364	368	11		

- Molecule 4 is a protein called Uncharacterized ABC transporter ATP-binding protein Rv1281c.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	608	Total	C	N	O	S	0	0
			4555	2856	828	859	12		

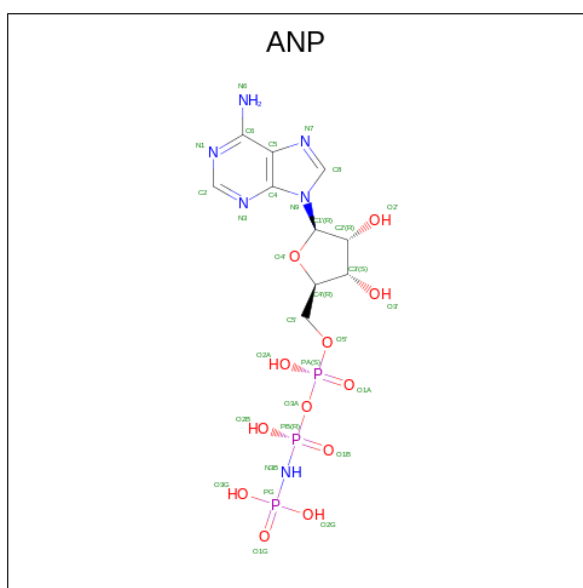
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	180	ASP	GLU	engineered mutation	UNP P9WQJ5
D	525	ASP	GLU	engineered mutation	UNP P9WQJ5

- Molecule 5 is a protein called Endogenous oligopeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	8	Total	C	N	O	0	0
			40	24	8	8		

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).

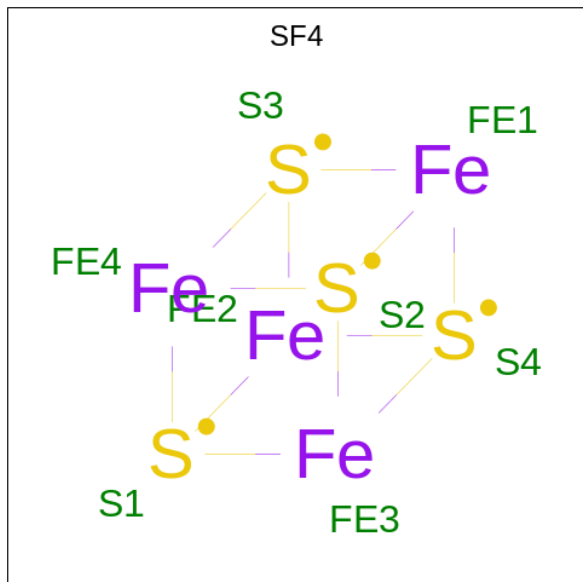


Mol	Chain	Residues	Atoms					AltConf
6	D	1	Total	C	N	O	P	0
			31	10	6	12	3	
6	D	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	D	2	Total	Mg	0
			2	2	

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

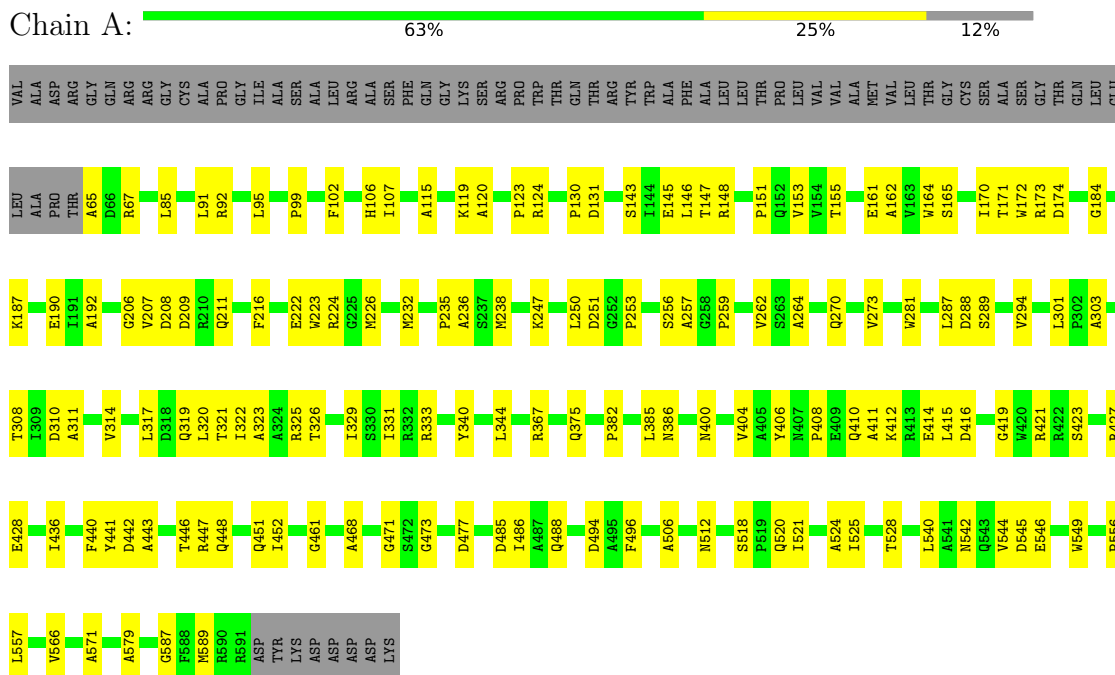


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
8	D	1	8	4	4	0

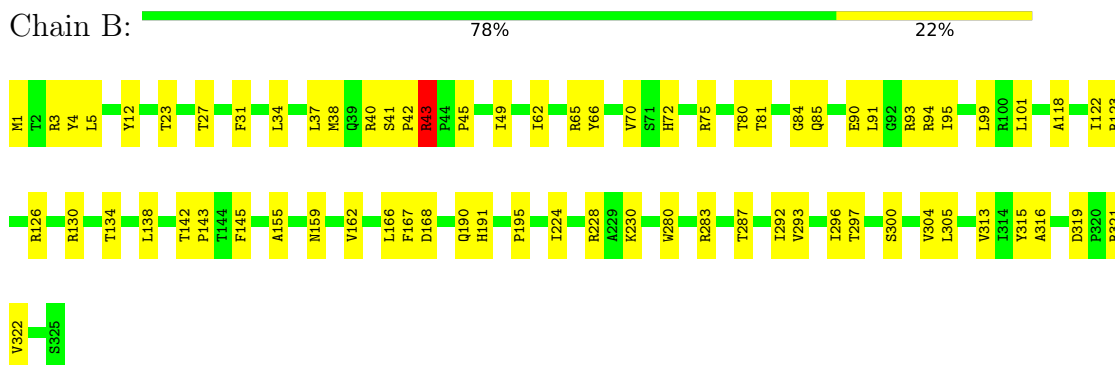
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Uncharacterized protein Rv1280c

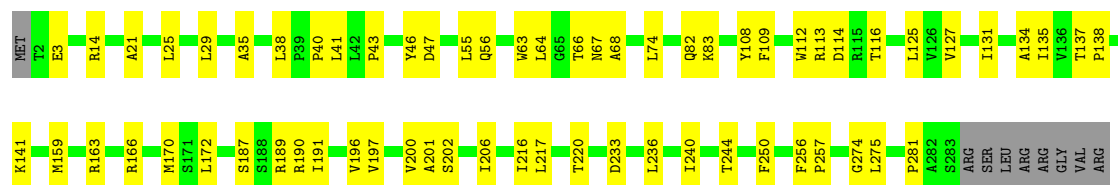


- Molecule 2: Putative peptide transport permease protein Rv1283c



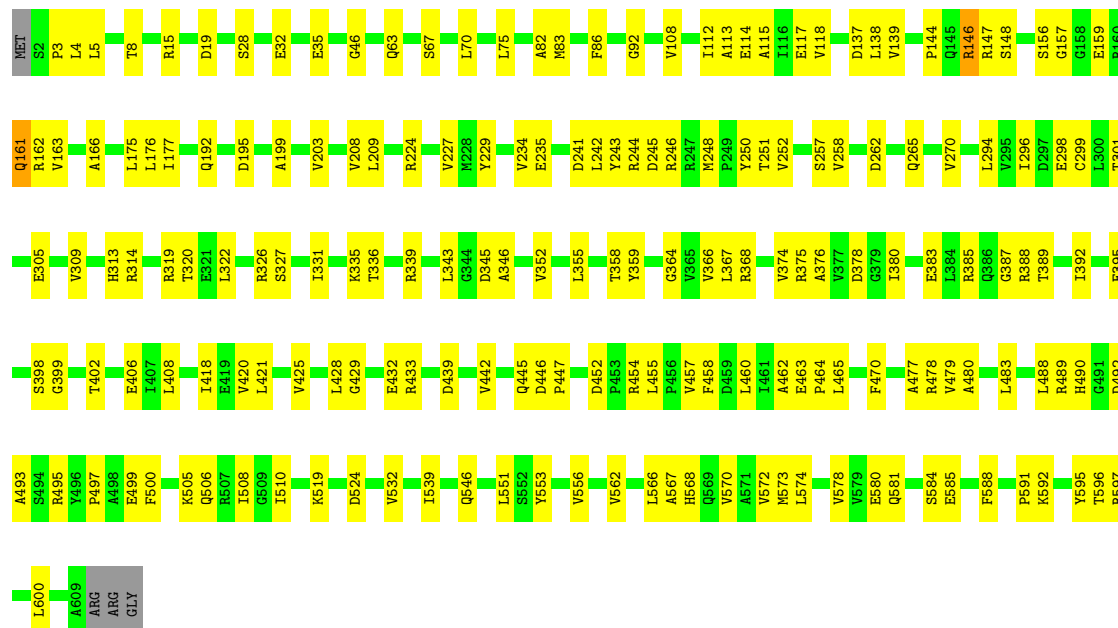
- Molecule 3: Putative peptide transport permease protein Rv1282c





- Molecule 4: Uncharacterized ABC transporter ATP-binding protein Rv1281c

Chain D: 69% 30%



- Molecule 5: Endogenous oligopeptide

Chain E: 88% 12%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	169227	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

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: ANP, SF4, MG

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	A	0.41	0/4089	0.52	0/5571
2	B	0.40	0/2523	0.52	0/3435
3	C	0.39	0/2173	0.50	0/2963
4	D	0.44	0/4625	0.54	0/6291
All	All	0.42	0/13410	0.52	0/18260

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	40	ARG	Sidechain
2	B	43	ARG	Sidechain

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	A	4003	0	3929	110	0
2	B	2475	0	2592	54	0
3	C	2130	0	2233	47	0
4	D	4555	0	4666	151	0
5	E	40	0	10	2	0
6	D	62	0	26	3	0
7	D	2	0	0	0	0
8	D	8	0	0	2	0
All	All	13275	0	13456	358	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 13.

The worst 5 of 358 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)
4:D:296:ILE:HG12	4:D:299:CYS:SG	2.02	0.99
4:D:364:GLY:H	4:D:368:ARG:HD3	1.27	0.99
4:D:392:ILE:HB	4:D:556:VAL:HG12	1.58	0.83
2:B:34:LEU:O	2:B:38:MET:HG3	1.84	0.76
4:D:352:VAL:HG22	4:D:418:ILE:HG22	1.69	0.75

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 PDB entries followed by that with respect to all EM entries.

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	A	525/599 (88%)	487 (93%)	38 (7%)	0	100	100
2	B	323/325 (99%)	318 (98%)	5 (2%)	0	100	100
3	C	280/291 (96%)	260 (93%)	20 (7%)	0	100	100
4	D	606/612 (99%)	561 (93%)	45 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1734/1827 (95%)	1626 (94%)	108 (6%)	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 PDB entries followed by that with respect to all EM entries.

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	A	411/467 (88%)	411 (100%)	0	100	100
2	B	255/255 (100%)	254 (100%)	1 (0%)	91	97
3	C	225/233 (97%)	225 (100%)	0	100	100
4	D	482/485 (99%)	478 (99%)	4 (1%)	81	93
All	All	1373/1440 (95%)	1368 (100%)	5 (0%)	91	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	43	ARG
4	D	146	ARG
4	D	161	GLN
4	D	313	HIS
4	D	478	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	161	GLN
4	D	565	HIS

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 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$
6	ANP	D	703	7	29,33,33	1.20	5 (17%)	31,52,52	1.13	4 (12%)
8	SF4	D	705	4	0,12,12	-	-	-		
6	ANP	D	701	7	29,33,33	1.20	5 (17%)	31,52,52	1.14	3 (9%)

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
6	ANP	D	703	7	-	4/14/38/38	0/3/3/3
8	SF4	D	705	4	-	-	0/6/5/5
6	ANP	D	701	7	-	2/14/38/38	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	701	ANP	PG-O1G	3.21	1.51	1.46
6	D	703	ANP	PG-O1G	3.20	1.51	1.46
6	D	701	ANP	PB-O1B	2.92	1.50	1.46
6	D	703	ANP	PB-O1B	2.90	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	701	ANP	PB-O2B	-2.22	1.50	1.56

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	703	ANP	O2B-PB-O1B	4.16	118.64	109.92
6	D	701	ANP	O2B-PB-O1B	4.13	118.58	109.92
6	D	701	ANP	C5-C6-N6	2.29	123.84	120.35
6	D	703	ANP	C5-C6-N6	2.25	123.77	120.35
6	D	703	ANP	O3G-PG-O1G	-2.05	108.31	113.45

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

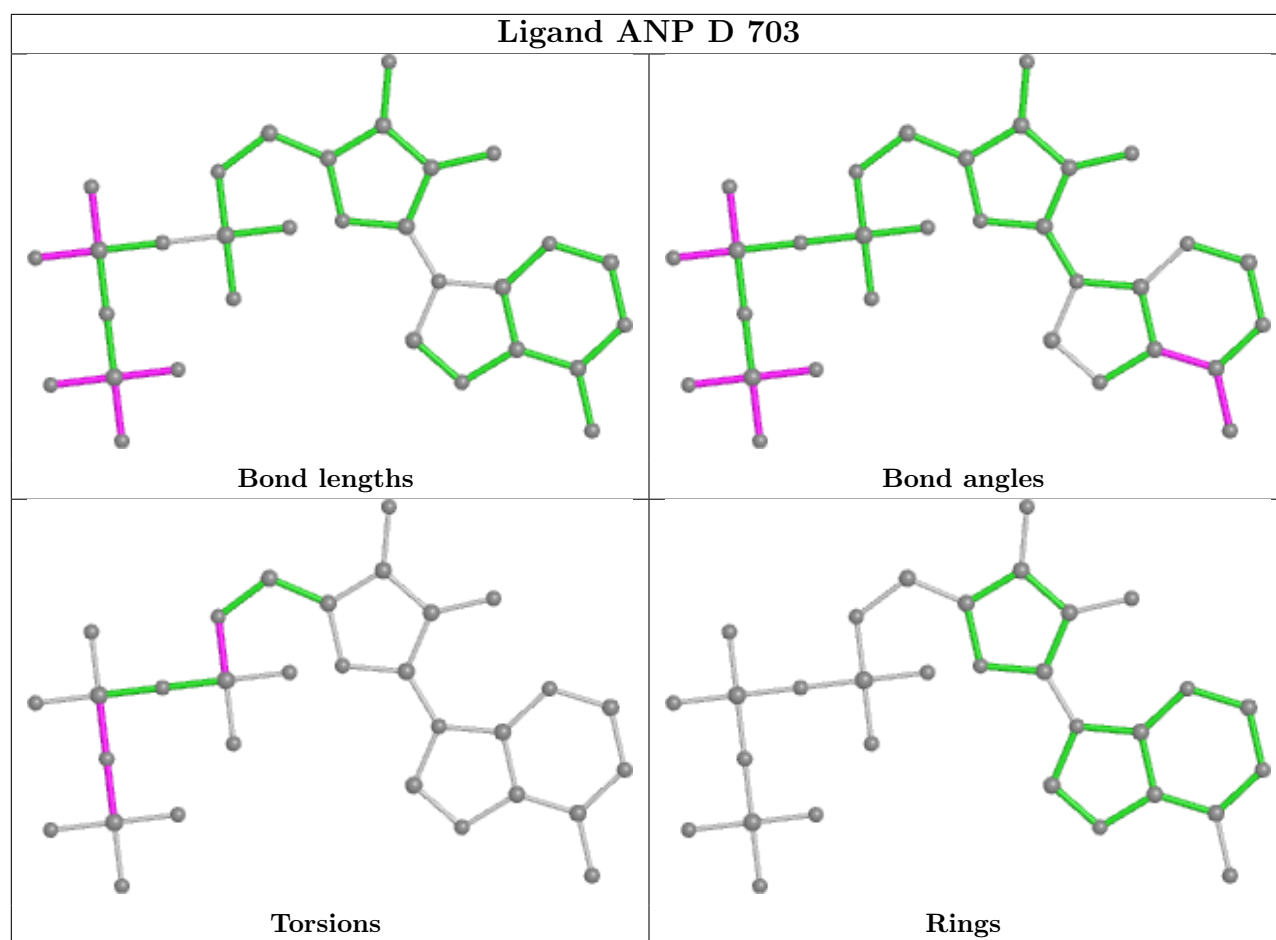
Mol	Chain	Res	Type	Atoms
6	D	701	ANP	PG-N3B-PB-O1B
6	D	701	ANP	PG-N3B-PB-O3A
6	D	703	ANP	PB-N3B-PG-O1G
6	D	703	ANP	PG-N3B-PB-O1B
6	D	703	ANP	PG-N3B-PB-O3A

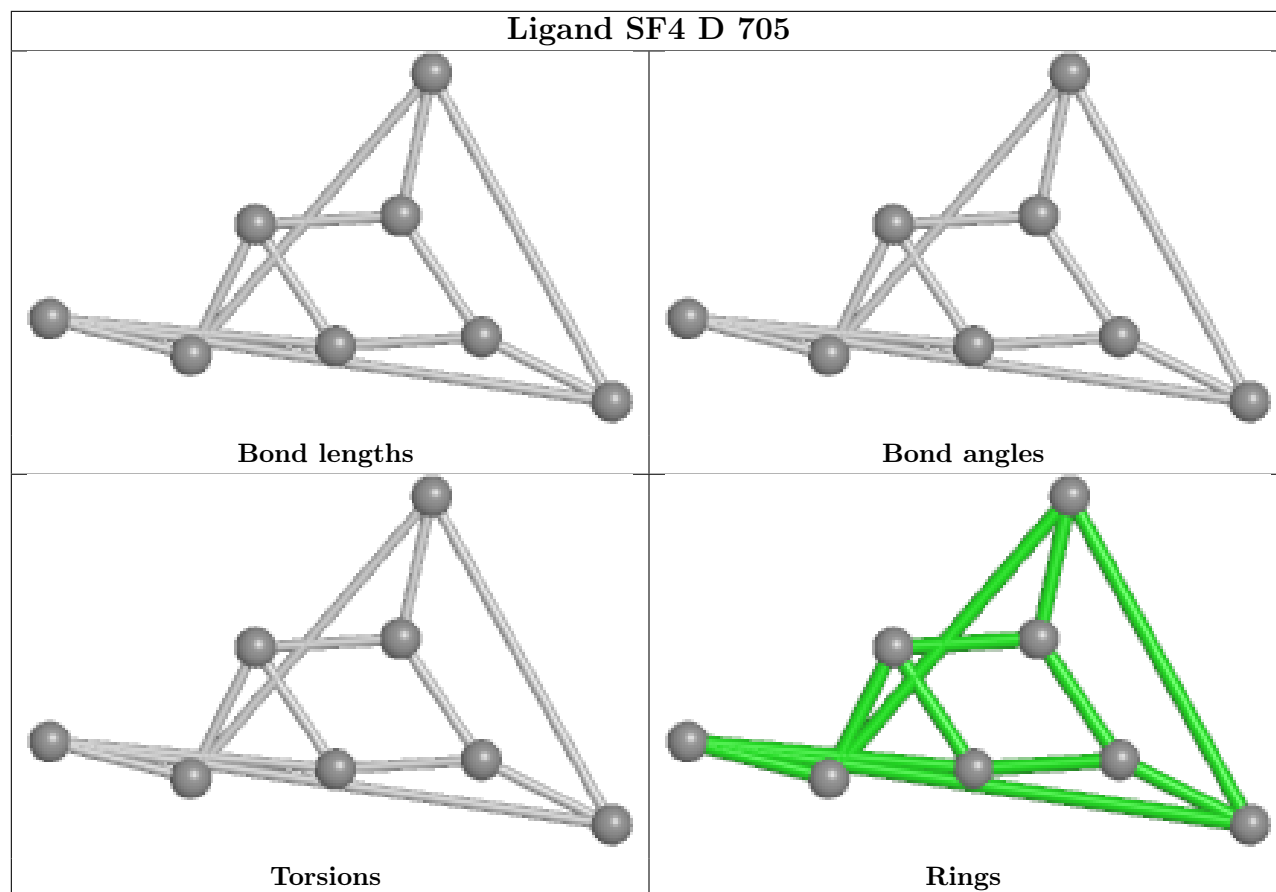
There are no ring outliers.

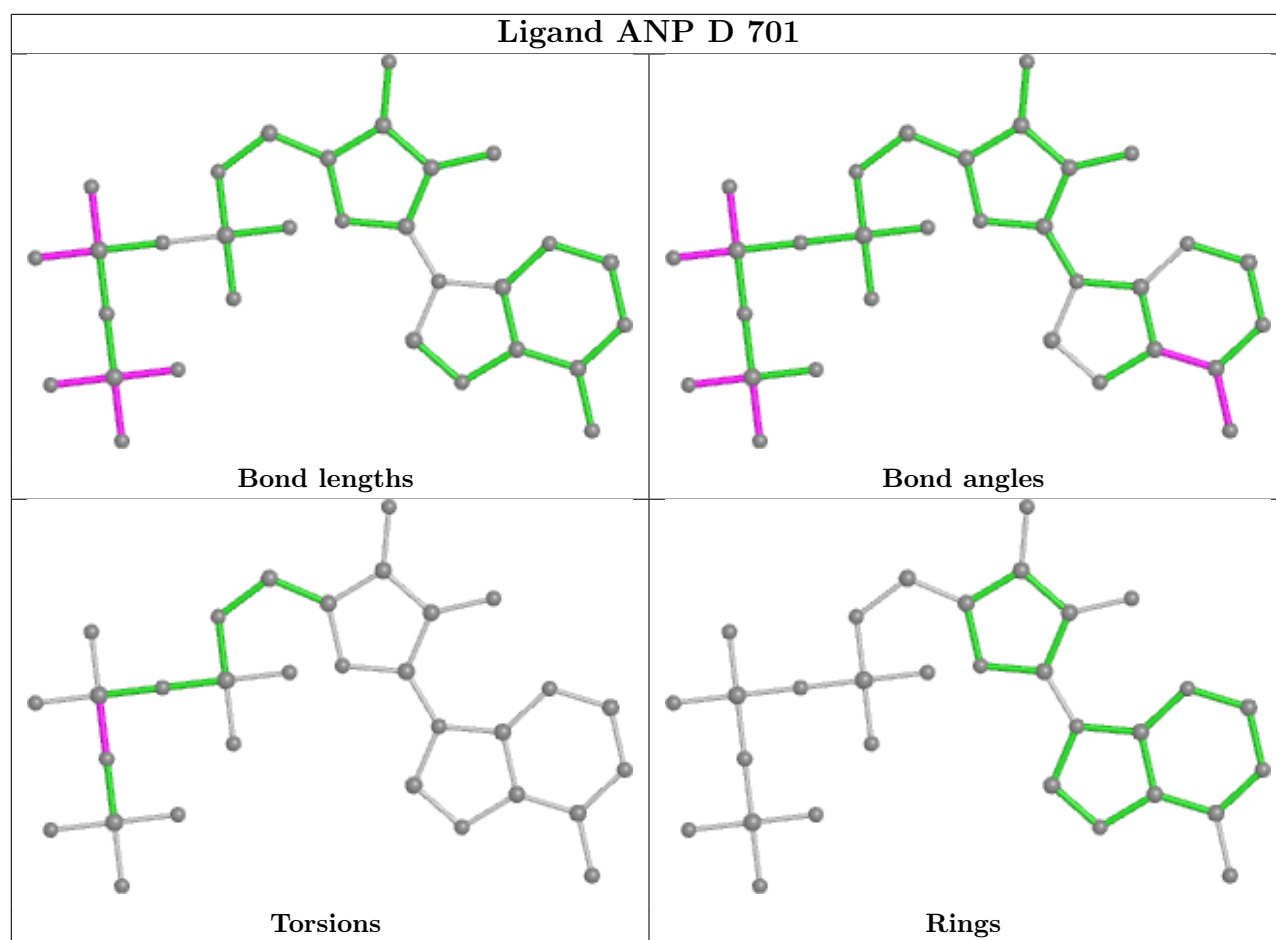
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	703	ANP	1	0
8	D	705	SF4	2	0
6	D	701	ANP	2	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.