



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2023 – 02:19 AM EDT

PDB ID : 2Q58
Title : *Cryptosporidium parvum* putative polyprenyl pyrophosphate synthase (cgd4_2550) in complex with zoledronate
Authors : Chruszcz, M.; Artz, J.; Zheng, H.; Dong, A.; Dunford, J.; Lew, J.; Zhao, Y.; Kozieradski, I.; Kavanaugh, K.L.; Opperman, U.; Sundstrom, M.; Weigelt, J.; Edwards, A.; Arrowsmith, C.; Bochkarev, A.; Hui, R.; Minor, W.; Structural Genomics Consortium (SGC)
Deposited on : 2007-05-31
Resolution : 2.37 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 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
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)

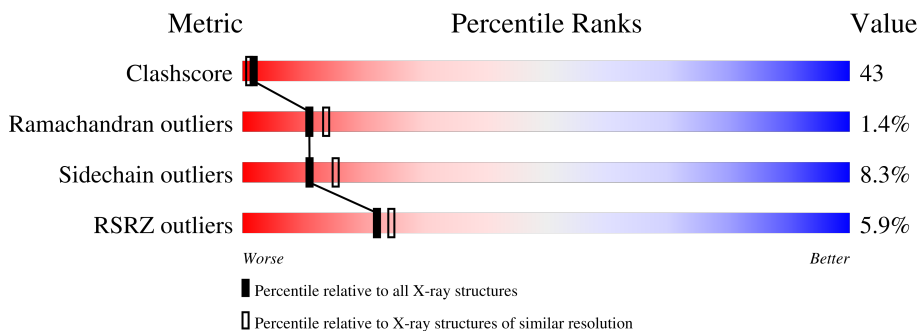
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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))
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	368	
1	B	368	

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.35

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 5370 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 Farnesyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	335	Total	C	N	O	S	0	0	0
			2655	1733	424	487	11			
1	B	329	Total	C	N	O	S	0	0	0
			2648	1723	422	492	11			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1001	MET	-	cloning artifact	UNP Q5CR09
A	1002	GLY	-	cloning artifact	UNP Q5CR09
A	1003	SER	-	cloning artifact	UNP Q5CR09
A	1004	SER	-	cloning artifact	UNP Q5CR09
A	1005	HIS	-	expression tag	UNP Q5CR09
A	1006	HIS	-	expression tag	UNP Q5CR09
A	1007	HIS	-	expression tag	UNP Q5CR09
A	1008	HIS	-	expression tag	UNP Q5CR09
A	1009	HIS	-	expression tag	UNP Q5CR09
A	1010	HIS	-	expression tag	UNP Q5CR09
A	1011	SER	-	cloning artifact	UNP Q5CR09
A	1012	SER	-	cloning artifact	UNP Q5CR09
A	1013	GLY	-	cloning artifact	UNP Q5CR09
A	1014	ARG	-	cloning artifact	UNP Q5CR09
A	1015	GLU	-	cloning artifact	UNP Q5CR09
A	1016	ASN	-	cloning artifact	UNP Q5CR09
A	1017	LEU	-	cloning artifact	UNP Q5CR09
A	1018	TYR	-	cloning artifact	UNP Q5CR09
A	1019	PHE	-	cloning artifact	UNP Q5CR09
A	1020	GLN	-	cloning artifact	UNP Q5CR09
A	1021	GLY	-	cloning artifact	UNP Q5CR09
B	2001	MET	-	cloning artifact	UNP Q5CR09
B	2002	GLY	-	cloning artifact	UNP Q5CR09
B	2003	SER	-	cloning artifact	UNP Q5CR09
B	2004	SER	-	cloning artifact	UNP Q5CR09

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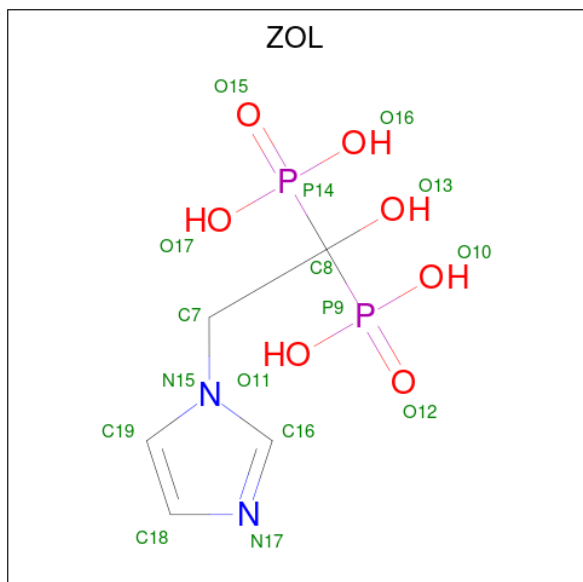
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Chain	Residue	Modelled	Actual	Comment	Reference
B	2005	HIS	-	expression tag	UNP Q5CR09
B	2006	HIS	-	expression tag	UNP Q5CR09
B	2007	HIS	-	expression tag	UNP Q5CR09
B	2008	HIS	-	expression tag	UNP Q5CR09
B	2009	HIS	-	expression tag	UNP Q5CR09
B	2010	HIS	-	expression tag	UNP Q5CR09
B	2011	SER	-	cloning artifact	UNP Q5CR09
B	2012	SER	-	cloning artifact	UNP Q5CR09
B	2013	GLY	-	cloning artifact	UNP Q5CR09
B	2014	ARG	-	cloning artifact	UNP Q5CR09
B	2015	GLU	-	cloning artifact	UNP Q5CR09
B	2016	ASN	-	cloning artifact	UNP Q5CR09
B	2017	LEU	-	cloning artifact	UNP Q5CR09
B	2018	TYR	-	cloning artifact	UNP Q5CR09
B	2019	PHE	-	cloning artifact	UNP Q5CR09
B	2020	GLN	-	cloning artifact	UNP Q5CR09
B	2021	GLY	-	cloning artifact	UNP Q5CR09

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Mg 3 3	0	0
2	B	3	Total Mg 3 3	0	0

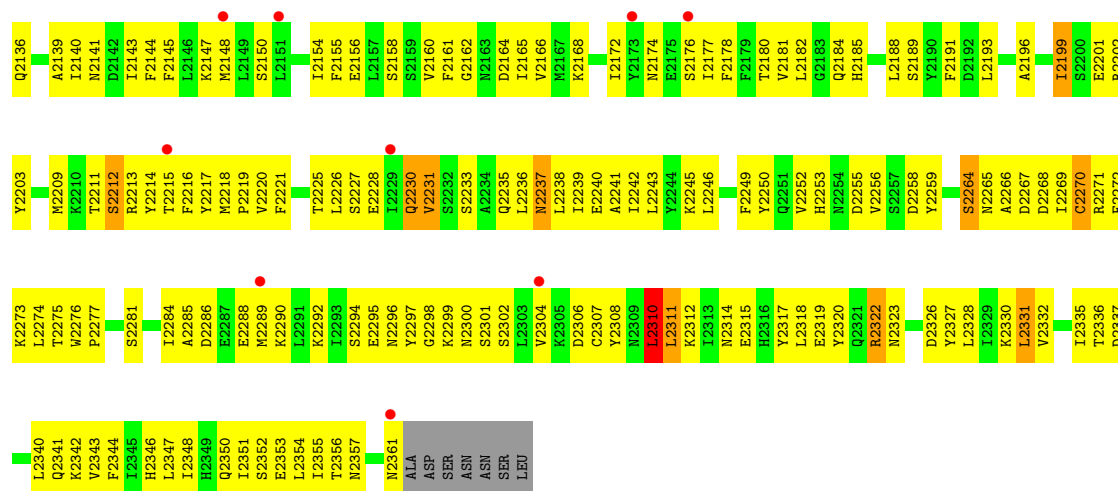
- Molecule 3 is ZOLEDRONIC ACID (three-letter code: ZOL) (formula: C₅H₁₀N₂O₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	16	5	2	7	2	0	0
3	B	1	16	5	2	7	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		
4	B	15	Total	O	0	0
			15	15		



4 Data and refinement statistics i

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	101.78Å 101.78Å 75.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.46 – 2.37 30.46 – 2.37	Depositor EDS
% Data completeness (in resolution range)	94.8 (30.46-2.37) 94.8 (30.46-2.37)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.36Å)	Xtrriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.216 , 0.238 0.209 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtrriage
Anisotropy	0.259	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 118.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.009 for -h,-k,l 0.032 for h,-h-k,-l 0.013 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5370	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZOL

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	0.27	0/2713	0.57	0/3678
1	B	0.28	0/2701	0.61	1/3649 (0.0%)
All	All	0.27	0/5414	0.59	1/7327 (0.0%)

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
1	A	0	9
1	B	0	6
All	All	0	15

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	2065	ASP	CB-CG-OD1	5.26	123.03	118.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1047	PRO	Peptide
1	A	1053	ARG	Peptide
1	A	1055	PRO	Peptide
1	A	1091	ASN	Peptide
1	A	1221	PHE	Peptide

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	2655	0	2561	219	0
1	B	2648	0	2590	235	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	16	0	6	3	0
3	B	16	0	7	1	0
4	A	14	0	0	0	0
4	B	15	0	0	2	0
All	All	5370	0	5164	449	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 43.

The worst 5 of 449 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:B:2110:LEU:C	1:B:2110:LEU:HD23	1.54	1.26
1:A:1270:CYS:O	1:A:1298:GLY:HA2	1.37	1.18
1:B:2110:LEU:HD23	1:B:2111:ILE:N	1.60	1.16
1:B:2024:ASP:CA	1:B:2025:TYR:HB2	1.78	1.12
1:B:2024:ASP:HA	1:B:2025:TYR:HB2	1.37	1.07

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	A	333/368 (90%)	270 (81%)	58 (17%)	5 (2%)	10	12
1	B	323/368 (88%)	273 (84%)	46 (14%)	4 (1%)	13	17
All	All	656/736 (89%)	543 (83%)	104 (16%)	9 (1%)	11	14

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1047	PRO
1	A	1092	ILE
1	B	2025	TYR
1	A	1338	ASP
1	B	2237	ASN

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	A	279/341 (82%)	254 (91%)	25 (9%)	9	12
1	B	286/341 (84%)	264 (92%)	22 (8%)	13	18
All	All	565/682 (83%)	518 (92%)	47 (8%)	11	15

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2045	LYS
1	B	2258	ASP
1	B	2058	GLU
1	B	2110	LEU
1	B	2267	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2136	GLN

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Mol	Chain	Res	Type
1	B	2185	HIS
1	B	2341	GLN
1	B	2323	ASN
1	B	2108	GLN

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 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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
3	ZOL	A	1	2	14,16,16	2.82	9 (64%)	20,26,26	1.46	4 (20%)
3	ZOL	B	2	2	14,16,16	2.85	9 (64%)	20,26,26	1.59	4 (20%)

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	ZOL	A	1	2	-	2/23/23/23	0/1/1/1
3	ZOL	B	2	2	-	1/23/23/23	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2	ZOL	P14-O15	6.30	1.60	1.50
3	A	1	ZOL	P14-O15	5.81	1.59	1.50
3	B	2	ZOL	P9-C8	-4.22	1.82	1.85
3	B	2	ZOL	C16-N17	-3.67	1.25	1.34
3	A	1	ZOL	C16-N17	-3.60	1.25	1.34

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	ZOL	C19-C18-N17	-3.67	101.13	107.57
3	B	2	ZOL	C19-C18-N17	-3.63	101.19	107.57
3	B	2	ZOL	P9-C8-P14	-2.73	107.92	112.81
3	A	1	ZOL	O16-P14-O15	-2.65	107.10	113.06
3	B	2	ZOL	O16-P14-O15	-2.37	107.72	113.06

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	ZOL	C8-C7-N15-C19
3	B	2	ZOL	C8-C7-N15-C19
3	A	1	ZOL	C8-C7-N15-C16

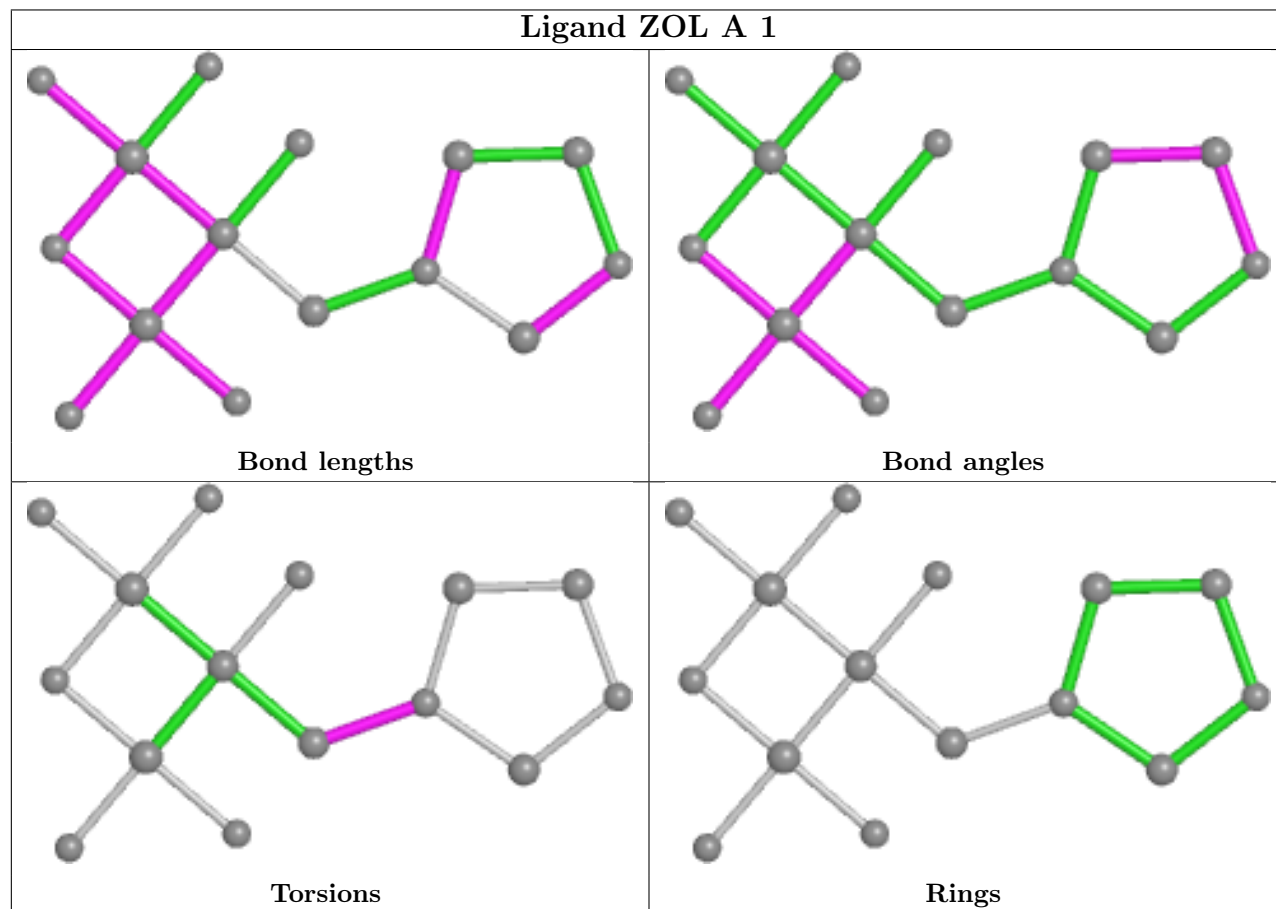
There are no ring outliers.

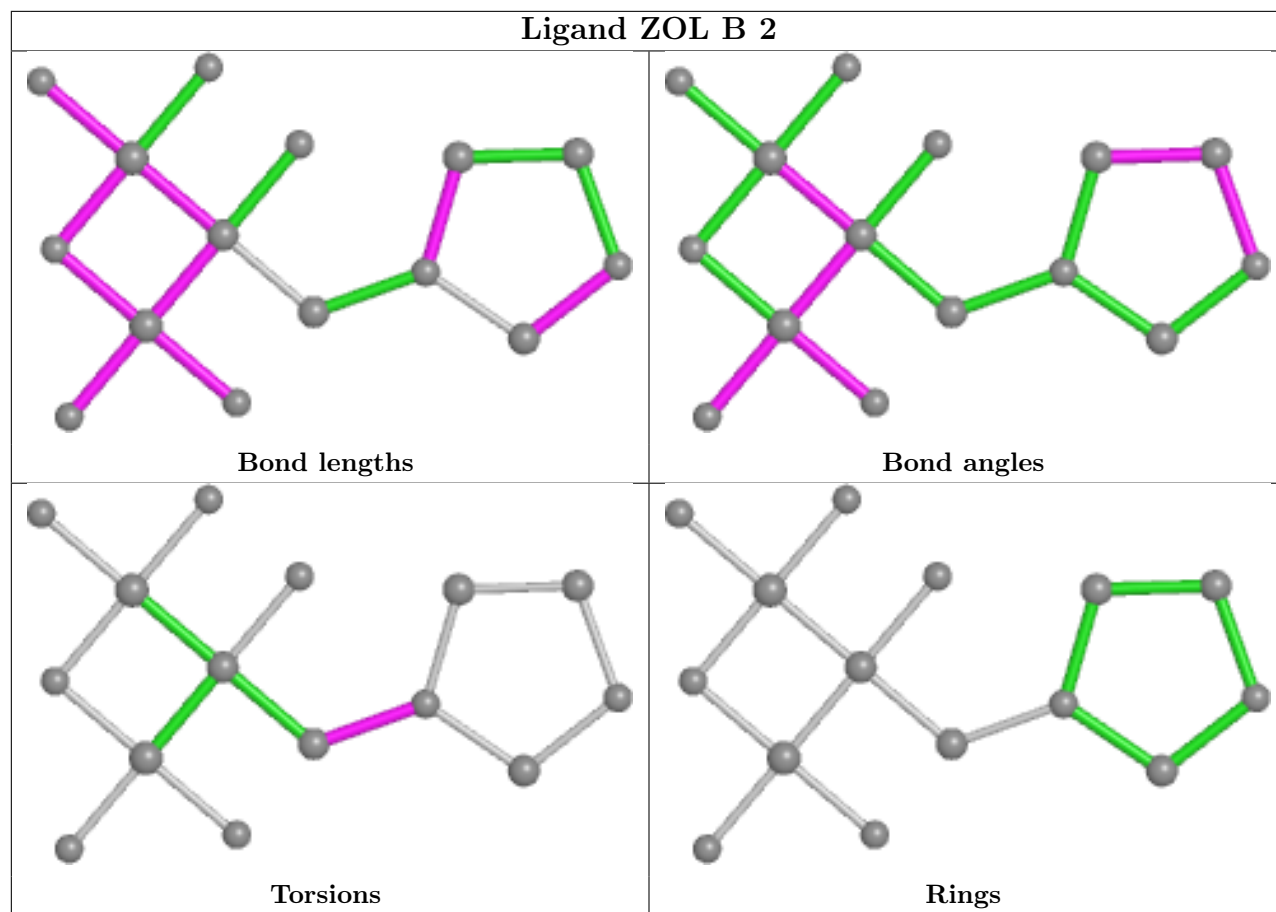
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	ZOL	3	0
3	B	2	ZOL	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 [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	A	335/368 (91%)	0.17	23 (6%) 16 18	24, 64, 113, 136	0
1	B	329/368 (89%)	0.04	16 (4%) 29 32	30, 59, 99, 157	0
All	All	664/736 (90%)	0.10	39 (5%) 22 24	24, 62, 107, 157	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1086	SER	5.2
1	B	2229	ILE	4.6
1	A	1311	LEU	4.2
1	B	2304	VAL	3.8
1	A	1217	TYR	3.5

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](#)

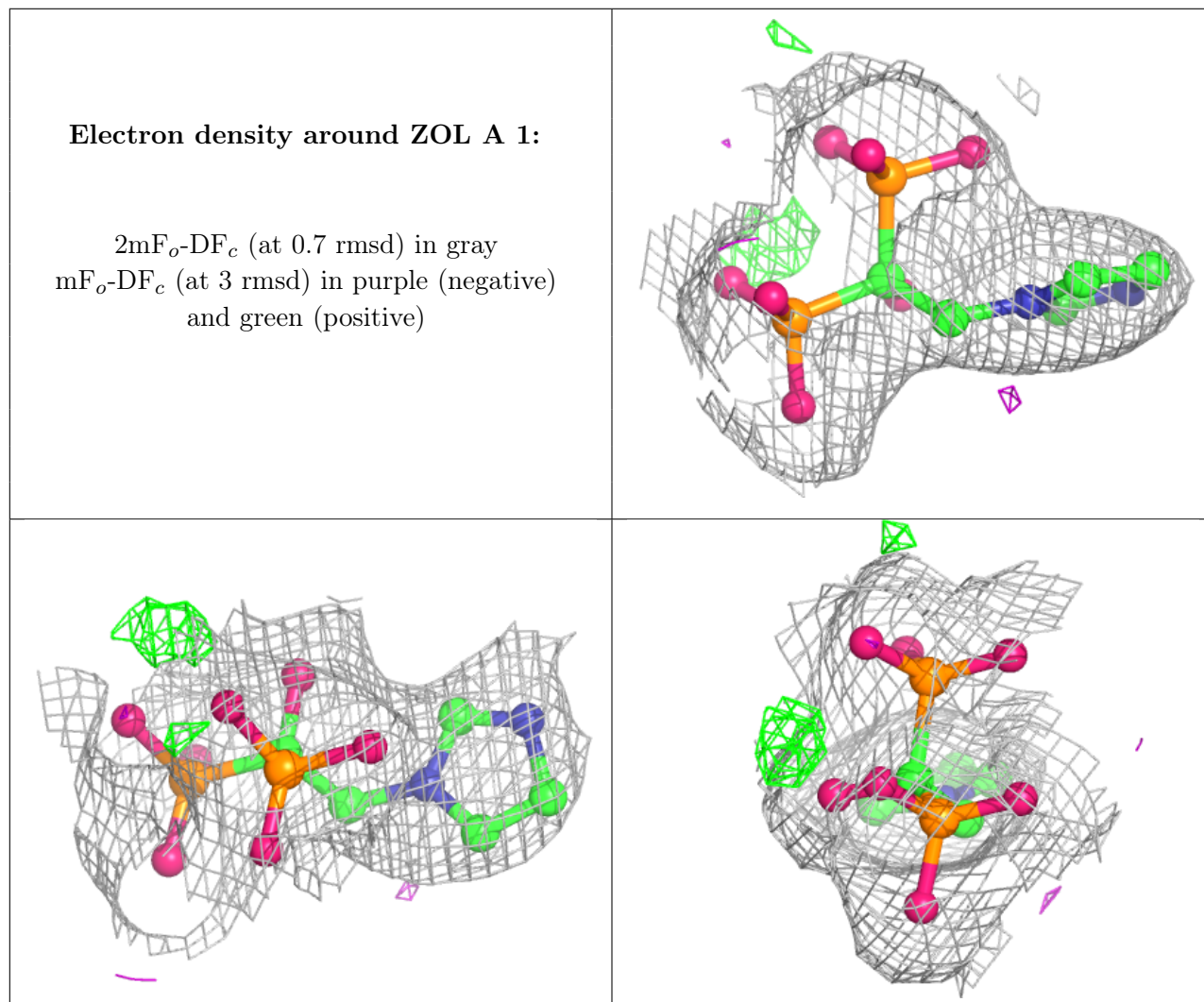
There are no monosaccharides in this entry.

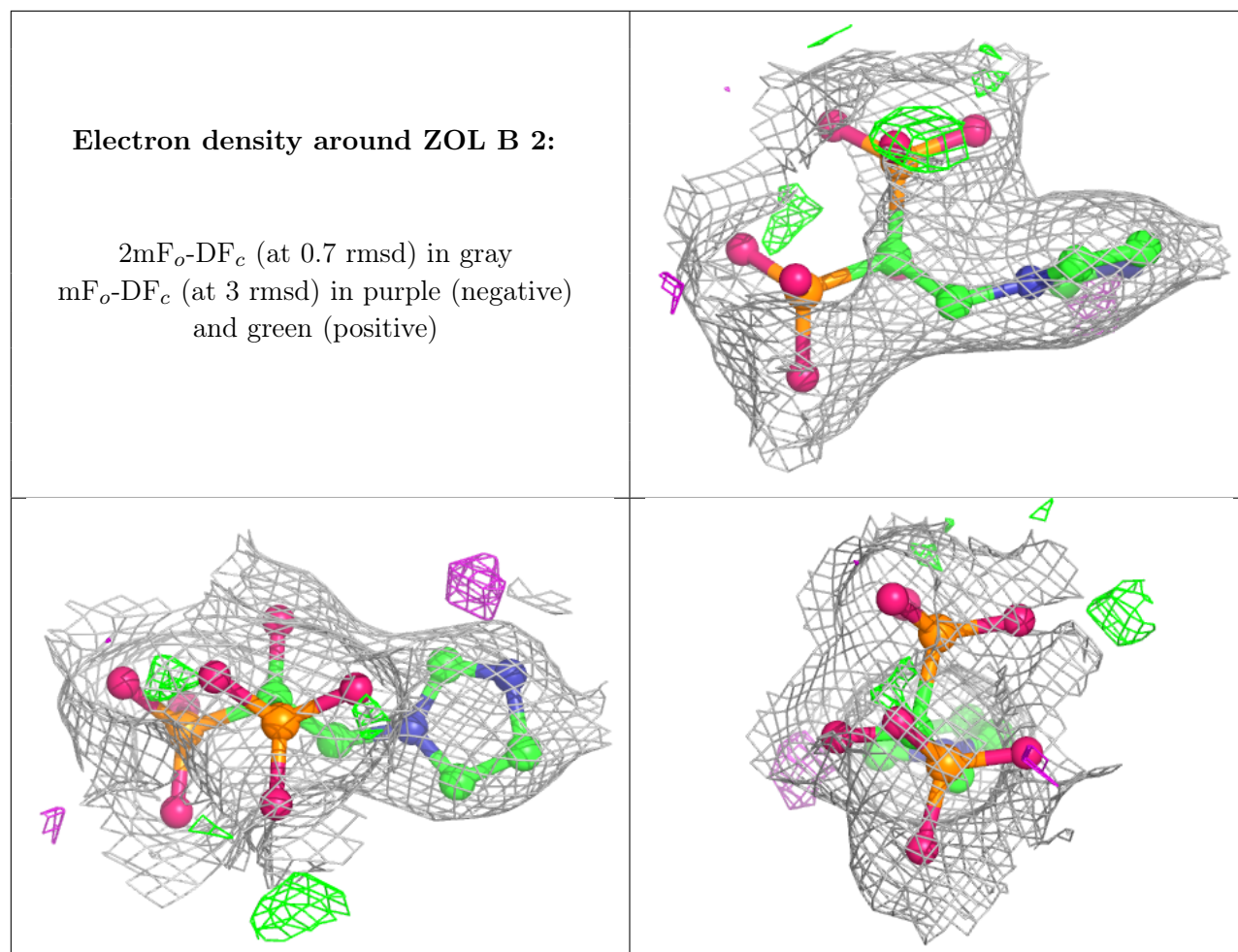
6.4 Ligands [i](#)

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
2	MG	A	5	1/1	0.82	0.06	30,30,30,30	0
2	MG	B	8	1/1	0.91	0.06	30,30,30,30	0
2	MG	B	7	1/1	0.95	0.14	33,33,33,33	0
2	MG	A	3	1/1	0.97	0.05	33,33,33,33	0
2	MG	B	6	1/1	0.97	0.12	33,33,33,33	0
3	ZOL	A	1	16/16	0.97	0.13	40,54,70,86	0
3	ZOL	B	2	16/16	0.98	0.19	40,53,65,66	0
2	MG	A	4	1/1	0.99	0.07	35,35,35,35	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.





6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.