



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2021 – 12:09 pm BST

PDB ID : 6YGU
Title : Crystal structure of the minimal Mtr4-Red1 complex (single chain) from *Chaetomium thermophilum*
Authors : Dobrev, N.; Ahmed, Y.L.; Sinning, I.
Deposited on : 2020-03-27
Resolution : 1.99 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

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 : 2.18
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) : 2.18

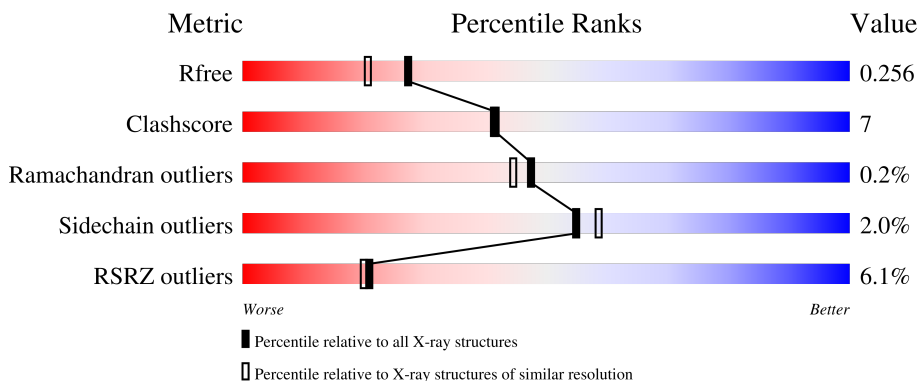
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	219	5% (Poor fit) 81% (0-1 outliers) 14% (2-3 outliers) . . (Not modelled)
1	C	219	8% (Poor fit) 81% (0-1 outliers) 17% (2-3 outliers) . (Not modelled)
2	B	86	3% (Poor fit) 65% (0-1 outliers) 12% (2-3 outliers) 23% (Not modelled)
2	D	86	3% (Poor fit) 67% (0-1 outliers) 7% (2-3 outliers) . (Not modelled) 24% (Not modelled)

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
3	ACT	A	901	-	-	X	-
4	EDO	A	905	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4711 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 ATP dependent RNA helicase (Dob1)-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	211	Total	C	N	O	S	0	2	0
			1702	1065	308	318	11			
1	C	215	Total	C	N	O	S	0	0	0
			1714	1070	311	321	12			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	653	MET	-	initiating methionine	UNP G0RZ64
A	866	GLY	-	expression tag	UNP G0RZ64
A	867	GLY	-	expression tag	UNP G0RZ64
A	868	SER	-	expression tag	UNP G0RZ64
A	869	GLY	-	expression tag	UNP G0RZ64
A	870	GLY	-	expression tag	UNP G0RZ64
A	871	SER	-	expression tag	UNP G0RZ64
C	653	MET	-	initiating methionine	UNP G0RZ64
C	866	GLY	-	expression tag	UNP G0RZ64
C	867	GLY	-	expression tag	UNP G0RZ64
C	868	SER	-	expression tag	UNP G0RZ64
C	869	GLY	-	expression tag	UNP G0RZ64
C	870	GLY	-	expression tag	UNP G0RZ64
C	871	SER	-	expression tag	UNP G0RZ64

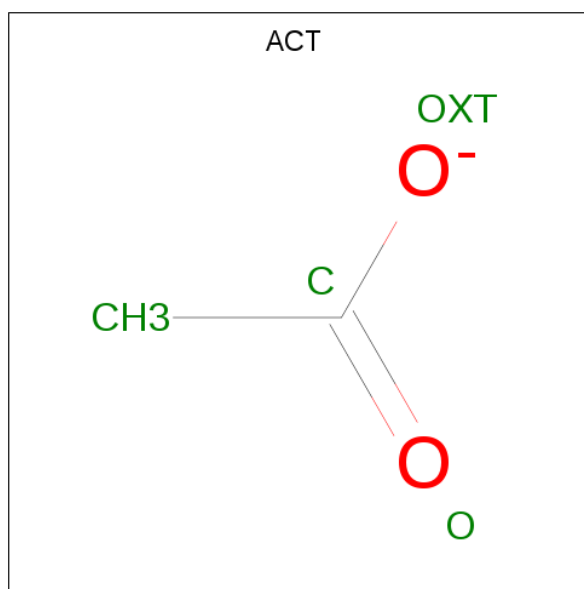
- Molecule 2 is a protein called Red1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	66	Total	C	N	O	S	0	0	0
			539	345	93	97	4			
2	D	65	Total	C	N	O	S	0	0	0
			534	342	92	96	4			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1081	ALA	-	insertion	UNP G0S1V1
B	1092	GLY	-	expression tag	UNP G0S1V1
B	1093	SER	-	expression tag	UNP G0S1V1
B	1094	HIS	-	expression tag	UNP G0S1V1
B	1095	HIS	-	expression tag	UNP G0S1V1
B	1096	HIS	-	expression tag	UNP G0S1V1
B	1097	HIS	-	expression tag	UNP G0S1V1
B	1098	HIS	-	expression tag	UNP G0S1V1
B	1099	HIS	-	expression tag	UNP G0S1V1
D	1081	ALA	-	insertion	UNP G0S1V1
D	1092	GLY	-	expression tag	UNP G0S1V1
D	1093	SER	-	expression tag	UNP G0S1V1
D	1094	HIS	-	expression tag	UNP G0S1V1
D	1095	HIS	-	expression tag	UNP G0S1V1
D	1096	HIS	-	expression tag	UNP G0S1V1
D	1097	HIS	-	expression tag	UNP G0S1V1
D	1098	HIS	-	expression tag	UNP G0S1V1
D	1099	HIS	-	expression tag	UNP G0S1V1

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	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	B	1	Total Zn 1 1	0	0
5	D	1	Total Zn 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	72	Total 72	O 72	0	0
6	B	35	Total 35	O 35	0	0
6	C	49	Total 49	O 49	0	0
6	D	24	Total 24	O 24	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.98Å 88.91Å 168.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.46 – 1.99 47.46 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.46-1.99) 100.0 (47.46-1.99)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.98Å)	Xtrriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.204 , 0.252 0.207 , 0.256	Depositor DCC
R_{free} test set	2395 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtrriage
Anisotropy	0.737	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4711	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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: ZN, EDO, 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	A	0.62	1/1742 (0.1%)	0.84	6/2358 (0.3%)
1	C	0.56	0/1751	0.67	2/2368 (0.1%)
2	B	0.62	0/558	0.69	0/756
2	D	0.81	2/553 (0.4%)	0.94	5/749 (0.7%)
All	All	0.63	3/4604 (0.1%)	0.78	13/6231 (0.2%)

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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1025	ARG	CG-CD	-9.20	1.28	1.51
2	D	1066	CYS	CB-SG	-7.99	1.68	1.82
1	A	678	VAL	CB-CG2	5.81	1.65	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	720	ARG	NE-CZ-NH2	14.50	127.55	120.30
2	D	1025	ARG	CA-CB-CG	-10.57	90.15	113.40
1	A	720	ARG	CG-CD-NE	-9.63	91.58	111.80
2	D	1025	ARG	NE-CZ-NH1	-8.79	115.91	120.30
2	D	1025	ARG	CG-CD-NE	-8.06	94.86	111.80
1	A	720	ARG	NE-CZ-NH1	-7.75	116.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	716	ARG	NE-CZ-NH1	6.00	123.30	120.30
2	D	1035	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	C	687	LYS	CA-CB-CG	5.79	126.13	113.40
2	D	1025	ARG	CB-CG-CD	5.78	126.62	111.60
1	C	717	ARG	CG-CD-NE	5.71	123.79	111.80
1	A	716	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	768	LYS	CB-CG-CD	5.52	125.96	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	719	GLU	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	1702	0	1697	25	0
1	C	1714	0	1704	24	0
2	B	539	0	499	7	2
2	D	534	0	494	7	0
3	A	4	0	3	3	0
3	B	4	0	3	0	0
4	A	24	0	36	6	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	72	0	0	5	0
6	B	35	0	0	3	1
6	C	49	0	0	2	0
6	D	24	0	0	0	0
All	All	4711	0	4448	63	2

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 7.

All (63) 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:A:814:LYS:NZ	6:A:1001:HOH:O	1.75	1.19
1:A:707:TRP:H	3:A:901:ACT:H2	1.17	1.05
2:D:1025:ARG:NH2	2:D:1046:TYR:O	2.14	0.80
1:C:795:PRO:HG2	1:C:811:ARG:HH12	1.46	0.80
1:A:814:LYS:HD2	6:A:1060:HOH:O	1.83	0.78
2:D:1025:ARG:HH12	2:D:1046:TYR:C	1.87	0.78
1:A:797:LYS:HG2	1:A:797:LYS:O	1.85	0.75
1:C:840:ASP:OD1	6:C:1001:HOH:O	2.08	0.71
1:C:753:LYS:HD3	1:C:756:GLN:NE2	2.08	0.69
1:A:807:GLU:OE1	1:A:810:ARG:NH2	2.28	0.66
1:A:827:ILE:HG12	4:A:905:EDO:H21	1.77	0.66
1:C:814:LYS:NZ	6:C:1002:HOH:O	2.28	0.66
1:C:753:LYS:HZ3	1:C:759:PRO:HA	1.63	0.63
1:C:795:PRO:HG2	1:C:811:ARG:NH1	2.15	0.61
1:A:716:ARG:HG2	1:A:727:TRP:CH2	2.37	0.60
1:C:801:GLY:HA3	1:C:805:ASP:HB2	1.83	0.59
1:C:716:ARG:HG2	1:C:727:TRP:CH2	2.37	0.59
1:A:707:TRP:N	3:A:901:ACT:H2	2.02	0.58
1:A:716:ARG:HD2	6:A:1016:HOH:O	2.04	0.57
1:A:820:GLN:OE1	4:A:905:EDO:O1	2.18	0.56
1:A:827:ILE:H	4:A:905:EDO:C2	2.18	0.56
2:D:1019:SER:O	2:D:1022:ARG:NH1	2.37	0.55
2:B:1035:ARG:NE	6:B:1201:HOH:O	2.06	0.55
1:C:654:ASP:OD1	1:C:655:GLU:N	2.31	0.55
1:C:773:ARG:NE	1:C:775:GLU:OE2	2.34	0.54
1:A:789:GLN:HG2	1:A:830:MET:HG2	1.90	0.54
1:C:795:PRO:CG	1:C:811:ARG:HH12	2.19	0.54
1:C:814:LYS:HD2	1:C:814:LYS:O	2.07	0.54
1:C:698:VAL:HG22	1:C:785:HIS:CG	2.43	0.53
2:B:1065:GLN:HB3	6:B:1229:HOH:O	2.09	0.53
2:B:1044:LEU:HD23	2:B:1080:PRO:HD3	1.90	0.53
2:B:1035:ARG:NH2	6:B:1201:HOH:O	2.42	0.52
2:D:1025:ARG:NH2	2:D:1028:ARG:HD3	2.23	0.52
1:A:717:ARG:HD2	4:A:906:EDO:H11	1.90	0.52
2:B:1058:PRO:O	2:B:1062:GLU:HB2	2.10	0.52
1:A:796:ASP:OD1	1:A:798:LYS:HG2	2.09	0.51
1:A:820:GLN:OE1	3:A:901:ACT:H3	2.12	0.50
1:A:665:ARG:NH2	1:A:669:ASP:OD1	2.45	0.50
1:C:716:ARG:HG2	1:C:727:TRP:CZ3	2.46	0.50
1:C:743:SER:OG	1:C:770:ASP:OD1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:ARG:NH2	6:A:1002:HOH:O	2.14	0.48
1:A:794:VAL:H	4:A:904:EDO:H12	1.77	0.48
1:C:698:VAL:HG22	1:C:785:HIS:ND1	2.29	0.47
1:C:742:SER:HA	1:C:765:VAL:HG22	1.97	0.47
1:C:758:ILE:HG13	1:C:759:PRO:HD2	1.97	0.47
1:C:792:LEU:HD21	1:C:819:VAL:HG21	1.96	0.46
1:C:753:LYS:NZ	1:C:760:ALA:H	2.14	0.46
1:C:757:CYS:HB2	1:C:783:CYS:SG	2.56	0.46
1:A:716:ARG:HG2	1:A:727:TRP:CZ3	2.51	0.46
2:B:1031:PRO:HB3	1:C:849:LYS:HG2	1.99	0.45
1:A:796:ASP:OD2	1:A:798:LYS:HE3	2.17	0.45
1:C:774:TRP:CE2	1:C:813:GLY:HA3	2.53	0.43
2:D:1025:ARG:HH11	2:D:1025:ARG:HD2	1.53	0.43
1:A:716:ARG:HB2	1:A:734:VAL:HG23	2.01	0.43
1:C:753:LYS:HZ3	1:C:760:ALA:H	1.67	0.42
2:D:1025:ARG:NH1	2:D:1046:TYR:C	2.66	0.42
2:B:1066:CYS:HB3	2:B:1070:CYS:HB2	2.02	0.41
2:D:1025:ARG:NH1	2:D:1046:TYR:HA	2.34	0.41
1:A:695:MET:HE2	1:A:697:VAL:HG22	2.02	0.41
1:A:796:ASP:O	1:A:799:SER:OG	2.32	0.40
1:A:803:MET:O	1:A:809:ARG:HD3	2.21	0.40
1:A:795:PRO:HG2	1:A:808:THR:HG21	2.03	0.40
4:A:905:EDO:H22	6:A:1045:HOH:O	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1066:CYS:SG	6:B:1201:HOH:O[4_556]	2.15	0.05
2:B:1035:ARG:NH2	2:B:1064:THR:O[4_456]	2.17	0.03

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	211/219 (96%)	204 (97%)	6 (3%)	1 (0%)	29	23
1	C	213/219 (97%)	208 (98%)	5 (2%)	0	100	100
2	B	64/86 (74%)	64 (100%)	0	0	100	100
2	D	63/86 (73%)	63 (100%)	0	0	100	100
All	All	551/610 (90%)	539 (98%)	11 (2%)	1 (0%)	47	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	720	ARG

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	196/198 (99%)	191 (97%)	5 (3%)	46	48
1	C	196/198 (99%)	190 (97%)	6 (3%)	40	40
2	B	59/77 (77%)	59 (100%)	0	100	100
2	D	59/77 (77%)	59 (100%)	0	100	100
All	All	510/550 (93%)	499 (98%)	11 (2%)	55	55

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	802	SER
1	A	819[A]	VAL
1	A	819[B]	VAL
1	A	846	LEU
1	A	848	ARG
1	C	665	ARG
1	C	713	PHE
1	C	721	ASN

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Mol	Chain	Res	Type
1	C	722	ASN
1	C	768	LYS
1	C	796	ASP

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

Mol	Chain	Res	Type
1	C	722	ASN
1	C	756	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 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	A	902	-	3,3,3	0.53	0	2,2,2	0.30	0
3	ACT	A	901	-	1,3,3	11.38	1 (100%)	0,3,3	0.00	-
4	EDO	C	901	-	3,3,3	0.52	0	2,2,2	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	904	-	3,3,3	0.48	0	2,2,2	0.39	0
4	EDO	A	905	-	3,3,3	0.38	0	2,2,2	0.32	0
4	EDO	B	1102	-	3,3,3	0.62	0	2,2,2	0.30	0
4	EDO	A	906	-	3,3,3	0.55	0	2,2,2	0.10	0
3	ACT	B	1101	-	1,3,3	7.60	1 (100%)	0,3,3	0.00	-
4	EDO	A	907	-	3,3,3	0.63	0	2,2,2	0.16	0
4	EDO	A	903	-	3,3,3	0.52	0	2,2,2	0.26	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	A	902	-	-	0/1/1/1	-
4	EDO	C	901	-	-	0/1/1/1	-
4	EDO	A	905	-	-	1/1/1/1	-
4	EDO	A	904	-	-	0/1/1/1	-
4	EDO	B	1102	-	-	0/1/1/1	-
4	EDO	A	906	-	-	1/1/1/1	-
4	EDO	A	907	-	-	1/1/1/1	-
4	EDO	A	903	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	ACT	CH3-C	11.38	1.63	1.48
3	B	1101	ACT	CH3-C	7.60	1.58	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	906	EDO	O1-C1-C2-O2
4	A	905	EDO	O1-C1-C2-O2
4	A	907	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	ACT	3	0
4	A	904	EDO	1	0
4	A	905	EDO	4	0
4	A	906	EDO	1	0

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, 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	211/219 (96%)	0.54	10 (4%) 31 30	29, 49, 92, 118	0
1	C	215/219 (98%)	0.59	18 (8%) 11 10	34, 53, 104, 117	0
2	B	66/86 (76%)	0.49	3 (4%) 33 32	33, 43, 67, 104	0
2	D	65/86 (75%)	0.34	3 (4%) 32 31	39, 51, 69, 78	0
All	All	557/610 (91%)	0.53	34 (6%) 21 20	29, 50, 94, 118	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	720	ARG	6.8
1	C	800	GLY	5.2
1	C	801	GLY	5.2
2	B	1081	ALA	5.0
1	C	756	GLN	4.9
1	C	796	ASP	4.3
2	D	1025	ARG	4.3
1	A	797	LYS	4.0
1	C	654	ASP	4.0
1	A	799	SER	3.7
2	B	1082	ALA	3.5
2	D	1035	ARG	3.4
1	A	798	LYS	3.4
1	C	724	ASN	3.2
1	C	769	ASN	3.2
1	C	717	ARG	3.1
1	C	752	LEU	3.1
1	C	720	ARG	3.1
2	D	1017	TYR	3.0
1	C	753	LYS	3.0
1	C	721	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	653	MET	2.9
1	C	656	ALA	2.8
1	A	656	ALA	2.7
1	C	767	GLN	2.7
1	A	768	LYS	2.5
1	C	798	LYS	2.4
1	A	657	LEU	2.4
1	C	723	PRO	2.4
1	A	767	GLN	2.3
1	C	754	ASP	2.2
2	B	1068	SER	2.1
1	A	654	ASP	2.1
1	A	717	ARG	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, 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.

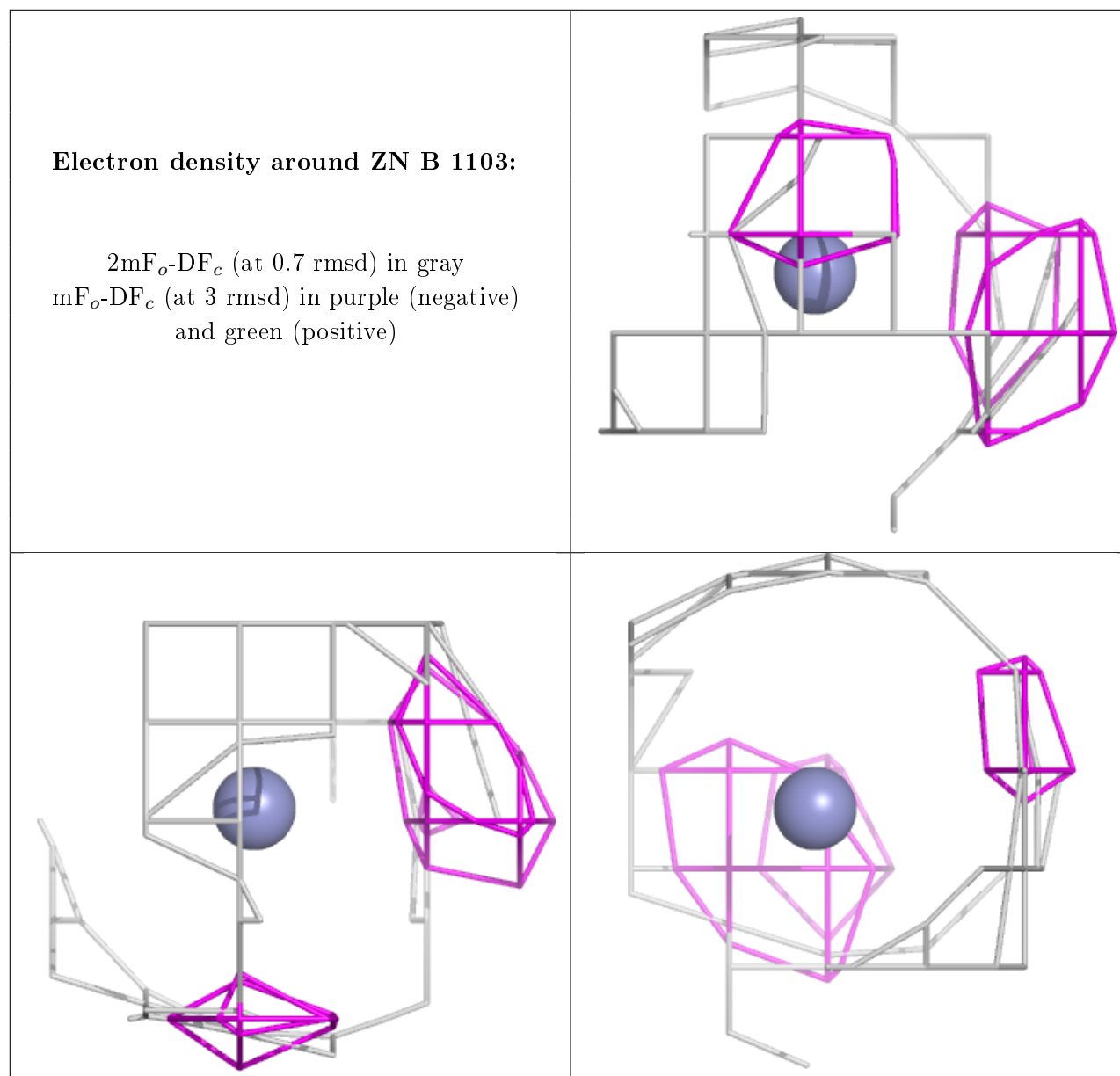
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	A	904	4/4	0.57	0.34	86,87,89,90	0
3	ACT	A	901	4/4	0.59	0.18	44,57,61,64	0
4	EDO	B	1102	4/4	0.70	0.16	55,62,68,72	0
4	EDO	C	901	4/4	0.78	0.19	74,77,77,78	0
4	EDO	A	907	4/4	0.79	0.14	63,65,67,69	0
4	EDO	A	902	4/4	0.79	0.19	70,71,74,80	0
3	ACT	B	1101	4/4	0.79	0.20	65,67,67,72	0
4	EDO	A	906	4/4	0.81	0.40	63,66,71,75	0
4	EDO	A	905	4/4	0.84	0.31	57,58,60,62	0
4	EDO	A	903	4/4	0.87	0.15	68,72,77,83	0

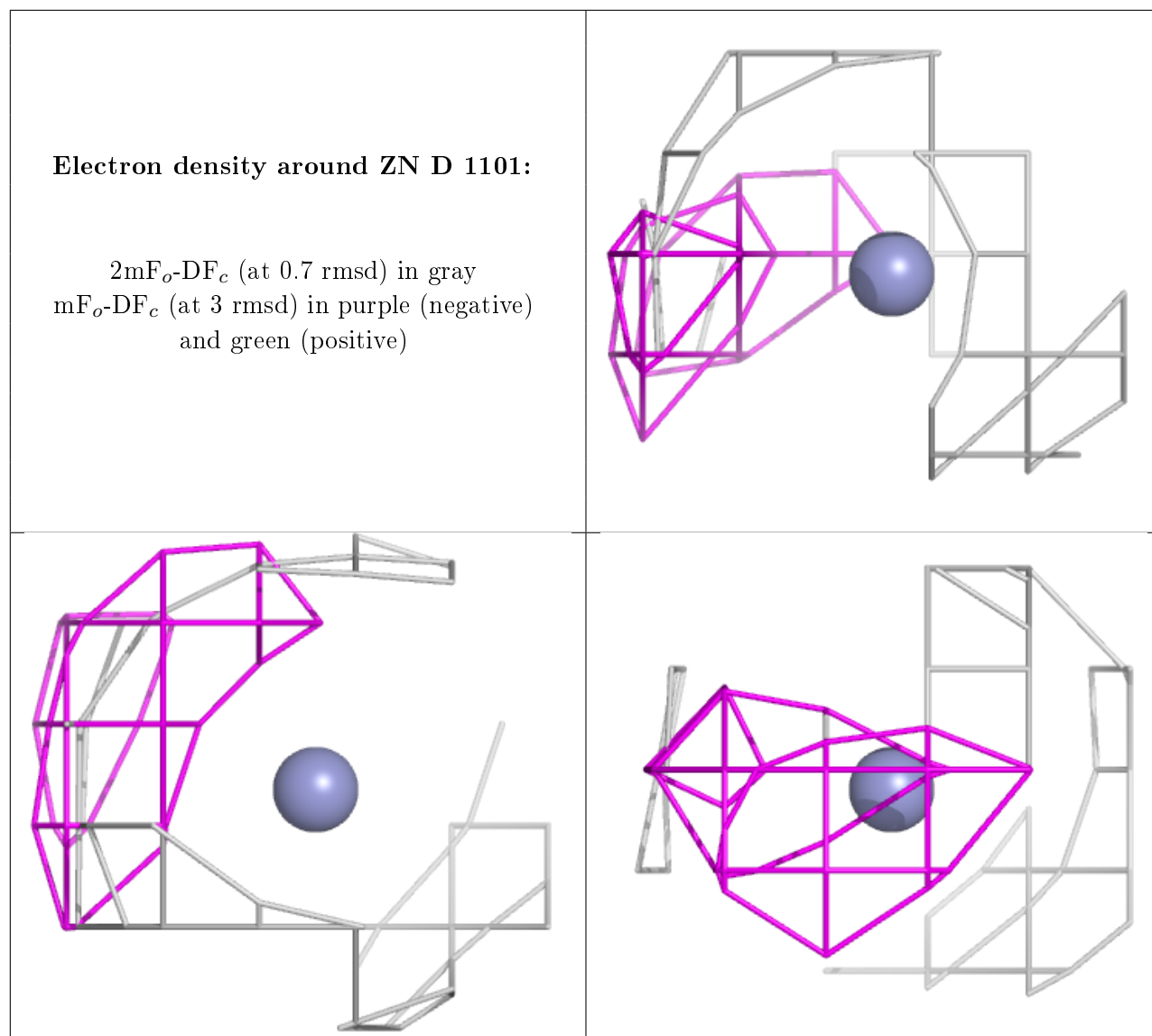
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	ZN	B	1103	1/1	0.99	0.08	50,50,50,50	0
5	ZN	D	1101	1/1	0.99	0.09	48,48,48,48	0

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.