



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2022 – 10:59 pm BST

PDB ID : 7Z00
Title : Crystal structure of Vibrio alkaline phosphatase in 1.0 M KBr
Authors : Markusson, S.; Hjorleifsson, J.G.; Kursula, P.; Asgeirsson, B.
Deposited on : 2022-02-21
Resolution : 2.60 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 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

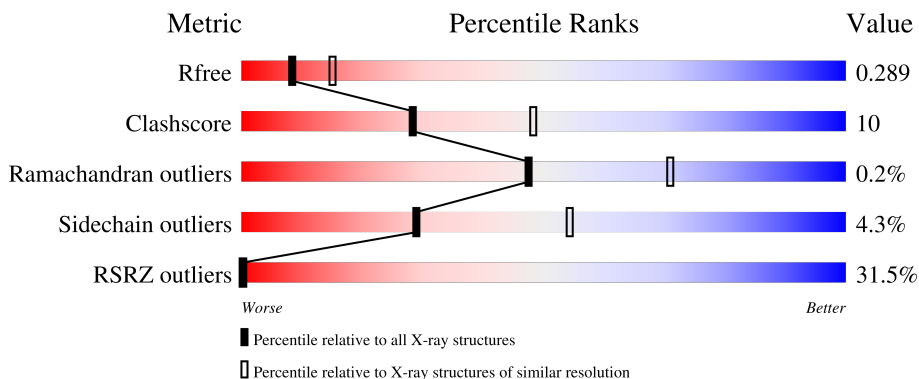
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	B	531	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7745 atoms, of which 3818 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 Alkaline phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	B	502	7732	2457	3818	668	776	13	0	7	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	503	SER	-	expression tag	UNP Q93P54
B	504	ALA	-	expression tag	UNP Q93P54
B	505	TRP	-	expression tag	UNP Q93P54
B	506	SER	-	expression tag	UNP Q93P54
B	507	HIS	-	expression tag	UNP Q93P54
B	508	PRO	-	expression tag	UNP Q93P54
B	509	GLN	-	expression tag	UNP Q93P54
B	510	PHE	-	expression tag	UNP Q93P54
B	511	GLU	-	expression tag	UNP Q93P54
B	512	LYS	-	expression tag	UNP Q93P54

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is BROMIDE ION (three-letter code: BR) (formula: Br) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Br	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Mg 2 2	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O P 5 4 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	3	Total O 3 3	0	0

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: Alkaline phosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	99.25Å 118.12Å 84.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.39 – 2.60 48.39 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.39-2.60) 88.0 (48.39-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.64 (at 2.61Å)	Xtriage
Refinement program	PHENIX dev_3958	Depositor
R, R_{free}	0.242 , 0.291 0.242 , 0.289	Depositor DCC
R_{free} test set	1557 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	61.4	Xtriage
Anisotropy	0.552	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7745	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% 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: PO4, MG, BR, ZN

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	B	0.37	1/4031 (0.0%)	0.58	5/5449 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	172	LYS	CE-NZ	8.25	1.69	1.49

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	LYS	CD-CE-NZ	-17.92	70.49	111.70
1	B	172	LYS	CB-CG-CD	7.25	130.45	111.60
1	B	332	LYS	CD-CE-NZ	-7.19	95.16	111.70
1	B	332	LYS	CB-CG-CD	-6.19	95.50	111.60
1	B	42	TYR	CA-CB-CG	-5.64	102.69	113.40

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	B	3914	3818	3769	76	3
2	B	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	B	2	0	0	0	0
5	B	5	0	0	0	0
6	B	3	0	0	4	0
All	All	3927	3818	3769	76	3

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 10.

All (76) 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:172:LYS:CE	1:B:172:LYS:NZ	1.69	1.53
1:B:172:LYS:NZ	1:B:172:LYS:CD	1.85	1.37
1:B:172:LYS:NZ	1:B:172:LYS:HD3	1.86	0.88
1:B:172:LYS:NZ	1:B:172:LYS:HD2	1.92	0.85
1:B:172:LYS:CD	1:B:172:LYS:HZ2	1.84	0.84
1:B:401:THR:OG1	6:B:701:HOH:O	1.86	0.82
1:B:389:ALA:O	1:B:393:ASN:ND2	2.14	0.81
1:B:172:LYS:HD2	1:B:172:LYS:HZ2	1.45	0.78
1:B:105:ALA:HB1	1:B:256:LEU:HD23	1.68	0.76
1:B:430:PRO:HB3	1:B:447:LEU:HD11	1.74	0.69
1:B:165:GLU:OE1	1:B:165:GLU:N	2.21	0.69
1:B:152:LEU:HD23	1:B:178:VAL:HG11	1.76	0.68
1:B:404:GLN:HG3	6:B:701:HOH:O	1.93	0.68
1:B:172:LYS:CD	1:B:172:LYS:HZ3	2.03	0.68
1:B:239:GLU:HA	1:B:239:GLU:OE1	1.94	0.67
1:B:190:LEU:HD22	1:B:193:GLU:OE1	1.96	0.66
1:B:317:GLU:OE1	1:B:466:THR:OG1	2.16	0.64
1:B:202:ALA:HA	1:B:207:MET:HE2	1.78	0.63
1:B:172:LYS:HD3	1:B:172:LYS:HZ3	1.58	0.61
1:B:456:GLN:HG3	1:B:458:ILE:HD12	1.84	0.59
1:B:98:LYS:HE2	1:B:498:LYS:HE3	1.85	0.58
1:B:253:LEU:O	1:B:257:SER:OG	2.20	0.57
1:B:105:ALA:CB	1:B:256:LEU:HD23	2.38	0.53
1:B:9:MET:HE2	1:B:295:ILE:HG13	1.89	0.53
1:B:105:ALA:HB1	1:B:256:LEU:CD2	2.38	0.52
1:B:372:ILE:O	1:B:376:GLN:HG3	2.10	0.52
1:B:70:THR:O	1:B:74:THR:HG23	2.09	0.52
1:B:12:ASP:O	1:B:273:ASP:N	2.43	0.51
1:B:114:LEU:HD12	1:B:114:LEU:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ALA:HB2	1:B:122:PHE:CE1	2.48	0.48
1:B:173:LEU:HD12	1:B:173:LEU:O	2.14	0.48
1:B:430:PRO:CB	1:B:447:LEU:HD11	2.43	0.47
1:B:156:ILE:HG23	1:B:191:LEU:HD11	1.97	0.47
1:B:107:GLY:HA3	1:B:256:LEU:HD11	1.97	0.47
1:B:433:ASN:O	6:B:703:HOH:O	2.20	0.47
1:B:93:GLU:OE1	1:B:98:LYS:HD3	2.14	0.47
1:B:408:VAL:O	1:B:444:ARG:NH1	2.47	0.46
1:B:138:ASP:O	1:B:142:THR:HG23	2.14	0.46
1:B:231:TYR:CZ	1:B:235:LYS:HE2	2.51	0.46
1:B:112:THR:OG1	1:B:113:ARG:N	2.49	0.45
1:B:43:GLN:HG3	1:B:299:TYR:OH	2.16	0.45
1:B:403:GLU:OE2	1:B:406:LYS:HD2	2.16	0.45
1:B:122:PHE:CE2	1:B:266:MET:HG3	2.52	0.45
1:B:231:TYR:OH	1:B:235:LYS:HE2	2.17	0.45
1:B:34:TYR:C	1:B:35:LYS:HG3	2.37	0.44
1:B:152:LEU:CD2	1:B:178:VAL:HG11	2.45	0.44
1:B:456:GLN:HG3	1:B:458:ILE:HB	1.98	0.44
1:B:332:LYS:HA	1:B:332:LYS:HD2	1.54	0.44
1:B:264:PHE:CD1	1:B:264:PHE:C	2.91	0.44
1:B:196:LYS:O	6:B:702:HOH:O	2.20	0.44
1:B:123:ALA:O	1:B:142:THR:HG21	2.17	0.43
1:B:57:PRO:HG2	1:B:60:ALA:HB3	1.99	0.43
1:B:34:TYR:C	1:B:35:LYS:CG	2.86	0.43
1:B:93:GLU:O	1:B:498:LYS:NZ	2.51	0.43
1:B:211:ALA:HB1	1:B:216:LEU:HD13	2.01	0.43
1:B:414:ASN:OD1	1:B:416:TYR:N	2.51	0.43
1:B:138:ASP:N	1:B:138:ASP:OD1	2.52	0.43
1:B:256:LEU:HD22	1:B:263:PHE:HB2	1.99	0.42
1:B:278:SER:OG	1:B:443:ASP:OD2	2.13	0.42
1:B:266:MET:HE3	1:B:266:MET:C	2.40	0.42
1:B:477:PRO:O	1:B:481:ILE:HG23	2.18	0.42
1:B:354:ALA:HB3	1:B:356:ASP:OD1	2.18	0.42
1:B:9:MET:HE1	1:B:295:ILE:HA	2.01	0.42
1:B:388:LEU:HD12	1:B:388:LEU:O	2.19	0.42
1:B:98:LYS:CE	1:B:498:LYS:HE3	2.50	0.42
1:B:489:HIS:ND1	1:B:490:HIS:N	2.69	0.41
1:B:9:MET:CE	1:B:295:ILE:HG13	2.49	0.41
1:B:153:ARG:HB3	1:B:222:TYR:CD1	2.55	0.41
1:B:264:PHE:CD1	1:B:265:LEU:N	2.89	0.41
1:B:166:THR:O	1:B:170:LEU:HD13	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:THR:HB	1:B:119:PRO:HD3	2.02	0.41
1:B:204:ASN:OD1	1:B:207:MET:HG3	2.20	0.41
1:B:385:PRO:HG2	1:B:406:LYS:HZ3	1.86	0.41
1:B:203:PHE:HD1	1:B:207:MET:CE	2.35	0.40
1:B:260:GLU:OE1	1:B:260:GLU:HA	2.21	0.40

All (3) 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)
1:B:2:GLU:OE2	1:B:163:LYS:NZ[8_545]	2.03	0.17
1:B:239:GLU:OE2	1:B:420:GLN:HE22[6_445]	1.43	0.17
1:B:239:GLU:OE2	1:B:420:GLN:NE2[6_445]	2.19	0.01

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	B	507/531 (96%)	483 (95%)	23 (4%)	1 (0%)	47 71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	477	PRO

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	B	422/443 (95%)	404 (96%)	18 (4%)	29 54

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2	GLU
1	B	23	GLU
1	B	78	SER
1	B	138	ASP
1	B	163	LYS
1	B	209	ASP
1	B	212	LYS
1	B	234	LYS
1	B	259	ASP
1	B	303	LYS
1	B	304	ASP
1	B	320	SER
1	B	376	GLN
1	B	379	ASP
1	B	394	LYS
1	B	450	ARG
1	B	479	GLU
1	B	490	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	366	GLN
1	B	420	GLN
1	B	500	GLN

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 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	$\# Z > 2$
5	PO4	B	606	2	4,4,4	0.88	0	6,6,6	0.50	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	B	502/531 (94%)	1.68	158 (31%) 0 0	59, 78, 100, 121	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	424[A]	LEU	14.9
1	B	373	SER	10.7
1	B	260	GLU	10.4
1	B	377	LYS	9.3
1	B	156	ILE	8.4
1	B	383	GLN	8.2
1	B	418	LEU	8.1
1	B	140	LEU	7.7
1	B	420	GLN	7.6
1	B	155	TRP	7.3
1	B	123	ALA	7.3
1	B	423	TYR	7.3
1	B	369	TYR	7.1
1	B	209	ASP	6.8
1	B	23	GLU	6.6
1	B	139	MET	6.5
1	B	343	ASP	6.1
1	B	218	GLY	6.1
1	B	379	ASP	6.1
1	B	146	VAL	6.0
1	B	106	THR	6.0
1	B	179	TYR	5.7
1	B	147	MET	5.7
1	B	214	ASP	5.5
1	B	358	LEU	5.3
1	B	370	GLY	5.3
1	B	30	PRO	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	314	ALA	5.2
1	B	171	GLU	5.2
1	B	380	LYS	5.1
1	B	416	TYR	5.1
1	B	176	GLY	5.0
1	B	299	TYR	4.9
1	B	191	LEU	4.9
1	B	440	PRO	4.7
1	B	201	LEU	4.6
1	B	142	THR	4.6
1	B	177	ASP	4.5
1	B	421	HIS	4.5
1	B	378	LEU	4.5
1	B	419	ALA	4.5
1	B	359	ASP	4.5
1	B	161	ASN	4.4
1	B	137	SER	4.4
1	B	443	ASP	4.3
1	B	217	LEU	4.2
1	B	255	ILE	4.2
1	B	153	ARG	4.2
1	B	355	PHE	4.2
1	B	427	GLU	4.1
1	B	22	LEU	4.1
1	B	444	ARG	4.1
1	B	148	LEU	4.0
1	B	438	PHE	3.9
1	B	14	MET	3.9
1	B	335	LYS	3.9
1	B	7	ILE	3.9
1	B	342	ALA	3.8
1	B	425	SER	3.8
1	B	417	ARG	3.8
1	B	395	ASN	3.8
1	B	319	GLY	3.7
1	B	354	ALA	3.7
1	B	391	ILE	3.7
1	B	222	TYR	3.6
1	B	381	SER	3.6
1	B	183	LYS	3.5
1	B	442	ASN	3.5
1	B	174	THR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	141	ALA	3.5
1	B	198	GLY	3.5
1	B	285	LEU	3.5
1	B	64	ASP	3.4
1	B	42	TYR	3.4
1	B	375	PHE	3.3
1	B	238	GLY	3.3
1	B	203	PHE	3.3
1	B	98	LYS	3.2
1	B	292	ASP	3.2
1	B	482	LEU	3.2
1	B	97	GLU	3.2
1	B	55	THR	3.2
1	B	348	PRO	3.2
1	B	428	GLU	3.1
1	B	484	VAL	3.1
1	B	356	ASP	3.1
1	B	145	ASP	3.1
1	B	237	SER	3.1
1	B	1	ALA	3.0
1	B	387	LYS	3.0
1	B	331	PRO	3.0
1	B	152	LEU	3.0
1	B	272	ILE	3.0
1	B	181	LYS	3.0
1	B	306	GLU	3.0
1	B	323	PHE	3.0
1	B	54	LEU	3.0
1	B	473	PHE	3.0
1	B	275	ALA	2.9
1	B	470	VAL	2.9
1	B	313	THR	2.8
1	B	479	GLU	2.8
1	B	368	TYR	2.8
1	B	65	SER	2.8
1	B	190	LEU	2.7
1	B	295	ILE	2.7
1	B	471	ASN	2.7
1	B	327	SER	2.7
1	B	454	THR	2.7
1	B	81	GLU	2.6
1	B	67	CYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	130	SER	2.6
1	B	339	GLU	2.6
1	B	131	LEU	2.6
1	B	185	LYS	2.6
1	B	288	LEU	2.6
1	B	107	GLY	2.5
1	B	219	LEU	2.5
1	B	96	LEU	2.5
1	B	297	THR	2.5
1	B	111	ASP	2.5
1	B	317	GLU	2.4
1	B	194	ALA	2.4
1	B	458	ILE	2.4
1	B	6	VAL	2.4
1	B	426	ALA	2.4
1	B	21	LEU	2.4
1	B	100	LYS	2.4
1	B	24	THR	2.4
1	B	208	LEU	2.4
1	B	336	ARG	2.4
1	B	39	THR	2.4
1	B	372	ILE	2.4
1	B	487	ILE	2.3
1	B	501	VAL	2.3
1	B	447	LEU	2.3
1	B	393	ASN	2.3
1	B	135	ILE	2.3
1	B	328	ASN	2.3
1	B	441	TYR	2.3
1	B	277	HIS	2.3
1	B	330	LEU	2.3
1	B	271	GLN	2.2
1	B	352	PHE	2.2
1	B	132	GLU	2.2
1	B	334	GLN	2.2
1	B	40	ALA	2.2
1	B	463	GLY	2.2
1	B	251	LYS	2.2
1	B	27	ASN	2.1
1	B	465	HIS	2.1
1	B	108	LEU	2.1
1	B	345	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	88[A]	GLN	2.1
1	B	270	GLY	2.1
1	B	291	PHE	2.1
1	B	376	GLN	2.0
1	B	210	ASP	2.0

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](#)

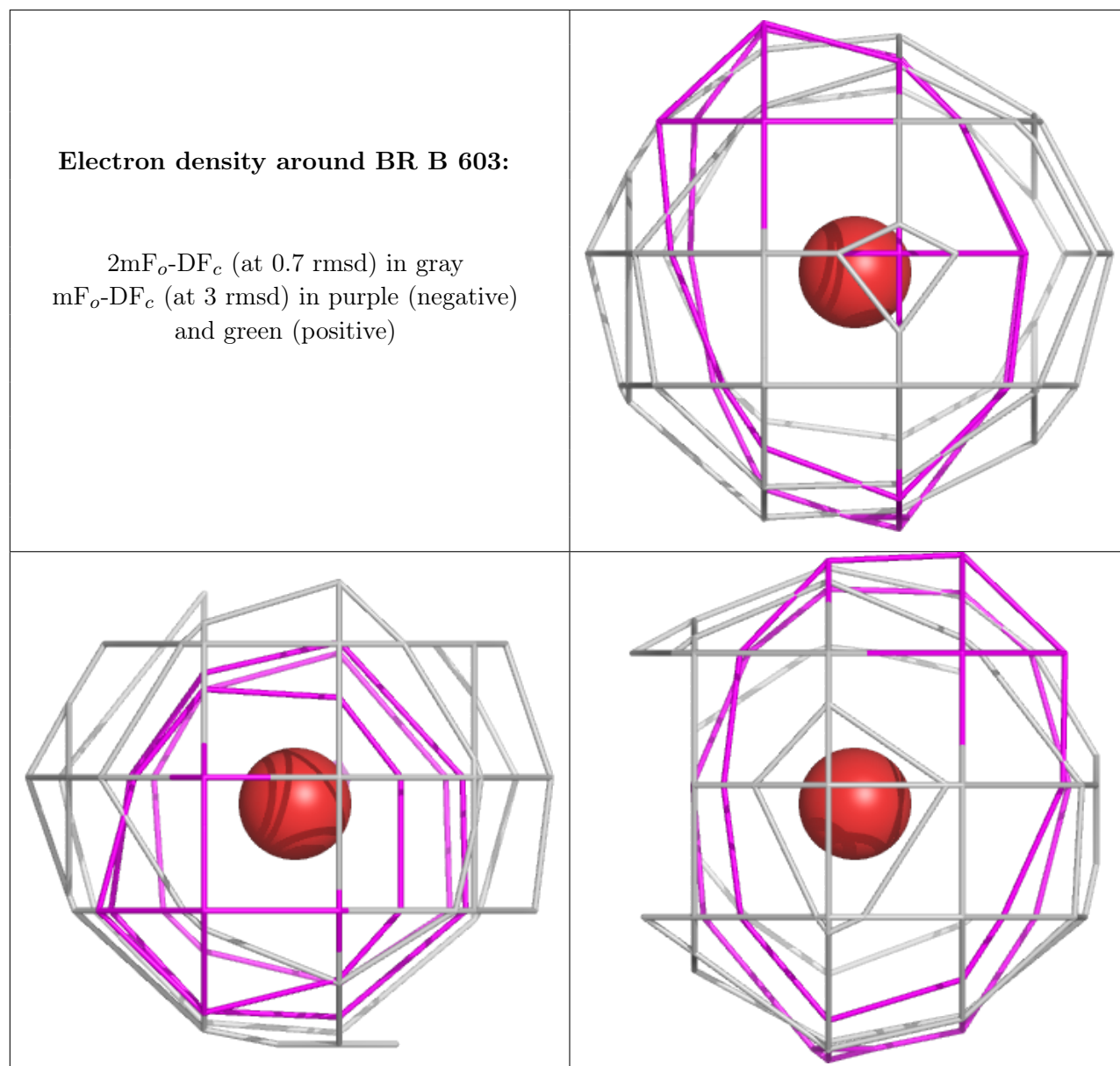
There are no monosaccharides in this entry.

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(Å ²)	Q<0.9
4	MG	B	605	1/1	0.69	0.20	73,73,73,73	0
2	ZN	B	601	1/1	0.78	0.11	67,67,67,67	0
5	PO4	B	606	5/5	0.88	0.18	63,64,66,69	0
2	ZN	B	602	1/1	0.93	0.16	64,64,64,64	0
4	MG	B	604	1/1	0.95	0.68	62,62,62,62	0
3	BR	B	603	1/1	0.98	0.12	92,92,92,92	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.