Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 04:30 PM EDT

PDB ID	:	3NU7
Title	:	WbpE, an Aminotransferase from Pseudomonas aeruginosa Involved in O-antigen Assembly in Complex with the Cofactor PMP
Authors	:	Larkin, A.; Olivier, N.B.; Imperiali, B.
Deposited on	:	2010-07-06
Resolution	:	1.95 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 (i) 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 (i)) were used in the production of this report:

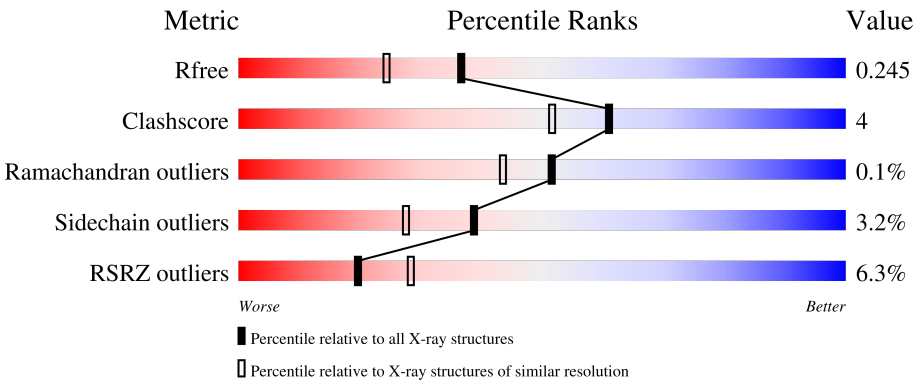
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 <=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	359	6% 90% 9% •
1	B	359	7% 89% 10% •

2 Entry composition (i)

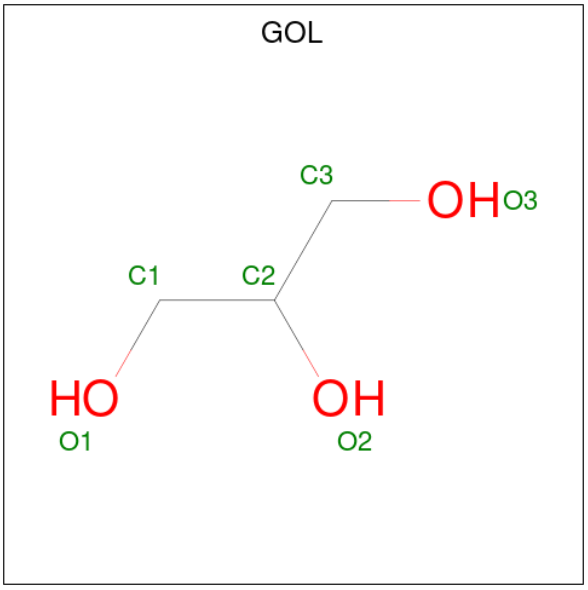
There are 4 unique types of molecules in this entry. The entry contains 5855 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aminotransferase WbpE.

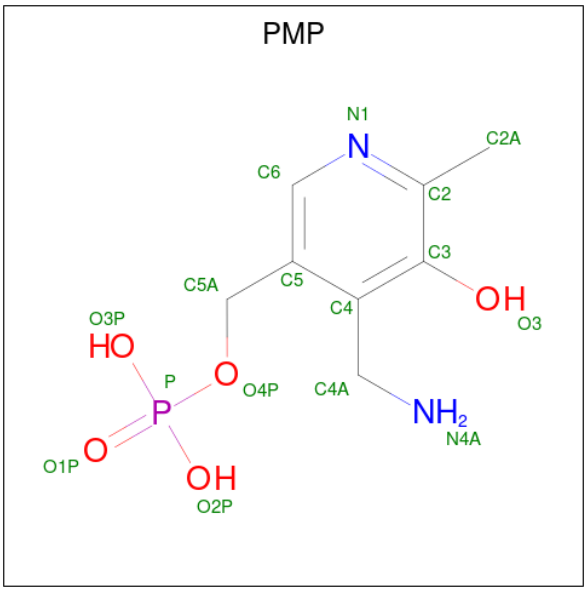
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	358	2703	1717	459	516	11	0	1	0
1	B	359	2725	1732	464	518	11	0	0	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0
2	B	1	6	3	3	0	0
2	B	1	6	3	3	0	0

- Molecule 3 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: $C_8H_{13}N_2O_5P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	16	8	2	5	1	0	0
			Total	C	N	O	P		
3	B	1	16	8	2	5	1	0	0

- Molecule 4 is water.

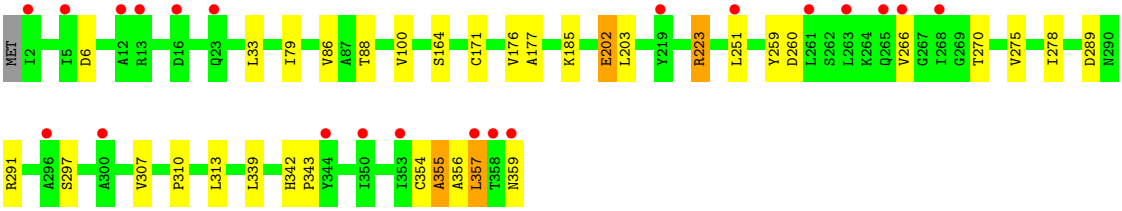
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	165	165	165	0	0
			Total	O		
4	B	212	212	212	0	0

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.

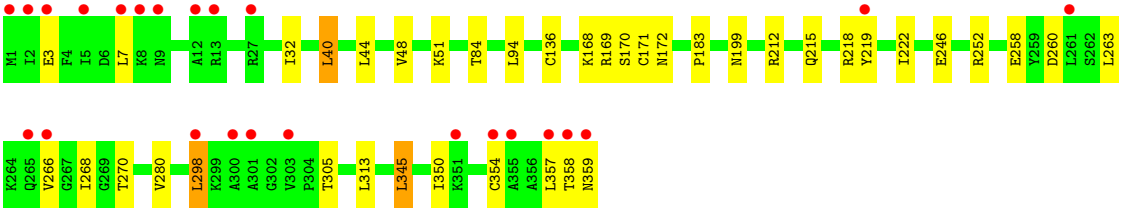
• Molecule 1: Aminotransferase WbpE

Chain A:



• Molecule 1: Aminotransferase WbpE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	78.28Å 149.29Å 54.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.66 – 1.95 42.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.66-1.95) 99.8 (42.00-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.24 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.199 , 0.245 0.199 , 0.245	Depositor DCC
R_{free} test set	2417 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.882	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5855	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, PMP

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	0.45	0/2756	0.58	0/3756
1	B	0.49	0/2775	0.62	0/3776
All	All	0.47	0/5531	0.60	0/7532

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 (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	2703	0	2696	16	1
1	B	2725	0	2740	32	0
2	A	6	0	8	1	0
2	B	12	0	16	2	0
3	A	16	0	10	2	0
3	B	16	0	10	1	0
4	A	165	0	0	1	1
4	B	212	0	0	0	0
All	All	5855	0	5480	49	1

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 4.

All (49) 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:212:ARG:HD2	2:B:362:GOL:O3	1.67	0.94
1:B:218:ARG:HE	1:B:219:TYR:H	1.13	0.89
1:B:266:VAL:HG11	1:B:358:THR:HG22	1.58	0.85
3:A:361:PMP:O4P	3:A:361:PMP:H4A1	1.83	0.78
1:B:84:THR:O	1:B:313:LEU:HD11	1.86	0.74
1:B:215:GLN:OE1	1:B:218:ARG:NH2	2.24	0.70
1:B:218:ARG:NE	1:B:219:TYR:H	1.91	0.67
1:B:266:VAL:HG11	1:B:358:THR:CG2	2.25	0.66
1:A:297:SER:OG	1:A:359:ASN:HB3	1.97	0.64
1:A:355:ALA:HA	1:A:357:LEU:HD23	1.79	0.64
1:B:354:CYS:O	1:B:358:THR:HG23	2.02	0.60
1:B:32:ILE:HB	2:B:360:GOL:H11	1.84	0.58
1:A:354:CYS:C	1:A:356:ALA:H	2.08	0.56
1:B:215:GLN:OE1	1:B:218:ARG:CZ	2.54	0.55
1:B:40:LEU:HD22	1:B:44:LEU:HG	1.89	0.55
1:A:223:ARG:NH1	4:A:495:HOH:O	2.35	0.54
1:A:164:SER:HB2	1:A:278:ILE:HB	1.90	0.53
1:B:3:GLU:HG2	1:B:7:LEU:HD22	1.91	0.53
1:B:169:ARG:NH2	1:B:246:GLU:OE2	2.42	0.52
1:B:218:ARG:HE	1:B:219:TYR:N	1.96	0.51
3:B:361:PMP:N4A	3:B:361:PMP:O4P	2.44	0.51
1:B:313:LEU:H	1:B:313:LEU:HD12	1.76	0.51
1:B:168:LYS:HE2	1:B:172:ASN:O	2.12	0.49
1:A:86:VAL:HA	1:A:313:LEU:HD21	1.94	0.49
1:B:345:LEU:HD13	1:B:350:ILE:HG13	1.97	0.47
1:B:48:VAL:HG13	1:B:172:ASN:HB2	1.96	0.46
1:A:185:LYS:NZ	3:A:361:PMP:H4A2	2.31	0.46
1:B:260:ASP:HA	1:B:270:THR:HG21	1.96	0.46
1:B:268:ILE:HD13	1:B:357:LEU:HD23	1.98	0.46
1:A:171:CYS:HA	1:A:177:ALA:CB	2.47	0.45
1:A:266:VAL:O	1:A:266:VAL:CG1	2.65	0.45
1:B:170:SER:O	1:B:171:CYS:HB2	2.18	0.44
1:B:252:ARG:HD3	1:B:280:VAL:O	2.16	0.44
1:B:313:LEU:HD12	1:B:313:LEU:N	2.32	0.43
1:B:136:CYS:SG	1:B:170:SER:HB2	2.58	0.43
1:B:298:LEU:HD11	1:B:357:LEU:HD12	2.01	0.43
1:B:51:LYS:HE3	1:B:199:ASN:O	2.19	0.43
2:A:360:GOL:H2	1:B:183:PRO:HB2	2.01	0.43
1:A:176:VAL:HG12	1:A:177:ALA:N	2.34	0.42
1:B:222:ILE:H	1:B:222:ILE:HG13	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:LYS:HB2	1:B:199:ASN:HA	2.01	0.42
1:A:260:ASP:HA	1:A:270:THR:HG21	2.00	0.42
1:A:79:ILE:HA	1:A:100:VAL:O	2.20	0.42
1:B:298:LEU:HD23	1:B:305:THR:HG21	2.02	0.41
1:A:291:ARG:HD3	1:A:307:VAL:HG21	2.02	0.41
1:A:310:PRO:HG3	1:B:219:TYR:CG	2.56	0.41
1:A:342:HIS:HB2	1:A:343:PRO:CD	2.51	0.41
1:B:84:THR:O	1:B:313:LEU:CD1	2.65	0.41
1:A:6:ASP:H	1:A:342:HIS:CD2	2.40	0.40

All (1) 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:A:202:GLU:OE2	4:A:519:HOH:O[4_445]	2.12	0.08

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	357/359 (99%)	346 (97%)	10 (3%)	1 (0%)	41 30
1	B	357/359 (99%)	346 (97%)	11 (3%)	0	100 100
All	All	714/718 (99%)	692 (97%)	21 (3%)	1 (0%)	51 43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	355	ALA

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	282/291 (97%)	271 (96%)	11 (4%)	32	19
1	B	285/291 (98%)	278 (98%)	7 (2%)	47	38
All	All	567/582 (97%)	549 (97%)	18 (3%)	39	27

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

Mol	Chain	Res	Type
1	A	33	LEU
1	A	88	THR
1	A	202	GLU
1	A	203	LEU
1	A	223	ARG
1	A	251	LEU
1	A	259	TYR
1	A	275	VAL
1	A	289	ASP
1	A	339	LEU
1	A	357	LEU
1	B	40	LEU
1	B	94	LEU
1	B	258	GLU
1	B	263	LEU
1	B	298	LEU
1	B	345	LEU
1	B	359	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	342	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)

5 ligands are modelled in this entry.

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	PMP	A	361	-	16,16,16	0.95	1 (6%)	22,23,23	1.21	1 (4%)
2	GOL	B	362	-	5,5,5	0.38	0	5,5,5	0.75	0
2	GOL	A	360	-	5,5,5	0.39	0	5,5,5	0.30	0
2	GOL	B	360	-	5,5,5	0.34	0	5,5,5	0.47	0
3	PMP	B	361	-	16,16,16	1.00	2 (12%)	22,23,23	1.33	4 (18%)

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	PMP	A	361	-	-	5/8/8/8	0/1/1/1
2	GOL	B	362	-	-	2/4/4/4	-
2	GOL	A	360	-	-	2/4/4/4	-
2	GOL	B	360	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PMP	B	361	-	-	5/8/8/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	361	PMP	C2-N1	2.31	1.38	1.33
3	A	361	PMP	C2-N1	2.16	1.37	1.33
3	B	361	PMP	C3-C2	-2.08	1.38	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	361	PMP	C5-C6-N1	-3.31	118.45	123.83
3	B	361	PMP	C5-C6-N1	-2.88	119.15	123.83
3	B	361	PMP	O3P-P-O4P	2.34	112.77	106.67
3	B	361	PMP	O2P-P-O4P	2.17	112.32	106.67
3	B	361	PMP	C2A-C2-N1	2.02	121.44	117.64

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	360	GOL	O1-C1-C2-C3
2	B	360	GOL	C1-C2-C3-O3
3	A	361	PMP	C4-C5-C5A-O4P
3	A	361	PMP	C6-C5-C5A-O4P
3	A	361	PMP	C5A-O4P-P-O2P
3	A	361	PMP	C5A-O4P-P-O3P
3	B	361	PMP	C4-C5-C5A-O4P
3	B	361	PMP	C6-C5-C5A-O4P
3	B	361	PMP	C5A-O4P-P-O2P
3	B	361	PMP	C5A-O4P-P-O3P
2	B	362	GOL	O1-C1-C2-C3
2	B	360	GOL	O1-C1-C2-O2
2	B	360	GOL	O2-C2-C3-O3
3	A	361	PMP	C5A-O4P-P-O1P
3	B	361	PMP	C5A-O4P-P-O1P
2	B	362	GOL	O1-C1-C2-O2
2	A	360	GOL	O1-C1-C2-C3
2	A	360	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	361	PMP	2	0
2	B	362	GOL	1	0
2	A	360	GOL	1	0
2	B	360	GOL	1	0
3	B	361	PMP	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 (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	358/359 (99%)	0.38	21 (5%)	22	30	16, 27, 48, 59	0
1	B	359/359 (100%)	0.42	24 (6%)	17	26	15, 24, 49, 61	0
All	All	717/718 (99%)	0.40	45 (6%)	20	28	15, 26, 49, 61	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	298	LEU	6.2
1	B	7	LEU	6.0
1	B	358	THR	4.3
1	A	296	ALA	4.0
1	B	1	MET	4.0
1	B	265	GLN	3.8
1	B	359	ASN	3.6
1	A	5	ILE	3.6
1	B	2	ILE	3.6
1	B	357	LEU	3.5
1	A	358	THR	3.5
1	A	265	GLN	3.5
1	A	268	ILE	3.4
1	B	355	ALA	3.4
1	B	300	ALA	3.2
1	A	251	LEU	3.2
1	B	354	CYS	3.1
1	A	2	ILE	3.0
1	B	5	ILE	3.0
1	B	261	LEU	3.0
1	A	219	TYR	2.8
1	A	13	ARG	2.8
1	B	301	ALA	2.8
1	A	12	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	300	ALA	2.6
1	A	357	LEU	2.5
1	B	303	VAL	2.5
1	B	266	VAL	2.4
1	A	261	LEU	2.4
1	A	344	TYR	2.4
1	B	8	LYS	2.3
1	B	351	LYS	2.2
1	A	359	ASN	2.2
1	A	350	ILE	2.2
1	A	353	ILE	2.2
1	B	13	ARG	2.2
1	B	219	TYR	2.2
1	A	263	LEU	2.1
1	A	266	VAL	2.1
1	B	12	ALA	2.1
1	A	23	GLN	2.1
1	B	27	ARG	2.1
1	A	16	ASP	2.1
1	B	3	GLU	2.1
1	B	9	ASN	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(Å^2)	Q<0.9
2	GOL	A	360	6/6	0.76	0.21	64,64,64,65	0
2	GOL	B	360	6/6	0.88	0.22	51,54,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	B	362	6/6	0.92	0.18	27,28,31,32	0
3	PMP	A	361	16/16	0.92	0.44	5,16,18,18	16
3	PMP	B	361	16/16	0.92	0.46	6,17,19,21	16

6.5 Other polymers (i)

There are no such residues in this entry.