



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:55 PM UTC

PDB ID : 4TOZ / pdb_00004toz
Title : MppA Periplasmic Murein Tripeptide Binding Protein, Unliganded Open Form
Authors : Jeffery, C.J.; Bhatt, F.
Deposited on : 2014-06-06
Resolution : 1.50 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

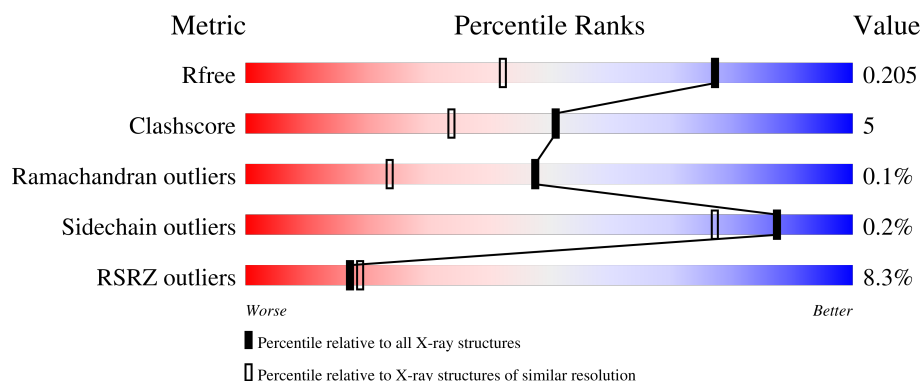
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	523	7% 88% 10% ..
1	B	523	9% 87% 11% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9803 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 Periplasmic murein peptide-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	0	0
			4074	2609	693	765	7			
1	B	515	Total	C	N	O	S	0	0	0
			4074	2608	695	764	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	359	ASP	GLU	conflict	UNP P77348
A	538	SER	-	expression tag	UNP P77348
A	539	ARG	-	expression tag	UNP P77348
A	540	HIS	-	expression tag	UNP P77348
A	541	HIS	-	expression tag	UNP P77348
A	542	HIS	-	expression tag	UNP P77348
A	543	HIS	-	expression tag	UNP P77348
A	544	HIS	-	expression tag	UNP P77348
A	545	HIS	-	expression tag	UNP P77348
B	359	ASP	GLU	conflict	UNP P77348
B	538	SER	-	expression tag	UNP P77348
B	539	ARG	-	expression tag	UNP P77348
B	540	HIS	-	expression tag	UNP P77348
B	541	HIS	-	expression tag	UNP P77348
B	542	HIS	-	expression tag	UNP P77348
B	543	HIS	-	expression tag	UNP P77348
B	544	HIS	-	expression tag	UNP P77348
B	545	HIS	-	expression tag	UNP P77348

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		

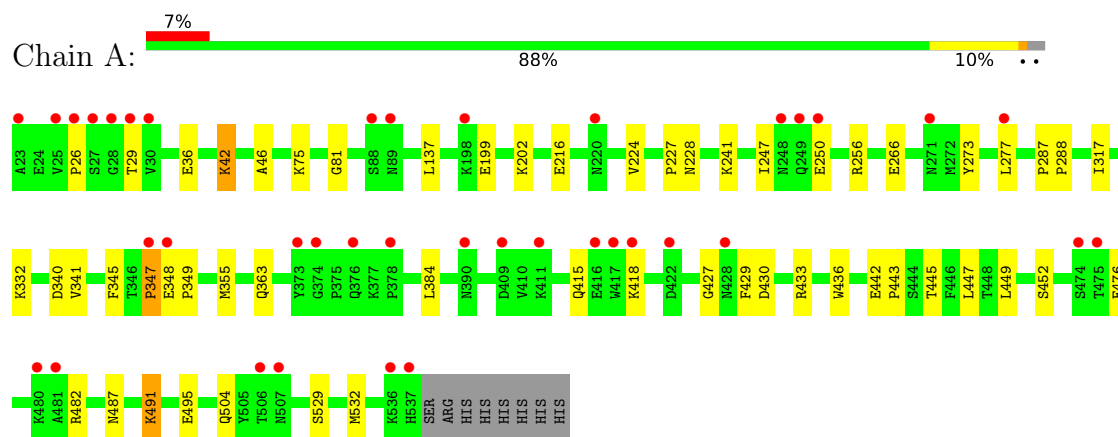
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	822	Total	O	0	0
			822	822		
3	B	825	Total	O	0	0
			825	825		

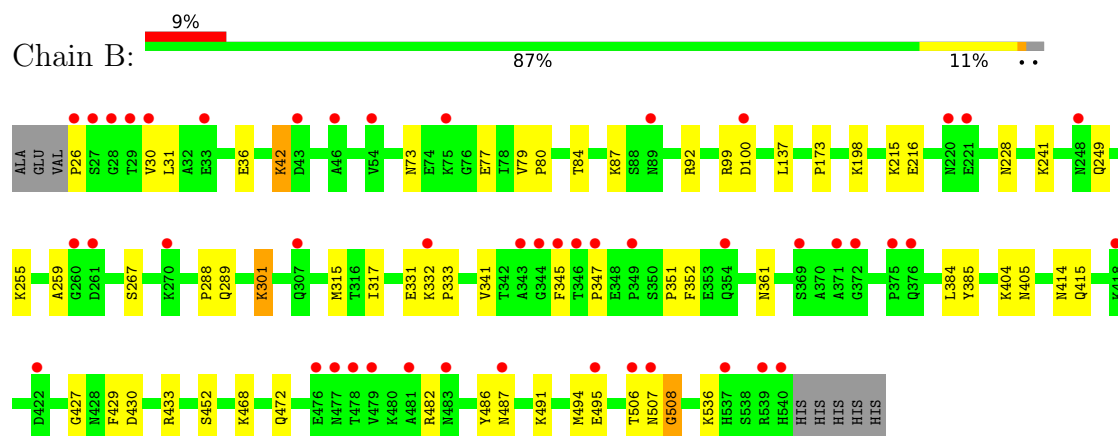
3 Residue-property plots [i](#)

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: Periplasmic murein peptide-binding protein



- Molecule 1: Periplasmic murein peptide-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.97Å 76.81Å 89.57Å 90.00° 91.58° 90.00°	Depositor
Resolution (Å)	50.00 – 1.50 50.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-1.50) 99.6 (50.00-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.82 (at 1.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.180 , 0.205 0.180 , 0.205	Depositor DCC
R_{free} test set	7968 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	11.6	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -k,-h,-l 0.008 for k,h,-l 0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9803	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: TRS

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	0.37	0/4178	0.84	9/5700 (0.2%)
1	B	0.34	0/4179	0.84	7/5700 (0.1%)
All	All	0.35	0/8357	0.84	16/11400 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	ILE	N-CA-C	-7.08	99.54	108.89
1	A	42	LYS	N-CA-C	6.81	121.19	113.01
1	A	452	SER	N-CA-C	6.66	119.39	111.33
1	B	452	SER	N-CA-C	6.59	119.31	111.33
1	B	317	ILE	N-CA-C	-6.33	100.53	108.89
1	B	508	GLY	N-CA-C	6.21	119.08	111.93
1	B	42	LYS	N-CA-C	5.61	119.61	112.87
1	A	447	LEU	N-CA-C	5.60	118.15	111.71
1	B	228	ASN	N-CA-C	-5.50	98.31	107.99
1	A	347	PRO	N-CA-C	5.44	119.73	111.19
1	A	430	ASP	N-CA-C	-5.42	104.32	111.96
1	A	81	GLY	N-CA-C	-5.35	100.51	113.18
1	B	430	ASP	N-CA-C	-5.29	104.50	111.96
1	A	228	ASN	N-CA-C	-5.26	98.73	107.99
1	B	198	LYS	N-CA-C	5.15	118.67	112.38
1	A	250	GLU	N-CA-C	5.14	118.33	111.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	4074	0	4048	39	0
1	B	4074	0	4043	45	0
2	A	8	0	12	0	0
3	A	822	0	0	13	0
3	B	825	0	0	12	0
All	All	9803	0	8103	84	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 5.

All (84) 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:529:SER:HA	1:A:532:MET:HE2	1.31	1.13
1:A:202:LYS:CE	3:A:2101:HOH:O	2.19	0.88
1:A:199:GLU:HB3	1:A:202:LYS:HE2	1.56	0.87
1:B:536:LYS:NZ	3:B:602:HOH:O	2.07	0.86
1:A:529:SER:CA	1:A:532:MET:HE2	2.13	0.76
1:B:100:ASP:OD2	3:B:601:HOH:O	2.05	0.73
1:A:36:GLU:HG2	1:A:241:LYS:HB3	1.70	0.73
1:B:36:GLU:HG2	1:B:241:LYS:HB3	1.72	0.70
1:A:202:LYS:NZ	3:A:2101:HOH:O	2.21	0.70
1:A:216:GLU:HG2	1:A:224:VAL:HB	1.73	0.69
1:B:345:PHE:CZ	1:B:347:PRO:HB3	2.28	0.68
1:A:202:LYS:HE3	3:A:2101:HOH:O	1.88	0.68
1:B:507:ASN:O	3:B:603:HOH:O	2.13	0.67
1:B:347:PRO:HA	1:B:487:ASN:OD1	1.95	0.66
1:A:491:LYS:NZ	1:A:491:LYS:HB2	2.13	0.63
1:A:504:GLN:NE2	3:A:2103:HOH:O	2.32	0.62
1:B:289:GLN:HG3	1:B:507:ASN:OD1	2.00	0.62
1:A:491:LYS:HB2	1:A:491:LYS:HZ2	1.64	0.62
1:A:476:GLU:HB2	1:A:482:ARG:HG2	1.83	0.61
1:A:75:LYS:HG3	3:A:2676:HOH:O	2.00	0.60
1:A:26:PRO:HG2	1:A:29:THR:OG1	2.02	0.60
1:B:301:LYS:HB3	1:B:301:LYS:NZ	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:ARG:HG2	1:B:486:TYR:CE2	2.39	0.57
1:B:137:LEU:HD23	1:B:137:LEU:C	2.30	0.56
1:B:404:LYS:HG3	3:B:643:HOH:O	2.05	0.56
1:A:348:GLU:HG2	1:A:349:PRO:HD2	1.87	0.56
1:A:227:PRO:HG2	3:A:2542:HOH:O	2.06	0.55
1:A:199:GLU:CD	3:A:2104:HOH:O	2.49	0.55
1:B:267:SER:HA	1:B:508:GLY:O	2.07	0.55
1:A:433:ARG:HD2	1:A:433:ARG:C	2.32	0.54
1:A:216:GLU:CG	1:A:224:VAL:HB	2.36	0.54
1:B:73:ASN:ND2	1:B:77:GLU:HB2	2.23	0.54
1:A:491:LYS:O	1:A:495:GLU:HG3	2.08	0.53
1:B:491:LYS:O	1:B:495:GLU:HG3	2.08	0.53
1:B:87:LYS:CG	3:B:605:HOH:O	2.56	0.52
1:A:202:LYS:HD2	3:A:2101:HOH:O	2.10	0.52
1:B:87:LYS:HG2	3:B:605:HOH:O	2.08	0.52
1:A:42:LYS:HD2	1:A:266:GLU:HG2	1.92	0.52
1:A:202:LYS:CD	3:A:2101:HOH:O	2.56	0.52
1:B:255:LYS:HD3	1:B:255:LYS:C	2.35	0.52
1:B:288:PRO:HG2	1:B:341:VAL:HG11	1.94	0.50
1:B:215:LYS:HG2	1:B:216:GLU:HG3	1.94	0.50
1:B:249:GLN:NE2	3:B:609:HOH:O	2.43	0.50
1:B:384:LEU:HD11	1:B:415:GLN:HG3	1.92	0.50
1:B:468:LYS:O	1:B:472:GLN:HG3	2.12	0.50
1:A:347:PRO:HA	1:A:487:ASN:OD1	2.12	0.50
1:B:73:ASN:HD21	1:B:77:GLU:HB2	1.77	0.49
1:A:418:LYS:HG2	3:A:2480:HOH:O	2.12	0.48
1:A:384:LEU:HD11	1:A:415:GLN:HG3	1.95	0.48
1:B:26:PRO:N	3:B:610:HOH:O	2.47	0.48
1:B:301:LYS:HB3	1:B:301:LYS:HZ3	1.79	0.47
1:B:433:ARG:HD2	1:B:433:ARG:C	2.40	0.47
1:A:287:PRO:HD2	3:A:2102:HOH:O	2.16	0.46
1:A:247:ILE:CD1	1:A:256:ARG:HH21	2.28	0.46
1:B:332:LYS:HD2	1:B:333:PRO:HD2	1.97	0.46
1:A:427:GLY:HA2	1:A:429:PHE:CE1	2.50	0.46
1:A:436:TRP:CD2	1:A:449:LEU:HD11	2.50	0.46
1:B:79:VAL:HB	1:B:80:PRO:HD2	1.97	0.45
1:B:315:MET:HE3	1:B:352:PHE:CE1	2.52	0.45
1:A:355:MET:HE1	1:A:363:GLN:OE1	2.17	0.45
1:B:84:THR:HG23	1:B:99:ARG:HB3	1.98	0.44
1:B:92:ARG:CZ	1:B:173:PRO:HG3	2.47	0.44
1:B:385:TYR:O	1:B:414:ASN:HA	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:TYR:CZ	1:A:277:LEU:HD11	2.53	0.44
1:B:42:LYS:HE2	3:B:922:HOH:O	2.17	0.44
1:B:267:SER:HB2	3:B:1134:HOH:O	2.18	0.43
1:B:341:VAL:HG13	3:B:614:HOH:O	2.17	0.43
1:A:340:ASP:OD1	1:A:341:VAL:HG13	2.18	0.43
1:A:345:PHE:CZ	1:A:347:PRO:HB3	2.53	0.42
1:B:255:LYS:NZ	1:B:259:ALA:HB2	2.34	0.42
1:B:331:GLU:HA	1:B:506:THR:CG2	2.49	0.42
1:B:30:VAL:HG12	1:B:31:LEU:N	2.34	0.42
1:B:361:ASN:OD1	1:B:405:ASN:HB3	2.19	0.42
1:B:427:GLY:HA2	1:B:429:PHE:CE1	2.55	0.42
1:A:288:PRO:HG3	1:A:332:LYS:HD3	2.02	0.42
1:B:80:PRO:HG2	3:B:900:HOH:O	2.20	0.41
1:B:84:THR:CG2	1:B:99:ARG:HB3	2.49	0.41
1:A:137:LEU:HD11	3:A:2678:HOH:O	2.19	0.41
1:A:287:PRO:CD	3:A:2102:HOH:O	2.68	0.41
1:B:331:GLU:HA	1:B:506:THR:HG21	2.01	0.41
1:A:345:PHE:HB2	1:A:443:PRO:HG3	2.03	0.41
1:A:442:GLU:O	1:A:445:THR:HG22	2.21	0.40
1:B:351:PRO:HD2	1:B:494:MET:SD	2.62	0.40
1:B:384:LEU:CD1	1:B:415:GLN:HG3	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	513/523 (98%)	504 (98%)	8 (2%)	1 (0%)	43	22
1	B	513/523 (98%)	507 (99%)	6 (1%)	0	100	100
All	All	1026/1046 (98%)	1011 (98%)	14 (1%)	1 (0%)	48	24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	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	438/446 (98%)	437 (100%)	1 (0%)	87	77
1	B	438/446 (98%)	437 (100%)	1 (0%)	87	77
All	All	876/892 (98%)	874 (100%)	2 (0%)	87	77

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	491	LYS
1	B	301	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	113	GLN
1	A	142	ASN
1	A	234	ASN
1	A	283	GLN
1	A	336	HIS
1	A	504	GLN
1	B	60	GLN
1	B	141	ASN
1	B	142	ASN
1	B	220	ASN
1	B	249	GLN
1	B	283	GLN
1	B	363	GLN

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Mol	Chain	Res	Type
1	B	428	ASN
1	B	504	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	$\# Z > 2$
2	TRS	A	2001	-	7,7,7	0.55	0	9,9,9	0.37	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
2	TRS	A	2001	-	-	0/9/9/9	-

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	A	515/523 (98%)	0.32	38 (7%) 20 22	7, 12, 26, 38	2 (0%)
1	B	515/523 (98%)	0.34	47 (9%) 15 15	6, 12, 25, 38	4 (0%)
All	All	1030/1046 (98%)	0.33	85 (8%) 17 19	6, 12, 25, 38	6 (0%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	507	ASN	5.6
1	B	100	ASP	5.1
1	B	479	VAL	5.0
1	B	478	THR	4.9
1	A	250	GLU	4.7
1	B	344	GLY	4.7
1	B	346	THR	4.4
1	A	28	GLY	4.3
1	B	345	PHE	4.2
1	A	89	ASN	4.1
1	B	347	PRO	4.1
1	B	343	ALA	4.0
1	B	54	VAL	3.7
1	B	248	ASN	3.7
1	A	537	HIS	3.6
1	B	332	LYS	3.6
1	A	480	LYS	3.6
1	B	33	GLU	3.5
1	B	354	GLN	3.4
1	B	418	LYS	3.4
1	A	248	ASN	3.3
1	B	30	VAL	3.3
1	A	418	LYS	3.2
1	B	539	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	537	HIS	3.2
1	A	23	ALA	3.2
1	B	481	ALA	3.1
1	A	198	LYS	3.0
1	A	376	GLN	3.0
1	B	46	ALA	2.9
1	B	89	ASN	2.9
1	B	477	ASN	2.9
1	B	376	GLN	2.8
1	A	29	THR	2.8
1	A	271	ASN	2.8
1	B	27	SER	2.7
1	A	507	ASN	2.7
1	A	475	THR	2.7
1	B	29	THR	2.7
1	B	487	ASN	2.6
1	B	483	ASN	2.6
1	A	249	GLN	2.6
1	B	221	GLU	2.6
1	B	260	GLY	2.6
1	A	416	GLU	2.5
1	A	374	GLY	2.5
1	A	30	VAL	2.5
1	B	506	THR	2.5
1	A	220	ASN	2.5
1	B	220	ASN	2.5
1	B	349	PRO	2.5
1	A	481	ALA	2.4
1	A	347	PRO	2.4
1	A	428	ASN	2.4
1	A	27	SER	2.4
1	A	474	SER	2.4
1	B	375	PRO	2.4
1	B	28	GLY	2.4
1	B	371	ALA	2.3
1	B	422	ASP	2.3
1	A	411	LYS	2.3
1	B	26	PRO	2.3
1	A	506	THR	2.3
1	A	373	TYR	2.3
1	A	378	PRO	2.3
1	A	26	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	307	GLN	2.2
1	A	277	LEU	2.2
1	B	372	GLY	2.1
1	A	422	ASP	2.1
1	B	43	ASP	2.1
1	B	270	LYS	2.1
1	A	88	SER	2.1
1	B	261	ASP	2.1
1	A	536	LYS	2.1
1	A	390	ASN	2.1
1	A	348	GLU	2.1
1	A	409	ASP	2.1
1	B	75	LYS	2.0
1	A	25	VAL	2.0
1	B	476	GLU	2.0
1	B	369	SER	2.0
1	A	417	TRP	2.0
1	B	540	HIS	2.0
1	B	495	GLU	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	TRS	A	2001	8/8	0.73	0.18	24,25,26,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.