



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:44 AM UTC

PDB ID : 5JIR / pdb_00005jir
Title : Crystal structure of Treponema pallidum protein Tp0624
Authors : Parker, M.L.; Boulanger, M.J.
Deposited on : 2016-04-22
Resolution : 1.70 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

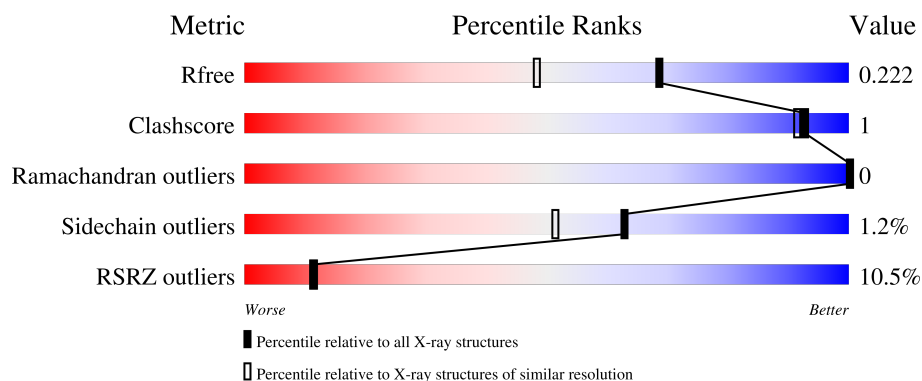
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	421	11% 94% ..
1	B	421	9% 92% ...

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6800 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 OOP family OmpA-OmpF porin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	405	Total	C	N	O	S	0	1	0
			3189	2007	586	586	10			
1	A	413	Total	C	N	O	S	0	0	0
			3233	2038	593	592	10			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	56	GLY	-	expression tag	UNP O83632
B	57	SER	-	expression tag	UNP O83632
B	58	MET	-	expression tag	UNP O83632
B	59	ALA	-	expression tag	UNP O83632
B	60	SER	-	expression tag	UNP O83632
A	56	GLY	-	expression tag	UNP O83632
A	57	SER	-	expression tag	UNP O83632
A	58	MET	-	expression tag	UNP O83632
A	59	ALA	-	expression tag	UNP O83632
A	60	SER	-	expression tag	UNP O83632

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	5	Total	Cl	0	0
			5	5		
3	A	3	Total	Cl	0	0
			3	3		

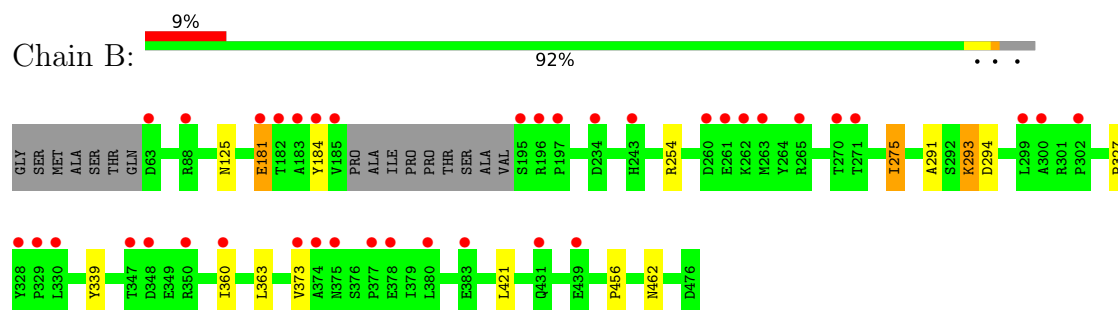
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	173	Total	O	0	0
			173	173		
4	A	173	Total	O	0	0
			173	173		

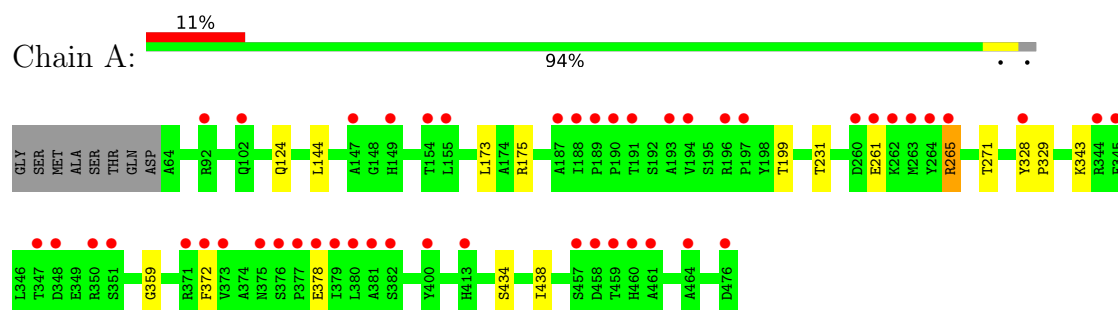
3 Residue-property plots [i](#)

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: OOP family OmpA-OmpF porin



- Molecule 1: OOP family OmpA-OmpF porin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.02Å 103.50Å 140.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.75 – 1.70 51.75 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (51.75-1.70) 97.2 (51.75-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.189 , 0.214 0.199 , 0.222	Depositor DCC
R_{free} test set	5075 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6800	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 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: CL, GOL

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	0.51	0/3300	0.74	1/4488 (0.0%)
1	B	0.54	0/3252	0.73	1/4417 (0.0%)
All	All	0.52	0/6552	0.73	2/8905 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	ASN	N-CA-C	7.92	122.39	109.72
1	A	359	GLY	N-CA-C	-5.38	105.38	112.81

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	3233	0	3281	8	0
1	B	3189	0	3227	10	0
2	A	18	0	24	1	0
2	B	6	0	8	0	0
3	A	3	0	0	0	0
3	B	5	0	0	0	0
4	A	173	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	173	0	0	1	0
All	All	6800	0	6540	19	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 1.

All (19) 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:343:LYS:NZ	4:A:601:HOH:O	2.22	0.72
1:B:254:ARG:NH1	4:B:601:HOH:O	2.24	0.70
1:B:327:PRO:HG3	1:B:360:ILE:HG23	1.78	0.64
1:A:124:GLN:NE2	4:A:604:HOH:O	2.30	0.64
1:B:275:ILE:HD13	1:B:294:ASP:HB3	1.84	0.59
1:A:261:GLU:OE1	1:A:265:ARG:NH1	2.35	0.58
1:B:327:PRO:HG3	1:B:360:ILE:CG2	2.34	0.57
1:B:291:ALA:HB1	1:B:293:LYS:HE2	1.93	0.51
1:B:373:VAL:HG11	1:B:421:LEU:CD1	2.43	0.48
1:B:327:PRO:CG	1:B:360:ILE:HG23	2.43	0.47
1:B:181:GLU:H	1:B:181:GLU:CD	2.26	0.44
1:B:456:PRO:O	1:B:462:ASN:HB3	2.17	0.43
1:B:339:TYR:CE1	1:B:363:LEU:HD11	2.53	0.43
1:A:175:ARG:NH2	4:A:605:HOH:O	2.32	0.42
1:A:328:TYR:HA	1:A:329:PRO:C	2.44	0.42
2:A:503:GOL:H12	4:A:634:HOH:O	2.18	0.42
1:A:144:LEU:HD11	1:A:173:LEU:HD23	2.02	0.42
1:A:199:THR:HG23	1:A:271:THR:HG23	2.03	0.41
1:A:434:SER:HA	1:A:438:ILE:O	2.20	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	411/421 (98%)	405 (98%)	6 (2%)	0	100	100
1	B	402/421 (96%)	395 (98%)	7 (2%)	0	100	100
All	All	813/842 (97%)	800 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	345/351 (98%)	341 (99%)	4 (1%)	63	51
1	B	340/351 (97%)	336 (99%)	4 (1%)	63	51
All	All	685/702 (98%)	677 (99%)	8 (1%)	63	51

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	181	GLU
1	B	184	TYR
1	B	275	ILE
1	B	293	LYS
1	A	231	THR
1	A	265	ARG
1	A	372	PHE
1	A	378	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	66	HIS
1	B	75	ASN
1	B	125	ASN
1	B	240	ASN
1	A	79	ASN

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Mol	Chain	Res	Type
1	A	102	GLN
1	A	167	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\# Z > 2$
2	GOL	B	501	-	5,5,5	0.35	0	5,5,5	0.91	0
2	GOL	A	501	-	5,5,5	0.53	0	5,5,5	0.25	0
2	GOL	A	502	-	5,5,5	0.41	0	5,5,5	0.47	0
2	GOL	A	503	-	5,5,5	0.39	0	5,5,5	0.52	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	GOL	B	501	-	-	2/4/4/4	-
2	GOL	A	501	-	-	2/4/4/4	-
2	GOL	A	502	-	-	3/4/4/4	-
2	GOL	A	503	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	GOL	O1-C1-C2-C3
2	A	502	GOL	O1-C1-C2-C3
2	A	501	GOL	O1-C1-C2-C3
2	A	503	GOL	C1-C2-C3-O3
2	B	501	GOL	O1-C1-C2-O2
2	A	502	GOL	O1-C1-C2-O2
2	A	503	GOL	O2-C2-C3-O3
2	A	502	GOL	O2-C2-C3-O3
2	A	503	GOL	O1-C1-C2-C3
2	A	501	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	GOL	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	413/421 (98%)	0.60	48 (11%) 9 9	12, 25, 49, 67	2 (0%)
1	B	405/421 (96%)	0.58	38 (9%) 14 14	9, 25, 48, 63	1 (0%)
All	All	818/842 (97%)	0.59	86 (10%) 11 11	9, 25, 49, 67	3 (0%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	THR	6.5
1	B	328	TYR	5.6
1	A	457	SER	5.3
1	A	194	VAL	5.2
1	B	185	VAL	5.1
1	A	187	ALA	5.0
1	A	189	PRO	4.9
1	B	263	MET	4.3
1	A	193	ALA	4.3
1	B	183	ALA	4.1
1	B	300	ALA	3.9
1	A	149	HIS	3.9
1	A	190	PRO	3.9
1	A	377	PRO	3.9
1	B	184	TYR	3.9
1	A	347	THR	3.7
1	B	329	PRO	3.7
1	A	263	MET	3.5
1	A	188	ILE	3.4
1	A	380	LEU	3.4
1	A	328	TYR	3.4
1	A	348	ASP	3.3
1	A	476	ASP	3.2
1	A	265	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	348	ASP	3.2
1	B	271	THR	3.1
1	A	350	ARG	3.1
1	A	372	PHE	3.0
1	A	379	ILE	2.9
1	B	182	THR	2.9
1	B	373	VAL	2.9
1	A	381	ALA	2.8
1	B	195	SER	2.8
1	B	377	PRO	2.8
1	B	63	ASP	2.8
1	A	460	HIS	2.8
1	B	299	LEU	2.8
1	B	380	LEU	2.8
1	A	155	LEU	2.7
1	A	147	ALA	2.7
1	B	88	ARG	2.7
1	A	196	ARG	2.7
1	A	382	SER	2.6
1	A	461	ALA	2.6
1	B	375	ASN	2.6
1	B	265	ARG	2.6
1	A	373	VAL	2.6
1	B	350	ARG	2.6
1	B	439	GLU	2.6
1	A	400	TYR	2.5
1	B	378	GLU	2.5
1	A	261	GLU	2.5
1	A	459	THR	2.5
1	A	197	PRO	2.5
1	A	264	TYR	2.5
1	A	464	ALA	2.5
1	B	347	THR	2.5
1	A	154	THR	2.5
1	A	260	ASP	2.4
1	B	270	THR	2.4
1	A	375	ASN	2.3
1	B	197	PRO	2.3
1	A	345	PHE	2.3
1	A	378	GLU	2.3
1	B	262	LYS	2.3
1	A	344	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	458	ASP	2.2
1	B	431	GLN	2.2
1	A	413	HIS	2.2
1	B	374	ALA	2.2
1	B	181	GLU	2.2
1	B	243	HIS	2.2
1	B	302	PRO	2.2
1	A	351	SER	2.2
1	B	196	ARG	2.1
1	B	234	ASP	2.1
1	A	376	SER	2.1
1	A	371	ARG	2.1
1	B	330	LEU	2.1
1	A	92	ARG	2.1
1	A	262	LYS	2.1
1	B	383	GLU	2.0
1	A	102	GLN	2.0
1	B	260	ASP	2.0
1	B	261	GLU	2.0
1	B	360	ILE	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(Å ²)	Q<0.9
2	GOL	A	503	6/6	0.76	0.16	30,36,40,41	0
2	GOL	A	502	6/6	0.89	0.12	22,40,40,41	0
2	GOL	B	501	6/6	0.90	0.09	27,32,33,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	A	501	6/6	0.92	0.10	27,27,33,35	0
3	CL	B	503	1/1	0.95	0.12	21,21,21,21	0
3	CL	A	506	1/1	0.95	0.10	30,30,30,30	0
3	CL	B	502	1/1	0.96	0.06	21,21,21,21	0
3	CL	B	506	1/1	0.98	0.04	26,26,26,26	0
3	CL	A	505	1/1	0.98	0.08	28,28,28,28	0
3	CL	B	505	1/1	0.98	0.07	24,24,24,24	0
3	CL	B	504	1/1	0.99	0.04	23,23,23,23	0
3	CL	A	504	1/1	0.99	0.10	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.