



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 11:17 AM EDT

PDB ID : 4OEV / pdb_00004oev
Title : Crystal structure of NikZ from *Campylobacter jejuni* in complex with Ni(II) ion
Authors : Lebrette, H.; Cavazza, C.
Deposited on : 2014-01-13
Resolution : 1.90 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

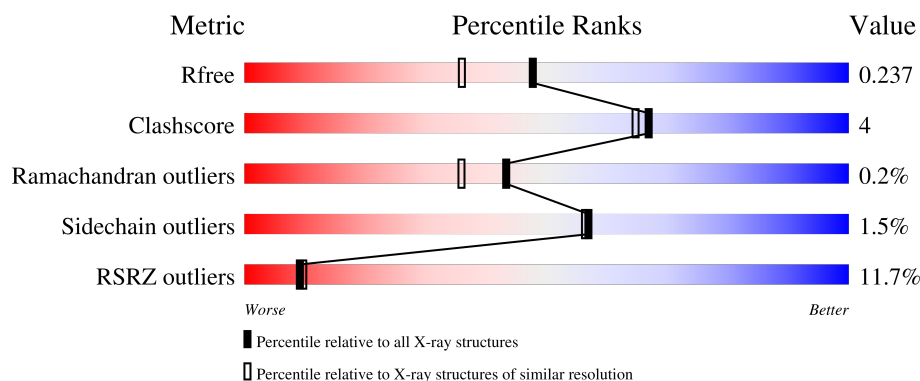
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	494	
1	B	494	

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	OXL	A	502	-	X	-	-
3	OXL	B	502	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8997 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.

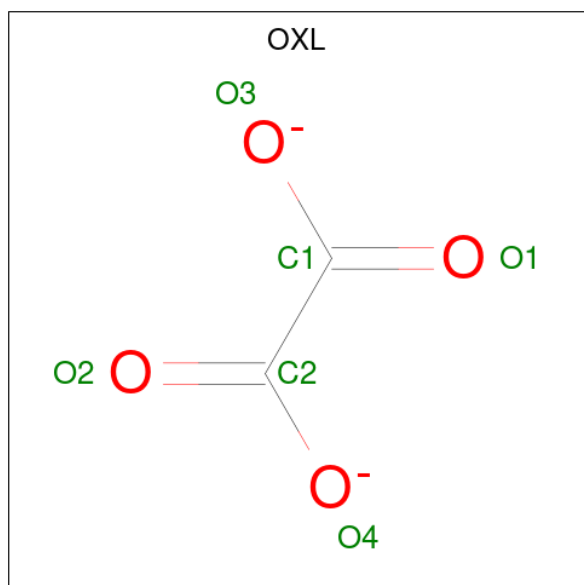
- Molecule 1 is a protein called Putative peptide ABC-transport system periplasmic peptide-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			4025	2612	665	744	4			
1	B	494	Total	C	N	O	S	0	0	0
			4025	2612	665	744	4			

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ni	0	0
			1	1		
2	B	1	Total	Ni	0	0
			1	1		

- Molecule 3 is OXALATE ION (CCD ID: OXL) (formula: C₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	2	4		
3	B	1	Total	C	O	0	0
			6	2	4		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

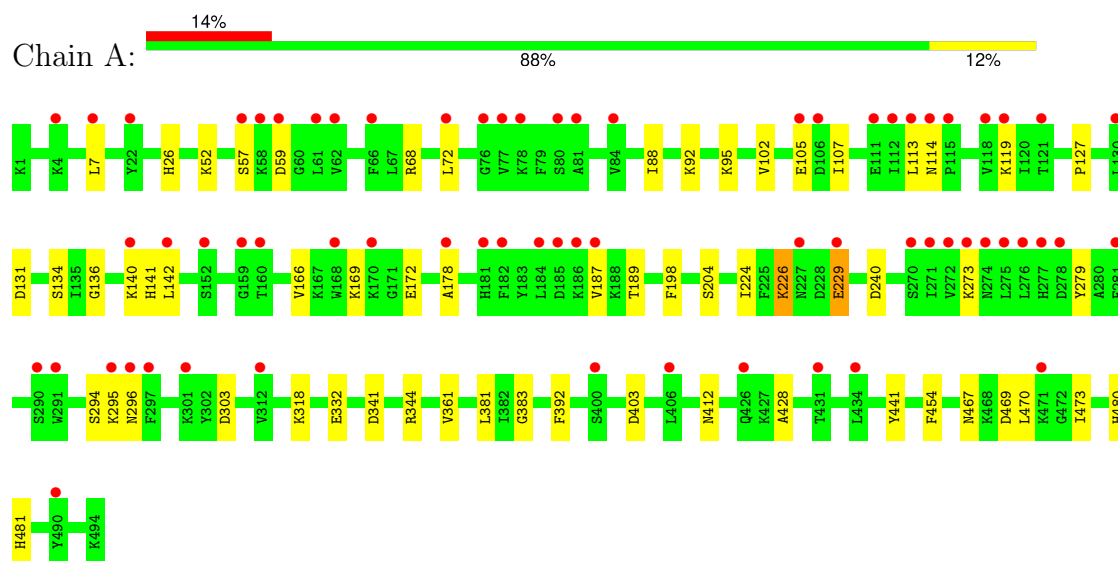
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	434	Total	O	0	0
			434	434		
5	B	463	Total	O	0	0
			463	463		

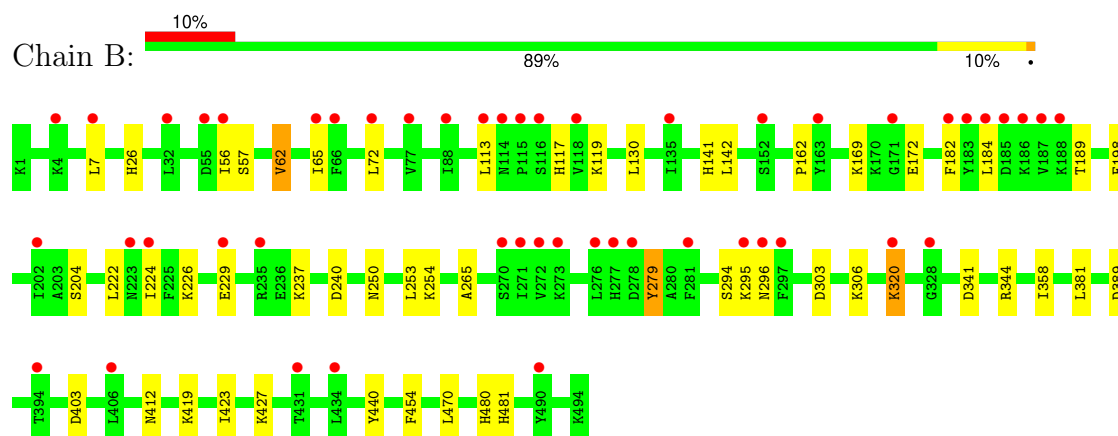
3 Residue-property plots

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: Putative peptide ABC-transport system periplasmic peptide-binding protein



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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	246.12Å 47.86Å 140.46Å 90.00° 114.60° 90.00°	Depositor
Resolution (Å)	45.23 – 1.90 45.23 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.23-1.90) 99.1 (45.23-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 1.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.202 , 0.235 0.203 , 0.237	Depositor DCC
R_{free} test set	5858 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 60.9	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	8997	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, OXL, 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	0.85	1/4130 (0.0%)	0.94	4/5582 (0.1%)
1	B	0.90	1/4130 (0.0%)	0.94	4/5582 (0.1%)
All	All	0.87	2/8260 (0.0%)	0.94	8/11164 (0.1%)

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
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	65	ILE	CA-CB	-5.75	1.47	1.54
1	A	383	GLY	CA-C	5.26	1.57	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	389	ASP	CA-C-N	5.95	125.63	119.56
1	B	389	ASP	C-N-CA	5.95	125.63	119.56
1	A	303	ASP	CA-C-N	5.39	125.21	119.28
1	A	303	ASP	C-N-CA	5.39	125.21	119.28
1	A	166	VAL	CB-CA-C	-5.28	107.22	111.71
1	B	279	TYR	N-CA-C	-5.25	107.41	112.97
1	B	62	VAL	N-CA-C	5.13	115.36	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	SER	N-CA-C	-5.06	107.11	113.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	454	PHE	Peptide
1	B	454	PHE	Peptide

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	4025	0	3981	34	0
1	B	4025	0	3981	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
4	A	12	0	16	1	0
4	B	24	0	32	0	0
5	A	434	0	0	11	0
5	B	463	0	0	3	0
All	All	8997	0	8010	60	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 4.

All (60) 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:113:LEU:HD11	1:A:119:LYS:HD2	1.65	0.78
1:A:229:GLU:H	1:A:229:GLU:CD	1.98	0.72
1:A:141:HIS:ND1	5:A:864:HOH:O	2.27	0.68
1:A:92:LYS:NZ	5:A:902:HOH:O	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LYS:HE3	1:A:68:ARG:HA	1.78	0.66
1:B:254:LYS:NZ	5:B:1039:HOH:O	2.30	0.64
1:B:7:LEU:HD13	1:B:189:THR:HG21	1.79	0.64
1:B:427:LYS:HD3	1:B:440:TYR:CE1	2.34	0.63
1:B:113:LEU:HD22	1:B:117:HIS:CE1	2.35	0.62
1:A:119:LYS:HE2	5:A:1017:HOH:O	2.01	0.61
1:A:169:LYS:HE2	1:A:172:GLU:OE2	2.02	0.59
1:B:403:ASP:HA	1:B:412:ASN:HB3	1.83	0.59
1:A:88:ILE:HG23	1:A:107:ILE:HD13	1.88	0.56
1:B:56:ILE:HD11	1:B:130:LEU:HD11	1.87	0.56
1:A:226:LYS:NZ	5:A:799:HOH:O	2.39	0.55
1:B:169:LYS:HE2	1:B:172:GLU:OE2	2.07	0.55
1:A:95:LYS:HE2	5:A:723:HOH:O	2.08	0.54
1:A:141:HIS:CD2	1:A:142:LEU:HG	2.43	0.53
1:A:204:SER:OG	1:A:224:ILE:HD11	2.08	0.53
1:B:237:LYS:NZ	5:B:888:HOH:O	2.41	0.52
1:A:318:LYS:NZ	5:A:1018:HOH:O	2.43	0.52
1:A:240:ASP:CG	1:A:480:HIS:HA	2.36	0.50
1:B:26:HIS:CD2	1:B:481:HIS:CD2	2.99	0.50
1:B:250:ASN:HB3	1:B:253:LEU:HB2	1.94	0.50
1:B:294:SER:C	1:B:296:ASN:H	2.19	0.50
1:A:105:GLU:OE1	4:A:503:GOL:H31	2.13	0.49
1:A:88:ILE:CG2	1:A:107:ILE:HD13	2.41	0.49
1:B:57:SER:HB3	1:B:62:VAL:HB	1.94	0.49
1:B:303:ASP:OD2	1:B:306:LYS:HG3	2.12	0.49
1:B:240:ASP:CG	1:B:480:HIS:HA	2.37	0.49
1:B:320:LYS:NZ	1:B:320:LYS:HB2	2.28	0.48
1:B:119:LYS:NZ	5:B:935:HOH:O	2.47	0.48
1:A:57:SER:OG	1:A:59:ASP:OD1	2.33	0.47
1:A:470:LEU:HD23	1:A:473:ILE:HD11	1.96	0.47
1:A:102:VAL:HG22	5:A:618:HOH:O	2.14	0.47
1:A:341:ASP:CG	1:A:344:ARG:HG3	2.41	0.46
1:A:114:ASN:HA	5:A:910:HOH:O	2.15	0.45
1:B:229:GLU:H	1:B:229:GLU:CD	2.24	0.45
1:B:204:SER:OG	1:B:224:ILE:HD11	2.15	0.45
1:B:162:PRO:HB3	1:B:182:PHE:CE2	2.51	0.45
1:A:294:SER:C	1:A:296:ASN:H	2.25	0.45
1:A:127:PRO:HD2	5:A:603:HOH:O	2.17	0.45
1:A:467:ASN:OD1	1:A:469:ASP:HB2	2.17	0.45
1:A:7:LEU:HG	1:A:189:THR:HG21	1.99	0.44
1:B:141:HIS:CD2	1:B:142:LEU:HG	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ASP:CG	1:B:344:ARG:HG3	2.42	0.44
1:A:428:ALA:HB1	1:A:441:TYR:CZ	2.53	0.44
1:A:273:LYS:HB3	1:A:273:LYS:HE2	1.86	0.43
1:A:136:GLY:N	5:A:774:HOH:O	2.46	0.43
1:A:403:ASP:HA	1:A:412:ASN:HB3	1.99	0.42
1:B:419:LYS:HE3	1:B:423:ILE:HD11	2.02	0.42
1:A:140:LYS:HE2	5:A:908:HOH:O	2.19	0.42
1:B:182:PHE:CE2	1:B:184:LEU:HB3	2.55	0.42
1:A:332:GLU:HA	1:A:361:VAL:O	2.19	0.42
1:B:62:VAL:HG11	1:B:119:LYS:HE2	2.02	0.41
1:A:26:HIS:CD2	1:A:481:HIS:CD2	3.08	0.41
1:A:131:ASP:HB3	1:A:392:PHE:HE2	1.86	0.41
1:B:265:ALA:HB2	1:B:358:ILE:HD13	2.02	0.40
1:A:178:ALA:HB1	1:A:187:VAL:HB	2.03	0.40
1:B:222:LEU:HA	1:B:222:LEU:HD23	1.87	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	492/494 (100%)	477 (97%)	14 (3%)	1 (0%)	43	36
1	B	492/494 (100%)	476 (97%)	15 (3%)	1 (0%)	43	36
All	All	984/988 (100%)	953 (97%)	29 (3%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	295	LYS
1	B	295	LYS

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	438/438 (100%)	432 (99%)	6 (1%)	59	59
1	B	438/438 (100%)	431 (98%)	7 (2%)	55	54
All	All	876/876 (100%)	863 (98%)	13 (2%)	57	56

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	198	PHE
1	A	226	LYS
1	A	229	GLU
1	A	279	TYR
1	A	381	LEU
1	B	72	LEU
1	B	198	PHE
1	B	226	LYS
1	B	279	TYR
1	B	320	LYS
1	B	381	LEU
1	B	470	LEU

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

Mol	Chain	Res	Type
1	A	97	ASN
1	A	149	ASN
1	B	181	HIS
1	B	284	ASN
1	B	352	GLN
1	B	426	GLN
1	B	430	ASN

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 ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	GOL	B	506	-	5,5,5	0.27	0	5,5,5	0.61	0
4	GOL	A	503	-	5,5,5	0.50	0	5,5,5	0.90	0
4	GOL	B	504	-	5,5,5	0.36	0	5,5,5	0.54	0
4	GOL	A	504	-	5,5,5	0.50	0	5,5,5	0.32	0
3	OXL	B	502	2	5,5,5	1.61	1 (20%)	6,6,6	2.72	2 (33%)
3	OXL	A	502	2	5,5,5	1.84	1 (20%)	6,6,6	2.47	2 (33%)
4	GOL	B	503	-	5,5,5	0.40	0	5,5,5	0.83	0
4	GOL	B	505	-	5,5,5	0.44	0	5,5,5	0.75	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	GOL	B	506	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	503	-	-	2/4/4/4	-
4	GOL	B	504	-	-	2/4/4/4	-
4	GOL	A	504	-	-	0/4/4/4	-
3	OXL	B	502	2	-	4/4/4/4	-
3	OXL	A	502	2	-	4/4/4/4	-
4	GOL	B	503	-	-	1/4/4/4	-
4	GOL	B	505	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	OXL	O1-C1	3.31	1.30	1.22
3	B	502	OXL	O1-C1	3.04	1.30	1.22

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	OXL	O4-C2-C1	5.41	123.33	112.83
3	A	502	OXL	O4-C2-C1	4.96	122.44	112.83
3	B	502	OXL	O3-C1-C2	2.61	117.90	112.83
3	A	502	OXL	O2-C2-C1	-2.13	116.20	120.63

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	OXL	O1-C1-C2-O2
3	A	502	OXL	O3-C1-C2-O2
3	B	502	OXL	O1-C1-C2-O2
3	B	502	OXL	O3-C1-C2-O2
3	B	502	OXL	O3-C1-C2-O4
4	A	503	GOL	O1-C1-C2-C3
4	B	504	GOL	O1-C1-C2-C3
4	B	506	GOL	O1-C1-C2-C3
4	B	506	GOL	C1-C2-C3-O3
3	B	502	OXL	O1-C1-C2-O4
3	A	502	OXL	O3-C1-C2-O4
4	B	506	GOL	O1-C1-C2-O2
4	B	506	GOL	O2-C2-C3-O3
3	A	502	OXL	O1-C1-C2-O4

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Mol	Chain	Res	Type	Atoms
4	B	505	GOL	O1-C1-C2-C3
4	A	503	GOL	O1-C1-C2-O2
4	B	504	GOL	O1-C1-C2-O2
4	B	503	GOL	O1-C1-C2-O2
4	B	505	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
4	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	494/494 (100%)	1.14	67 (13%)	7 7	23, 44, 66, 80	0
1	B	494/494 (100%)	1.03	49 (9%)	13 13	22, 41, 60, 82	0
All	All	988/988 (100%)	1.09	116 (11%)	9 10	22, 43, 64, 82	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	113	LEU	4.7
1	A	72	LEU	4.1
1	A	114	ASN	4.0
1	A	281	PHE	4.0
1	A	278	ASP	3.9
1	A	112	ILE	3.9
1	B	281	PHE	3.8
1	A	58	LYS	3.6
1	B	182	PHE	3.6
1	A	4	LYS	3.4
1	B	431	THR	3.4
1	B	113	LEU	3.3
1	A	186	LYS	3.3
1	A	115	PRO	3.3
1	B	184	LEU	3.2
1	B	272	VAL	3.1
1	A	184	LEU	3.1
1	A	182	PHE	3.1
1	B	223	ASN	3.1
1	A	181	HIS	3.0
1	B	187	VAL	3.0
1	A	273	LYS	3.0
1	B	66	PHE	3.0
1	B	273	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	271	ILE	3.0
1	A	277	HIS	2.9
1	A	77	VAL	2.9
1	A	62	VAL	2.9
1	A	229	GLU	2.9
1	A	168	TRP	2.9
1	A	142	LEU	2.9
1	A	406	LEU	2.9
1	A	78	LYS	2.8
1	B	114	ASN	2.8
1	A	431	THR	2.8
1	A	271	ILE	2.8
1	A	295	LYS	2.7
1	A	160	THR	2.7
1	B	185	ASP	2.7
1	B	490	TYR	2.7
1	A	66	PHE	2.6
1	A	400	SER	2.6
1	B	277	HIS	2.6
1	A	7	LEU	2.6
1	A	434	LEU	2.6
1	A	426	GLN	2.6
1	A	272	VAL	2.6
1	A	22	TYR	2.6
1	A	471	LYS	2.6
1	B	116	SER	2.6
1	A	76	GLY	2.5
1	A	185	ASP	2.5
1	B	4	LYS	2.5
1	A	490	TYR	2.5
1	A	270	SER	2.5
1	B	186	LYS	2.5
1	A	111	GLU	2.4
1	B	56	ILE	2.4
1	B	434	LEU	2.4
1	B	229	GLU	2.4
1	B	171	GLY	2.4
1	A	119	LYS	2.4
1	A	84	VAL	2.4
1	B	278	ASP	2.3
1	A	121	THR	2.3
1	B	394	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	152	SER	2.3
1	A	105	GLU	2.3
1	B	183	TYR	2.3
1	B	88	ILE	2.3
1	B	115	PRO	2.3
1	A	276	LEU	2.3
1	B	7	LEU	2.3
1	A	81	ALA	2.3
1	A	118	VAL	2.3
1	B	77	VAL	2.3
1	A	227	ASN	2.3
1	B	296	ASN	2.3
1	A	275	LEU	2.3
1	A	297	PHE	2.2
1	B	270	SER	2.2
1	B	65	ILE	2.2
1	A	61	LEU	2.2
1	B	406	LEU	2.2
1	A	290	SER	2.2
1	A	187	VAL	2.2
1	B	297	PHE	2.2
1	B	135	ILE	2.2
1	B	202	ILE	2.2
1	A	140	LYS	2.2
1	A	301	LYS	2.2
1	A	106	ASP	2.2
1	A	57	SER	2.2
1	A	130	LEU	2.2
1	B	163	TYR	2.1
1	A	312	VAL	2.1
1	A	152	SER	2.1
1	B	72	LEU	2.1
1	A	296	ASN	2.1
1	B	118	VAL	2.1
1	B	328	GLY	2.1
1	A	170	LYS	2.1
1	B	188	LYS	2.1
1	B	295	LYS	2.1
1	B	32	LEU	2.1
1	A	59	ASP	2.1
1	A	159	GLY	2.1
1	A	274	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	291	TRP	2.1
1	B	276	LEU	2.1
1	A	178	ALA	2.1
1	B	235	ARG	2.1
1	B	224	ILE	2.0
1	B	320	LYS	2.0
1	B	55	ASP	2.0
1	A	80	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	GOL	B	503	6/6	0.79	0.20	42,48,49,53	0
4	GOL	B	504	6/6	0.79	0.25	65,66,67,67	0
4	GOL	A	503	6/6	0.84	0.15	44,47,49,51	0
4	GOL	B	505	6/6	0.84	0.15	53,55,57,58	0
4	GOL	B	506	6/6	0.87	0.16	51,58,60,62	0
4	GOL	A	504	6/6	0.88	0.14	46,53,57,60	0
3	OXL	B	502	6/6	0.94	0.10	23,24,29,32	0
3	OXL	A	502	6/6	0.95	0.10	21,25,32,35	0
2	NI	A	501	1/1	0.99	0.04	27,27,27,27	0
2	NI	B	501	1/1	0.99	0.03	26,26,26,26	0

6.5 Other polymers ⓘ

There are no such residues in this entry.