



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2022 – 03:36 PM EST

PDB ID : 7ULA
Title : Structure of the Pseudomonas putida AlgKX modification and secretion complex
Authors : Gheorghita, A.A.; Li, E.Y.; Pfoh, R.; Howell, P.L.
Deposited on : 2022-04-04
Resolution : 2.46 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
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)	:	2.31.2

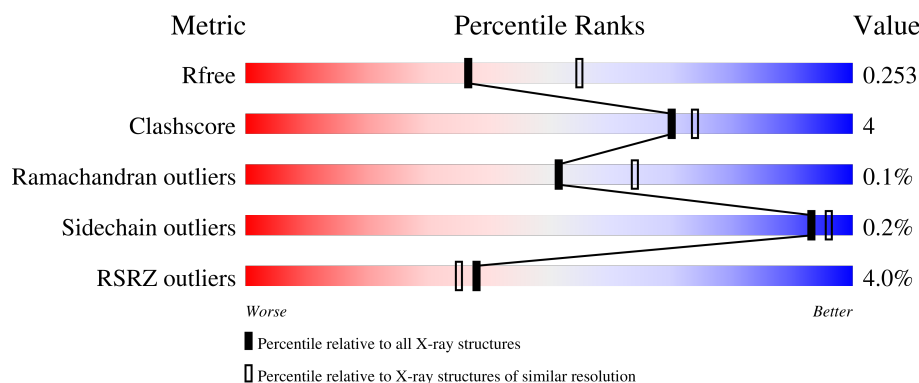
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.46 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	461	 6% 62% 6% 31%
2	A	487	 80% 8% 12%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5702 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 Alginate biosynthesis protein AlgK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	316	Total	C	N	O	S	0	2	0
			2321	1448	415	455	3			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	32	MET	-	initiating methionine	UNP Q88NC7
B	485	LEU	-	expression tag	UNP Q88NC7
B	486	GLU	-	expression tag	UNP Q88NC7
B	487	HIS	-	expression tag	UNP Q88NC7
B	488	HIS	-	expression tag	UNP Q88NC7
B	489	HIS	-	expression tag	UNP Q88NC7
B	490	HIS	-	expression tag	UNP Q88NC7
B	491	HIS	-	expression tag	UNP Q88NC7
B	492	HIS	-	expression tag	UNP Q88NC7

- Molecule 2 is a protein called Alginate biosynthesis protein AlgX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	430	Total	C	N	O	S	0	0	0
			3323	2096	569	641	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	480	LEU	-	expression tag	UNP Q88ND0
A	481	GLU	-	expression tag	UNP Q88ND0
A	482	HIS	-	expression tag	UNP Q88ND0
A	483	HIS	-	expression tag	UNP Q88ND0
A	484	HIS	-	expression tag	UNP Q88ND0
A	485	HIS	-	expression tag	UNP Q88ND0
A	486	HIS	-	expression tag	UNP Q88ND0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	487	HIS	-	expression tag	UNP Q88ND0

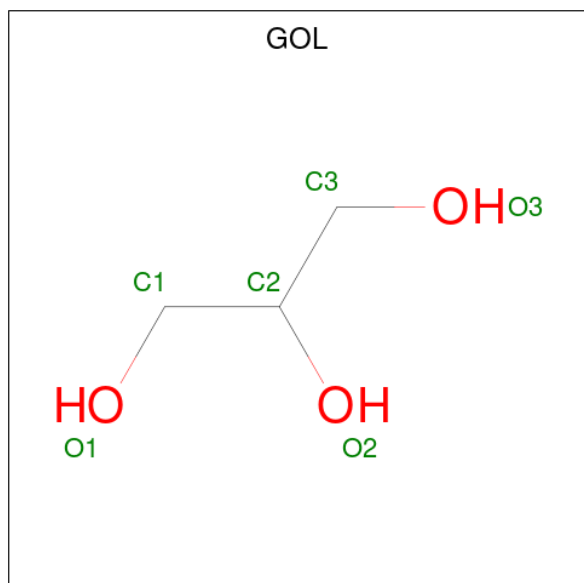
- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Ni 2 2	0	0
3	A	4	Total Ni 4 4	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

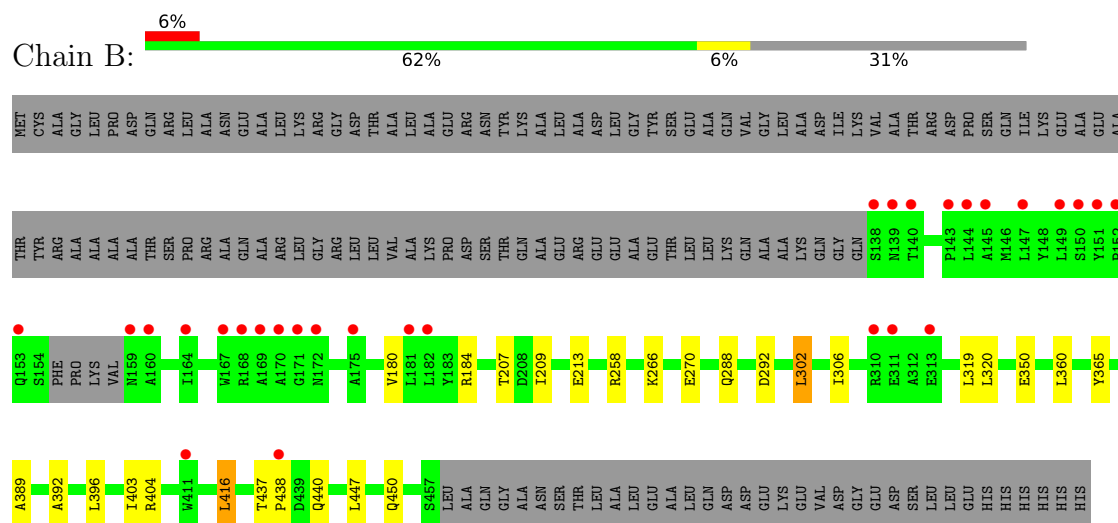
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	5	Total	O	0	0
			5	5		
6	A	22	Total	O	0	0
			22	22		

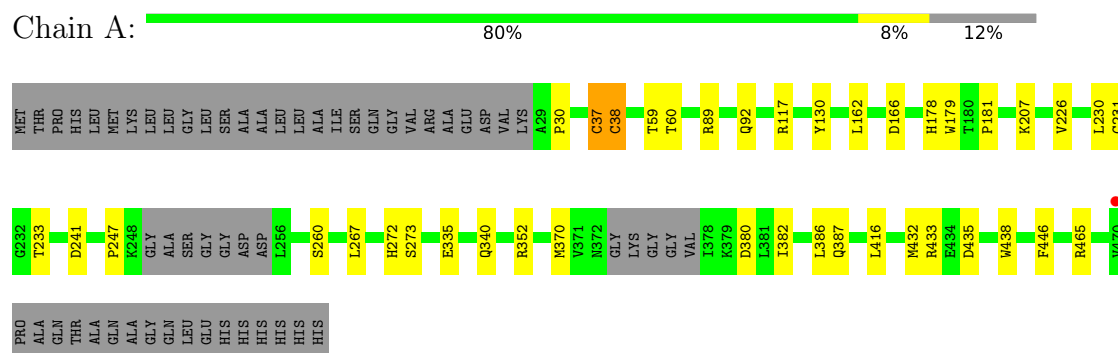
3 Residue-property plots

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: Alginate biosynthesis protein AlgK



• Molecule 2: Alginate biosynthesis protein AlgX



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.95Å 169.95Å 143.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.00 – 2.46 46.00 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.00-2.46) 99.9 (46.00-2.46)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874+SVN	Depositor
R, R_{free}	0.215 , 0.254 0.215 , 0.253	Depositor DCC
R_{free} test set	1916 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.9	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	0.95	EDS
Total number of atoms	5702	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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, NI

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	0.32	0/2367	0.54	3/3227 (0.1%)
2	A	0.33	0/3398	0.54	0/4615
All	All	0.32	0/5765	0.54	3/7842 (0.0%)

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
2	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	447	LEU	CB-CG-CD2	-5.73	101.25	111.00
1	B	416	LEU	CB-CG-CD2	-5.29	102.00	111.00
1	B	302	LEU	CA-CB-CG	5.21	127.28	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	37	CYS	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	B	2321	0	2166	16	0
2	A	3323	0	3106	25	0
3	A	4	0	0	0	0
3	B	2	0	0	0	0
4	B	1	0	0	0	0
5	A	24	0	32	0	0
6	A	22	0	0	0	0
6	B	5	0	0	0	0
All	All	5702	0	5304	39	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 (39) 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)
2:A:433:ARG:HD3	2:A:438:TRP:CG	2.20	0.76
1:B:450:GLN:HG2	2:A:30:PRO:HG3	1.77	0.66
2:A:370:MET:HG3	2:A:446:PHE:HB3	1.77	0.66
2:A:380:ASP:OD2	2:A:382:ILE:HD11	1.96	0.64
1:B:207:THR:HG22	1:B:209:ILE:HG22	1.80	0.63
2:A:207:LYS:HE2	2:A:247:PRO:HB3	1.80	0.63
1:B:437:THR:OG1	1:B:440:GLN:HG3	1.99	0.61
2:A:387:GLN:HG3	2:A:465:ARG:HG2	1.83	0.58
1:B:180:VAL:O	1:B:184:ARG:HG3	2.08	0.54
2:A:386:LEU:HB2	2:A:432:MET:HG2	1.90	0.52
1:B:258[B]:ARG:HH21	1:B:292:ASP:HB3	1.75	0.51
2:A:433:ARG:HD3	2:A:438:TRP:CD1	2.44	0.51
2:A:89:ARG:NH2	2:A:335:GLU:OE2	2.44	0.51
2:A:340:GLN:NE2	2:A:416:LEU:HD22	2.26	0.51
2:A:207:LYS:HD2	2:A:260:SER:OG	2.11	0.50
1:B:319:LEU:HD22	1:B:350:GLU:HG2	1.95	0.49
1:B:437:THR:HB	1:B:438:PRO:HD2	1.95	0.48
1:B:266:LYS:O	1:B:270:GLU:HG3	2.12	0.48
1:B:288:GLN:HG2	1:B:320:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:LEU:HD23	1:B:306:ILE:HD11	1.98	0.46
1:B:404:ARG:HA	2:A:37:CYS:HB2	1.98	0.45
2:A:433:ARG:HD3	2:A:438:TRP:CD2	2.51	0.45
2:A:352:ARG:HE	2:A:352:ARG:HB2	1.53	0.44
1:B:184:ARG:NH1	1:B:213:GLU:OE1	2.51	0.44
2:A:178:HIS:HA	2:A:272:HIS:CE1	2.53	0.43
2:A:181:PRO:HG2	2:A:241:ASP:O	2.18	0.43
2:A:162:LEU:HD13	2:A:166:ASP:O	2.18	0.43
1:B:396:LEU:HG	1:B:403:ILE:HD12	2.01	0.43
2:A:59:THR:HA	2:A:60:THR:HA	1.80	0.42
2:A:267:LEU:HD21	2:A:273:SER:HB3	2.02	0.42
2:A:433:ARG:NE	2:A:435:ASP:OD1	2.49	0.42
2:A:117:ARG:HD2	2:A:130:TYR:CD1	2.55	0.42
1:B:389:ALA:O	1:B:392:ALA:HB3	2.20	0.41
2:A:89:ARG:NH1	2:A:92:GLN:OE1	2.47	0.41
2:A:37:CYS:O	2:A:38:CYS:HB2	2.20	0.41
1:B:360:LEU:HD12	1:B:365:TYR:HD2	1.84	0.41
2:A:226:VAL:O	2:A:230:LEU:HD23	2.21	0.40
2:A:231:CYS:O	2:A:233:THR:HG23	2.21	0.40
1:B:416:LEU:HD23	1:B:416:LEU:HA	1.73	0.40

There are no symmetry-related clashes.

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	314/461 (68%)	306 (98%)	8 (2%)	0	100	100
2	A	424/487 (87%)	411 (97%)	12 (3%)	1 (0%)	47	57
All	All	738/948 (78%)	717 (97%)	20 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	38	CYS

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	213/357 (60%)	213 (100%)	0	100	100
2	A	339/403 (84%)	338 (100%)	1 (0%)	92	95
All	All	552/760 (73%)	551 (100%)	1 (0%)	93	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	179	TRP

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

Mol	Chain	Res	Type
2	A	262	ASN

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

Of 11 ligands modelled in this entry, 7 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
5	GOL	A	508	-	5,5,5	0.86	0	5,5,5	0.98	0
5	GOL	A	506	-	5,5,5	1.13	1 (20%)	5,5,5	0.94	0
5	GOL	A	505	-	5,5,5	1.00	0	5,5,5	0.99	0
5	GOL	A	507	-	5,5,5	0.72	0	5,5,5	1.02	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
5	GOL	A	508	-	-	0/4/4/4	-
5	GOL	A	506	-	-	0/4/4/4	-
5	GOL	A	505	-	-	2/4/4/4	-
5	GOL	A	507	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	506	GOL	O2-C2	-2.15	1.37	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	505	GOL	O1-C1-C2-C3
5	A	507	GOL	C1-C2-C3-O3
5	A	505	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	507	GOL	O2-C2-C3-O3

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	316/461 (68%)	0.48	29 (9%) 9 6	50, 74, 128, 149	0
2	A	430/487 (88%)	0.12	1 (0%) 95 95	44, 62, 93, 122	0
All	All	746/948 (78%)	0.28	30 (4%) 38 35	44, 66, 118, 149	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	170	ALA	6.9
1	B	151	TYR	4.4
1	B	144	LEU	3.9
1	B	152	PRO	3.8
1	B	171	GLY	3.7
1	B	160	ALA	3.7
1	B	167	TRP	3.6
1	B	149	LEU	3.6
1	B	313	GLU	3.5
1	B	175	ALA	3.4
1	B	150	SER	3.4
1	B	169	ALA	3.2
1	B	143	PRO	3.1
1	B	159	ASN	3.1
1	B	145	ALA	2.9
1	B	138	SER	2.9
1	B	182	LEU	2.8
1	B	164	ILE	2.7
1	B	140	THR	2.7
1	B	153	GLN	2.6
1	B	147	LEU	2.6
1	B	438	PRO	2.4
1	B	311	GLU	2.4
1	B	172	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	168	ARG	2.3
2	A	470	VAL	2.2
1	B	139	ASN	2.1
1	B	310	ARG	2.1
1	B	181	LEU	2.1
1	B	411	TRP	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
5	GOL	A	508	6/6	0.70	0.27	66,80,81,100	0
3	NI	B	501	1/1	0.74	0.15	132,132,132,132	0
3	NI	A	502	1/1	0.80	0.10	135,135,135,135	0
5	GOL	A	507	6/6	0.82	0.24	63,70,74,88	0
3	NI	A	503	1/1	0.86	0.21	127,127,127,127	0
5	GOL	A	506	6/6	0.87	0.40	72,74,79,81	0
3	NI	B	502	1/1	0.89	0.09	116,116,116,116	0
3	NI	A	504	1/1	0.89	0.11	116,116,116,116	0
5	GOL	A	505	6/6	0.89	0.28	71,73,80,83	0
4	CL	B	503	1/1	0.94	0.17	88,88,88,88	0
3	NI	A	501	1/1	0.95	0.08	121,121,121,121	0

6.5 Other polymers [i](#)

There are no such residues in this entry.