wwPDB X-ray Structure Validation Summary Report (i)

Jun 27, 2023 – 01:34 pm BST

PDB ID	:	8ORN
Title	:	Crystal structure of Xanthomonas campestris pv. campestris LolA-LolB complex
Authors	:	Furlanetto, V.; Divne, C.
Deposited on	:	2023-04-14
Resolution	:	2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (1)) were used in the production of this report:

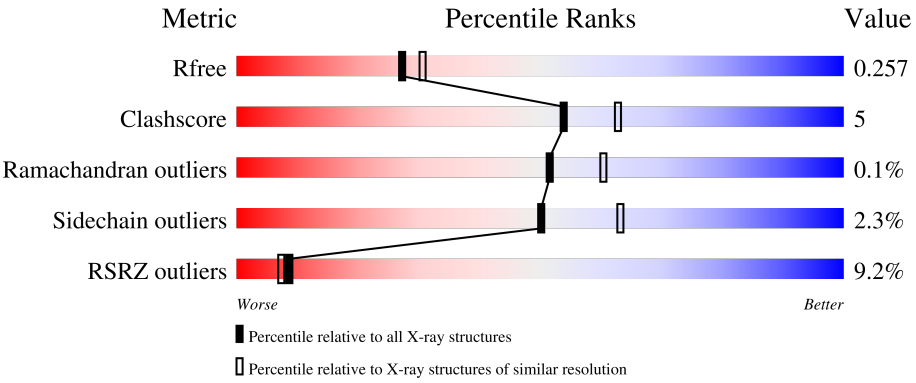
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	204	9% 74% 16% 9%
1	C	204	12% 76% 14% 9%
2	B	212	6% 73% 11% 15%
2	D	212	6% 79% 6% 15%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5711 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 Outer-membrane lipoprotein carrier protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	1	0
			1448	909	260	277	2			
1	C	185	Total	C	N	O	S	0	0	0
			1440	904	257	277	2			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP B0RT42
A	189	ALA	-	expression tag	UNP B0RT42
A	190	GLU	-	expression tag	UNP B0RT42
A	191	ASN	-	expression tag	UNP B0RT42
A	192	LEU	-	expression tag	UNP B0RT42
A	193	TYR	-	expression tag	UNP B0RT42
A	194	PHE	-	expression tag	UNP B0RT42
A	195	GLN	-	expression tag	UNP B0RT42
A	196	SER	-	expression tag	UNP B0RT42
A	197	HIS	-	expression tag	UNP B0RT42
A	198	HIS	-	expression tag	UNP B0RT42
A	199	HIS	-	expression tag	UNP B0RT42
A	200	HIS	-	expression tag	UNP B0RT42
A	201	HIS	-	expression tag	UNP B0RT42
A	202	HIS	-	expression tag	UNP B0RT42
C	-1	MET	-	initiating methionine	UNP B0RT42
C	189	ALA	-	expression tag	UNP B0RT42
C	190	GLU	-	expression tag	UNP B0RT42
C	191	ASN	-	expression tag	UNP B0RT42
C	192	LEU	-	expression tag	UNP B0RT42
C	193	TYR	-	expression tag	UNP B0RT42
C	194	PHE	-	expression tag	UNP B0RT42
C	195	GLN	-	expression tag	UNP B0RT42
C	196	SER	-	expression tag	UNP B0RT42
C	197	HIS	-	expression tag	UNP B0RT42

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Chain	Residue	Modelled	Actual	Comment	Reference
C	198	HIS	-	expression tag	UNP B0RT42
C	199	HIS	-	expression tag	UNP B0RT42
C	200	HIS	-	expression tag	UNP B0RT42
C	201	HIS	-	expression tag	UNP B0RT42
C	202	HIS	-	expression tag	UNP B0RT42

- Molecule 2 is a protein called Outer-membrane lipoprotein LolB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	0	0
			1393	862	267	263	1			
2	D	180	Total	C	N	O	S	0	0	0
			1393	862	267	263	1			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP B0RUA2
B	199	ALA	-	expression tag	UNP B0RUA2
B	200	GLU	-	expression tag	UNP B0RUA2
B	201	ASN	-	expression tag	UNP B0RUA2
B	202	LEU	-	expression tag	UNP B0RUA2
B	203	TYR	-	expression tag	UNP B0RUA2
B	204	PHE	-	expression tag	UNP B0RUA2
B	205	GLN	-	expression tag	UNP B0RUA2
B	206	SER	-	expression tag	UNP B0RUA2
B	207	HIS	-	expression tag	UNP B0RUA2
B	208	HIS	-	expression tag	UNP B0RUA2
B	209	HIS	-	expression tag	UNP B0RUA2
B	210	HIS	-	expression tag	UNP B0RUA2
B	211	HIS	-	expression tag	UNP B0RUA2
B	212	HIS	-	expression tag	UNP B0RUA2
D	1	MET	-	initiating methionine	UNP B0RUA2
D	199	ALA	-	expression tag	UNP B0RUA2
D	200	GLU	-	expression tag	UNP B0RUA2
D	201	ASN	-	expression tag	UNP B0RUA2
D	202	LEU	-	expression tag	UNP B0RUA2
D	203	TYR	-	expression tag	UNP B0RUA2
D	204	PHE	-	expression tag	UNP B0RUA2
D	205	GLN	-	expression tag	UNP B0RUA2
D	206	SER	-	expression tag	UNP B0RUA2
D	207	HIS	-	expression tag	UNP B0RUA2

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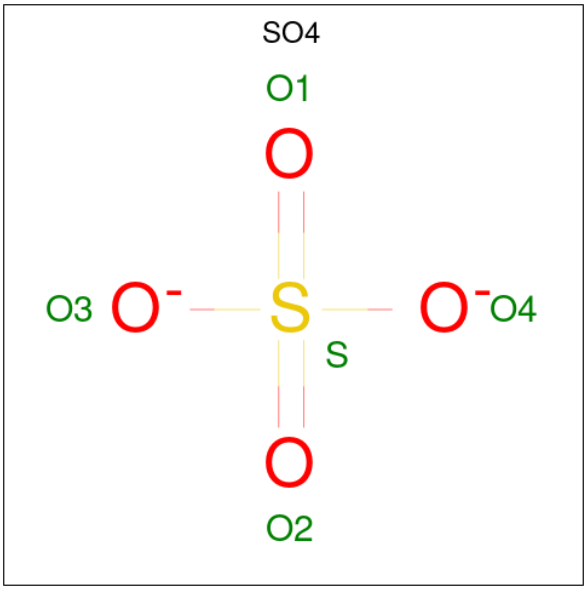
Chain	Residue	Modelled	Actual	Comment	Reference
D	208	HIS	-	expression tag	UNP B0RUA2
D	209	HIS	-	expression tag	UNP B0RUA2
D	210	HIS	-	expression tag	UNP B0RUA2
D	211	HIS	-	expression tag	UNP B0RUA2
D	212	HIS	-	expression tag	UNP B0RUA2

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

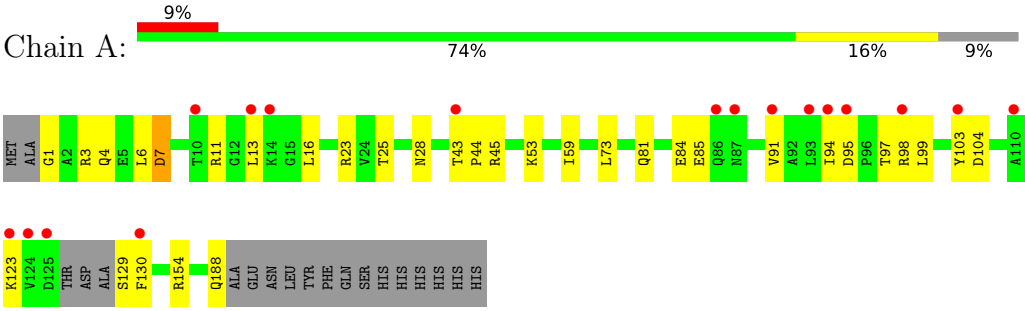
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total O 3 3	0	0
4	B	7	Total O 7 7	0	0
4	C	4	Total O 4 4	0	0
4	D	13	Total O 13 13	0	0

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.

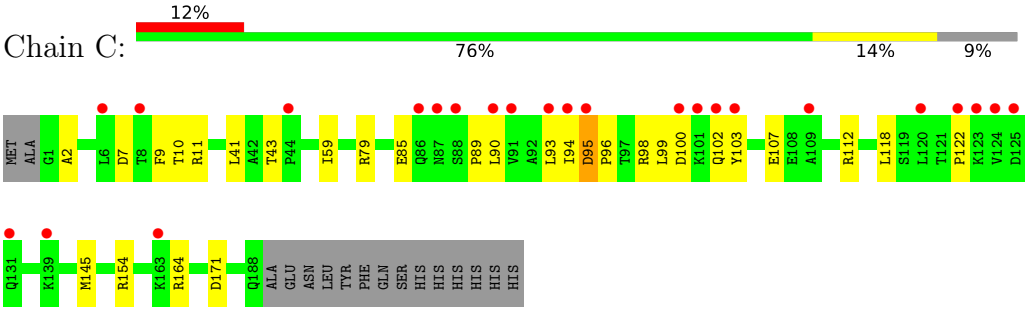
• Molecule 1: Outer-membrane lipoprotein carrier protein

Chain A:



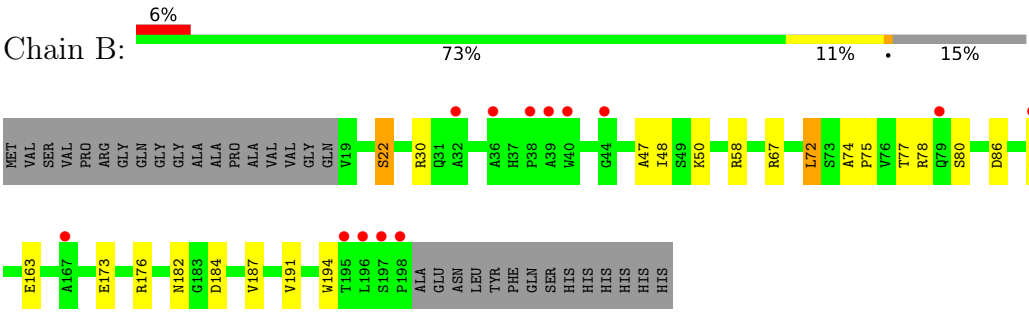
• Molecule 1: Outer-membrane lipoprotein carrier protein

Chain C:



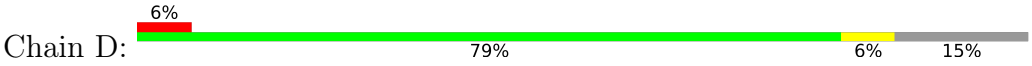
• Molecule 2: Outer-membrane lipoprotein LolB

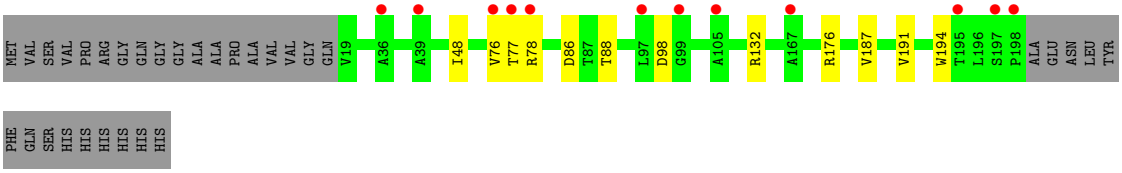
Chain B:



• Molecule 2: Outer-membrane lipoprotein LolB

Chain D:




MET VAL SER VAL PRO ARG GLY GLN GLY GLY ALA ALA PRO ALA VAL VAL GLY GLN
V19 A36 A39 I48 V76 T77 R78 D86 T87 T88 L97 D98 G99 A105 R132 A167 R176 V187 V191 W194 T195 L196 S197 P198
ALA GLU ASN LEU TYR
PHE GLN SER HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	137.51Å 137.51Å 145.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.40 – 2.20 48.40 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.40-2.20) 99.9 (48.40-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.221 , 0.261 0.217 , 0.257	Depositor DCC
R_{free} test set	1997 reflections (3.84%)	wwPDB-VP
Wilson B-factor (Å^2)	66.4	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.020 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5711	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.43	0/1479	0.68	0/1998
1	C	0.40	0/1468	0.69	1/1984 (0.1%)
2	B	0.48	0/1427	0.72	1/1947 (0.1%)
2	D	0.47	0/1427	0.72	0/1947
All	All	0.44	0/5801	0.70	2/7876 (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
1	A	0	3
1	C	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	107	GLU	N-CA-CB	-5.79	100.19	110.60
2	B	72	LEU	CA-CB-CG	-5.61	102.40	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23[A]	ARG	Sidechain
1	A	23[B]	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	45	ARG	Sidechain
1	C	100	ASP	Peptide

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	1448	0	1429	19	0
1	C	1440	0	1416	24	0
2	B	1393	0	1341	14	1
2	D	1393	0	1341	8	0
3	B	5	0	0	0	0
3	D	5	0	0	0	0
4	A	3	0	0	0	0
4	B	7	0	0	0	0
4	C	4	0	0	0	0
4	D	13	0	0	0	0
All	All	5711	0	5527	59	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 5.

The worst 5 of 59 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:C:7:ASP:O	1:C:11:ARG:HG3	1.65	0.95
2:B:58:ARG:O	2:B:72:LEU:HD12	1.74	0.86
1:C:59:ILE:HD13	2:D:76:VAL:HG12	1.59	0.85
1:C:85:GLU:OE1	1:C:102:GLN:NE2	2.11	0.84
1:A:85:GLU:O	1:A:103:TYR:OH	2.00	0.77

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)
2:B:67:ARG:NH2	2:B:86:ASP:OD2[3_665]	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	182/204 (89%)	174 (96%)	8 (4%)	0	100 100
1	C	181/204 (89%)	168 (93%)	13 (7%)	0	100 100
2	B	178/212 (84%)	176 (99%)	1 (1%)	1 (1%)	25 26
2	D	178/212 (84%)	174 (98%)	4 (2%)	0	100 100
All	All	719/832 (86%)	692 (96%)	26 (4%)	1 (0%)	51 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	75	PRO

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	151/166 (91%)	145 (96%)	6 (4%)	31 40
1	C	150/166 (90%)	148 (99%)	2 (1%)	69 81
2	B	138/162 (85%)	136 (99%)	2 (1%)	67 80
2	D	138/162 (85%)	135 (98%)	3 (2%)	52 65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	577/656 (88%)	564 (98%)	13 (2%)	50 63

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	98	ASP
1	C	95	ASP
2	D	176	ARG
2	D	98	ASP
2	D	132	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
2	B	62	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	SO4	D	301	-	4,4,4	0.19	0	6,6,6	0.20	0
3	SO4	B	301	-	4,4,4	0.08	0	6,6,6	0.33	0

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, 95^{th} 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	185/204 (90%)	0.60	18 (9%) 7 6	52, 77, 131, 148	0
1	C	185/204 (90%)	0.77	24 (12%) 3 3	53, 85, 131, 152	0
2	B	180/212 (84%)	0.50	13 (7%) 15 14	49, 61, 86, 111	0
2	D	180/212 (84%)	0.36	12 (6%) 17 16	48, 61, 91, 123	0
All	All	730/832 (87%)	0.56	67 (9%) 9 7	48, 67, 122, 152	0

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	94	ILE	9.0
1	A	94	ILE	7.9
1	C	87	ASN	5.4
1	A	124	VAL	5.4
1	C	103	TYR	5.3

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 monosaccharides 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, 95^{th} 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
3	SO4	B	301	5/5	0.91	0.13	76,81,95,102	0
3	SO4	D	301	5/5	0.93	0.16	79,81,92,94	0

6.5 Other polymers (i)

There are no such residues in this entry.