Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 08:21 PM GMT

PDB ID	:	4Y7O
Title	:	T6SS protein TssM C-terminal domain (869-1107) from EAEC
Authors	:	Nguyen, V.S.; Spinelli, S.; Durand, E.; Roussel, A.; Cambillau, C.
Deposited on	:	2015-02-15
Resolution	:	2.24 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

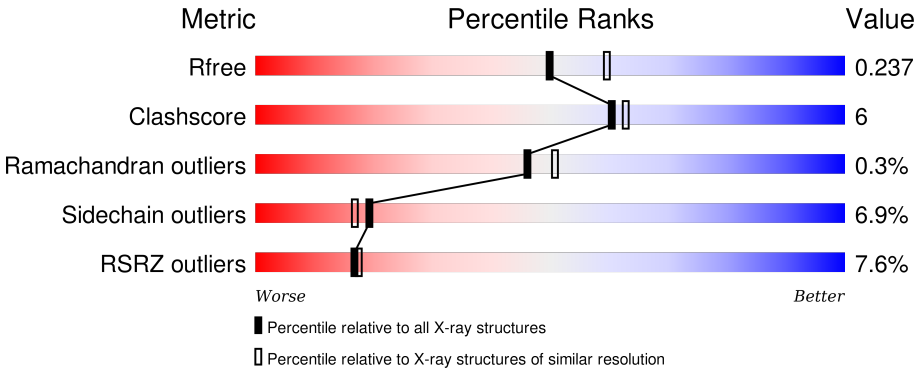
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

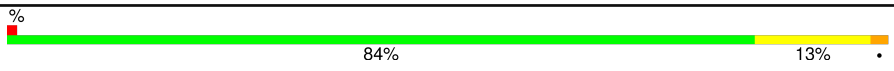
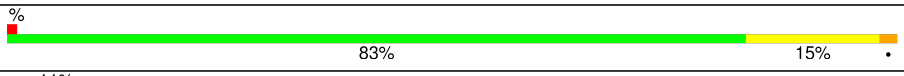
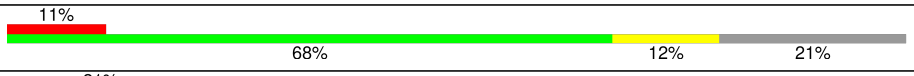
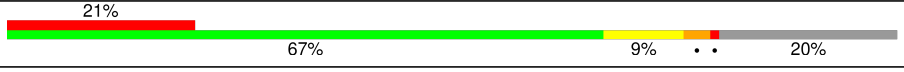
The reported resolution of this entry is 2.24 Å.

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}	91344	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	240	
1	B	240	
2	C	155	
2	D	155	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5901 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 Type VI secretion protein IcmF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1841	1176	322	339	4			
1	B	239	Total	C	N	O	S	0	0	0
			1839	1172	324	339	4			

- Molecule 2 is a protein called Type VI secretion system protein VasD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	123	Total	C	N	O	S	0	0	0
			924	589	159	174	2			
2	D	124	Total	C	N	O	S	0	0	0
			914	583	150	179	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	GLY	-	expression tag	UNP H4VA93
D	1	GLY	-	expression tag	UNP H4VA93

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is water.

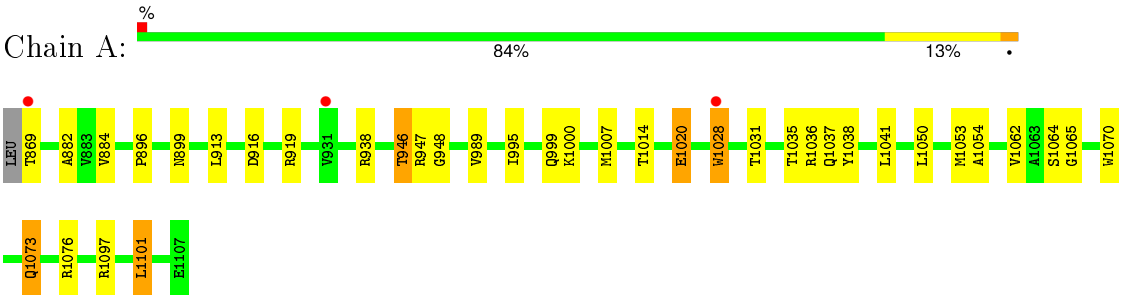
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	158	Total O 158 158	0	0
4	B	156	Total O 156 156	0	0
4	C	33	Total O 33 33	0	0
4	D	32	Total O 32 32	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

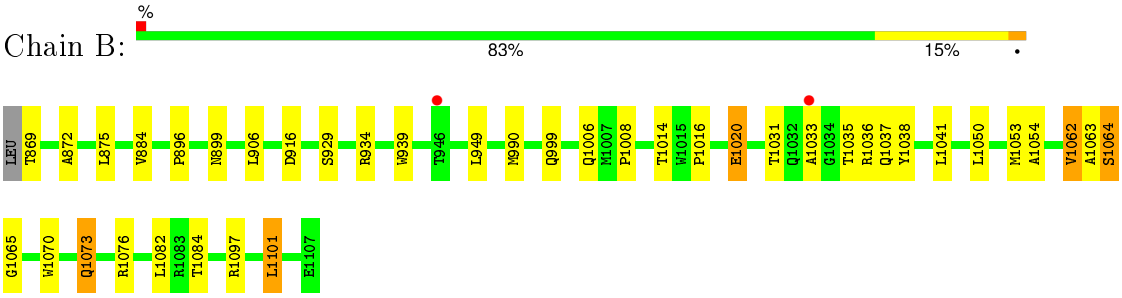
- Molecule 1: Type VI secretion protein IcmF

Chain A:



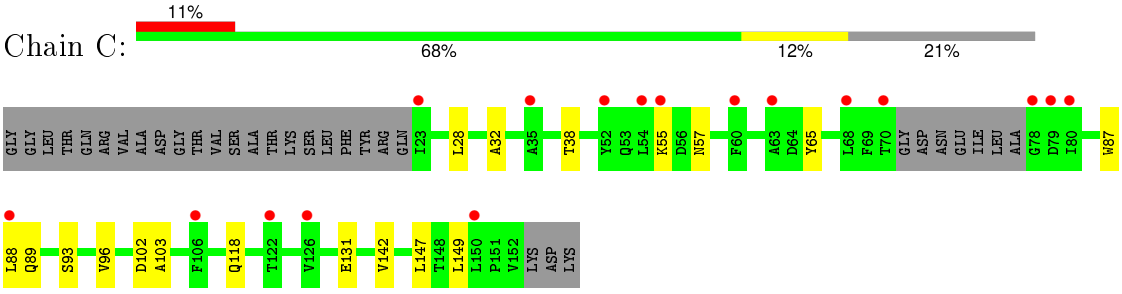
- Molecule 1: Type VI secretion protein IcmF

Chain B:



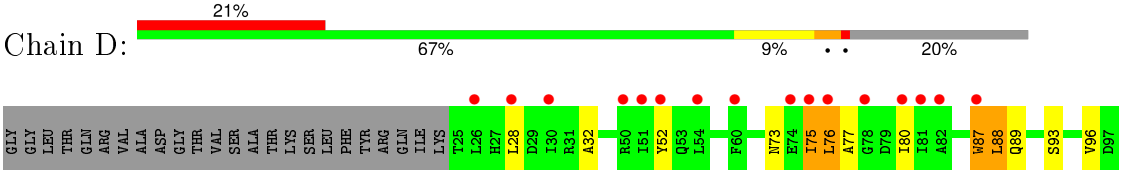
- Molecule 2: Type VI secretion system protein VasD

Chain C:



- Molecule 2: Type VI secretion system protein VasD

Chain D:




N98
P99
L100
D101
ASP
AIA
A104
T107
G108
V109
A110
F113
L114
D117
T122
V125
V126
L127
D130
E131
L132
R138
L139
I140
E141
V142
L147
T148
L149
L150
PRO
VAL
LYS
ASP
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	85.47Å 85.47Å 256.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.34 – 2.24 49.34 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.34-2.24) 99.7 (49.34-2.24)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.25Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.204 , 0.224 0.211 , 0.237	Depositor DCC
R_{free} test set	2321 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	48.6	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 52.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 46408 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5901	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN

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	0/1888	0.75	2/2580 (0.1%)
1	B	0.51	0/1886	0.69	0/2577
2	C	0.48	0/940	0.72	0/1282
2	D	0.45	0/929	0.77	1/1272 (0.1%)
All	All	0.49	0/5643	0.73	3/7711 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	130	ASP	C-N-CA	7.84	141.31	121.70
1	A	946	THR	N-CA-C	-6.31	93.97	111.00
1	A	947	ARG	C-N-CA	6.17	135.26	122.30

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	1841	0	1802	22	0
1	B	1839	0	1791	24	0
2	C	924	0	915	8	0
2	D	914	0	877	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	158	0	0	0	0
4	B	156	0	0	1	0
4	C	33	0	0	1	0
4	D	32	0	0	0	0
All	All	5901	0	5385	61	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 6.

All (61) 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:1073:GLN:HE21	1:A:1073:GLN:H	1.13	0.93
1:B:1073:GLN:HE21	1:B:1073:GLN:H	1.17	0.92
1:A:1031:THR:HG22	2:C:89:GLN:HE22	1.44	0.82
1:A:999:GLN:HE22	1:A:1014:THR:H	1.25	0.81
1:A:896:PRO:O	1:A:1097:ARG:HD2	1.81	0.81
1:B:999:GLN:HE22	1:B:1014:THR:H	1.29	0.79
1:B:896:PRO:O	1:B:1097:ARG:HD2	1.84	0.77
1:A:1028:TRP:HZ3	1:A:1073:GLN:NE2	1.85	0.74
1:B:1073:GLN:NE2	1:B:1073:GLN:H	1.90	0.69
2:D:32:ALA:HB2	2:D:88:LEU:HD23	1.74	0.68
2:C:142:VAL:HG22	2:C:147:LEU:HD23	1.75	0.67
2:D:127:LEU:HD21	2:D:149:LEU:HG	1.76	0.66
1:A:1073:GLN:H	1:A:1073:GLN:NE2	1.90	0.66
1:A:882:ALA:HB1	1:A:919:ARG:HH21	1.63	0.64
1:A:1050:LEU:HA	1:A:1053:MET:HE2	1.79	0.63
1:B:1050:LEU:HA	1:B:1053:MET:HE2	1.81	0.62
1:A:1062:VAL:HG13	1:A:1065:GLY:HA3	1.82	0.61
1:A:1028:TRP:CZ3	1:A:1073:GLN:NE2	2.67	0.60
1:A:882:ALA:HB1	1:A:919:ARG:NH2	2.18	0.59
1:B:884:VAL:HG22	1:B:1101:LEU:HD13	1.85	0.58
1:B:1062:VAL:HG22	1:B:1063:ALA:HA	1.85	0.58
2:D:73:ASN:HB3	2:D:76:LEU:HB2	1.85	0.57
1:A:1041:LEU:HD11	1:A:1053:MET:HE1	1.89	0.55
1:A:884:VAL:HG22	1:A:1101:LEU:HD13	1.88	0.55
1:B:934:ARG:HD3	1:B:939:TRP:CE2	2.43	0.53
2:D:131:GLU:O	2:D:138:ARG:HD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:THR:C	1:A:948:GLY:HA2	2.30	0.52
1:A:1020:GLU:CD	1:A:1020:GLU:H	2.12	0.52
1:B:1020:GLU:H	1:B:1020:GLU:CD	2.14	0.51
1:B:899:ASN:HB2	1:B:1097:ARG:NH2	2.27	0.50
1:B:1036:ARG:NH2	1:B:1073:GLN:HG3	2.26	0.50
1:A:899:ASN:HB2	1:A:1097:ARG:NH2	2.27	0.50
1:A:1007:MET:HB2	2:C:65:TYR:CE1	2.48	0.48
1:A:989:VAL:HG13	1:A:1028:TRP:HD1	1.79	0.48
1:B:1041:LEU:HD11	1:B:1053:MET:HE1	1.95	0.48
2:C:142:VAL:HG22	2:C:147:LEU:CD2	2.42	0.48
1:B:1006:GLN:HG2	4:B:1339:HOH:O	2.12	0.47
2:D:130:ASP:HB2	2:D:131:GLU:HB2	1.95	0.47
2:D:77:ALA:O	2:D:80:ILE:HG22	2.15	0.46
2:D:73:ASN:HD21	2:D:75:ILE:HD12	1.79	0.46
1:B:872:ALA:HB2	1:B:949:LEU:HD22	1.97	0.46
1:B:1065:GLY:HA2	1:B:1082:LEU:O	2.16	0.45
1:B:1064:SER:HB2	1:B:1084:THR:OG1	2.17	0.45
2:D:28:LEU:HB2	2:D:96:VAL:HB	1.99	0.45
2:C:32:ALA:HB2	2:C:88:LEU:HD21	1.99	0.45
1:A:1038:TYR:HE2	1:A:1053:MET:HE3	1.82	0.44
2:C:118:GLN:HG2	4:C:312:HOH:O	2.17	0.44
2:C:55:LYS:HE3	2:C:103:ALA:HB1	1.98	0.44
1:A:1036:ARG:NH2	1:A:1073:GLN:HG3	2.32	0.44
1:B:1054:ALA:HB2	1:B:1070:TRP:CE2	2.53	0.44
1:A:995:ILE:HG12	1:A:1000:LYS:HG2	2.00	0.44
2:C:28:LEU:HB2	2:C:96:VAL:HB	1.99	0.43
1:B:990:MET:O	2:D:87:TRP:HH2	2.01	0.43
1:B:1038:TYR:HE2	1:B:1053:MET:HE3	1.82	0.43
2:D:52:TYR:HD2	2:D:80:ILE:HD12	1.82	0.43
1:A:1054:ALA:HB2	1:A:1070:TRP:CE2	2.54	0.43
1:B:1063:ALA:HB1	1:B:1064:SER:HA	2.01	0.42
1:B:990:MET:O	2:D:87:TRP:CH2	2.73	0.42
1:B:906:LEU:HD13	1:B:1016:PRO:HG3	2.03	0.41
1:B:1033:ALA:HB3	1:B:1036:ARG:HD3	2.02	0.41
1:B:1008:PRO:HD3	2:D:114:LEU:HD12	2.04	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	237/240 (99%)	229 (97%)	8 (3%)	0	100	100
1	B	237/240 (99%)	229 (97%)	8 (3%)	0	100	100
2	C	119/155 (77%)	115 (97%)	3 (2%)	1 (1%)	24	20
2	D	120/155 (77%)	117 (98%)	2 (2%)	1 (1%)	24	20
All	All	713/790 (90%)	690 (97%)	21 (3%)	2 (0%)	46	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	131	GLU
2	C	102	ASP

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	188/195 (96%)	176 (94%)	12 (6%)	22	20
1	B	187/195 (96%)	174 (93%)	13 (7%)	19	16
2	C	96/129 (74%)	90 (94%)	6 (6%)	22	20
2	D	93/129 (72%)	85 (91%)	8 (9%)	13	9
All	All	564/648 (87%)	525 (93%)	39 (7%)	19	17

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	869	THR
1	A	913	LEU
1	A	916	ASP
1	A	938	ARG
1	A	1020	GLU
1	A	1028	TRP
1	A	1035	THR
1	A	1037	GLN
1	A	1064	SER
1	A	1073	GLN
1	A	1076	ARG
1	A	1101	LEU
1	B	869	THR
1	B	875	LEU
1	B	916	ASP
1	B	929	SER
1	B	1020	GLU
1	B	1031	THR
1	B	1035	THR
1	B	1037	GLN
1	B	1062	VAL
1	B	1064	SER
1	B	1073	GLN
1	B	1076	ARG
1	B	1101	LEU
2	C	38	THR
2	C	57	ASN
2	C	87	TRP
2	C	93	SER
2	C	131	GLU
2	C	149	LEU
2	D	75	ILE
2	D	76	LEU
2	D	87	TRP
2	D	88	LEU
2	D	89	GLN
2	D	93	SER
2	D	131	GLU
2	D	141	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	999	GLN
1	A	1073	GLN
1	A	1098	ASN
1	B	999	GLN
1	B	1073	GLN
1	B	1098	ASN
2	C	57	ASN
2	C	89	GLN
2	D	53	GLN
2	D	73	ASN
2	D	89	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	239/240 (99%)	0.08	3 (1%) 79 81	34, 48, 76, 104	0
1	B	239/240 (99%)	-0.01	2 (0%) 87 87	35, 48, 84, 103	0
2	C	123/155 (79%)	0.77	17 (13%) 4 4	50, 75, 102, 112	5 (4%)
2	D	124/155 (80%)	1.13	33 (26%) 1 1	55, 85, 114, 131	4 (3%)
All	All	725/790 (91%)	0.35	55 (7%) 17 17	34, 56, 101, 131	9 (1%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	60	PHE	6.5
1	B	946	THR	5.9
2	D	80	ILE	4.7
2	D	126	VAL	4.4
2	D	81	ILE	4.3
2	D	148	THR	4.2
2	D	100	LEU	4.1
2	C	60	PHE	4.1
2	D	149	LEU	4.1
2	D	98	MET	3.9
2	D	142	VAL	3.8
2	D	26	LEU	3.6
1	A	931	VAL	3.4
2	C	150	LEU	3.3
2	D	99	PRO	3.3
2	D	132	LEU	3.3
2	D	109	VAL	3.2
2	D	54	LEU	3.2
2	C	88	LEU	3.0
2	C	78	GLY	2.9
2	C	106	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	51	ILE	2.9
2	D	139	LEU	2.9
2	D	87	TRP	2.8
2	C	70	THR	2.8
2	D	125	VAL	2.8
1	A	1028	TRP	2.8
2	D	76	LEU	2.7
2	D	122	THR	2.7
2	C	23	ILE	2.7
2	C	80	ILE	2.7
2	D	147	LEU	2.6
2	D	75	ILE	2.6
2	C	35	ALA	2.6
2	D	50	ARG	2.5
2	C	68	LEU	2.5
2	D	82	ALA	2.4
1	A	869	THR	2.4
1	B	1033	ALA	2.4
2	D	110	ALA	2.4
2	D	28	LEU	2.4
2	D	117	ASP	2.4
2	C	55	LYS	2.4
2	D	113	PHE	2.3
2	C	126	VAL	2.3
2	C	63	ALA	2.3
2	D	78	GLY	2.3
2	D	107	THR	2.2
2	C	52	TYR	2.2
2	C	122	THR	2.2
2	D	52	TYR	2.2
2	C	54	LEU	2.2
2	C	79	ASP	2.1
2	D	74	GLU	2.1
2	D	30	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	ZN	B	1201	1/1	0.96	0.13	-0.38	89,89,89,89	0
3	ZN	A	1202	1/1	0.99	0.13	-1.21	47,47,47,47	0
3	ZN	C	201	1/1	0.98	0.04	-	83,83,83,83	0
3	ZN	A	1201	1/1	0.96	0.04	-	103,103,103,103	0

6.5 Other polymers (i)

There are no such residues in this entry.