Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 04:59 pm BST

PDB ID	:	1ZWY
Title	:	Crystal structure of protein VC0702 from Vibrio cholerae
Authors	:	Chang, C.; Wu, R.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2005-06-06
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 following versions of software and data (see references ⓘ) were used in the production of this report:

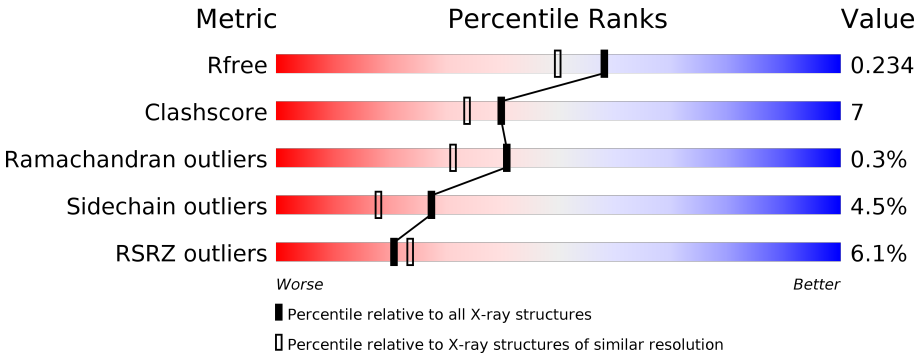
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 on 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	185	9% 77% 11% • 11%
1	B	185	4% 83% 12% • •
1	C	185	7% 79% 11% • 7%
1	D	185	3% 77% 14% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6062 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 Hypothetical UPF0244 protein VC0702.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	Se	0	4	0
			1313	829	231	247	1	5			
1	B	180	Total	C	N	O	S	Se	0	3	0
			1431	907	254	263	1	6			
1	C	172	Total	C	N	O	S	Se	0	4	0
			1377	871	244	256	1	5			
1	D	173	Total	C	N	O	S	Se	0	2	0
			1374	868	244	256	1	5			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASN	-	CLONING ARTIFACT	UNP Q9KU27
A	0	ALA	-	CLONING ARTIFACT	UNP Q9KU27
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9KU27
A	10	MSE	MET	MODIFIED RESIDUE	UNP Q9KU27
A	55	MSE	MET	MODIFIED RESIDUE	UNP Q9KU27
A	97	MSE	MET	MODIFIED RESIDUE	UNP Q9KU27
A	114	MSE	MET	MODIFIED RESIDUE	UNP Q9KU27
A	133	MSE	MET	MODIFIED RESIDUE	UNP Q9KU27
B	-1	ASN	-	CLONING ARTIFACT	UNP Q9KU27
B	0	ALA	-	CLONING ARTIFACT	UNP Q9KU27
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9KU27
B	10	MSE	MET	MODIFIED RESIDUE	UNP Q9KU27
B	55	MSE	MET	MODIFIED RESIDUE	UNP Q9KU27
B	97	MSE	MET	MODIFIED RESIDUE	UNP Q9KU27
B	114	MSE	MET	MODIFIED RESIDUE	UNP Q9KU27
B	133	MSE	MET	MODIFIED RESIDUE	UNP Q9KU27
C	-1	ASN	-	CLONING ARTIFACT	UNP Q9KU27
C	0	ALA	-	CLONING ARTIFACT	UNP Q9KU27
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q9KU27
C	10	MSE	MET	MODIFIED RESIDUE	UNP Q9KU27
C	55	MSE	MET	MODIFIED RESIDUE	UNP Q9KU27

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Chain	Residue	Modelled	Actual	Comment	Reference
C	97	MSE	MET	MODIFIED RESIDUE	UNP Q9KU27
C	114	MSE	MET	MODIFIED RESIDUE	UNP Q9KU27
C	133	MSE	MET	MODIFIED RESIDUE	UNP Q9KU27
D	-1	ASN	-	CLONING ARTIFACT	UNP Q9KU27
D	0	ALA	-	CLONING ARTIFACT	UNP Q9KU27
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q9KU27
D	10	MSE	MET	MODIFIED RESIDUE	UNP Q9KU27
D	55	MSE	MET	MODIFIED RESIDUE	UNP Q9KU27
D	97	MSE	MET	MODIFIED RESIDUE	UNP Q9KU27
D	114	MSE	MET	MODIFIED RESIDUE	UNP Q9KU27
D	133	MSE	MET	MODIFIED RESIDUE	UNP Q9KU27

- Molecule 2 is water.

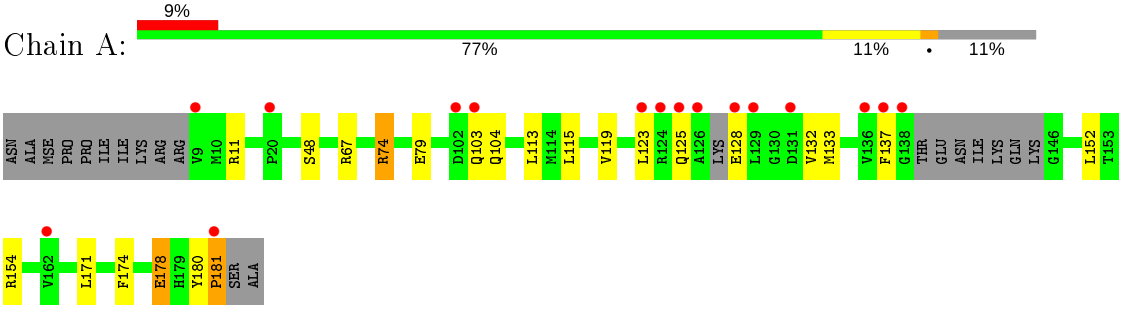
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	100	Total O 100 100	0	0
2	B	168	Total O 168 168	0	0
2	C	122	Total O 122 122	0	0
2	D	177	Total O 177 177	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

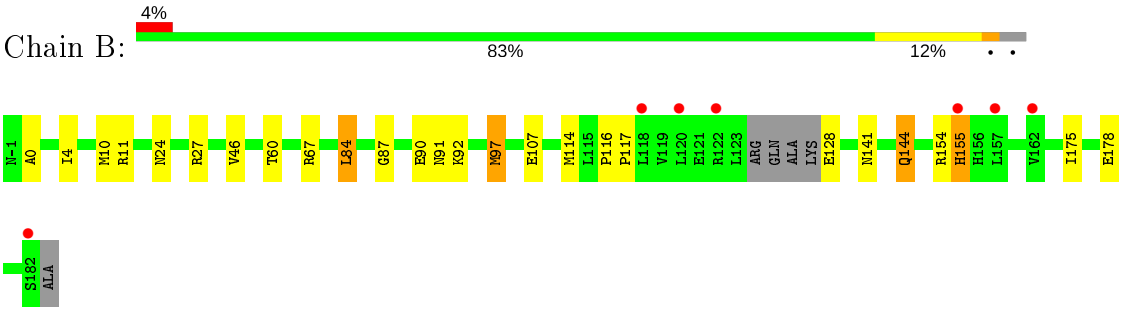
- Molecule 1: Hypothetical UPF0244 protein VC0702

Chain A:



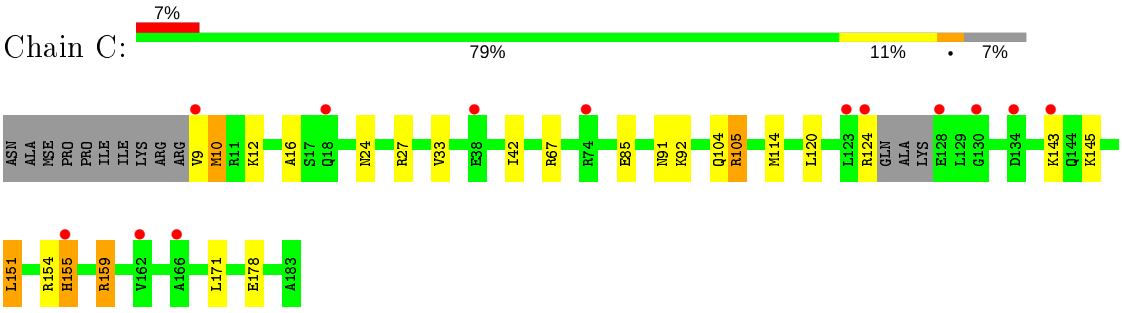
- Molecule 1: Hypothetical UPF0244 protein VC0702

Chain B:



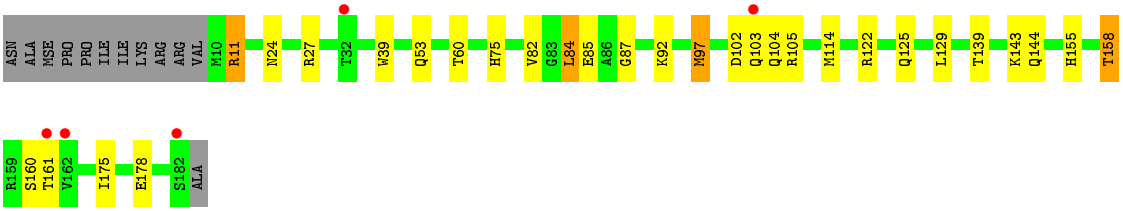
- Molecule 1: Hypothetical UPF0244 protein VC0702

Chain C:



- Molecule 1: Hypothetical UPF0244 protein VC0702

Chain D:


ASN
ALA
MSE
PRO
PRO
ILE
ILE
LYS
ARG
ARG
VAL
M10
R11
N24
R27
T32
W39
Q53
T60
H75
V82
G83
L84
E85
A86
G87
K92
M97
D102
Q103
Q104
R105
M114
R122
Q125
L129
T139
K143
Q144
H155
T158
R159
S160
T161
V162
I175
E178
S182
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.40Å 105.35Å 75.27Å 90.00° 104.57° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 36.43 – 1.88	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.00-1.90) 97.4 (36.43-1.88)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.180 , 0.226 0.195 , 0.234	Depositor DCC
R_{free} test set	3212 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 55.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6062	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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

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	0.64	0/1345	0.69	1/1811 (0.1%)
1	B	0.81	0/1464	0.80	2/1972 (0.1%)
1	C	0.68	0/1412	0.69	1/1901 (0.1%)
1	D	0.85	0/1404	0.76	0/1894
All	All	0.75	0/5625	0.74	4/7578 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	11	ARG	NE-CZ-NH2	-7.99	116.30	120.30
1	A	181	PRO	N-CA-CB	7.44	112.23	103.30
1	B	97	MSE	CG-SE-CE	-6.55	84.50	98.90
1	C	105	ARG	NE-CZ-NH2	-6.42	117.09	120.30

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	1313	0	1300	14	0
1	B	1431	0	1443	22	0
1	C	1377	0	1379	20	0
1	D	1374	0	1373	30	0
2	A	100	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	168	0	0	2	0
2	C	122	0	0	3	0
2	D	177	0	0	3	0
All	All	6062	0	5495	80	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 7.

All (80) 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:B:84[B]:LEU:HG	1:B:97:MSE:HE1	1.18	1.14
1:B:84[B]:LEU:HG	1:B:97:MSE:CE	1.83	1.09
1:A:133:MSE:SE	1:A:137:PHE:HE2	2.00	0.94
1:B:84[B]:LEU:CG	1:B:97:MSE:HE1	1.97	0.94
1:B:155[B]:HIS:HB3	1:C:155[B]:HIS:HB3	1.47	0.93
2:C:208:HOH:O	1:D:92:LYS:HE2	1.68	0.91
1:D:11:ARG:HG3	1:D:39:TRP:CZ3	2.12	0.85
1:C:104[A]:GLN:HE21	1:C:105:ARG:H	1.28	0.81
1:D:104[B]:GLN:HE21	1:D:105:ARG:H	1.26	0.80
1:B:144:GLN:HB3	2:B:331:HOH:O	1.84	0.77
1:C:159:ARG:NH1	2:C:192:HOH:O	2.18	0.76
1:D:53:GLN:HE22	1:D:129:LEU:H	1.35	0.74
1:B:24:ASN:ND2	1:B:27:ARG:HH21	1.86	0.72
1:C:33[A]:VAL:HG21	1:C:171:LEU:HD13	1.69	0.72
2:C:208:HOH:O	1:D:92:LYS:CE	2.32	0.69
1:A:115:LEU:HD22	1:A:133:MSE:HE1	1.75	0.69
1:B:67:ARG:NH1	1:B:67:ARG:HG2	2.07	0.68
1:D:139:THR:HG22	1:D:143:LYS:HE2	1.77	0.67
1:B:91:ASN:HD21	1:B:114:MSE:HE2	1.58	0.66
1:C:9:VAL:O	1:C:10:MSE:HB2	1.96	0.66
1:A:133:MSE:SE	1:A:137:PHE:CE2	2.91	0.65
1:D:122:ARG:HD2	1:D:125:GLN:NE2	2.11	0.64
1:A:115:LEU:HD22	1:A:133:MSE:CE	2.28	0.64
1:C:91:ASN:HB2	1:C:120:LEU:HD11	1.79	0.63
1:D:53:GLN:NE2	1:D:129:LEU:H	1.98	0.60
1:D:11:ARG:CG	1:D:39:TRP:CZ3	2.84	0.60
1:C:145:LYS:HD3	1:C:151:LEU:HD11	1.83	0.60
1:C:92[B]:LYS:HE2	1:C:114:MSE:HG3	1.85	0.58
1:B:67:ARG:HH11	1:B:67:ARG:HG2	1.69	0.58
1:B:46:VAL:O	1:B:67:ARG:NH1	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:LYS:HD3	1:C:42:ILE:CD1	2.33	0.58
1:D:139:THR:HG22	1:D:143:LYS:CE	2.33	0.58
1:D:158:THR:HG22	1:D:161:THR:H	1.69	0.58
1:D:102:ASP:OD1	1:D:103:GLN:HG2	2.02	0.58
1:D:158:THR:CG2	1:D:160:SER:OG	2.52	0.57
1:A:178:GLU:H	1:A:178:GLU:CD	2.08	0.57
1:C:67:ARG:HE	1:C:85:GLU:CD	2.08	0.57
1:B:84[B]:LEU:CD2	1:B:97:MSE:HE1	2.35	0.56
1:D:122:ARG:HD2	1:D:125:GLN:HE21	1.70	0.54
1:D:11:ARG:HG2	1:D:39:TRP:CE3	2.44	0.54
1:A:104:GLN:HB3	1:A:174:PHE:CE1	2.43	0.53
1:B:24:ASN:HD21	1:B:27:ARG:HH21	1.56	0.53
1:D:60:THR:OG1	1:D:87:GLY:HA3	2.09	0.53
1:D:75:HIS:HE1	2:D:211:HOH:O	1.92	0.53
1:B:155[B]:HIS:CB	1:C:155[B]:HIS:HB3	2.31	0.52
1:B:154:ARG:O	1:B:155[B]:HIS:HB2	2.10	0.51
1:D:92:LYS:HE3	1:D:114:MSE:HG3	1.93	0.51
1:A:154:ARG:HG3	1:B:175:ILE:CG2	2.41	0.49
1:C:24:ASN:HD22	1:C:27:ARG:NH1	2.09	0.49
1:D:122:ARG:HH11	1:D:125:GLN:HE22	1.60	0.49
1:B:10:MSE:SE	2:B:269:HOH:O	2.80	0.49
1:A:119:VAL:HG11	1:A:133:MSE:HE2	1.95	0.49
1:D:158:THR:HG21	1:D:160:SER:OG	2.13	0.48
1:C:104[A]:GLN:NE2	1:C:105:ARG:H	2.04	0.48
1:C:154:ARG:NH1	1:D:175:ILE:O	2.47	0.47
1:D:85:GLU:OE1	2:D:254:HOH:O	2.20	0.47
1:A:11:ARG:HG3	1:A:79:GLU:HB2	1.96	0.47
1:D:122:ARG:HH11	1:D:125:GLN:NE2	2.11	0.47
1:D:11:ARG:CG	1:D:39:TRP:CE3	2.97	0.47
1:D:24:ASN:ND2	1:D:27:ARG:HH11	2.12	0.46
1:C:104[A]:GLN:HE21	1:C:105:ARG:N	2.06	0.46
1:B:92:LYS:HE3	1:B:114:MSE:HG3	1.99	0.45
1:B:155[B]:HIS:HB3	1:C:155[B]:HIS:CB	2.32	0.45
1:B:60:THR:OG1	1:B:87:GLY:HA3	2.16	0.45
1:A:74:ARG:HE	1:A:74:ARG:HB2	1.65	0.44
1:B:0:ALA:O	1:D:75:HIS:HD2	2.01	0.44
1:B:90:GLU:HG3	1:B:91:ASN:H	1.83	0.43
1:A:137:PHE:HZ	1:A:152:LEU:HD21	1.84	0.42
1:D:155:HIS:ND1	2:D:317:HOH:O	2.22	0.42
1:A:48:SER:HB3	1:A:67:ARG:CZ	2.50	0.42
1:D:97:MSE:N	1:D:97:MSE:SE	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:TYR:O	1:A:181:PRO:CB	2.67	0.41
1:C:16:ALA:HB1	1:C:67:ARG:HB3	2.01	0.41
1:C:91:ASN:CB	1:C:120:LEU:HD11	2.49	0.41
1:A:128:GLU:O	1:A:132:VAL:HG23	2.20	0.41
1:C:33[A]:VAL:HG21	1:C:171:LEU:CD1	2.44	0.41
1:D:82:VAL:HG12	1:D:84[A]:LEU:HD22	2.03	0.41
1:D:104[B]:GLN:HG3	1:D:105:ARG:N	2.36	0.41
1:B:116:PRO:HA	1:B:117:PRO:HD3	1.97	0.40
1:C:33[A]:VAL:CG2	1:C:171:LEU:HD13	2.46	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	A	163/185 (88%)	161 (99%)	2 (1%)	0	100 100
1	B	179/185 (97%)	176 (98%)	3 (2%)	0	100 100
1	C	172/185 (93%)	167 (97%)	2 (1%)	3 (2%)	9 2
1	D	173/185 (94%)	170 (98%)	3 (2%)	0	100 100
All	All	687/740 (93%)	674 (98%)	10 (2%)	3 (0%)	41 24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	10	MSE
1	C	155[A]	HIS
1	C	155[B]	HIS

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	142/151 (94%)	135 (95%)	7 (5%)	25 15
1	B	156/151 (103%)	146 (94%)	10 (6%)	17 8
1	C	150/151 (99%)	145 (97%)	5 (3%)	38 29
1	D	148/151 (98%)	141 (95%)	7 (5%)	26 16
All	All	596/604 (99%)	567 (95%)	29 (5%)	27 15

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ARG
1	A	103	GLN
1	A	113	LEU
1	A	123	LEU
1	A	125	GLN
1	A	171	LEU
1	A	178	GLU
1	B	4	ILE
1	B	84[A]	LEU
1	B	84[B]	LEU
1	B	107	GLU
1	B	128	GLU
1	B	141	ASN
1	B	144	GLN
1	B	155[A]	HIS
1	B	155[B]	HIS
1	B	178	GLU
1	C	124	ARG
1	C	143	LYS
1	C	151	LEU
1	C	159	ARG
1	C	178	GLU
1	D	11	ARG
1	D	84[A]	LEU

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Mol	Chain	Res	Type
1	D	84[B]	LEU
1	D	97	MSE
1	D	144	GLN
1	D	158	THR
1	D	178	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	24	ASN
1	A	70	ASN
1	B	24	ASN
1	B	70	ASN
1	B	104	GLN
1	B	141	ASN
1	C	24	ASN
1	C	70	ASN
1	C	179	HIS
1	D	18	GLN
1	D	19	ASN
1	D	24	ASN
1	D	53	GLN
1	D	70	ASN
1	D	75	HIS
1	D	125	GLN
1	D	144	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

There are no ligands in this entry.

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	160/185 (86%)	0.60	16 (10%) 7 8	15, 24, 42, 54	0
1	B	174/185 (94%)	0.17	7 (4%) 38 41	10, 18, 36, 42	0
1	C	167/185 (90%)	0.48	13 (7%) 13 14	13, 23, 33, 42	0
1	D	168/185 (90%)	0.16	5 (2%) 50 53	11, 16, 30, 38	0
All	All	669/740 (90%)	0.35	41 (6%) 21 24	10, 20, 35, 54	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	VAL	8.8
1	A	137	PHE	6.3
1	C	9	VAL	5.6
1	C	124	ARG	4.8
1	C	123	LEU	4.2
1	A	181	PRO	3.8
1	A	126	ALA	3.5
1	A	129	LEU	3.4
1	A	123	LEU	3.4
1	D	182	SER	3.0
1	C	128	GLU	2.9
1	A	136	VAL	2.9
1	B	182	SER	2.8
1	D	103	GLN	2.8
1	A	125	GLN	2.8
1	A	20	PRO	2.8
1	B	162	VAL	2.8
1	B	120	LEU	2.6
1	A	131	ASP	2.5
1	C	155[A]	HIS	2.5
1	C	74	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	18	GLN	2.4
1	A	128	GLU	2.4
1	A	138	GLY	2.4
1	B	155[A]	HIS	2.3
1	A	162	VAL	2.3
1	C	38	GLU	2.3
1	B	157	LEU	2.3
1	A	124	ARG	2.3
1	D	162	VAL	2.3
1	C	166	ALA	2.3
1	C	162	VAL	2.2
1	D	161	THR	2.2
1	A	102	ASP	2.2
1	C	134	ASP	2.2
1	A	103	GLN	2.1
1	B	118	LEU	2.1
1	C	143	LYS	2.1
1	C	130	GLY	2.1
1	B	122	ARG	2.0
1	D	32	THR	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.