Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:58 AM GMT

PDB ID	:	2VH1
Title	:	CRYSTAL STRUCTURE OF BACTERIAL CELL DIVISION PROTEIN FTSQ FROM E.COLI
Authors	:	Van Den Ent, F.; Vinkenvleugel, T.; Ind, A.; West, P.; Veprintsev, D.; Naninga, N.; Den Blaauwen, T.; Lowe, J.
Deposited on	:	2007-11-16
Resolution	:	2.70 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:

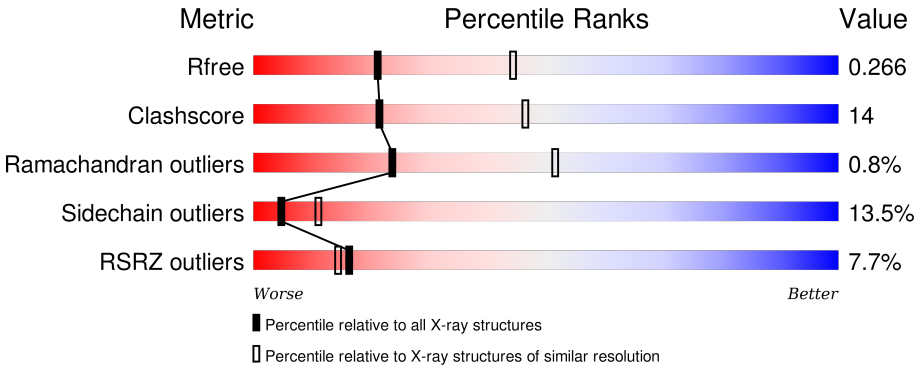
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	220	5% 66% 22% • • 8%
1	B	220	10% 58% 24% 7% • 10%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3234 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 CELL DIVISION PROTEIN FTSQ.

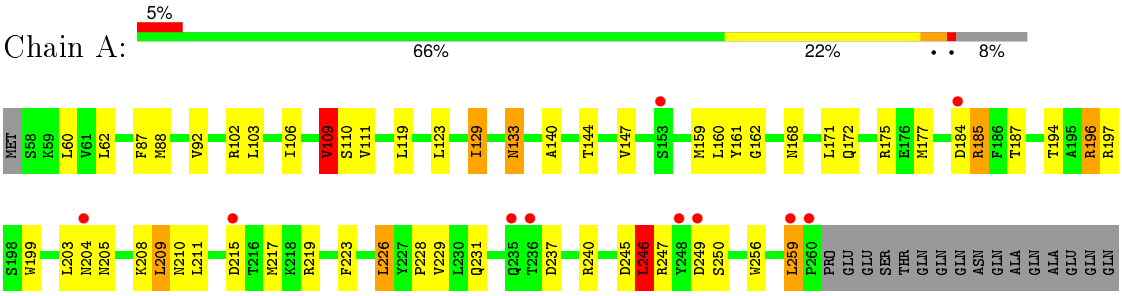
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1640	1034	296	303	7			
1	B	198	Total	C	N	O	S	0	0	1
			1594	1005	287	295	7			

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 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.

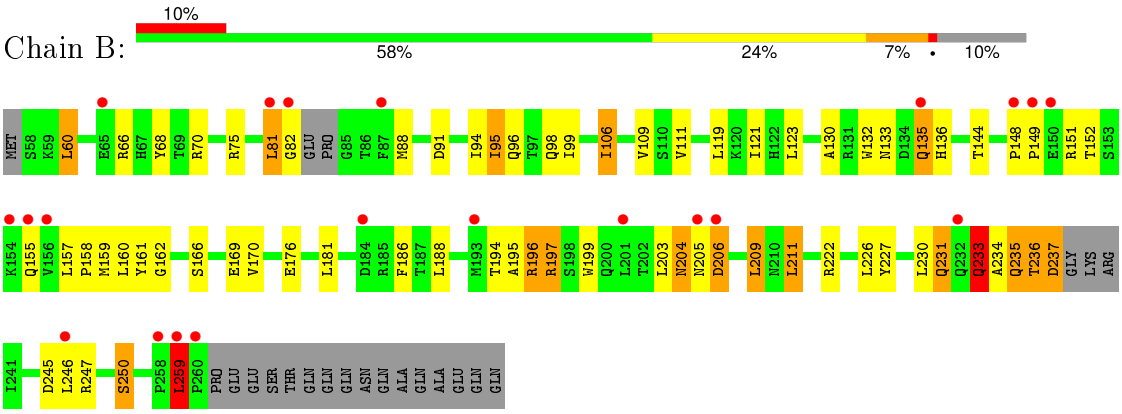
- Molecule 1: CELL DIVISION PROTEIN FTSQ

Chain A:



- Molecule 1: CELL DIVISION PROTEIN FTSQ

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	147.84Å 147.84Å 69.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.35 – 2.70 27.04 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (36.35-2.70) 97.9 (27.04-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.237 , 0.288 0.225 , 0.266	Depositor DCC
R_{free} test set	6606 reflections (39.36%)	DCC
Wilson B-factor (Å^2)	64.6	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 66.1	EDS
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 23390 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	3234	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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

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	0.61	0/1674	0.82	5/2268 (0.2%)
1	B	0.83	4/1624 (0.2%)	0.80	3/2198 (0.1%)
All	All	0.73	4/3298 (0.1%)	0.81	8/4466 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	GLY	C-O	21.79	1.58	1.23
1	B	233	GLN	CD-NE2	7.83	1.52	1.32
1	B	233	GLN	CD-OE1	5.28	1.35	1.24
1	B	259	LEU	C-N	-5.26	1.24	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	246	LEU	CA-CB-CG	8.31	134.41	115.30
1	B	246	LEU	CA-CB-CG	7.06	131.54	115.30
1	A	109	VAL	CB-CA-C	-6.28	99.47	111.40
1	A	259	LEU	CA-CB-CG	6.14	129.43	115.30
1	B	82	GLY	CA-C-O	-5.38	110.92	120.60
1	B	197	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	A	60	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	226	LEU	CA-CB-CG	5.05	126.92	115.30

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	1640	0	1643	38	0
1	B	1594	0	1592	55	0
All	All	3234	0	3235	91	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 14.

All (91) 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:205:ASN:H	1:B:206:ASP:HA	1.12	1.10
1:B:205:ASN:N	1:B:206:ASP:HA	1.79	0.95
1:B:132:TRP:O	1:B:136:HIS:HB2	1.72	0.90
1:B:204:ASN:H	1:B:204:ASN:HD22	1.22	0.82
1:B:233:GLN:HB3	1:B:237:ASP:HB2	1.61	0.82
1:A:129:ILE:HD11	1:A:171:LEU:HD11	1.62	0.82
1:B:169:GLU:CD	1:B:197:ARG:HH12	1.87	0.77
1:A:133:ASN:ND2	1:A:162:GLY:H	1.82	0.77
1:B:133:ASN:HD21	1:B:162:GLY:H	1.33	0.76
1:B:133:ASN:ND2	1:B:162:GLY:H	1.88	0.71
1:A:223:PHE:HB2	1:A:246:LEU:HD21	1.72	0.70
1:B:194:THR:HG22	1:B:195:ALA:N	2.07	0.70
1:B:66:ARG:HD3	1:B:123:LEU:HD12	1.73	0.69
1:B:245:ASP:OD2	1:B:247:ARG:HB3	1.92	0.69
1:A:133:ASN:HD22	1:A:162:GLY:H	1.40	0.68
1:A:194:THR:O	1:A:196:ARG:O	2.12	0.68
1:A:106:ILE:HG21	1:A:109:VAL:HG22	1.74	0.68
1:A:92:VAL:HG22	1:A:111:VAL:HG12	1.75	0.67
1:B:194:THR:HG22	1:B:195:ALA:H	1.61	0.65
1:A:129:ILE:CD1	1:A:171:LEU:HD11	2.26	0.65
1:B:204:ASN:HD22	1:B:204:ASN:N	1.96	0.63
1:B:206:ASP:OD1	1:B:206:ASP:N	2.32	0.61
1:A:109:VAL:HG13	1:A:123:LEU:HD23	1.84	0.60
1:B:132:TRP:O	1:B:136:HIS:CB	2.49	0.59
1:A:187:THR:HB	1:A:204:ASN:HB3	1.85	0.58
1:A:245:ASP:OD1	1:A:247:ARG:HB2	2.04	0.58
1:B:106:ILE:HG21	1:B:109:VAL:HG22	1.85	0.58
1:A:219:ARG:HD3	1:A:246:LEU:O	2.04	0.57
1:B:205:ASN:N	1:B:206:ASP:CA	2.63	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ALA:O	1:A:175:ARG:NH1	2.38	0.57
1:B:231:GLN:HG2	1:B:234:ALA:HB2	1.88	0.56
1:B:227:TYR:HA	1:B:230:LEU:HD12	1.87	0.56
1:A:87:PHE:CE2	1:A:88:MET:HE2	2.41	0.56
1:B:169:GLU:OE2	1:B:197:ARG:NH1	2.39	0.55
1:A:129:ILE:HD11	1:A:171:LEU:CD1	2.36	0.54
1:A:209:LEU:HD21	1:A:246:LEU:CD2	2.36	0.54
1:B:135:GLN:HG2	1:B:136:HIS:CD2	2.43	0.54
1:A:133:ASN:HD22	1:A:161:TYR:HA	1.73	0.53
1:A:184:ASP:O	1:A:185:ARG:HB2	2.09	0.52
1:A:133:ASN:HD22	1:A:162:GLY:N	2.08	0.51
1:B:166:SER:O	1:B:170:VAL:HG23	2.11	0.51
1:B:106:ILE:HG21	1:B:109:VAL:CG2	2.41	0.51
1:B:235:GLN:HG2	1:B:259:LEU:O	2.11	0.51
1:B:70:ARG:HH21	1:B:151:ARG:HD3	1.76	0.50
1:B:169:GLU:OE1	1:B:197:ARG:NH1	2.37	0.50
1:A:87:PHE:CZ	1:A:88:MET:HE2	2.47	0.50
1:B:194:THR:CG2	1:B:195:ALA:N	2.75	0.49
1:A:109:VAL:HG13	1:A:123:LEU:CD2	2.43	0.48
1:B:245:ASP:OD2	1:B:247:ARG:CB	2.62	0.48
1:A:133:ASN:HB3	1:A:161:TYR:CD2	2.49	0.47
1:B:181:LEU:HB3	1:B:186:PHE:HB2	1.95	0.47
1:B:60:LEU:HD21	1:B:121:ILE:HD12	1.96	0.47
1:B:155:GLN:NE2	1:B:157:LEU:HD21	2.29	0.47
1:B:194:THR:O	1:B:196:ARG:O	2.33	0.47
1:A:203:LEU:O	1:A:205:ASN:O	2.34	0.47
1:A:185:ARG:O	1:A:185:ARG:HG2	2.15	0.46
1:A:249:ASP:O	1:A:250:SER:OG	2.27	0.46
1:A:256:TRP:CE2	1:B:250:SER:HA	2.51	0.46
1:A:211:LEU:O	1:A:219:ARG:NH2	2.46	0.45
1:B:91:ASP:O	1:B:95:ILE:HG23	2.16	0.45
1:B:95:ILE:HD12	1:B:99:ILE:CD1	2.46	0.45
1:B:130:ALA:HB2	1:B:158:PRO:HG2	1.99	0.45
1:B:91:ASP:HB3	1:B:94:ILE:HD12	1.99	0.44
1:B:109:VAL:HG13	1:B:123:LEU:HD23	2.00	0.44
1:A:228:PRO:O	1:A:231:GLN:HB3	2.18	0.44
1:A:87:PHE:CZ	1:A:88:MET:CE	3.00	0.43
1:B:68:TYR:HE1	1:B:152:THR:HB	1.82	0.43
1:A:184:ASP:O	1:A:185:ARG:CB	2.65	0.43
1:B:209:LEU:HD22	1:B:211:LEU:HD13	1.99	0.43
1:A:210:ASN:OD1	1:A:247:ARG:HD3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:TRP:O	1:B:136:HIS:CA	2.67	0.43
1:B:194:THR:C	1:B:196:ARG:O	2.57	0.43
1:B:195:ALA:C	1:B:196:ARG:O	2.55	0.43
1:A:177:MET:HE1	1:A:199:TRP:CE3	2.54	0.43
1:B:194:THR:CG2	1:B:195:ALA:H	2.28	0.43
1:B:170:VAL:HA	1:B:199:TRP:HH2	1.84	0.43
1:A:194:THR:C	1:A:196:ARG:O	2.58	0.42
1:A:237:ASP:CG	1:B:222:ARG:HH12	2.23	0.42
1:A:102:ARG:O	1:A:103:LEU:HD23	2.18	0.42
1:A:87:PHE:CE2	1:A:88:MET:CE	3.03	0.42
1:B:222:ARG:O	1:B:226:LEU:HB2	2.20	0.42
1:B:148:PRO:HA	1:B:149:PRO:HD3	1.86	0.41
1:B:111:VAL:HG13	1:B:121:ILE:HG12	2.01	0.41
1:B:95:ILE:HG13	1:B:96:GLN:N	2.35	0.41
1:B:81:LEU:HD11	1:B:98:GLN:HG3	2.01	0.41
1:B:133:ASN:HD22	1:B:161:TYR:HA	1.85	0.41
1:B:203:LEU:HB3	1:B:204:ASN:H	1.58	0.41
1:A:133:ASN:ND2	1:A:162:GLY:N	2.59	0.41
1:B:148:PRO:HD2	1:B:151:ARG:HG3	2.02	0.41
1:B:81:LEU:HD21	1:B:94:ILE:HG22	2.02	0.40
1:A:249:ASP:O	1:A:250:SER:CB	2.69	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	201/220 (91%)	187 (93%)	12 (6%)	2 (1%)	19 45
1	B	192/220 (87%)	170 (88%)	21 (11%)	1 (0%)	34 63
All	All	393/440 (89%)	357 (91%)	33 (8%)	3 (1%)	24 51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	ARG
1	A	133	ASN
1	B	236	THR

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	177/192 (92%)	155 (88%)	22 (12%)	6 13
1	B	172/192 (90%)	147 (86%)	25 (14%)	4 10
All	All	349/384 (91%)	302 (86%)	47 (14%)	5 11

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	LEU
1	A	109	VAL
1	A	110	SER
1	A	119	LEU
1	A	129	ILE
1	A	144	THR
1	A	147	VAL
1	A	159	MET
1	A	160	LEU
1	A	168	ASN
1	A	172	GLN
1	A	196	ARG
1	A	197	ARG
1	A	208	LYS
1	A	209	LEU
1	A	215	ASP
1	A	217	MET
1	A	226	LEU
1	A	229	VAL
1	A	240	ARG

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Mol	Chain	Res	Type
1	A	246	LEU
1	A	259	LEU
1	B	60	LEU
1	B	75	ARG
1	B	81	LEU
1	B	88	MET
1	B	95	ILE
1	B	106	ILE
1	B	119	LEU
1	B	135	GLN
1	B	144	THR
1	B	159	MET
1	B	160	LEU
1	B	176	GLU
1	B	188	LEU
1	B	196	ARG
1	B	204	ASN
1	B	206	ASP
1	B	209	LEU
1	B	211	LEU
1	B	231	GLN
1	B	233	GLN
1	B	235	GLN
1	B	236	THR
1	B	237	ASP
1	B	250	SER
1	B	259	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	122	HIS
1	A	133	ASN
1	A	168	ASN
1	A	231	GLN
1	B	76	GLN
1	B	122	HIS
1	B	133	ASN
1	B	135	GLN
1	B	136	HIS
1	B	155	GLN

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Mol	Chain	Res	Type
1	B	204	ASN
1	B	235	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	203/220 (92%)	0.43	10 (4%) 33 32	49, 58, 63, 75	0
1	B	198/220 (90%)	0.55	21 (10%) 8 6	49, 58, 64, 74	0
All	All	401/440 (91%)	0.49	31 (7%) 16 14	49, 58, 64, 75	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	ASP	6.7
1	B	258	PRO	5.6
1	A	260	PRO	5.0
1	B	232	GLN	4.7
1	A	215	ASP	4.5
1	B	259	LEU	4.2
1	B	81	LEU	4.2
1	A	259	LEU	4.2
1	A	236	THR	4.0
1	A	204	ASN	3.3
1	B	82	GLY	3.3
1	B	184	ASP	3.2
1	A	184	ASP	3.1
1	B	206	ASP	3.1
1	B	260	PRO	3.1
1	A	235	GLN	3.0
1	B	154	LYS	2.9
1	B	149	PRO	2.8
1	B	155	GLN	2.8
1	B	156	VAL	2.7
1	B	150	GLU	2.7
1	A	153	SER	2.7
1	B	246	LEU	2.5
1	A	248	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	87	PHE	2.4
1	B	135	GLN	2.4
1	B	65	GLU	2.3
1	B	193	MET	2.3
1	B	205	ASN	2.2
1	B	201	LEU	2.1
1	B	148	PRO	2.1

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.