Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	6K9N
Title	:	Rice_OTUB_like_catalytic domain
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Deposited on	:	2019-06-17
Resolution	:	2.27 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 (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:

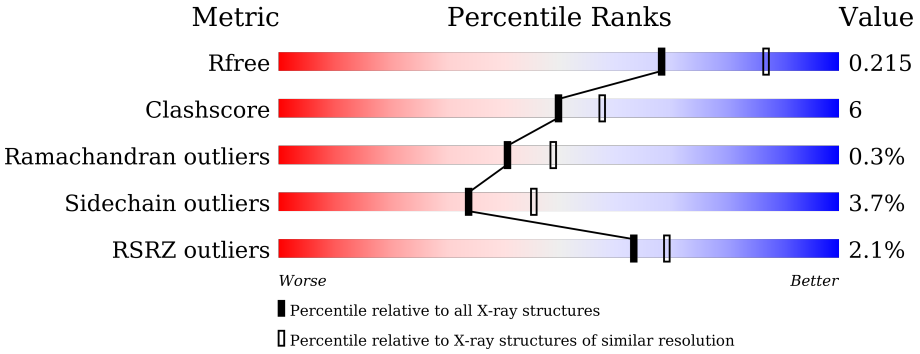
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.27 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	251	.% 86% 10% • •
1	B	251	2% 80% 13% • •
1	C	251	2% 77% 18% •
1	D	251	2% 79% 17% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8278 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 Ubiquitin thioesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	242	1955	1249	321	377	8	0	0	0
1	B	241	1951	1247	320	376	8	0	0	0
1	C	240	1943	1243	319	373	8	0	0	0
1	D	243	1957	1251	321	377	8	0	0	0

- Molecule 2 is water.

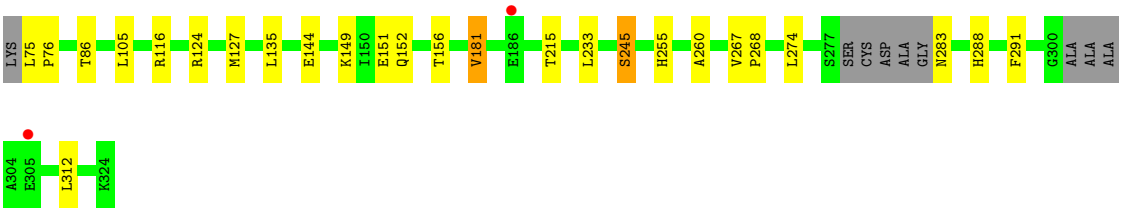
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	146	146	146	0	0
2	B	106	106	106	0	0
2	C	108	108	108	0	0
2	D	112	112	112	0	0

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.

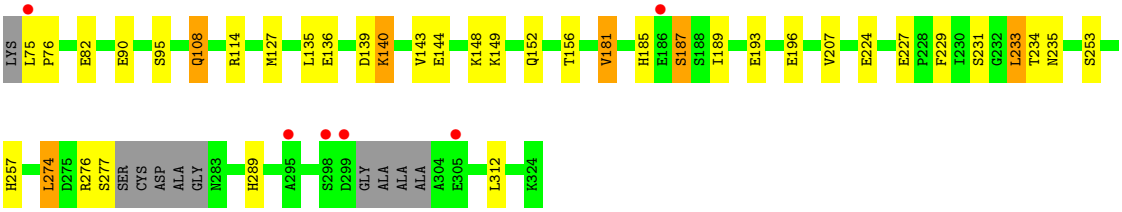
• Molecule 1: Ubiquitin thioesterase

Chain A:



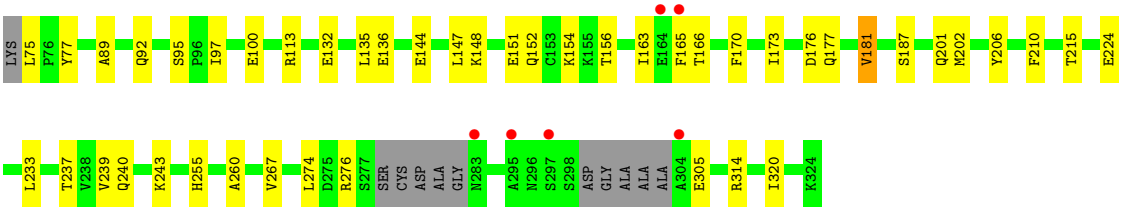
• Molecule 1: Ubiquitin thioesterase

Chain B:



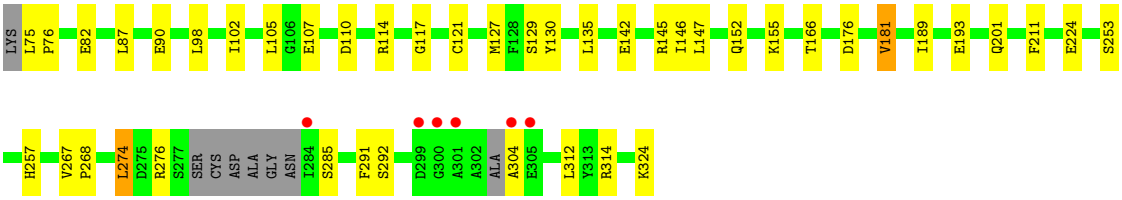
• Molecule 1: Ubiquitin thioesterase

Chain C:



• Molecule 1: Ubiquitin thioesterase

Chain D:


LYS
L75
P76
E82
L87
E90
L98
I102
L105
G106
E107
D110
R114
G117
C121
M127
F128
S129
Y130
L135
E142
R145
I146
L147
Q152
K155
T166
D176
V181
I189
E193
Q201
F211
E224
S253
H257
V267
P268
L274
D275
R276
S277
SER
CYS
ASP
ALA
GLY
ASN
I284
S285
F291
S292
D299
G300
A301
A302
ALA
A304
E305
L312
Y313
R314
K324

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.69Å 144.81Å 155.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.38 – 2.27 47.38 – 2.27	Depositor EDS
% Data completeness (in resolution range)	98.0 (47.38-2.27) 98.0 (47.38-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.73 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.186 , 0.217 0.185 , 0.215	Depositor DCC
R_{free} test set	3027 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	36.1	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8278	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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 (i)

5.1 Standard geometry (i)

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	0.30	0/1997	0.54	0/2693
1	B	0.29	0/1993	0.54	0/2688
1	C	0.29	0/1985	0.51	0/2677
1	D	0.29	0/1999	0.51	0/2696
All	All	0.29	0/7974	0.52	0/10754

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1955	0	1897	17	0
1	B	1951	0	1894	23	0
1	C	1943	0	1890	25	0
1	D	1957	0	1901	25	0
2	A	146	0	0	6	1
2	B	106	0	0	7	0
2	C	108	0	0	5	0
2	D	112	0	0	6	1
All	All	8278	0	7582	89	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 6.

All (89) 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:196:GLU:OE1	2:B:401:HOH:O	1.82	0.95
1:B:276:ARG:O	2:B:402:HOH:O	1.83	0.95
1:C:100:GLU:OE2	2:C:401:HOH:O	1.84	0.93
1:C:176:ASP:OD2	2:C:402:HOH:O	1.89	0.87
1:D:82:GLU:OE1	2:D:401:HOH:O	1.94	0.84
1:D:224:GLU:OE2	2:D:402:HOH:O	1.97	0.83
1:D:314:ARG:NH2	2:D:403:HOH:O	2.17	0.77
1:B:82:GLU:OE2	1:B:114:ARG:NH1	2.23	0.71
1:B:136:GLU:OE1	2:B:403:HOH:O	2.10	0.70
1:B:127:MET:HG3	1:B:207:VAL:HG11	1.76	0.68
1:D:155:LYS:HE3	2:D:406:HOH:O	1.96	0.65
1:A:151:GLU:OE1	2:A:401:HOH:O	2.13	0.65
1:C:154:LYS:NZ	2:C:404:HOH:O	2.24	0.64
1:D:274:LEU:HB3	1:D:314:ARG:HG2	1.79	0.62
1:B:108:GLN:NE2	2:B:407:HOH:O	2.32	0.62
1:C:163:ILE:HD12	1:C:165:PHE:HB3	1.83	0.60
1:B:189:ILE:HG23	1:B:193:GLU:HB3	1.83	0.59
1:C:97:ILE:HD11	1:C:276:ARG:HG2	1.84	0.59
1:D:142:GLU:OE1	2:D:404:HOH:O	2.17	0.58
1:C:239:VAL:O	1:C:243:LYS:HG2	2.03	0.57
1:C:233:LEU:HD11	1:C:255:HIS:CE1	2.40	0.57
1:D:90:GLU:OE1	1:D:114:ARG:NH2	2.34	0.56
1:D:146:ILE:HD12	1:D:147:LEU:N	2.22	0.55
1:C:135:LEU:HB2	1:C:181:VAL:HG22	1.89	0.54
1:A:144:GLU:OE1	2:A:402:HOH:O	2.18	0.54
1:B:289:HIS:HE1	2:B:413:HOH:O	1.91	0.54
1:A:233:LEU:HD11	1:A:255:HIS:CE1	2.44	0.53
1:D:75:LEU:HG	1:D:76:PRO:HD3	1.91	0.53
1:D:135:LEU:HB2	1:D:181:VAL:HG22	1.90	0.53
1:C:176:ASP:OD1	2:C:403:HOH:O	2.18	0.52
1:D:105:LEU:HD21	1:D:312:LEU:HD13	1.91	0.52
1:C:237:THR:OG1	1:C:240:GLN:HG3	2.09	0.52
1:A:75:LEU:O	1:A:116:ARG:NH2	2.41	0.52
1:B:75:LEU:N	1:B:76:PRO:HD2	2.25	0.52
1:A:152:GLN:O	1:A:156:THR:HG23	2.09	0.51
1:D:145:ARG:NH2	1:D:146:ILE:HG23	2.25	0.51
1:D:82:GLU:OE2	1:D:114:ARG:NH1	2.43	0.51
1:C:202:MET:O	1:C:206:TYR:HD1	1.93	0.50
1:B:140:LYS:O	1:B:143:VAL:N	2.43	0.50
1:B:144:GLU:O	1:B:148:LYS:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:N	1:A:76:PRO:HD2	2.28	0.49
1:B:152:GLN:O	1:B:156:THR:HG23	2.13	0.48
1:C:152:GLN:O	1:C:156:THR:HG23	2.13	0.48
1:C:77:TYR:OH	1:C:201:GLN:HG3	2.13	0.48
1:B:229:PHE:O	1:B:233:LEU:HB2	2.14	0.48
1:A:124:ARG:HG3	1:A:127:MET:HE2	1.96	0.47
1:A:215:THR:HG23	1:A:260:ALA:HB3	1.96	0.47
1:D:107:GLU:O	1:D:324:LYS:HD3	2.13	0.47
1:D:152:GLN:HG2	1:D:155:LYS:NZ	2.29	0.47
1:C:274:LEU:HD23	1:C:314:ARG:HD3	1.97	0.47
1:C:187:SER:HB2	2:C:437:HOH:O	2.15	0.47
1:A:135:LEU:HB2	1:A:181:VAL:HG22	1.96	0.47
1:C:147:LEU:O	1:C:151:GLU:HG2	2.15	0.46
1:D:87:LEU:HG	1:D:102:ILE:HD13	1.97	0.45
1:D:130:TYR:OH	1:D:146:ILE:HG12	2.17	0.45
1:B:75:LEU:HD23	1:B:76:PRO:HD3	1.99	0.45
1:B:234:THR:HG22	1:B:235:ASN:H	1.81	0.44
1:D:253:SER:HB3	1:D:257:HIS:HB2	1.99	0.44
1:D:127:MET:HB2	1:D:211:PHE:HE2	1.81	0.44
1:B:274:LEU:HB2	1:B:312:LEU:HD11	2.00	0.44
1:B:135:LEU:HB2	1:B:181:VAL:HG22	2.00	0.44
1:C:132:GLU:O	1:C:136:GLU:HG3	2.18	0.44
1:A:116:ARG:HD3	1:B:90:GLU:O	2.18	0.43
1:A:274:LEU:HB2	1:A:312:LEU:HD11	1.99	0.43
1:A:149:LYS:HD2	1:A:149:LYS:HA	1.78	0.43
1:B:227:GLU:OE2	2:B:404:HOH:O	2.21	0.43
1:B:276:ARG:O	1:B:277:SER:HB3	2.18	0.43
1:C:144:GLU:O	1:C:148:LYS:HG3	2.19	0.43
1:C:89:ALA:O	1:C:92:GLN:HG2	2.18	0.42
1:D:304:ALA:N	2:D:415:HOH:O	2.52	0.42
1:D:117:GLY:HA2	1:D:121:CYS:SG	2.59	0.42
1:C:148:LYS:O	1:C:152:GLN:HG3	2.18	0.42
1:C:215:THR:HG23	1:C:260:ALA:HB3	2.01	0.42
1:D:268:PRO:HB3	1:D:292:SER:HB3	2.02	0.42
1:C:170:PHE:HB3	1:C:210:PHE:HB2	2.01	0.42
1:C:173:ILE:O	1:C:177:GLN:HG2	2.20	0.42
1:A:288:HIS:HE1	2:A:403:HOH:O	2.02	0.42
1:B:253:SER:HB3	1:B:257:HIS:HB2	2.02	0.41
1:B:108:GLN:NE2	2:B:416:HOH:O	2.52	0.41
1:A:268:PRO:HA	1:A:291:PHE:O	2.21	0.41
1:D:268:PRO:HA	1:D:291:PHE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:THR:HG21	2:A:444:HOH:O	2.21	0.41
1:A:245:SER:HB2	2:A:418:HOH:O	2.20	0.41
1:C:97:ILE:HD11	1:C:276:ARG:CG	2.50	0.41
1:B:234:THR:HG22	1:B:235:ASN:N	2.36	0.40
1:D:189:ILE:HG13	1:D:193:GLU:HB3	2.03	0.40
1:C:113:ARG:HB3	1:C:320:ILE:HB	2.03	0.40
1:A:86:THR:HG22	2:A:441:HOH:O	2.22	0.40
1:D:98:LEU:HD22	1:D:274:LEU:HD22	2.02	0.40

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:A:407:HOH:O	2:D:492:HOH:O[4_445]	2.00	0.20

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	236/251 (94%)	233 (99%)	3 (1%)	0	100	100
1	B	235/251 (94%)	225 (96%)	7 (3%)	3 (1%)	12	11
1	C	234/251 (93%)	225 (96%)	9 (4%)	0	100	100
1	D	237/251 (94%)	231 (98%)	6 (2%)	0	100	100
All	All	942/1004 (94%)	914 (97%)	25 (3%)	3 (0%)	41	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	187	SER
1	B	139	ASP

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Mol	Chain	Res	Type
1	B	185	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	216/220 (98%)	211 (98%)	5 (2%)	50	65
1	B	216/220 (98%)	206 (95%)	10 (5%)	27	35
1	C	215/220 (98%)	208 (97%)	7 (3%)	38	51
1	D	215/220 (98%)	205 (95%)	10 (5%)	26	34
All	All	862/880 (98%)	830 (96%)	32 (4%)	34	45

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	LEU
1	A	181	VAL
1	A	245	SER
1	A	267	VAL
1	A	283	ASN
1	B	95	SER
1	B	108	GLN
1	B	140	LYS
1	B	149	LYS
1	B	181	VAL
1	B	187	SER
1	B	224	GLU
1	B	231	SER
1	B	233	LEU
1	B	274	LEU
1	C	75	LEU
1	C	95	SER
1	C	166	THR
1	C	181	VAL
1	C	224	GLU

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Mol	Chain	Res	Type
1	C	267	VAL
1	C	305	GLU
1	D	110	ASP
1	D	129	SER
1	D	166	THR
1	D	176	ASP
1	D	181	VAL
1	D	201	GLN
1	D	267	VAL
1	D	274	LEU
1	D	276	ARG
1	D	285	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	B	287	ASN
1	D	287	ASN
1	D	296	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 (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	A	242/251 (96%)	-0.30	2 (0%)	86	89	22, 34, 55, 92	0
1	B	241/251 (96%)	-0.09	6 (2%)	57	63	27, 41, 64, 100	0
1	C	240/251 (95%)	-0.06	6 (2%)	57	63	29, 41, 63, 95	0
1	D	243/251 (96%)	-0.09	6 (2%)	57	63	25, 39, 64, 96	0
All	All	966/1004 (96%)	-0.13	20 (2%)	63	69	22, 39, 63, 100	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	301	ALA	6.0
1	C	165	PHE	5.4
1	B	298	SER	4.2
1	B	305	GLU	4.1
1	D	300	GLY	3.4
1	B	186	GLU	3.4
1	A	186	GLU	3.3
1	D	284	ILE	3.1
1	B	295	ALA	2.9
1	B	299	ASP	2.9
1	A	305	GLU	2.9
1	D	299	ASP	2.8
1	C	304	ALA	2.8
1	C	283	ASN	2.6
1	C	297	SER	2.6
1	B	75	LEU	2.3
1	C	295	ALA	2.2
1	D	304	ALA	2.1
1	C	164	GLU	2.1
1	D	305	GLU	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 monosaccharides 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.