Full wwPDB X-ray Structure Validation Report (i)

May 23, 2020 – 03:31 pm BST

PDB ID	:	4RG9
Title	:	Crystal structure of APC3-APC16 complex (Selenomethionine Derivative)
Authors	:	Yamaguchi, M.; Yu, S.; Miller, D.J.; Schulman, B.A.
Deposited on	:	2014-09-29
Resolution	:	3.25 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 following versions of software and data (see references (1)) were used in the production of this report:

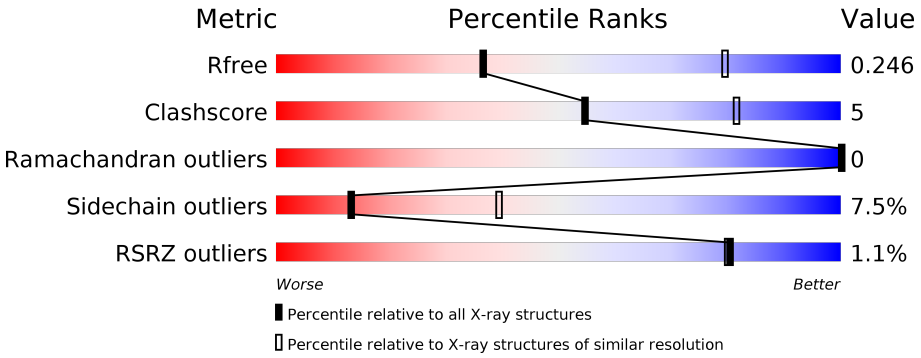
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 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	560	% 72% 11% • 16%
1	B	560	% 70% 12% • 16%
2	S	43	74% 5% • 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7542 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 cycle protein 27 homolog.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	Se	0	0	0
			3607	2311	596	674	17	9			
1	B	472	Total	C	N	O	S	Se	0	0	0
			3659	2349	611	673	17	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P30260
A	0	SER	-	EXPRESSION TAG	UNP P30260
B	-1	GLY	-	EXPRESSION TAG	UNP P30260
B	0	SER	-	EXPRESSION TAG	UNP P30260

- Molecule 2 is a protein called Anaphase-promoting complex subunit 16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	35	Total	C	N	O	Se	0	0	0
			276	178	47	50	1			

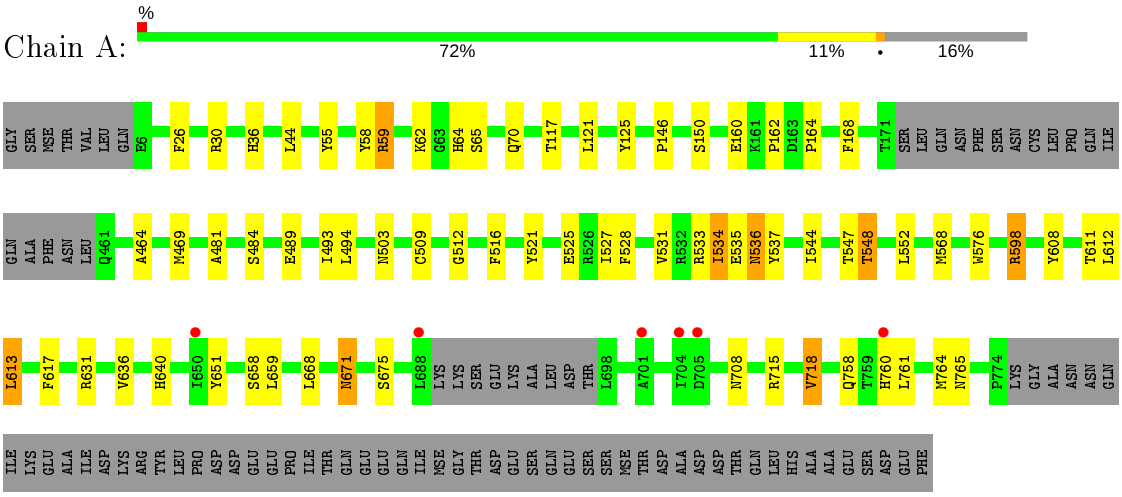
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	73	MSE	-	INITIATING METHIONINE	UNP Q96DE5
S	110	GLU	-	EXPRESSION TAG	UNP Q96DE5
S	111	ASN	-	EXPRESSION TAG	UNP Q96DE5
S	112	LEU	-	EXPRESSION TAG	UNP Q96DE5
S	113	TYR	-	EXPRESSION TAG	UNP Q96DE5
S	114	PHE	-	EXPRESSION TAG	UNP Q96DE5
S	115	GLN	-	EXPRESSION TAG	UNP Q96DE5

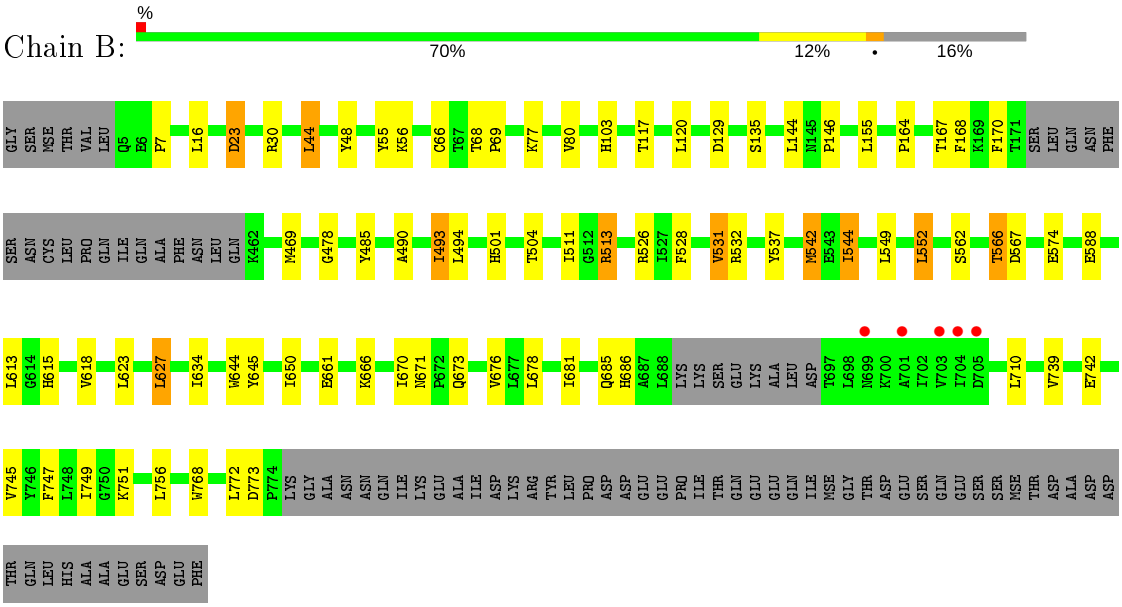
3 Residue-property plots (i)

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.

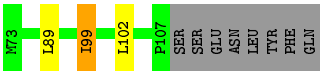
- Molecule 1: Cell division cycle protein 27 homolog



- Molecule 1: Cell division cycle protein 27 homolog



- Molecule 2: Anaphase-promoting complex subunit 16


M73
L89
I99
L102
P107
SER
SER
GLU
ASN
LEU
TYR
PHE
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	116.02Å 116.02Å 184.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.94 – 3.25 49.94 – 3.25	Depositor EDS
% Data completeness (in resolution range)	94.2 (49.94-3.25) 94.2 (49.94-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.210 , 0.248 0.212 , 0.246	Depositor DCC
R_{free} test set	1813 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	76.7	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 37.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7542	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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	0.33	0/3683	0.54	0/4992
1	B	0.34	0/3739	0.55	1/5064 (0.0%)
2	S	0.38	0/279	0.59	0/373
All	All	0.34	0/7701	0.54	1/10429 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	542	MSE	CA-CB-CG	-5.00	104.80	113.30

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	3607	0	3330	38	0
1	B	3659	0	3422	42	0
2	S	276	0	265	3	0
All	All	7542	0	7017	75	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 5.

All (75) 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:55:TYR:O	1:A:59:ARG:HG2	1.96	0.66
1:A:535:GLU:O	1:A:536:ASN:ND2	2.32	0.63
1:A:512:GLY:HA2	1:A:527:ILE:HD11	1.80	0.61
1:B:673:GLN:OE1	1:B:747:PHE:CE2	2.54	0.61
1:B:742:GLU:O	1:B:745:VAL:HG12	2.01	0.60
1:A:760:HIS:O	1:A:764:MSE:HB2	2.03	0.58
1:B:164:PRO:HA	1:B:167:THR:HG22	1.85	0.58
1:A:59:ARG:HG3	1:B:537:TYR:HB3	1.85	0.58
1:A:537:TYR:HA	1:A:568:MSE:HE1	1.85	0.57
1:B:478:GLY:N	1:B:493:ILE:HD11	2.19	0.57
1:B:562:SER:O	1:B:566:THR:HB	2.05	0.57
1:A:568:MSE:HE2	1:B:55:TYR:CE1	2.40	0.56
1:B:501:HIS:O	1:B:504:THR:HG22	2.06	0.55
1:A:528:PHE:HA	1:A:531:VAL:HG12	1.90	0.54
1:B:645:TYR:HB3	1:B:678:LEU:HD23	1.90	0.53
1:A:146:PRO:HB2	1:A:469:MSE:HE1	1.91	0.53
1:B:739:VAL:HG23	1:B:739:VAL:O	2.09	0.52
1:B:645:TYR:HB3	1:B:678:LEU:CD2	2.39	0.52
1:B:528:PHE:O	1:B:531:VAL:HG12	2.10	0.51
1:B:513:ARG:HA	1:B:544:ILE:HD11	1.92	0.51
1:B:478:GLY:CA	1:B:493:ILE:HD11	2.41	0.51
1:A:503:ASN:O	1:A:534:ILE:HD13	2.11	0.51
1:B:168:PHE:C	1:B:469:MSE:HE3	2.31	0.51
1:B:673:GLN:O	1:B:676:VAL:HG22	2.11	0.51
1:A:761:LEU:O	1:A:765:ASN:ND2	2.44	0.50
1:A:150:SER:HG	1:B:23:ASP:CG	2.14	0.50
1:A:162:PRO:O	1:A:164:PRO:HD3	2.12	0.49
1:B:80:VAL:HG21	1:B:120:LEU:HD11	1.94	0.49
1:A:58:TYR:O	1:A:62:LYS:HB2	2.13	0.49
1:A:489:GLU:O	1:A:493:ILE:HG12	2.13	0.49
1:A:26:PHE:O	1:A:30:ARG:HG2	2.12	0.48
1:A:758:GLN:CG	1:A:761:LEU:HD13	2.43	0.48
1:B:745:VAL:O	1:B:749:ILE:HG13	2.13	0.48
1:A:668:LEU:HA	1:A:671:ASN:O	2.14	0.48
1:A:168:PHE:C	1:A:469:MSE:HE3	2.34	0.47
1:B:566:THR:HG22	1:B:567:ASP:N	2.28	0.47
1:A:516:PHE:CD2	1:A:548:THR:HG22	2.49	0.47
1:B:146:PRO:HB2	1:B:469:MSE:HE1	1.97	0.47
1:A:598:ARG:HG3	2:S:89:LEU:HD22	1.95	0.47
1:B:666:LYS:O	1:B:670:ILE:HG12	2.14	0.46
1:B:645:TYR:CD2	1:B:678:LEU:HD23	2.50	0.46
1:B:485:TYR:CD1	1:B:671:ASN:OD1	2.69	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:ALA:O	1:B:494:LEU:HG	2.16	0.46
1:A:761:LEU:N	1:A:761:LEU:HD12	2.31	0.46
1:B:566:THR:CG2	1:B:567:ASP:N	2.79	0.46
1:A:651:TYR:CD1	1:A:659:LEU:HD11	2.51	0.45
1:B:681:ILE:O	1:B:685:GLN:HG3	2.15	0.45
1:A:613:LEU:HD22	1:A:617:PHE:CE2	2.52	0.45
1:A:608:TYR:CE2	1:A:612:LEU:HD11	2.52	0.45
1:A:715:ARG:O	1:A:718:VAL:HG12	2.17	0.44
1:A:150:SER:OG	1:B:23:ASP:CG	2.55	0.44
1:A:761:LEU:O	1:A:764:MSE:HB3	2.18	0.44
1:B:623:LEU:HD23	1:B:650:ILE:HG23	2.00	0.43
1:A:611:THR:HG1	1:A:640:HIS:CD2	2.36	0.43
1:B:615:HIS:O	1:B:618:VAL:HG22	2.19	0.43
1:A:544:ILE:O	1:A:548:THR:HG23	2.19	0.43
1:A:481:ALA:O	1:A:484:SER:O	2.37	0.43
1:A:576:TRP:CH2	2:S:89:LEU:HD21	2.54	0.42
1:B:168:PHE:C	1:B:469:MSE:CE	2.88	0.42
1:B:627:LEU:HD11	1:B:650:ILE:HG21	2.01	0.42
1:A:521:TYR:HB2	1:A:552:LEU:HD21	2.02	0.41
1:B:532:ARG:HD3	1:B:542:MSE:SE	2.69	0.41
1:A:30:ARG:NH2	1:B:504:THR:HG21	2.35	0.41
1:B:68:THR:OG1	1:B:69:PRO:HD2	2.20	0.41
1:A:651:TYR:CG	1:A:659:LEU:HD11	2.55	0.41
1:B:44:LEU:HD22	1:B:48:TYR:CE1	2.55	0.41
1:B:55:TYR:CD1	1:B:56:LYS:N	2.89	0.41
1:B:549:LEU:O	1:B:552:LEU:O	2.39	0.41
1:B:634:ILE:HD13	1:B:644:TRP:CE2	2.56	0.41
1:A:121:LEU:HD22	1:A:125:TYR:CE2	2.56	0.41
2:S:99:ILE:HA	2:S:102:LEU:HB2	2.03	0.41
1:A:528:PHE:HZ	1:A:544:ILE:HD11	1.87	0.40
1:B:494:LEU:HD11	1:B:511:ILE:HG13	2.04	0.40
1:B:661:GLU:OE2	1:B:710:LEU:HB2	2.22	0.40
1:A:464:ALA:HB3	1:B:7:PRO:HG2	2.03	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	465/560 (83%)	436 (94%)	29 (6%)	0	100	100
1	B	466/560 (83%)	433 (93%)	33 (7%)	0	100	100
2	S	33/43 (77%)	33 (100%)	0	0	100	100
All	All	964/1163 (83%)	902 (94%)	62 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	355/473 (75%)	330 (93%)	25 (7%)	15	43
1	B	365/473 (77%)	335 (92%)	30 (8%)	11	36
2	S	26/36 (72%)	25 (96%)	1 (4%)	33	62
All	All	746/982 (76%)	690 (92%)	56 (8%)	13	39

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	44	LEU
1	A	59	ARG
1	A	64	HIS
1	A	65	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	70	GLN
1	A	117	THR
1	A	160	GLU
1	A	494	LEU
1	A	509	CYS
1	A	525	GLU
1	A	533	ARG
1	A	534	ILE
1	A	536	ASN
1	A	547	THR
1	A	548	THR
1	A	598	ARG
1	A	613	LEU
1	A	631	ARG
1	A	636	VAL
1	A	658	SER
1	A	671	ASN
1	A	675	SER
1	A	708	ASN
1	A	718	VAL
1	B	16	LEU
1	B	23	ASP
1	B	30	ARG
1	B	44	LEU
1	B	66	CYS
1	B	77	LYS
1	B	103	HIS
1	B	117	THR
1	B	129	ASP
1	B	135	SER
1	B	144	LEU
1	B	155	LEU
1	B	170	PHE
1	B	493	ILE
1	B	513	ARG
1	B	526	ARG
1	B	531	VAL
1	B	544	ILE
1	B	552	LEU
1	B	566	THR
1	B	574	GLU
1	B	588	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	613	LEU
1	B	627	LEU
1	B	686	HIS
1	B	751	LYS
1	B	756	LEU
1	B	768	TRP
1	B	772	LEU
1	B	773	ASP
2	S	99	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	708	ASN
1	B	671	ASN

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	462/560 (82%)	-0.10	6 (1%) 77 75	47, 87, 125, 202	0
1	B	463/560 (82%)	-0.12	5 (1%) 80 80	52, 75, 116, 195	0
2	S	33/43 (76%)	-0.25	0 100 100	62, 84, 115, 125	0
All	All	958/1163 (82%)	-0.11	11 (1%) 80 80	47, 80, 125, 202	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	705	ASP	4.1
1	B	701	ALA	3.6
1	A	705	ASP	3.0
1	A	688	LEU	2.7
1	B	699	ASN	2.6
1	A	760	HIS	2.4
1	A	701	ALA	2.4
1	B	703	VAL	2.3
1	A	704	ILE	2.2
1	B	704	ILE	2.1
1	A	650	ILE	2.1

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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.