



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:57 AM GMT

PDB ID : 3NMX
Title : Crystal structure of APC complexed with Asef
Authors : Zhang, Z.; Chen, L.; Gao, L.; Lin, K.; Wu, G.
Deposited on : 2010-06-22
Resolution : 2.30 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

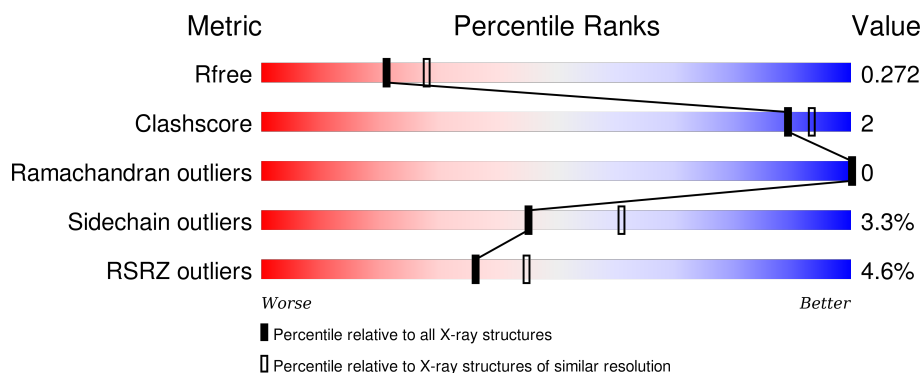
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 $\leq 5\%$. 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	354	<div> <div>3%</div> <div>85% 6% 8%</div> </div>
1	B	354	<div> <div>2%</div> <div>86% 6% 8%</div> </div>
1	C	354	<div> <div>7%</div> <div>84% 6% 9%</div> </div>
2	D	25	<div> <div>16%</div> <div>40% 12% 48%</div> </div>
2	E	25	<div> <div>40% 12% 48%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	25	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a green segment on the left labeled '48%', a yellow segment in the middle, and a grey segment on the right labeled '48%'. A small black dot is located at the boundary between the yellow and grey segments.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8318 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 APC variant protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	6	0	0
			2513	1565	454	468	26			
1	B	325	Total	C	N	O	S	0	0	0
			2515	1568	453	468	26			
1	C	323	Total	C	N	O	S	0	0	0
			2503	1559	453	466	25			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	398	MET	-	EXPRESSION TAG	UNP Q4LE70
A	399	GLY	-	EXPRESSION TAG	UNP Q4LE70
A	400	HIS	-	EXPRESSION TAG	UNP Q4LE70
A	401	HIS	-	EXPRESSION TAG	UNP Q4LE70
A	402	HIS	-	EXPRESSION TAG	UNP Q4LE70
A	403	HIS	-	EXPRESSION TAG	UNP Q4LE70
A	404	HIS	-	EXPRESSION TAG	UNP Q4LE70
A	405	HIS	-	EXPRESSION TAG	UNP Q4LE70
A	406	MET	-	EXPRESSION TAG	UNP Q4LE70
B	398	MET	-	EXPRESSION TAG	UNP Q4LE70
B	399	GLY	-	EXPRESSION TAG	UNP Q4LE70
B	400	HIS	-	EXPRESSION TAG	UNP Q4LE70
B	401	HIS	-	EXPRESSION TAG	UNP Q4LE70
B	402	HIS	-	EXPRESSION TAG	UNP Q4LE70
B	403	HIS	-	EXPRESSION TAG	UNP Q4LE70
B	404	HIS	-	EXPRESSION TAG	UNP Q4LE70
B	405	HIS	-	EXPRESSION TAG	UNP Q4LE70
B	406	MET	-	EXPRESSION TAG	UNP Q4LE70
C	398	MET	-	EXPRESSION TAG	UNP Q4LE70
C	399	GLY	-	EXPRESSION TAG	UNP Q4LE70
C	400	HIS	-	EXPRESSION TAG	UNP Q4LE70
C	401	HIS	-	EXPRESSION TAG	UNP Q4LE70
C	402	HIS	-	EXPRESSION TAG	UNP Q4LE70

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Chain	Residue	Modelled	Actual	Comment	Reference
C	403	HIS	-	EXPRESSION TAG	UNP Q4LE70
C	404	HIS	-	EXPRESSION TAG	UNP Q4LE70
C	405	HIS	-	EXPRESSION TAG	UNP Q4LE70
C	406	MET	-	EXPRESSION TAG	UNP Q4LE70

- Molecule 2 is a protein called Rho guanine nucleotide exchange factor 4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	13	Total	C	N	O	0	0	0
			90	55	15	20			
2	E	13	Total	C	N	O	0	0	0
			90	55	15	20			
2	F	13	Total	C	N	O	0	0	0
			90	55	15	20			

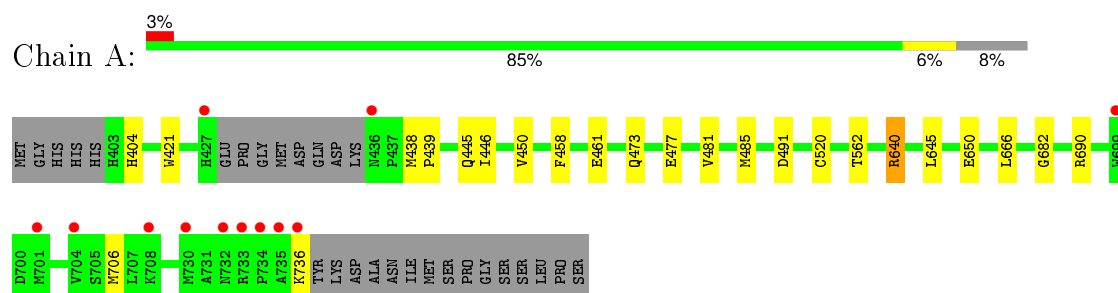
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	166	Total	O	0	0
			166	166		
3	B	190	Total	O	0	0
			190	190		
3	C	120	Total	O	0	0
			120	120		
3	D	13	Total	O	0	0
			13	13		
3	E	15	Total	O	0	0
			15	15		
3	F	13	Total	O	0	0
			13	13		

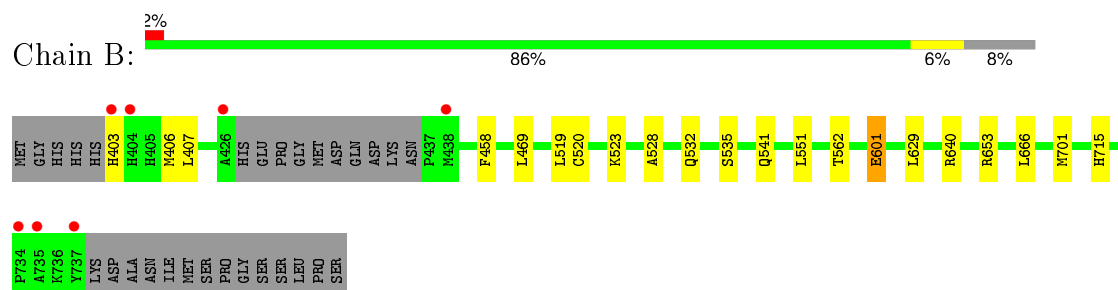
3 Residue-property plots [i](#)

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.

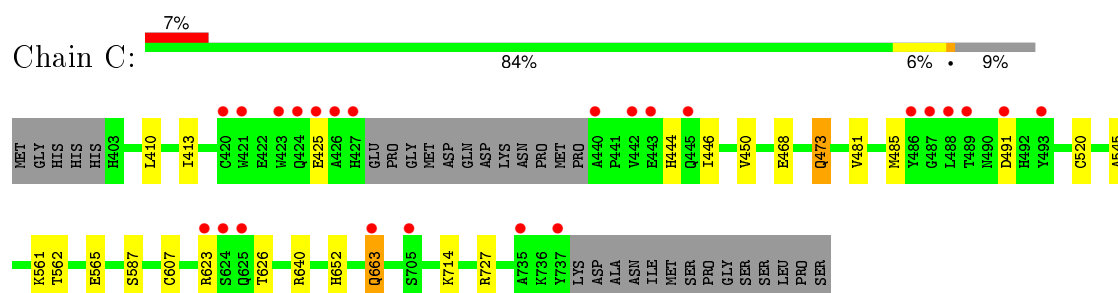
- Molecule 1: APC variant protein



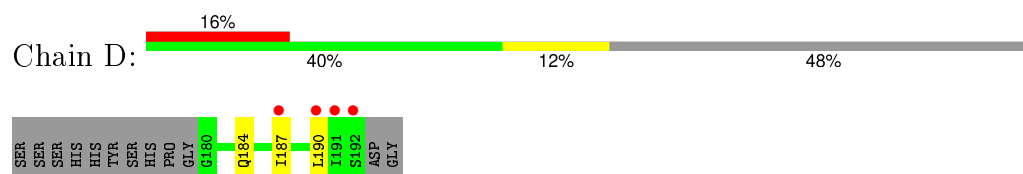
- Molecule 1: APC variant protein



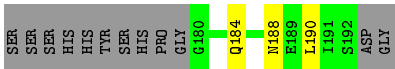
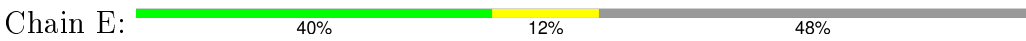
- Molecule 1: APC variant protein



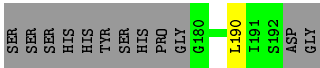
- Molecule 2: Rho guanine nucleotide exchange factor 4



- Molecule 2: Rho guanine nucleotide exchange factor 4



- Molecule 2: Rho guanine nucleotide exchange factor 4



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.79Å 92.18Å 107.84Å 90.00° 93.77° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 43.61 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.5 (50.00-2.30) 90.6 (43.61-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	14.22 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.208 , 0.254 0.227 , 0.272	Depositor DCC
R_{free} test set	2923 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 57893 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8318	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.30	0/2551	0.45	0/3448
1	B	0.30	0/2554	0.45	0/3451
1	C	0.30	0/2541	0.45	0/3433
2	D	0.40	0/89	0.44	0/118
2	E	0.37	0/89	0.44	0/118
2	F	0.40	0/89	0.39	0/118
All	All	0.30	0/7913	0.45	0/10686

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

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	2513	0	2534	17	0
1	B	2515	0	2540	10	0
1	C	2503	0	2523	14	0
2	D	90	0	88	3	0
2	E	90	0	88	3	0
2	F	90	0	88	1	0
3	A	166	0	0	0	0
3	B	190	0	0	0	0
3	C	120	0	0	0	0
3	D	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	15	0	0	0	0
3	F	13	0	0	0	0
All	All	8318	0	7861	37	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 2.

All (37) 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:690:ARG:HG2	1:C:468:GLU:OE1	1.75	0.86
1:A:421:TRP:HZ2	1:A:477:GLU:HG3	1.59	0.68
1:A:520:CYS:O	1:A:562:THR:HG21	1.99	0.62
1:C:561:LYS:O	1:C:565:GLU:HG2	2.00	0.62
1:A:421:TRP:HZ2	1:A:477:GLU:CG	2.13	0.61
1:A:473:GLN:O	1:A:477:GLU:HB2	2.03	0.58
2:E:190:LEU:HD22	2:F:190:LEU:HD22	1.85	0.57
1:A:690:ARG:CG	1:C:468:GLU:OE2	2.53	0.57
1:C:473:GLN:HE21	1:C:473:GLN:H	1.53	0.56
2:D:184:GLN:HE21	2:D:187:ILE:HD11	1.70	0.56
1:A:666:LEU:HD12	1:A:706:MET:SD	2.46	0.55
1:C:663:GLN:HE21	1:C:663:GLN:H	1.55	0.55
1:B:520:CYS:O	1:B:562:THR:HG21	2.08	0.54
1:A:690:ARG:HD2	1:C:468:GLU:OE2	2.09	0.51
1:C:520:CYS:O	1:C:562:THR:HG21	2.10	0.51
1:B:458:PHE:CE2	2:E:190:LEU:HD21	2.46	0.49
1:A:690:ARG:HG2	1:C:468:GLU:CD	2.33	0.49
2:E:184:GLN:HE22	2:E:188:ASN:ND2	2.10	0.48
1:B:407:LEU:HD13	1:B:469:LEU:HD22	1.96	0.47
1:C:473:GLN:NE2	1:C:473:GLN:H	2.12	0.46
1:C:607:CYS:HB3	1:C:652:HIS:CE1	2.50	0.46
1:A:650:GLU:H	1:B:715:HIS:CE1	2.34	0.46
1:A:640:ARG:HH11	1:A:682:GLY:HA3	1.82	0.45
1:A:458:PHE:CE2	2:D:190:LEU:HD21	2.52	0.44
1:B:528:ALA:O	1:B:532:GLN:HG2	2.18	0.43
1:B:519:LEU:HD23	1:B:551:LEU:HD21	1.99	0.43
1:B:403:HIS:HD2	1:B:406:MET:HB2	1.83	0.43
1:C:413:ILE:HA	1:C:446:ILE:HD11	2.01	0.43
1:A:650:GLU:H	1:B:715:HIS:HE1	1.67	0.42
1:B:601:GLU:HG2	1:B:601:GLU:H	1.65	0.42
1:C:481:VAL:O	1:C:485:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:VAL:HG13	1:A:485:MET:HE2	2.02	0.41
1:A:690:ARG:HG3	1:C:468:GLU:OE2	2.20	0.41
1:B:535:SER:O	1:B:541:GLN:NE2	2.50	0.41
1:A:458:PHE:CZ	2:D:190:LEU:HD21	2.57	0.40
1:C:545:ALA:HB3	1:C:587:SER:HB3	2.03	0.40
1:A:438:MET:HA	1:A:439:PRO:HD3	1.92	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	322/354 (91%)	320 (99%)	2 (1%)	0	100	100
1	B	321/354 (91%)	317 (99%)	4 (1%)	0	100	100
1	C	319/354 (90%)	316 (99%)	3 (1%)	0	100	100
2	D	11/25 (44%)	10 (91%)	1 (9%)	0	100	100
2	E	11/25 (44%)	10 (91%)	1 (9%)	0	100	100
2	F	11/25 (44%)	10 (91%)	1 (9%)	0	100	100
All	All	995/1137 (88%)	983 (99%)	12 (1%)	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	274/300 (91%)	265 (97%)	9 (3%)	45	61
1	B	275/300 (92%)	268 (98%)	7 (2%)	55	73
1	C	273/300 (91%)	261 (96%)	12 (4%)	35	46
2	D	9/19 (47%)	9 (100%)	0	100	100
2	E	9/19 (47%)	9 (100%)	0	100	100
2	F	9/19 (47%)	9 (100%)	0	100	100
All	All	849/957 (89%)	821 (97%)	28 (3%)	45	61

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	404	HIS
1	A	445	GLN
1	A	446	ILE
1	A	450	VAL
1	A	461	GLU
1	A	491	ASP
1	A	640	ARG
1	A	645	LEU
1	A	736	LYS
1	B	523	LYS
1	B	601	GLU
1	B	629	LEU
1	B	640	ARG
1	B	653	ARG
1	B	666	LEU
1	B	701	MET
1	C	410	LEU
1	C	425	GLU
1	C	444	HIS
1	C	450	VAL
1	C	473	GLN
1	C	491	ASP
1	C	623	ARG
1	C	626	THR
1	C	640	ARG
1	C	663	GLN
1	C	714	LYS
1	C	727	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	652	HIS
1	B	403	HIS
1	B	405	HIS
1	B	715	HIS
1	B	732	ASN
1	C	405	HIS
1	C	473	GLN
1	C	663	GLN
1	C	728	ASN
2	E	188	ASN
2	F	184	GLN
2	F	188	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 carbohydrates 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 ⓘ

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, 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	326/354 (92%)	0.19	12 (3%) 45 54	13, 30, 54, 78	19 (5%)
1	B	325/354 (91%)	0.09	7 (2%) 65 73	11, 29, 55, 79	16 (4%)
1	C	323/354 (91%)	0.39	24 (7%) 17 25	20, 45, 88, 168	10 (3%)
2	D	13/25 (52%)	1.33	4 (30%) 1 1	25, 30, 59, 76	0
2	E	13/25 (52%)	0.10	0 100 100	12, 19, 40, 53	3 (23%)
2	F	13/25 (52%)	0.61	0 100 100	17, 28, 54, 71	0
All	All	1013/1137 (89%)	0.24	47 (4%) 36 45	11, 33, 68, 168	48 (4%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	735	ALA	6.2
1	C	427	HIS	6.2
1	C	421	TRP	5.3
1	C	442	VAL	5.0
1	C	486	TYR	4.4
1	C	420	CYS	3.9
1	A	733	ARG	3.7
1	A	736	LYS	3.7
1	C	489	THR	3.5
1	C	424	GLN	3.3
1	C	443	GLU	3.1
2	D	190	LEU	3.1
1	C	426	ALA	3.1
1	B	403	HIS	3.1
1	C	488	LEU	3.0
1	B	734	PRO	3.0
1	A	734	PRO	3.0
1	A	735	ALA	3.0
1	C	445	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	438	MET	2.9
1	C	625	GLN	2.9
1	A	708	LYS	2.9
1	C	705	SER	2.8
1	A	699	TRP	2.8
1	C	623	ARG	2.8
1	B	737	TYR	2.7
1	A	427	HIS	2.7
2	D	192	SER	2.7
1	A	732	ASN	2.6
1	C	487	GLY	2.6
1	B	404	HIS	2.6
1	C	737	TYR	2.5
1	C	491	ASP	2.5
1	A	701	MET	2.5
1	C	493	TYR	2.5
1	A	704	VAL	2.4
1	B	426	ALA	2.4
1	A	436	ASN	2.4
1	C	735	ALA	2.3
2	D	191	ILE	2.3
1	C	440	ALA	2.2
1	C	423	TRP	2.2
1	C	425	GLU	2.2
1	A	730	MET	2.1
2	D	187	ILE	2.1
1	C	663	GLN	2.0
1	C	624	SER	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.