wwPDB X-ray Structure Validation Summary Report (i)

Aug 20, 2023 – 02:29 AM EDT

PDB ID	:	2H66
Title	:	The Crystal Structure of Plasmodium Vivax 2-Cys peroxiredoxin
Authors	:	Wernimont, A.K.; Dong, A.; Zhao, Y.; Lew, J.; Melone, M.; Kozieradzki, I.; Weigelt, J.; Sundstrom, M.; Edwards, A.M.; Arrowsmith, C.H.; Bochkarev, A.; Hui, R.; Artz, J.D.; Structural Genomics Consortium (SGC)
Deposited on	:	2006-05-30
Resolution	:	2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

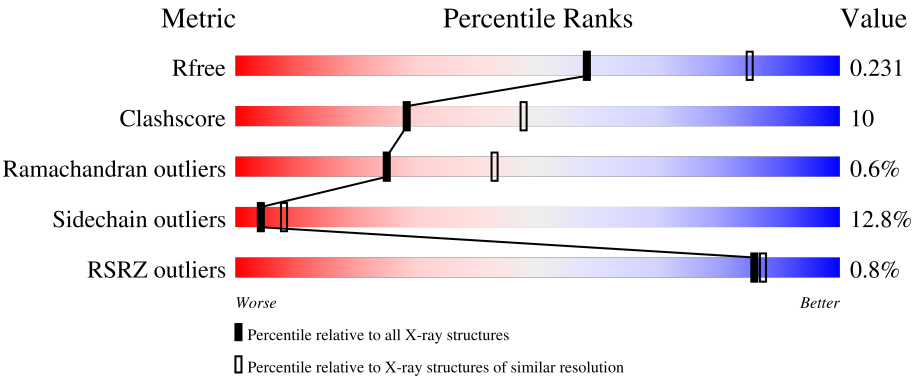
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	213	52% 22% 5% 22%
1	B	213	60% 15% 6% 20%
1	C	213	61% 15% 20%
1	D	213	62% 15% 21%
1	E	213	56% 15% 24%

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Mol	Chain	Length	Quality of chain
1	F	213	2% 54% 20% 5% 21%
1	G	213	57% 16% 7% 20%
1	H	213	% 58% 18% 22%
1	I	213	% 63% 14% 6% 17%
1	J	213	54% 18% 23%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13448 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 PV-PF14_0368.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	0	0	0
			1325	862	216	244	3			
1	B	171	Total	C	N	O	S	0	0	0
			1346	875	219	248	4			
1	C	170	Total	C	N	O	S	0	0	0
			1333	865	217	247	4			
1	D	169	Total	C	N	O	S	0	0	0
			1335	868	218	246	3			
1	E	161	Total	C	N	O	S	0	0	0
			1273	830	207	233	3			
1	F	168	Total	C	N	O	S	0	0	0
			1331	865	217	245	4			
1	G	171	Total	C	N	O	S	0	0	0
			1346	875	219	248	4			
1	H	167	Total	C	N	O	S	0	0	0
			1322	861	216	242	3			
1	I	177	Total	C	N	O	S	0	0	0
			1395	906	229	256	4			
1	J	163	Total	C	N	O	S	0	0	0
			1288	839	211	235	3			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	10	Total	O	0	0
			10	10		
2	B	8	Total	O	0	0
			8	8		
2	C	23	Total	O	0	0
			23	23		
2	D	14	Total	O	0	0
			14	14		

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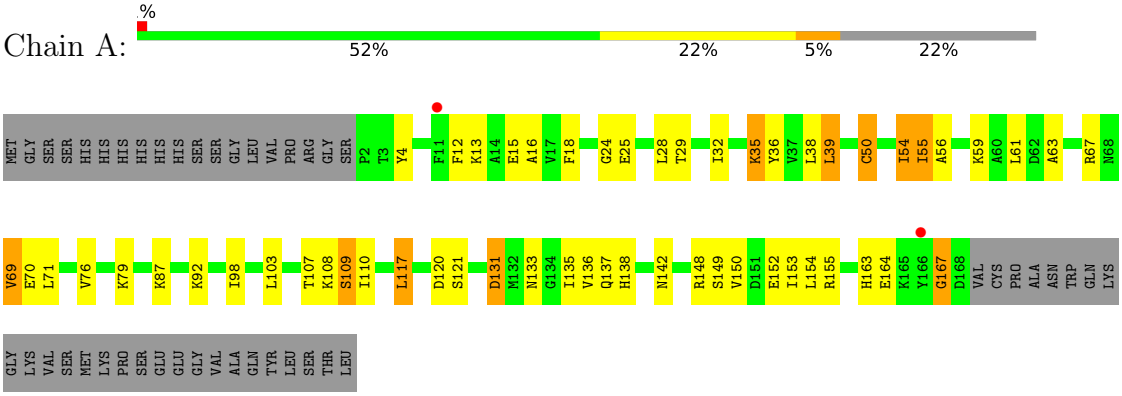
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	12	Total O 12 12	0	0
2	F	12	Total O 12 12	0	0
2	G	10	Total O 10 10	0	0
2	H	18	Total O 18 18	0	0
2	I	23	Total O 23 23	0	0
2	J	24	Total O 24 24	0	0

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.

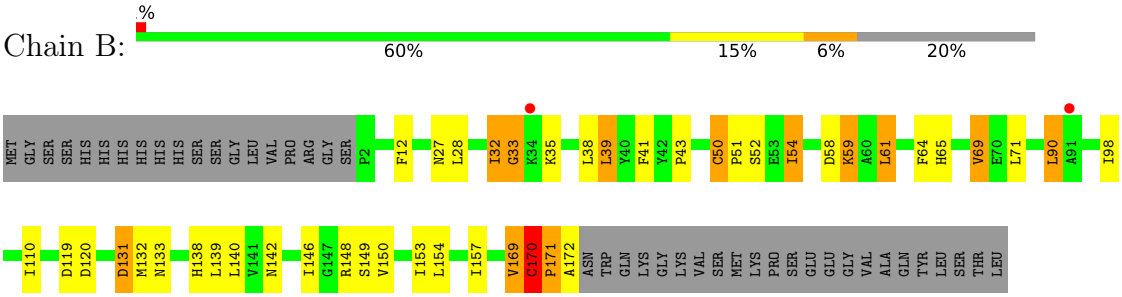
• Molecule 1: PV-PF14_0368

Chain A:



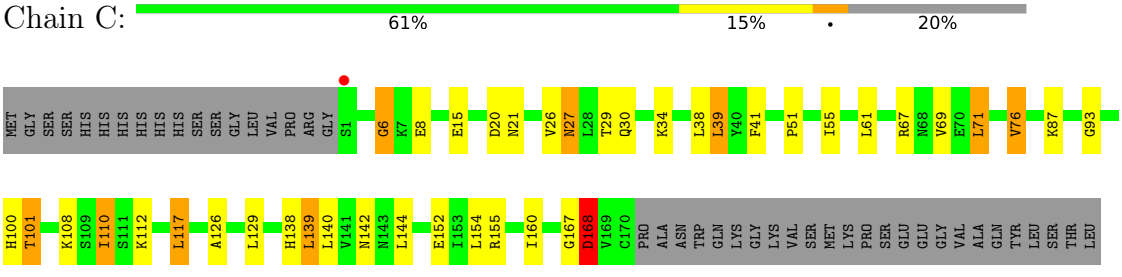
• Molecule 1: PV-PF14_0368

Chain B:



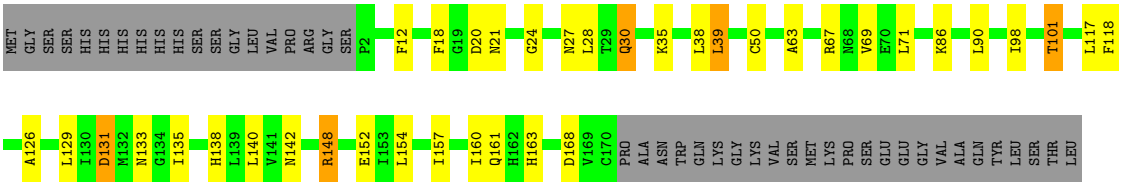
• Molecule 1: PV-PF14_0368

Chain C:



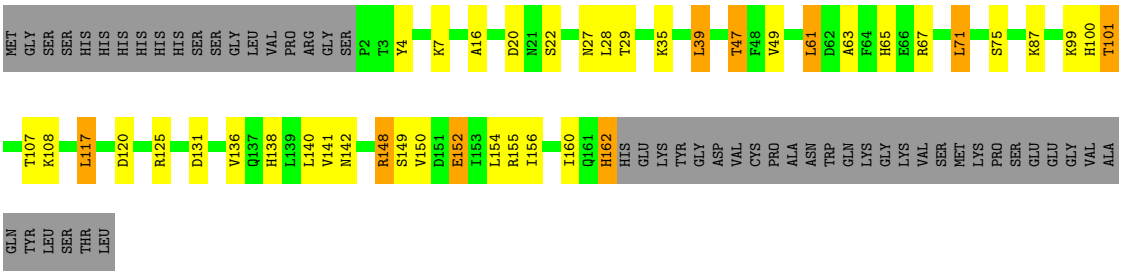
• Molecule 1: PV-PF14_0368

Chain D:



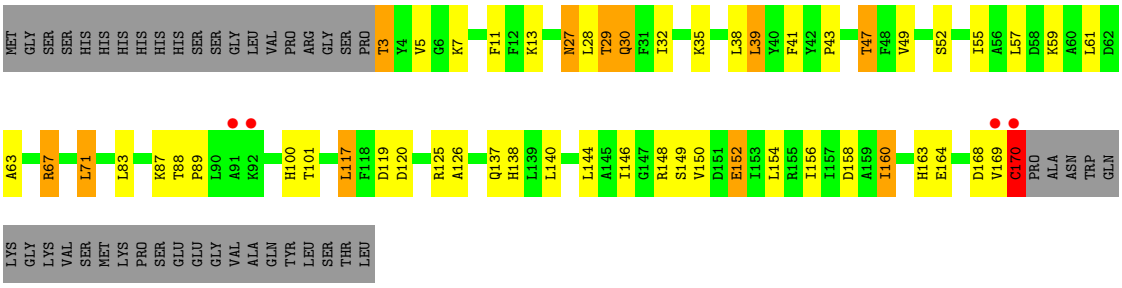
• Molecule 1: PV-PF14_0368

Chain E:



• Molecule 1: PV-PF14_0368

Chain F:

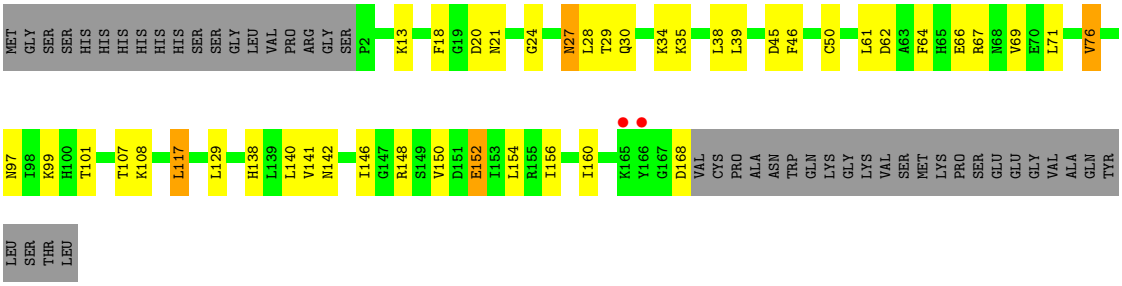


• Molecule 1: PV-PF14_0368

Chain G:

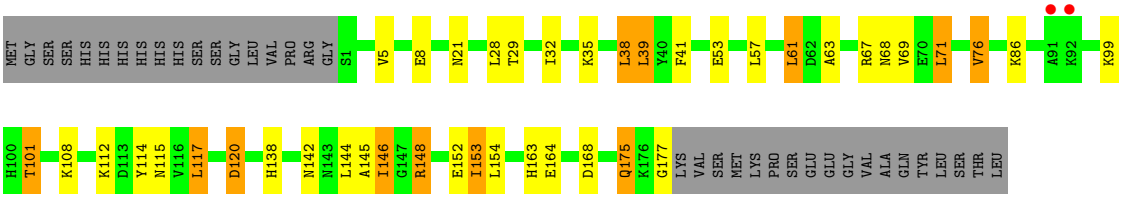
• Molecule 1: PV-PF14_0368

Chain H:



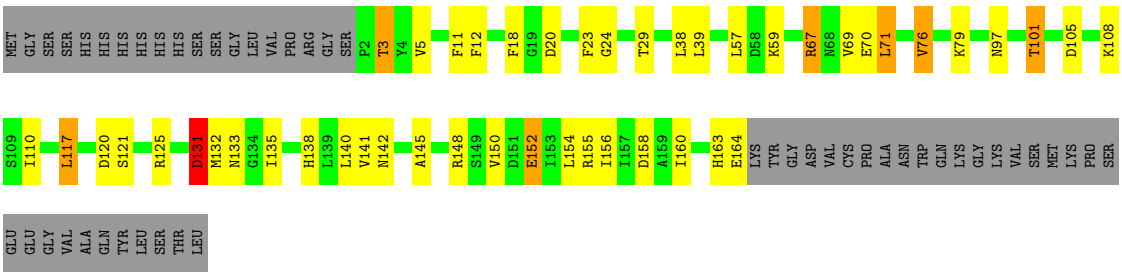
- Molecule 1: PV-PF14_0368

Chain I:



- Molecule 1: PV-PF14_0368

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.55Å 149.59Å 131.91Å 90.00° 104.88° 90.00°	Depositor
Resolution (Å)	41.56 – 2.50 40.25 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.7 (41.56-2.50) 94.7 (40.25-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.194 , 0.232 0.194 , 0.231	Depositor DCC
R_{free} test set	4302 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 35.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13448	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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	0.72	0/1355	0.78	1/1834 (0.1%)
1	B	0.75	1/1377 (0.1%)	0.82	2/1867 (0.1%)
1	C	0.82	1/1363 (0.1%)	0.87	3/1849 (0.2%)
1	D	0.72	1/1365 (0.1%)	0.76	2/1848 (0.1%)
1	E	0.78	2/1301 (0.2%)	0.81	2/1762 (0.1%)
1	F	0.84	3/1360 (0.2%)	0.80	0/1841
1	G	0.76	1/1377 (0.1%)	0.81	1/1867 (0.1%)
1	H	0.85	3/1352 (0.2%)	0.80	2/1830 (0.1%)
1	I	0.84	2/1428 (0.1%)	0.79	0/1937
1	J	0.83	1/1317 (0.1%)	0.84	1/1784 (0.1%)
All	All	0.79	15/13595 (0.1%)	0.81	14/18419 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3
1	C	0	2
All	All	0	5

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	168	ASP	C-O	12.44	1.47	1.23
1	F	170	CYS	C-O	10.16	1.42	1.23
1	E	162	HIS	C-O	7.80	1.38	1.23
1	I	177	GLY	CA-C	7.35	1.63	1.51
1	F	152	GLU	CG-CD	7.34	1.62	1.51

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	168	ASP	OD1-CG-OD2	-7.21	109.60	123.30
1	E	39	LEU	CA-CB-CG	6.44	130.12	115.30
1	G	28	LEU	CA-CB-CG	6.29	129.77	115.30
1	C	139	LEU	CA-CB-CG	6.01	129.13	115.30
1	B	170	CYS	C-N-CD	-5.78	107.88	120.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	169	VAL	Peptide
1	B	170	CYS	Peptide
1	B	33	GLY	Peptide
1	C	168	ASP	Sidechain
1	C	6	GLY	Peptide

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	1325	0	1327	29	0
1	B	1346	0	1342	24	0
1	C	1333	0	1316	27	0
1	D	1335	0	1331	25	0
1	E	1273	0	1286	25	0
1	F	1331	0	1334	34	0
1	G	1346	0	1342	35	0
1	H	1322	0	1325	18	0
1	I	1395	0	1386	40	0
1	J	1288	0	1294	30	0
2	A	10	0	0	0	0
2	B	8	0	0	0	0
2	C	23	0	0	3	0
2	D	14	0	0	1	0
2	E	12	0	0	3	0
2	F	12	0	0	0	0
2	G	10	0	0	2	0
2	H	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	23	0	0	4	0
2	J	24	0	0	1	0
All	All	13448	0	13283	260	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 10.

The worst 5 of 260 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:171:PRO:HB2	1:B:172:ALA:O	1.43	1.16
1:F:149:SER:HB3	1:F:152:GLU:HG3	1.30	1.08
1:E:16:ALA:HB3	2:E:203:HOH:O	1.60	1.00
1:B:32:ILE:HD13	1:B:33:GLY:H	1.31	0.95
1:I:67:ARG:CZ	2:I:204:HOH:O	2.16	0.93

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	165/213 (78%)	153 (93%)	10 (6%)	2 (1%)	13 24
1	B	169/213 (79%)	158 (94%)	8 (5%)	3 (2%)	8 14
1	C	168/213 (79%)	157 (94%)	9 (5%)	2 (1%)	13 24
1	D	167/213 (78%)	160 (96%)	7 (4%)	0	100 100
1	E	159/213 (75%)	153 (96%)	6 (4%)	0	100 100
1	F	166/213 (78%)	156 (94%)	10 (6%)	0	100 100
1	G	169/213 (79%)	162 (96%)	6 (4%)	1 (1%)	25 43
1	H	165/213 (78%)	160 (97%)	5 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	I	175/213 (82%)	166 (95%)	8 (5%)	1 (1%)	25 43
1	J	161/213 (76%)	155 (96%)	5 (3%)	1 (1%)	25 43
All	All	1664/2130 (78%)	1580 (95%)	74 (4%)	10 (1%)	25 43

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	GLY
1	C	168	ASP
1	G	21	ASN
1	I	145	ALA
1	C	167	GLY

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	145/184 (79%)	124 (86%)	21 (14%)	3 6
1	B	147/184 (80%)	125 (85%)	22 (15%)	3 5
1	C	144/184 (78%)	125 (87%)	19 (13%)	4 7
1	D	145/184 (79%)	135 (93%)	10 (7%)	15 30
1	E	140/184 (76%)	122 (87%)	18 (13%)	4 8
1	F	146/184 (79%)	123 (84%)	23 (16%)	2 4
1	G	147/184 (80%)	124 (84%)	23 (16%)	2 4
1	H	144/184 (78%)	126 (88%)	18 (12%)	4 8
1	I	151/184 (82%)	135 (89%)	16 (11%)	6 13
1	J	141/184 (77%)	126 (89%)	15 (11%)	6 13
All	All	1450/1840 (79%)	1265 (87%)	185 (13%)	4 8

5 of 185 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	27	ASN
1	H	39	LEU
1	G	38	LEU
1	G	117	LEU
1	H	101	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	27	ASN
1	I	138	HIS
1	H	30	GLN
1	I	21	ASN
1	I	175	GLN

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

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	167/213 (78%)	-0.16	2 (1%) 79 80	34, 49, 67, 84	0
1	B	171/213 (80%)	-0.15	2 (1%) 79 80	36, 47, 67, 85	0
1	C	170/213 (79%)	-0.21	1 (0%) 89 90	30, 41, 59, 73	0
1	D	169/213 (79%)	-0.21	0 100 100	32, 48, 61, 70	0
1	E	161/213 (75%)	-0.30	0 100 100	33, 45, 61, 76	0
1	F	168/213 (78%)	-0.13	4 (2%) 59 62	33, 46, 65, 86	0
1	G	171/213 (80%)	-0.18	0 100 100	33, 47, 62, 67	0
1	H	167/213 (78%)	-0.34	2 (1%) 79 80	26, 41, 61, 84	0
1	I	177/213 (83%)	-0.21	2 (1%) 80 82	30, 43, 58, 65	0
1	J	163/213 (76%)	-0.40	0 100 100	27, 37, 51, 64	0
All	All	1684/2130 (79%)	-0.23	13 (0%) 86 87	26, 44, 62, 86	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	166	TYR	3.5
1	I	92	LYS	3.2
1	A	11	PHE	2.9
1	F	92	LYS	2.8
1	B	91	ALA	2.7

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 (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.