WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:03 AM GMT

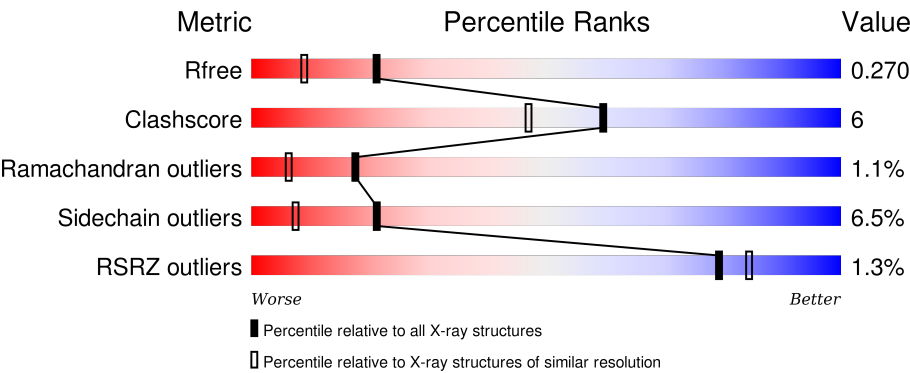|		
PDB ID	:	2VPF
Title	:	VASCULAR ENDOTHELIAL GROWTH FACTOR REFINED TO 1.93 ANGSTROMS RESOLUTION
Authors	:	Muller, Y.A.; De Vos, A.M.
Deposited on	:	1997-07-29
Resolution	:	1.93 Å(reported)

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 1.93 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 | Percentile Ranks | Value

Rfree — 0.270
Clashscore — 6
Ramachandran outliers — 1.1%
Sidechain outliers — 6.5%
RSRZ outliers — 1.3%

Worse | *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	2910 (1.96-1.92)
Clashscore	102246	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)
RSRZ outliers	91569	2915 (1.96-1.92)

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	102	% 78% 16% • 5%
1	B	102	% 75% 18% • 6%
1	C	102	2% 77% 11% • • 9%
1	D	102	4% 71% 18% 5% 7%
1	E	102	81% 11% • 6%

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Mol	Chain	Length	Quality of chain
1	F	102	74% 18% 6%
1	G	102	70% 19% 7%
1	H	102	80% 10% 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6782 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 VASCULAR ENDOTHELIAL GROWTH FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	97	Total 776	C 487	N 131	O 145	S 13	0	0	0
1	B	96	Total 775	C 487	N 131	O 144	S 13	0	0	0
1	C	93	Total 752	C 472	N 126	O 141	S 13	0	0	0
1	D	95	Total 766	C 481	N 129	O 143	S 13	0	0	0
1	E	96	Total 775	C 487	N 131	O 144	S 13	0	0	0
1	F	96	Total 771	C 484	N 130	O 144	S 13	0	0	0
1	G	95	Total 766	C 481	N 129	O 143	S 13	0	0	0
1	H	94	Total 761	C 478	N 128	O 142	S 13	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	102	Total 102	O 102	0	0
2	B	95	Total 95	O 95	0	0
2	C	52	Total 52	O 52	0	0
2	D	68	Total 68	O 68	0	0
2	E	96	Total 96	O 96	0	0
2	F	78	Total 78	O 78	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	56	Total 56	O 56	0	0
2	H	93	Total 93	O 93	0	0

3 Residue-property plots ⓘ

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: VASCULAR ENDOTHELIAL GROWTH FACTOR
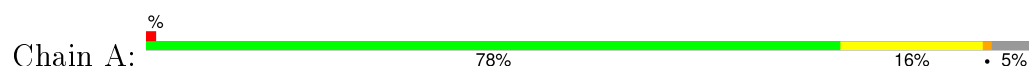
- Molecule 1: VASCULAR ENDOTHELIAL GROWTH FACTOR

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- Molecule 1: VASCULAR ENDOTHELIAL GROWTH FACTOR

- Molecule 1: VASCULAR ENDOTHELIAL GROWTH FACTOR

GLY GLN ASN HIS HIS E13 V20 Y21 Q22 R23 C26 L32 Q37 I43 F47 K48 P49 M55 D63 E72 M81 R82 I83 K84 Q87 I91 Q98 K101 K108 ASP

● Molecule 1: VASCULAR ENDOTHELIAL GROWTH FACTOR

%

Chain G: 70%   19% · · 7%

GLY GLN ASN HIS HIS E13 V20 Q37 E38 Y39 P40 D41 E42 I43 E44 Y45 I46 F47 K48 M55 G59 C60 V69 P70 E73 M78 R82 I83 K84 E93 L97 Q98 H99 N100 R105 P106 K107 LYS ASP

● Molecule 1: VASCULAR ENDOTHELIAL GROWTH FACTOR

Chain H: 80%   10% · 8%

GLY GLN ASN HIS HIS GLU V14 V15 Y21 Q22 R23 L32 V33 D34 D41 K48 C51 M55 N62 D63 Q98 K107 LYS ASP
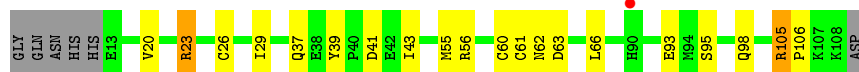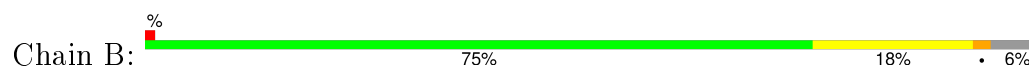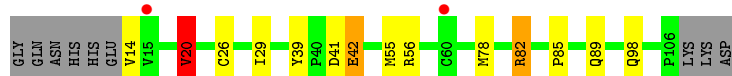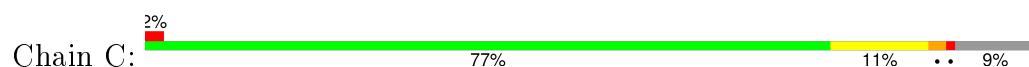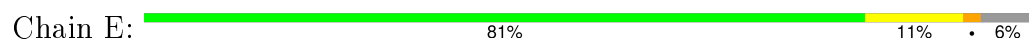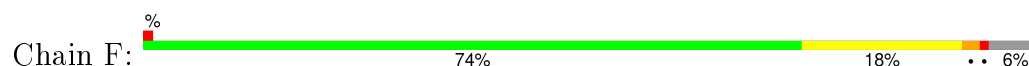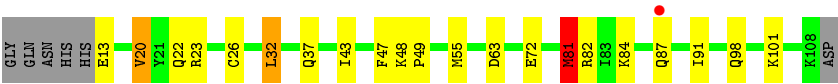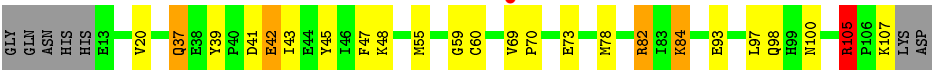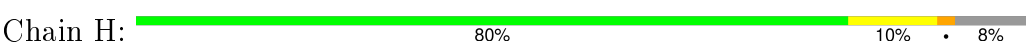
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	45.47Å　68.47Å　85.82Å 105.44°　93.71°　101.49°	Depositor
Resolution (Å)	16.00　–　1.93 64.31　–　1.90	Depositor EDS
% Data completeness (in resolution range)	94.0 (16.00-1.93) 84.9 (64.31-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.64 (at 1.90Å)	Xtriage
Refinement program	REFMAC, X-PLOR	Depositor
R, R_{free}	0.209　,　0.272 0.207　,　0.270	Depositor DCC
R_{free} test set	7074 reflections (11.44%)	DCC
Wilson B-factor (Å^2)	29.9	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 60.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Outliers	0 of 70694 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6782	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (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	0.61	0/794	1.38	8/1071 (0.7%)
1	B	0.59	0/793	1.33	6/1068 (0.6%)
1	C	0.53	0/770	1.22	5/1039 (0.5%)
1	D	0.50	0/784	1.20	3/1057 (0.3%)
1	E	0.59	0/793	1.22	3/1068 (0.3%)
1	F	0.58	0/789	1.27	6/1064 (0.6%)
1	G	0.46	0/784	1.13	2/1057 (0.2%)
1	H	0.59	0/779	1.29	3/1050 (0.3%)
All	All	0.56	0/6286	1.26	36/8474 (0.4%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	23	ARG	NE-CZ-NH1	15.08	127.84	120.30
1	F	81	MET	CA-CB-CG	10.22	130.68	113.30
1	B	23	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	C	82	ARG	NE-CZ-NH1	-9.25	115.68	120.30
1	B	56	ARG	NE-CZ-NH2	9.10	124.85	120.30
1	A	23	ARG	CD-NE-CZ	8.80	135.93	123.60
1	A	105	ARG	NE-CZ-NH2	-8.71	115.95	120.30
1	C	56	ARG	NE-CZ-NH2	7.91	124.26	120.30
1	F	23	ARG	NE-CZ-NH2	-7.45	116.57	120.30
1	D	23	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	A	72	GLU	OE1-CD-OE2	-6.81	115.12	123.30
1	C	20	VAL	CB-CA-C	-6.68	98.70	111.40
1	H	34	ASP	CB-CG-OD2	-6.68	112.28	118.30
1	A	23	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	D	20	VAL	CB-CA-C	-6.32	99.40	111.40
1	E	23	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	C	56	ARG	NE-CZ-NH1	-6.27	117.17	120.30
1	H	34	ASP	CB-CG-OD1	6.18	123.86	118.30
1	F	87	GLN	CA-C-N	6.05	128.30	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	20	VAL	CB-CA-C	-5.94	100.11	111.40
1	A	39	TYR	CB-CG-CD1	5.82	124.49	121.00
1	C	42	GLU	OE1-CD-OE2	5.81	130.28	123.30
1	B	105	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	B	23	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	G	37	GLN	CB-CG-CD	5.47	125.83	111.60
1	B	39	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	D	56	ARG	CD-NE-CZ	5.42	131.18	123.60
1	A	41	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	23	ARG	CG-CD-NE	5.28	122.88	111.80
1	F	87	GLN	N-CA-C	5.26	125.21	111.00
1	H	23	ARG	CD-NE-CZ	5.21	130.89	123.60
1	E	39	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	E	82	ARG	CB-CA-C	5.18	120.75	110.40
1	G	105	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	41	ASP	CB-CG-OD1	5.14	122.92	118.30
1	F	20	VAL	N-CA-CB	5.13	122.80	111.50

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	776	0	732	7	0
1	B	775	0	741	12	0
1	C	752	0	713	11	0
1	D	766	0	728	13	0
1	E	775	0	741	7	0
1	F	771	0	730	9	0
1	G	766	0	729	14	0
1	H	761	0	727	9	0
2	A	102	0	0	1	0
2	B	95	0	0	3	0
2	C	52	0	0	4	0
2	D	68	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	96	0	0	0	0
2	F	78	0	0	2	0
2	G	56	0	0	1	0
2	H	93	0	0	0	0
All	All	6782	0	5841	67	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 6.

All (67) 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:F:81:MET:HE3	1:F:91:ILE:HD12	1.68	0.76
1:G:60:CYS:HG	1:H:51:CYS:HG	0.76	0.75
1:G:55:MET:H	1:G:98:GLN:HE21	1.35	0.75
1:C:39:TYR:HB3	1:C:42:GLU:HG3	1.69	0.73
1:D:69:VAL:HB	1:D:70:PRO:HD2	1.72	0.71
1:H:55:MET:H	1:H:98:GLN:HE21	1.41	0.69
1:E:23:ARG:HD2	2:F:156:HOH:O	1.93	0.67
1:G:39:TYR:HB3	1:G:42:GLU:HG3	1.78	0.66
1:H:55:MET:H	1:H:98:GLN:NE2	1.96	0.64
1:A:23:ARG:HD2	2:B:142:HOH:O	1.97	0.64
1:B:55:MET:H	1:B:98:GLN:HE21	1.47	0.62
1:G:47:PHE:CE1	1:G:82:ARG:HD2	2.34	0.61
1:G:59:GLY:HA2	1:H:32:LEU:HG	1.81	0.61
1:G:47:PHE:HE1	1:G:82:ARG:HD2	1.64	0.61
1:B:55:MET:H	1:B:98:GLN:NE2	1.99	0.60
1:G:55:MET:H	1:G:98:GLN:NE2	1.99	0.59
2:C:160:HOH:O	1:D:23:ARG:HD2	2.03	0.58
1:C:14:VAL:HG13	1:D:77:THR:HG22	1.84	0.58
1:D:86:HIS:HD2	2:D:151:HOH:O	1.88	0.56
1:B:105:ARG:NH1	1:E:41:ASP:HB3	2.21	0.56
1:E:55:MET:H	1:E:98:GLN:NE2	2.05	0.55
1:D:103:GLU:HG2	1:D:105:ARG:HG2	1.88	0.55
1:F:47:PHE:HE1	1:F:82:ARG:HE	1.56	0.54
1:G:78:MET:HG2	1:H:15:VAL:HB	1.89	0.54
1:D:69:VAL:HB	1:D:70:PRO:CD	2.39	0.52
1:C:82:ARG:HG3	2:C:158:HOH:O	2.10	0.52
1:C:20:VAL:HG11	1:D:52:VAL:HG12	1.92	0.51
1:G:60:CYS:CB	1:H:51:CYS:HG	2.24	0.49
1:G:73:GLU:HB3	1:G:97:LEU:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:TYR:HB3	1:C:42:GLU:CG	2.41	0.49
1:F:55:MET:H	1:F:98:GLN:HE21	1.60	0.49
1:D:103:GLU:OE2	1:D:105:ARG:HD2	2.13	0.49
1:C:55:MET:H	1:C:98:GLN:NE2	2.10	0.48
1:C:29:ILE:HD13	2:C:136:HOH:O	2.11	0.48
1:F:13:GLU:N	2:F:160:HOH:O	2.45	0.48
1:G:41:ASP:HB2	2:G:145:HOH:O	2.13	0.48
1:D:66:LEU:O	1:D:107:LYS:HE2	2.14	0.47
1:D:63:ASP:HB3	1:D:66:LEU:HD12	1.97	0.46
1:A:55:MET:H	1:A:98:GLN:NE2	2.12	0.46
1:A:78:MET:HB3	1:B:20:VAL:HG21	1.98	0.46
1:E:83:ILE:HG12	1:E:89:GLN:CG	2.46	0.46
2:A:119:HOH:O	1:B:23:ARG:HD2	2.15	0.45
1:F:55:MET:H	1:F:98:GLN:NE2	2.14	0.45
1:E:55:MET:H	1:E:98:GLN:HE21	1.64	0.45
1:G:45:TYR:CE1	1:G:84:LYS:HG3	2.52	0.45
1:C:98:GLN:NE2	2:C:111:HOH:O	2.49	0.45
1:D:75:ASN:HD21	1:F:22:GLN:NE2	2.15	0.45
1:B:105:ARG:CZ	1:E:41:ASP:HB3	2.47	0.45
1:B:37:GLN:NE2	2:B:138:HOH:O	2.50	0.44
1:F:63:ASP:OD2	1:H:48:LYS:NZ	2.44	0.44
1:G:69:VAL:HG21	1:G:105:ARG:NE	2.31	0.44
1:F:48:LYS:HA	1:F:49:PRO:C	2.37	0.44
1:H:21:TYR:HE1	1:H:62:ASN:HD22	1.65	0.43
1:E:59:GLY:HA2	1:F:32:LEU:HG	1.99	0.43
1:D:64:GLU:O	1:D:107:LYS:HE3	2.19	0.43
1:C:78:MET:HG2	1:D:15:VAL:HB	1.99	0.43
1:C:55:MET:H	1:C:98:GLN:HE21	1.65	0.43
1:A:18:MET:O	1:A:22:GLN:HG3	2.19	0.42
1:A:14:VAL:HG21	1:B:93:GLU:OE2	2.20	0.42
1:G:69:VAL:HB	1:G:70:PRO:HD2	2.01	0.41
1:C:42:GLU:OE1	1:C:82:ARG:NH1	2.53	0.41
1:A:44:GLU:CD	1:A:44:GLU:H	2.24	0.41
1:B:98:GLN:NE2	2:B:116:HOH:O	2.53	0.41
1:B:61:CYS:O	1:B:62:ASN:HB2	2.21	0.41
1:A:55:MET:H	1:A:98:GLN:HE21	1.68	0.40
1:B:95:SER:HB3	1:H:41:ASP:HA	2.02	0.40
1:B:66:LEU:HD23	1:B:106:PRO:HA	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	95/102 (93%)	92 (97%)	2 (2%)	1 (1%)	17	6
1	B	94/102 (92%)	90 (96%)	2 (2%)	2 (2%)	9	2
1	C	91/102 (89%)	90 (99%)	0	1 (1%)	17	6
1	D	93/102 (91%)	89 (96%)	3 (3%)	1 (1%)	17	6
1	E	94/102 (92%)	93 (99%)	0	1 (1%)	17	6
1	F	94/102 (92%)	90 (96%)	3 (3%)	1 (1%)	17	6
1	G	93/102 (91%)	88 (95%)	5 (5%)	0	100	100
1	H	92/102 (90%)	87 (95%)	4 (4%)	1 (1%)	17	6
All	All	746/816 (91%)	719 (96%)	19 (2%)	8 (1%)	17	6

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	26	CYS
1	A	26	CYS
1	B	26	CYS
1	E	26	CYS
1	B	63	ASP
1	C	26	CYS
1	F	26	CYS
1	H	63	ASP

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	89/96 (93%)	85 (96%)	4 (4%)	34	18
1	B	90/96 (94%)	87 (97%)	3 (3%)	45	31
1	C	88/96 (92%)	84 (96%)	4 (4%)	34	18
1	D	89/96 (93%)	79 (89%)	10 (11%)	7	1
1	E	90/96 (94%)	86 (96%)	4 (4%)	35	18
1	F	89/96 (93%)	81 (91%)	8 (9%)	12	2
1	G	89/96 (93%)	78 (88%)	11 (12%)	6	1
1	H	89/96 (93%)	87 (98%)	2 (2%)	60	50
All	All	713/768 (93%)	667 (94%)	46 (6%)	21	7

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	37	GLN
1	A	43	ILE
1	A	90	HIS
1	B	29	ILE
1	B	43	ILE
1	B	60	CYS
1	C	20	VAL
1	C	41	ASP
1	C	85	PRO
1	C	89	GLN
1	D	20	VAL
1	D	22	GLN
1	D	52	VAL
1	D	60	CYS
1	D	73	GLU
1	D	82	ARG
1	D	87	GLN
1	D	89	GLN
1	D	103	GLU
1	D	105	ARG
1	E	37	GLN
1	E	73	GLU
1	E	82	ARG
1	E	108	LYS
1	F	20	VAL
1	F	32	LEU

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Mol	Chain	Res	Type
1	F	37	GLN
1	F	43	ILE
1	F	72	GLU
1	F	81	MET
1	F	84	LYS
1	F	101	LYS
1	G	20	VAL
1	G	37	GLN
1	G	42	GLU
1	G	43	ILE
1	G	48	LYS
1	G	82	ARG
1	G	84	LYS
1	G	93	GLU
1	G	100	ASN
1	G	105	ARG
1	G	107	LYS
1	H	32	LEU
1	H	63	ASP

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	98	GLN
1	B	98	GLN
1	C	87	GLN
1	C	89	GLN
1	C	98	GLN
1	D	89	GLN
1	D	98	GLN
1	E	98	GLN
1	F	22	GLN
1	F	89	GLN
1	F	98	GLN
1	G	98	GLN
1	H	98	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 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 (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(Å²)	Q<0.9
1	A	97/102 (95%)	0.01	1 (1%)	84	88	32, 39, 55, 68	0
1	B	96/102 (94%)	0.10	1 (1%)	84	88	30, 40, 64, 71	0
1	C	93/102 (91%)	0.27	2 (2%)	65	73	34, 48, 64, 73	0
1	D	95/102 (93%)	0.44	4 (4%)	40	49	41, 50, 65, 70	0
1	E	96/102 (94%)	0.03	0	100	100	32, 41, 56, 63	0
1	F	96/102 (94%)	0.03	1 (1%)	84	88	32, 43, 68, 77	0
1	G	95/102 (93%)	0.26	1 (1%)	82	87	41, 50, 66, 73	0
1	H	94/102 (92%)	0.07	0	100	100	30, 41, 60, 63	0
All	All	762/816 (93%)	0.15	10 (1%)	79	84	30, 44, 64, 77	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	ASP	3.9
1	D	102	CYS	3.3
1	D	104	CYS	3.0
1	B	90	HIS	2.7
1	C	60	CYS	2.5
1	C	15	VAL	2.5
1	D	66	LEU	2.4
1	D	67	GLU	2.3
1	G	69	VAL	2.1
1	F	87	GLN	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.