



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:28 am BST

PDB ID : 2FJH
Title : Structure of the B20-4 Fab, a phage derived Fab fragment, in complex with VEGF
Authors : Wiesmann, C.
Deposited on : 2006-01-02
Resolution : 3.10 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
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

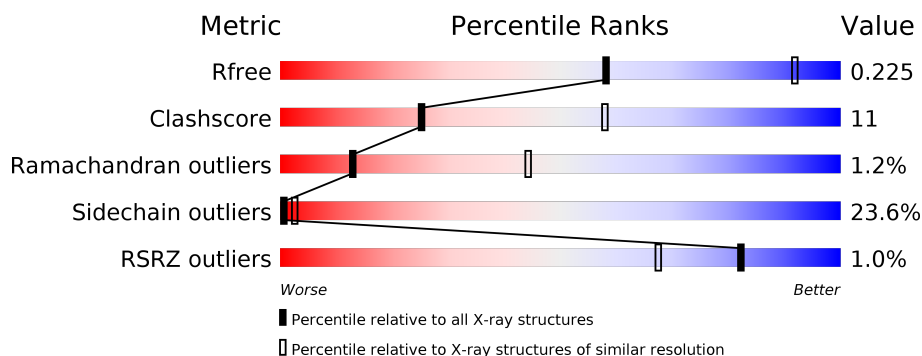
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 $\leq 5\%$. 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	V	102	<div> <div></div> <div>68%23%6%.</div> </div>
1	W	102	<div> <div>2%</div> <div>68%19%9%5%</div> </div>
2	A	214	<div> <div>2%</div> <div>55%37%7%.</div> </div>
2	L	214	<div> <div></div> <div>60%30%9%</div> </div>
3	B	228	<div> <div>%</div> <div>63%30%. .</div> </div>
3	H	228	<div> <div></div> <div>60%32%. .</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8103 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 A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	V	98	Total	C	N	O	S	0	0	0
			797	499	135	150	13			
1	W	97	Total	C	N	O	S	0	0	0
			787	493	132	149	13			


- Molecule 2 is a protein called Fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1632	1016	279	331	6			
2	A	211	Total	C	N	O	S	0	0	0
			1613	1006	276	326	5			

- Molecule 3 is a protein called Fab fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	219	Total	C	N	O	S	0	0	0
			1637	1038	274	318	7			
3	B	219	Total	C	N	O	S	0	0	0
			1637	1038	274	318	7			

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.

- Chain V: 

Amino Acid	Count
GLY	1
GLI	1
ASN	1
HIS	1
HI2	1
K16	1
Y20	1
Q22	1
C26	1
F36	1
Q37	1
D41	1
E42	1
I43	1
E44	1
Y45	1
K48	1
P49	1
S50	1
R56	1
M62	1
D63	1
E64	1
E67	1
T71	1
E72	1
E73	1
S74	1
N75	1
M81	1
Q87	1
L97	1
E103	1
C104	1
R105	1
P107	1
K108	1
K109	1

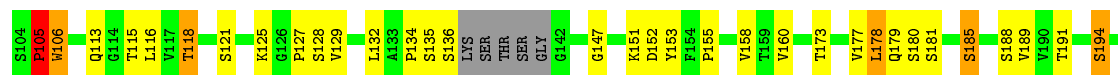
- Chain W:
-
- | Amino Acid | Percentage |
|------------|------------|
| GLY | 2% |
| GLN | 68% |
| ASN | 19% |
| HIS | 9% |
| HIS | 5% |
| F13 | |
| V14 | |
| V15 | |
| K16 | |
| F17 | |
| F17 | |
| M18 | |
| D19 | |
| Q22 | |
| R23 | |
| I29 | |
| D34 | |
| D41 | |
| Y45 | |
| I46 | |
| F47 | |
| K48 | |
| P49 | |
| S50 | |
| R56 | |
| D63 | |
| E67 | |
| G68 | |
| V69 | |
| I76 | |
| Q79 | |
| R82 | |
| I83 | |
| K84 | |
| Q87 | |
| M94 | |
| S95 | |
| F96 | |
| L97 | |
| K107 | |
| I108 | |
| D109 | |

- Chain L:
-
- | Category | Percentage |
|---------------------|------------|
| Category 1 (Green) | 60% |
| Category 2 (Yellow) | 30% |
| Category 3 (Orange) | 9% |
- Legend: 60% 30% 9%
- Chain L: D1, I2, P8, S9, S10, L11, V15, G16, D17, R18, V19, T20, R24, Q27, V28, I29, R30, R31, S32, L33, K39, P40, Y49, A50, A51, S52, M53, S56, R61, S65, F71, T72, L73, D82, F83, Q80, S91, N92, T93, S94, T102, K103, R108, T109, A110, D122, E123, K124, L125, K126, S131, G134, L135, L136, M137, Y140, P141, R142, K145, K149, L154, Q155, M158, S159, Q160, V163, T164, E165, Q166, D167, S168, K169, Y173, S174, L175, L181, S182, K183, A184, D185, K188, H189, K190, A193, C194, H198, Q199, G200, L201, S202, C214

- Chain A:
-
- 2% 55% 37% 7%
- D1 I2 Q3 M4 T5 Q6 S7 P8 S9 S10 L11 S14 R18 V19 T20 I21 T22 C23 R24 A25 S26 Q27 V28 I29 R30 R31 S32 L33 Q37 Q38 K39 P40 S60 R61 P62 S67 D70 F71 T72 L73 T74 I75 Q79 P80 R81 D82 F83 Q89 Q90 S91 N92 T93 F98 G99 Q100 G101 T102 R108 T109 P113 I117 D122 E123 Q124 L125 S131 L135 N138 F139 Q147 W148 K149 V150 D151 M152 A153 L154 Q155 S156 G157 M158 S162 W163 T164 E165 K169 D170 L171 S172 T172 Y173 S177 T178 L179 K183 A184 D185 Y186 F187 F188



- Molecule 3: Fab fragment heavy chain



- Molecule 3: Fab fragment heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	165.54Å 165.54Å 150.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.10 39.90 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.00-3.10) 98.0 (39.90-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.198 , 0.239 0.188 , 0.225	Depositor DCC
R_{free} test set	2120 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	95.4	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 80.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8103	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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, 0.333 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	V	0.69	0/816	0.84	4/1099 (0.4%)
1	W	0.46	0/805	0.78	5/1084 (0.5%)
2	A	0.44	0/1645	0.76	5/2233 (0.2%)
2	L	0.64	0/1664	0.91	5/2258 (0.2%)
3	B	0.47	0/1682	0.76	1/2299 (0.0%)
3	H	0.54	0/1682	0.81	2/2299 (0.1%)
All	All	0.54	0/8294	0.81	22/11272 (0.2%)

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
3	H	0	1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	167	ASP	CB-CG-OD2	6.84	124.46	118.30
1	W	41	ASP	CB-CG-OD2	6.53	124.17	118.30
2	A	70	ASP	CB-CG-OD2	6.19	123.88	118.30
2	A	82	ASP	CB-CG-OD2	6.12	123.81	118.30
1	W	109	ASP	CB-CG-OD2	6.06	123.76	118.30
2	L	17	ASP	CB-CG-OD2	5.96	123.66	118.30
2	L	142	ARG	NE-CZ-NH1	5.90	123.25	120.30
2	L	1	ASP	CB-CG-OD2	5.64	123.37	118.30
2	L	82	ASP	CB-CG-OD2	5.54	123.28	118.30
1	V	41	ASP	CB-CG-OD2	5.51	123.26	118.30
1	W	63	ASP	CB-CG-OD2	5.46	123.22	118.30
2	A	122	ASP	CB-CG-OD2	5.43	123.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	151	ASP	CB-CG-OD2	5.39	123.15	118.30
1	W	19	ASP	CB-CG-OD2	5.34	123.11	118.30
1	W	34	ASP	CB-CG-OD2	5.30	123.07	118.30
3	H	152	ASP	CB-CG-OD2	5.28	123.05	118.30
1	V	63	ASP	CB-CG-OD2	5.22	123.00	118.30
1	V	20	VAL	CB-CA-C	-5.13	101.65	111.40
3	H	105	PRO	CA-C-N	-5.13	105.92	117.20
3	B	216	ASP	CB-CG-OD2	5.12	122.91	118.30
1	V	109	ASP	CB-CG-OD2	5.11	122.89	118.30
2	A	170	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	105	PRO	Peptide

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	V	797	0	758	7	0
1	W	787	0	751	9	0
2	A	1613	0	1588	46	0
2	L	1632	0	1601	49	0
3	B	1637	0	1586	34	0
3	H	1637	0	1585	34	0
All	All	8103	0	7869	171	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 11.

All (171) 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)
2:L:2:ILE:HD13	2:L:29:ILE:HD11	1.48	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:50:ALA:HB3	2:L:53:ASN:HD21	1.36	0.91
3:B:179:GLN:HE22	3:B:185:SER:HB3	1.37	0.89
3:B:179:GLN:NE2	3:B:185:SER:HB3	1.88	0.88
2:L:164:THR:HG22	2:L:174:SER:H	1.43	0.83
2:L:40:PRO:HG3	2:L:165:GLU:HG2	1.60	0.82
2:L:158:ASN:ND2	2:L:158:ASN:H	1.79	0.81
2:L:112:ALA:HB1	2:L:201:LEU:HD13	1.65	0.79
2:L:83:PHE:HZ	2:L:165:GLU:HG3	1.50	0.77
2:L:164:THR:CG2	2:L:174:SER:H	1.97	0.77
3:H:30:ASN:HD22	3:H:74:THR:HG21	1.50	0.76
3:H:35:HIS:HD2	3:H:47:TRP:HE1	1.36	0.74
2:A:198:HIS:CD2	2:A:200:GLY:H	2.07	0.73
1:W:67:GLU:OE2	1:W:108:LYS:HB2	1.88	0.73
2:A:198:HIS:HD2	2:A:200:GLY:H	1.35	0.72
2:L:108:ARG:HD3	2:L:109:THR:O	1.91	0.71
2:A:4:MET:HA	2:A:4:MET:CE	2.21	0.70
2:L:198:HIS:CD2	2:L:200:GLY:H	2.10	0.70
2:L:49:TYR:O	2:L:53:ASN:ND2	2.28	0.67
3:H:127:PRO:HB3	3:H:153:TYR:HB3	1.76	0.67
2:A:4:MET:HA	2:A:4:MET:HE3	1.77	0.66
3:B:43:LYS:HG3	3:B:44:GLY:N	2.11	0.66
1:V:67:GLU:HG2	1:V:107:LYS:HG3	1.78	0.66
2:A:30:ARG:HE	2:A:92:ASN:HD21	1.43	0.65
3:B:29:ILE:H	3:B:77:ASN:HD21	1.45	0.65
2:L:40:PRO:HG3	2:L:165:GLU:CG	2.28	0.64
3:H:30:ASN:ND2	3:H:74:THR:HG21	2.14	0.63
2:L:124:GLN:HE22	2:L:131:SER:HB2	1.63	0.62
1:V:67:GLU:HG2	1:V:107:LYS:CG	2.28	0.62
2:A:29:ILE:HG13	2:A:90:GLN:HG3	1.82	0.62
3:B:35:HIS:CD2	3:B:47:TRP:HE1	2.18	0.61
3:H:208:HIS:HD2	3:H:211:SER:OG	1.84	0.60
2:A:155:GLN:HB3	2:A:158:ASN:HD21	1.66	0.60
2:A:6:GLN:HB2	2:A:100:GLN:HE22	1.66	0.59
2:A:30:ARG:HB2	2:A:92:ASN:ND2	2.17	0.59
3:H:30:ASN:HD22	3:H:74:THR:CG2	2.13	0.59
2:A:170:ASP:OD1	2:A:172:THR:HG23	2.03	0.59
3:B:151:LYS:HA	3:B:185:SER:HB2	1.84	0.58
2:L:122:ASP:HB2	3:H:222:LYS:HZ2	1.69	0.58
2:L:61:ARG:HG2	2:L:61:ARG:HH11	1.68	0.57
3:H:151:LYS:HA	3:H:185:SER:HB2	1.87	0.57
2:L:123:GLU:O	2:L:126:LYS:HB2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:84:LYS:HB3	1:W:87:GLN:HB2	1.87	0.56
2:A:113:PRO:HB3	2:A:139:PHE:HB3	1.87	0.56
2:L:167:ASP:OD2	2:L:169:LYS:N	2.19	0.56
3:B:43:LYS:HG3	3:B:44:GLY:H	1.71	0.55
2:A:193:ALA:HB2	2:A:208:SER:HB3	1.87	0.55
3:B:35:HIS:HD2	3:B:47:TRP:HE1	1.53	0.55
2:L:2:ILE:HG12	2:L:27:GLN:HG2	1.88	0.55
1:V:71:THR:HG21	1:V:103:GLU:HG3	1.88	0.55
2:A:62:PHE:CE1	2:A:75:ILE:HG12	2.42	0.55
3:B:101:HIS:H	3:B:101:HIS:CD2	2.26	0.54
2:L:83:PHE:CZ	2:L:165:GLU:HG3	2.36	0.54
2:A:108:ARG:HD3	2:A:109:THR:O	2.07	0.54
2:L:122:ASP:HB2	3:H:222:LYS:NZ	2.23	0.54
3:B:91:THR:HG23	3:B:118:THR:HA	1.91	0.53
2:L:142:ARG:HH11	2:L:142:ARG:HG3	1.72	0.53
2:L:193:ALA:HA	2:L:208:SER:HB3	1.91	0.53
3:H:29:ILE:H	3:H:77:ASN:HD21	1.56	0.53
3:B:6:GLU:N	3:B:113:GLN:OE1	2.32	0.53
2:L:112:ALA:HB1	2:L:201:LEU:CD1	2.38	0.53
2:A:3:GLN:HB2	2:A:26:SER:HB3	1.91	0.52
2:L:142:ARG:CG	2:L:142:ARG:HH11	2.23	0.52
3:B:38:ARG:HD3	3:B:48:VAL:HG22	1.90	0.52
2:L:24:ARG:HH11	2:L:24:ARG:HB2	1.75	0.52
3:B:122:ALA:HB3	3:B:154:PHE:CE1	2.46	0.51
3:H:83:MET:HE2	3:H:86:LEU:HD21	1.92	0.51
1:W:45:TYR:CD1	1:W:82:ARG:HB3	2.46	0.51
2:A:89:GLN:HB2	2:A:98:PHE:CD2	2.46	0.50
2:L:31:ARG:NH2	2:L:52:SER:HB3	2.27	0.50
1:W:16:LYS:HD2	3:B:59:ASN:HD21	1.77	0.50
2:A:158:ASN:ND2	2:A:158:ASN:H	2.10	0.49
2:A:21:ILE:HG12	2:A:102:THR:HG21	1.94	0.49
2:A:138:ASN:HA	2:A:173:TYR:O	2.13	0.49
3:B:94:TYR:O	3:B:114:GLY:HA2	2.12	0.49
2:L:142:ARG:NH1	2:L:142:ARG:HG3	2.28	0.49
3:B:208:HIS:NE2	3:B:210:PRO:HG2	2.27	0.48
2:A:198:HIS:HD2	2:A:200:GLY:N	2.06	0.48
2:A:193:ALA:CB	2:A:208:SER:HB3	2.44	0.48
2:A:61:ARG:NH2	2:A:82:ASP:OD1	2.46	0.48
2:L:158:ASN:H	2:L:158:ASN:HD22	1.58	0.48
2:A:29:ILE:CG1	2:A:90:GLN:HG3	2.44	0.47
3:B:43:LYS:CG	3:B:44:GLY:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:160:VAL:HG11	3:H:188:SER:CB	2.45	0.47
3:H:35:HIS:CD2	3:H:47:TRP:HE1	2.24	0.47
2:L:163:VAL:HG22	2:L:175:LEU:HD12	1.96	0.47
2:A:6:GLN:OE1	2:A:99:GLY:HA3	2.15	0.47
1:V:48:LYS:HB3	1:V:81:MET:HB3	1.95	0.47
3:H:194:SER:O	3:H:197:LEU:HB2	2.15	0.47
2:A:8:PRO:O	2:A:102:THR:HG23	2.14	0.47
2:A:29:ILE:HG13	2:A:90:GLN:CG	2.45	0.47
3:B:6:GLU:HA	3:B:21:SER:O	2.15	0.47
3:B:29:ILE:O	3:B:53:PRO:HG2	2.15	0.47
1:W:23:ARG:NH1	2:A:92:ASN:O	2.36	0.47
3:H:129:VAL:O	3:H:217:LYS:HD3	2.15	0.47
2:L:122:ASP:H	3:H:222:LYS:NZ	2.13	0.47
2:A:186:TYR:HD2	2:A:192:TYR:CZ	2.32	0.46
2:A:6:GLN:HB2	2:A:100:GLN:NE2	2.29	0.46
2:L:141:PRO:O	2:L:198:HIS:HE1	1.99	0.46
2:A:186:TYR:CD2	2:A:192:TYR:CZ	3.03	0.46
3:H:209:LYS:N	3:H:210:PRO:HD2	2.31	0.46
2:L:33:LEU:HD22	2:L:71:PHE:CG	2.51	0.46
1:W:69:VAL:HG11	1:W:108:LYS:HD2	1.98	0.46
2:A:61:ARG:HH21	2:A:82:ASP:CG	2.19	0.46
3:H:132:LEU:HB2	3:H:147:GLY:CA	2.46	0.46
2:L:155:GLN:HB3	2:L:158:ASN:HD21	1.81	0.46
3:B:176:ALA:HA	3:B:186:LEU:HB3	1.98	0.46
2:L:29:ILE:HG12	2:L:90:GLN:HG3	1.98	0.46
1:V:97:LEU:HA	1:V:97:LEU:HD12	1.70	0.46
3:B:43:LYS:CG	3:B:44:GLY:H	2.29	0.46
1:W:19:ASP:O	1:W:23:ARG:HD3	2.17	0.45
3:H:173:THR:HG23	3:H:188:SER:HB2	1.97	0.45
2:L:140:TYR:CG	2:L:141:PRO:HA	2.50	0.45
2:L:145:LYS:HB3	2:L:145:LYS:HE2	1.82	0.45
2:L:166:GLN:HB2	2:L:173:TYR:CE2	2.52	0.45
3:B:68:PHE:N	3:B:68:PHE:CD1	2.85	0.45
3:B:73:ASP:OD2	3:B:76:LYS:HE3	2.16	0.45
3:B:86:LEU:HB3	3:B:119:VAL:HG21	1.98	0.45
1:W:45:TYR:CE1	1:W:82:ARG:HB3	2.52	0.44
3:H:99:TRP:NE1	3:H:105:PRO:HA	2.32	0.44
1:V:22:GLN:HG2	3:H:105:PRO:HB2	1.99	0.44
2:A:7:SER:HA	2:A:8:PRO:HA	1.82	0.44
2:L:190:LYS:HD3	2:L:210:ASN:HB3	1.99	0.44
2:A:148:TRP:CE2	2:A:179:LEU:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:29:ILE:H	3:B:77:ASN:ND2	2.13	0.43
3:H:6:GLU:OE2	3:H:94:TYR:O	2.37	0.43
2:A:169:LYS:HB2	2:A:169:LYS:HE2	1.69	0.43
2:L:181:LEU:HD12	2:L:185:ASP:HB3	2.00	0.43
2:L:29:ILE:HG13	2:L:90:GLN:HG2	1.99	0.43
2:L:31:ARG:HH22	2:L:52:SER:HB3	1.82	0.43
2:A:33:LEU:HD13	2:A:71:PHE:CD1	2.54	0.43
3:B:208:HIS:CD2	3:B:211:SER:OG	2.72	0.43
3:H:51:ILE:O	3:H:53:PRO:HD3	2.19	0.43
2:A:79:GLN:CB	2:A:80:PRO:HD2	2.48	0.43
2:A:28:VAL:O	2:A:29:ILE:HD13	2.18	0.43
3:B:106:TRP:CE3	3:B:106:TRP:N	2.83	0.43
2:L:167:ASP:OD2	2:L:168:SER:N	2.52	0.43
3:B:154:PHE:HA	3:B:155:PRO:HA	1.84	0.42
2:L:8:PRO:O	2:L:102:THR:HG23	2.19	0.42
1:V:42:GLU:HB3	1:V:45:TYR:HD1	1.84	0.42
2:A:201:LEU:HD13	2:A:201:LEU:H	1.83	0.42
2:A:2:ILE:CD1	2:A:93:THR:HB	2.49	0.42
2:A:29:ILE:O	2:A:29:ILE:HG23	2.19	0.42
3:H:132:LEU:HB2	3:H:147:GLY:C	2.40	0.42
3:H:178:LEU:HA	3:H:178:LEU:HD23	1.79	0.42
3:H:155:PRO:O	3:H:208:HIS:HE1	2.01	0.42
3:B:68:PHE:N	3:B:68:PHE:HD1	2.17	0.42
3:H:91:THR:HG23	3:H:118:THR:HA	2.01	0.42
3:H:27:PHE:CE2	3:H:98:ARG:HD3	2.55	0.42
2:A:153:ALA:O	2:A:155:GLN:NE2	2.52	0.42
3:H:179:GLN:C	3:H:181:SER:N	2.73	0.42
3:B:186:LEU:HD12	3:B:186:LEU:C	2.41	0.41
1:W:48:LYS:HA	1:W:49:PRO:C	2.39	0.41
3:H:68:PHE:N	3:H:68:PHE:CD1	2.87	0.41
3:H:208:HIS:CD2	3:H:211:SER:OG	2.68	0.41
2:A:147:GLN:HE21	2:A:154:LEU:HB2	1.86	0.41
3:B:152:ASP:HB3	3:B:183:LEU:HD23	2.02	0.41
2:A:124:GLN:HG3	3:B:130:PHE:CE2	2.55	0.41
3:B:162:TRP:O	3:B:163:ASN:C	2.59	0.41
2:L:188:LYS:HD2	2:L:188:LYS:HA	1.96	0.41
2:A:198:HIS:CD2	2:A:200:GLY:N	2.82	0.41
2:A:79:GLN:HB3	2:A:80:PRO:HD2	2.03	0.41
2:L:137:ASN:ND2	3:H:191:THR:HG21	2.35	0.41
2:L:30:ARG:NH1	2:L:92:ASN:HD21	2.19	0.41
3:B:134:PRO:HG2	3:B:221:PRO:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:30:ARG:HB3	2:A:31:ARG:H	1.79	0.40
3:H:32:SER:HB2	3:H:99:TRP:O	2.21	0.40
3:H:20:LEU:HA	3:H:20:LEU:HD23	1.78	0.40
2:L:2:ILE:CD1	2:L:29:ILE:HD11	2.35	0.40
2:L:30:ARG:HH11	2:L:92:ASN:HD21	1.69	0.40
2:L:2:ILE:HD12	2:L:93:THR:HB	2.02	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	V	96/102 (94%)	91 (95%)	2 (2%)	3 (3%)	4	23
1	W	95/102 (93%)	85 (90%)	8 (8%)	2 (2%)	7	30
2	A	209/214 (98%)	197 (94%)	10 (5%)	2 (1%)	15	49
2	L	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
3	B	215/228 (94%)	196 (91%)	17 (8%)	2 (1%)	17	52
3	H	215/228 (94%)	200 (93%)	11 (5%)	4 (2%)	8	33
All	All	1042/1088 (96%)	970 (93%)	59 (6%)	13 (1%)	13	44

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	106	TRP
1	V	87	GLN
1	W	107	LYS
3	B	212	ASN
1	V	62	ASN
3	H	223	SER

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Mol	Chain	Res	Type
1	W	63	ASP
3	B	101	HIS
1	V	26	CYS
3	H	134	PRO
3	H	180	SER
2	A	30	ARG
2	A	40	PRO

5.3.2 Protein sidechains ⓘ

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	V	93/96 (97%)	75 (81%)	18 (19%)	1	6
1	W	92/96 (96%)	74 (80%)	18 (20%)	1	6
2	A	185/187 (99%)	134 (72%)	51 (28%)	0	1
2	L	187/187 (100%)	140 (75%)	47 (25%)	0	1
3	B	180/188 (96%)	142 (79%)	38 (21%)	1	5
3	H	180/188 (96%)	136 (76%)	44 (24%)	0	2
All	All	917/942 (97%)	701 (76%)	216 (24%)	1	2

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	12	HIS
1	V	16	LYS
1	V	20	VAL
1	V	36	PHE
1	V	37	GLN
1	V	42	GLU
1	V	43	ILE
1	V	48	LYS
1	V	50	SER
1	V	56	ARG
1	V	62	ASN

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Mol	Chain	Res	Type
1	V	64	GLU
1	V	67	GLU
1	V	73	GLU
1	V	75	ASN
1	V	97	LEU
1	V	105	ARG
1	V	108	LYS
2	L	9	SER
2	L	11	LEU
2	L	15	VAL
2	L	18	ARG
2	L	20	THR
2	L	27	GLN
2	L	28	VAL
2	L	29	ILE
2	L	30	ARG
2	L	39	LYS
2	L	52	SER
2	L	53	ASN
2	L	56	SER
2	L	61	ARG
2	L	65	SER
2	L	72	THR
2	L	73	LEU
2	L	83	PHE
2	L	90	GLN
2	L	91	SER
2	L	94	SER
2	L	103	LYS
2	L	108	ARG
2	L	123	GLU
2	L	125	LEU
2	L	126	LYS
2	L	134	CYS
2	L	135	LEU
2	L	142	ARG
2	L	145	LYS
2	L	149	LYS
2	L	154	LEU
2	L	158	ASN
2	L	159	SER
2	L	160	GLN

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Mol	Chain	Res	Type
2	L	164	THR
2	L	165	GLU
2	L	181	LEU
2	L	183	LYS
2	L	185	ASP
2	L	194	CYS
2	L	199	GLN
2	L	201	LEU
2	L	203	SER
2	L	206	THR
2	L	207	LYS
2	L	208	SER
3	H	1	GLU
3	H	3	GLN
3	H	4	LEU
3	H	7	SER
3	H	11	LEU
3	H	12	VAL
3	H	19	ARG
3	H	43	LYS
3	H	45	LEU
3	H	55	SER
3	H	64	VAL
3	H	67	ARG
3	H	71	SER
3	H	76	LYS
3	H	85	SER
3	H	98	ARG
3	H	103	THR
3	H	106	TRP
3	H	113	GLN
3	H	115	THR
3	H	116	LEU
3	H	118	THR
3	H	121	SER
3	H	125	LYS
3	H	128	SER
3	H	135	SER
3	H	136	SER
3	H	158	VAL
3	H	177	VAL
3	H	178	LEU

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Mol	Chain	Res	Type
3	H	185	SER
3	H	189	VAL
3	H	194	SER
3	H	197	LEU
3	H	201	THR
3	H	203	ILE
3	H	204	CYS
3	H	205	ASN
3	H	207	ASN
3	H	209	LYS
3	H	214	LYS
3	H	217	LYS
3	H	223	SER
3	H	224	CYS
1	W	14	VAL
1	W	18	MET
1	W	22	GLN
1	W	29	ILE
1	W	41	ASP
1	W	48	LYS
1	W	50	SER
1	W	56	ARG
1	W	69	VAL
1	W	76	ILE
1	W	79	GLN
1	W	82	ARG
1	W	84	LYS
1	W	94	MET
1	W	95	SER
1	W	97	LEU
1	W	107	LYS
1	W	108	LYS
2	A	1	ASP
2	A	9	SER
2	A	11	LEU
2	A	14	SER
2	A	18	ARG
2	A	20	THR
2	A	22	THR
2	A	24	ARG
2	A	27	GLN
2	A	28	VAL

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Mol	Chain	Res	Type
2	A	29	ILE
2	A	30	ARG
2	A	31	ARG
2	A	32	SER
2	A	37	GLN
2	A	39	LYS
2	A	60	SER
2	A	61	ARG
2	A	67	SER
2	A	73	LEU
2	A	83	PHE
2	A	89	GLN
2	A	90	GLN
2	A	100	GLN
2	A	108	ARG
2	A	117	ILE
2	A	122	ASP
2	A	125	LEU
2	A	131	SER
2	A	135	LEU
2	A	149	LYS
2	A	154	LEU
2	A	156	SER
2	A	158	ASN
2	A	162	SER
2	A	164	THR
2	A	165	GLU
2	A	171	SER
2	A	177	SER
2	A	183	LYS
2	A	185	ASP
2	A	188	LYS
2	A	190	LYS
2	A	197	THR
2	A	199	GLN
2	A	201	LEU
2	A	203	SER
2	A	205	VAL
2	A	206	THR
2	A	210	ASN
2	A	211	ARG
3	B	1	GLU

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Mol	Chain	Res	Type
3	B	4	LEU
3	B	5	VAL
3	B	6	GLU
3	B	11	LEU
3	B	12	VAL
3	B	13	GLN
3	B	18	LEU
3	B	19	ARG
3	B	25	SER
3	B	28	THR
3	B	55	SER
3	B	65	LYS
3	B	71	SER
3	B	76	LYS
3	B	85	SER
3	B	98	ARG
3	B	102	SER
3	B	106	TRP
3	B	113	GLN
3	B	115	THR
3	B	116	LEU
3	B	118	THR
3	B	124	THR
3	B	125	LYS
3	B	135	SER
3	B	158	VAL
3	B	164	SER
3	B	178	LEU
3	B	185	SER
3	B	187	SER
3	B	189	VAL
3	B	204	CYS
3	B	209	LYS
3	B	213	THR
3	B	214	LYS
3	B	217	LYS
3	B	222	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	53	ASN

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Mol	Chain	Res	Type
2	L	89	GLN
2	L	92	ASN
2	L	124	GLN
2	L	147	GLN
2	L	158	ASN
2	L	160	GLN
2	L	198	HIS
3	H	30	ASN
3	H	35	HIS
3	H	77	ASN
3	H	208	HIS
2	A	92	ASN
2	A	100	GLN
2	A	158	ASN
2	A	198	HIS
3	B	3	GLN
3	B	35	HIS
3	B	39	GLN
3	B	59	ASN
3	B	77	ASN
3	B	101	HIS
3	B	207	ASN
3	B	208	HIS

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, 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	V	98/102 (96%)	-0.49	0 100 100	37, 52, 86, 125	0
1	W	97/102 (95%)	-0.07	2 (2%) 63 43	36, 53, 78, 94	0
2	A	211/214 (98%)	-0.07	5 (2%) 59 37	35, 53, 66, 84	0
2	L	214/214 (100%)	-0.41	0 100 100	34, 52, 71, 257	0
3	B	219/228 (96%)	-0.21	3 (1%) 75 56	29, 54, 74, 101	0
3	H	219/228 (96%)	-0.19	1 (0%) 91 81	33, 53, 77, 161	0
All	All	1058/1088 (97%)	-0.23	11 (1%) 82 67	29, 53, 75, 257	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	192	TYR	3.5
3	B	17	SER	3.2
2	A	149	LYS	3.1
3	B	13	GLN	2.5
1	W	109	ASP	2.5
3	H	1	GLU	2.4
2	A	189	HIS	2.2
2	A	148	TRP	2.2
2	A	190	LYS	2.1
3	B	119	VAL	2.1
1	W	47	PHE	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 [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.