Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2024 – 04:42 pm BST

PDB ID	:	8QP6
Title	:	Crystal structure of Hepatitis C Virus E1 glycoprotein epitope 314-324 scaffold design 1W4K_08 in complex with neutralizing antibody F(ab) fragment IGH526
Authors	:	Nagarathinam, K.; Krey, T.
Deposited on	:	2023-09-30
Resolution	:	2.59 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

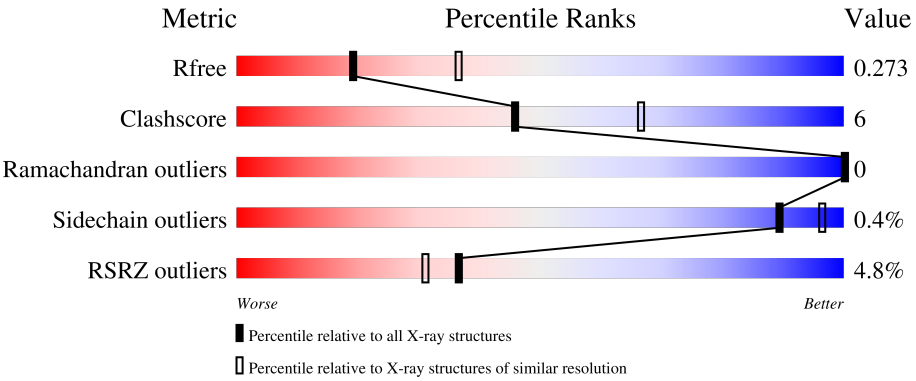
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.59 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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	60	10% 45% 5% 50%
1	D	60	27% 70%
1	G	60	2% 25% 75%
1	J	60	15% 53% 47%
2	B	486	2% 39% 6% 55%

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Mol	Chain	Length	Quality of chain
2	C	486	2% 39% 5% 56%
2	E	486	2% 40% 5% 55%
2	F	486	% 38% 6% 56%
2	H	486	2% 40% 5% 55%
2	I	486	% 37% 7% 56%
2	K	486	2% 37% 8% 55%
2	L	486	% 37% 7% 56%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13211 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 1W4K_08.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	30	Total	C	N	O	S	0	0	0
			206	134	36	34	2			
1	G	15	Total	C	N	O	S	0	0	0
			112	73	21	16	2			
1	D	18	Total	C	N	O	S	0	0	0
			128	83	24	19	2			
1	J	32	Total	C	N	O	S	0	0	0
			215	139	39	35	2			

- Molecule 2 is a protein called F(ab) IGH526.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	220	Total	C	N	O	S	0	0	0
			1617	1023	273	315	6			
2	C	213	Total	C	N	O	S	0	0	0
			1511	948	252	307	4			
2	E	219	Total	C	N	O	S	0	0	0
			1615	1028	269	312	6			
2	H	219	Total	C	N	O	S	0	0	0
			1615	1024	271	314	6			
2	I	212	Total	C	N	O	S	0	0	0
			1513	952	254	303	4			
2	F	213	Total	C	N	O	S	0	0	0
			1541	966	256	315	4			
2	K	219	Total	C	N	O	S	0	0	0
			1605	1029	266	304	6			
2	L	212	Total	C	N	O	S	0	0	0
			1526	957	254	311	4			

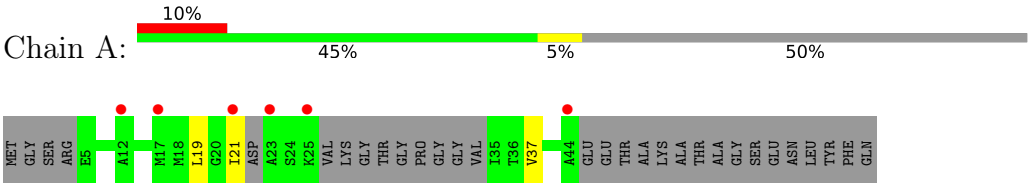
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total O 2 2	0	0
3	C	2	Total O 2 2	0	0
3	H	2	Total O 2 2	0	0
3	F	1	Total O 1 1	0	0

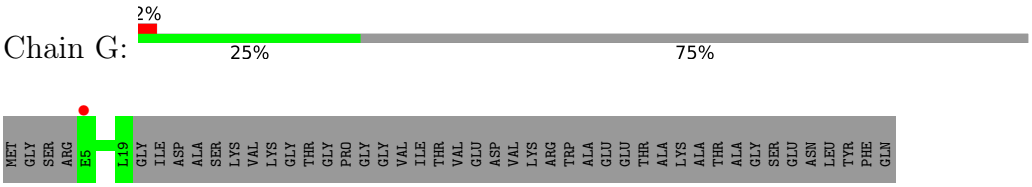
3 Residue-property plots (i)

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.

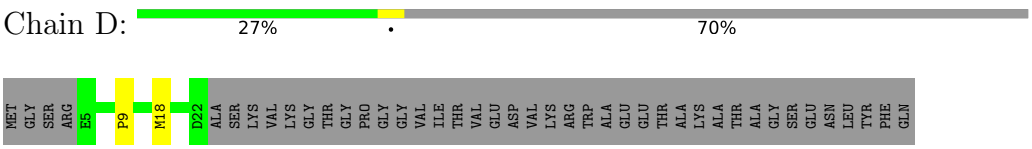
• Molecule 1: 1W4K_08



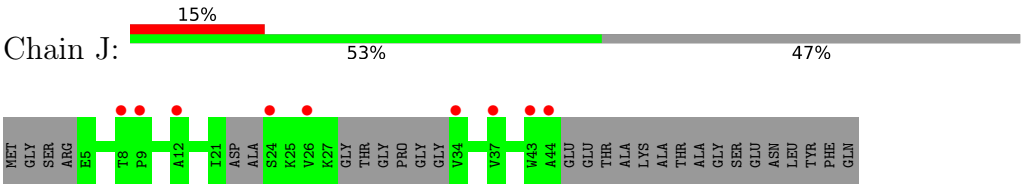
• Molecule 1: 1W4K_08



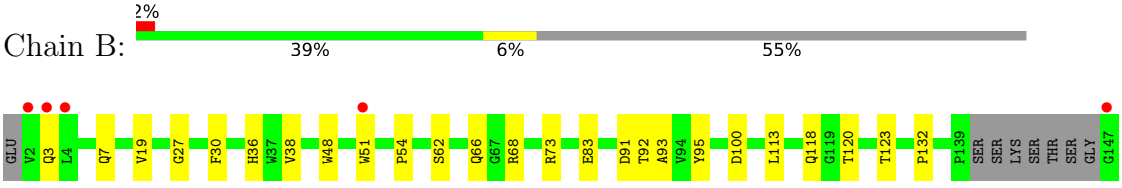
• Molecule 1: 1W4K_08

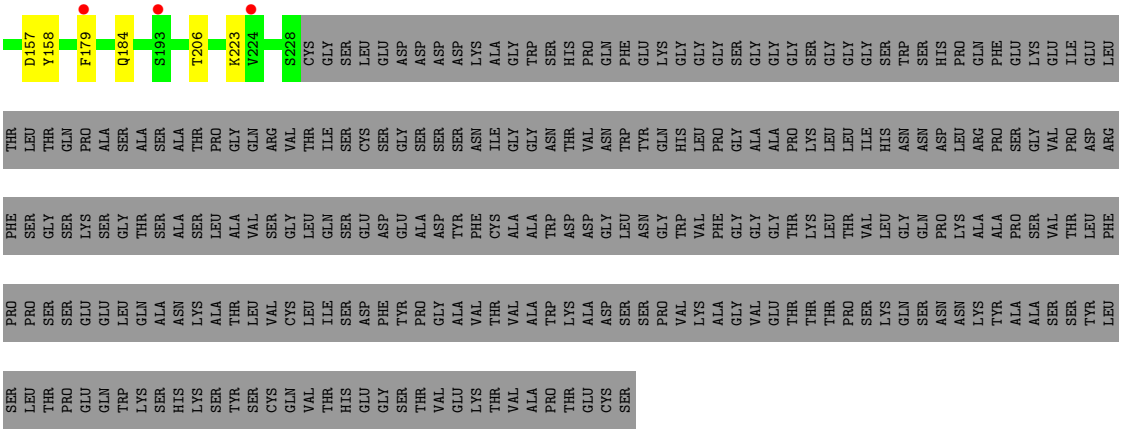


• Molecule 1: 1W4K_08



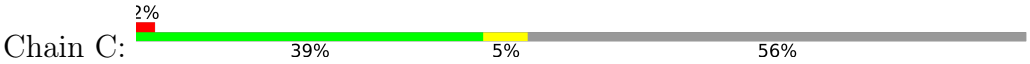
• Molecule 2: F(ab) IGH526

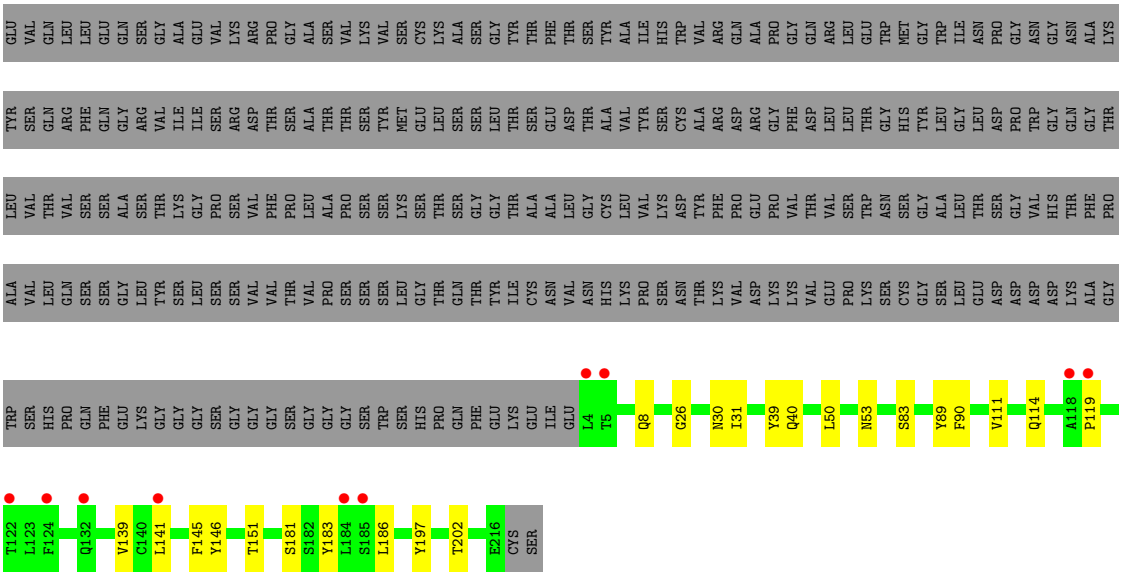




• Molecule 2: F(ab) IGH526

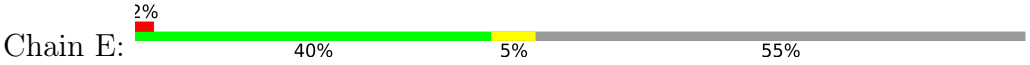
Chain C:

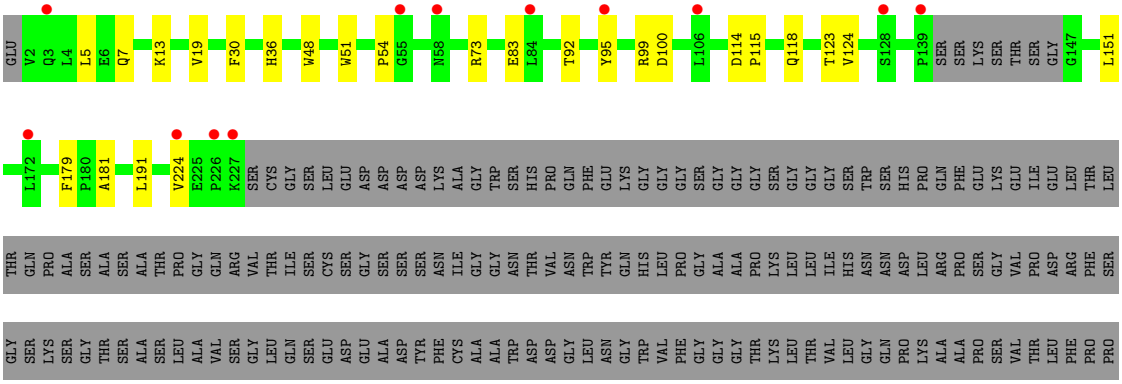


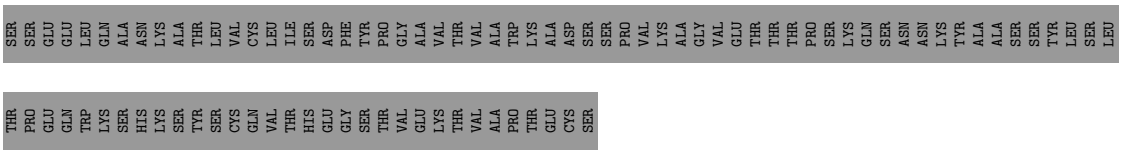


• Molecule 2: F(ab) IGH526

Chain E:

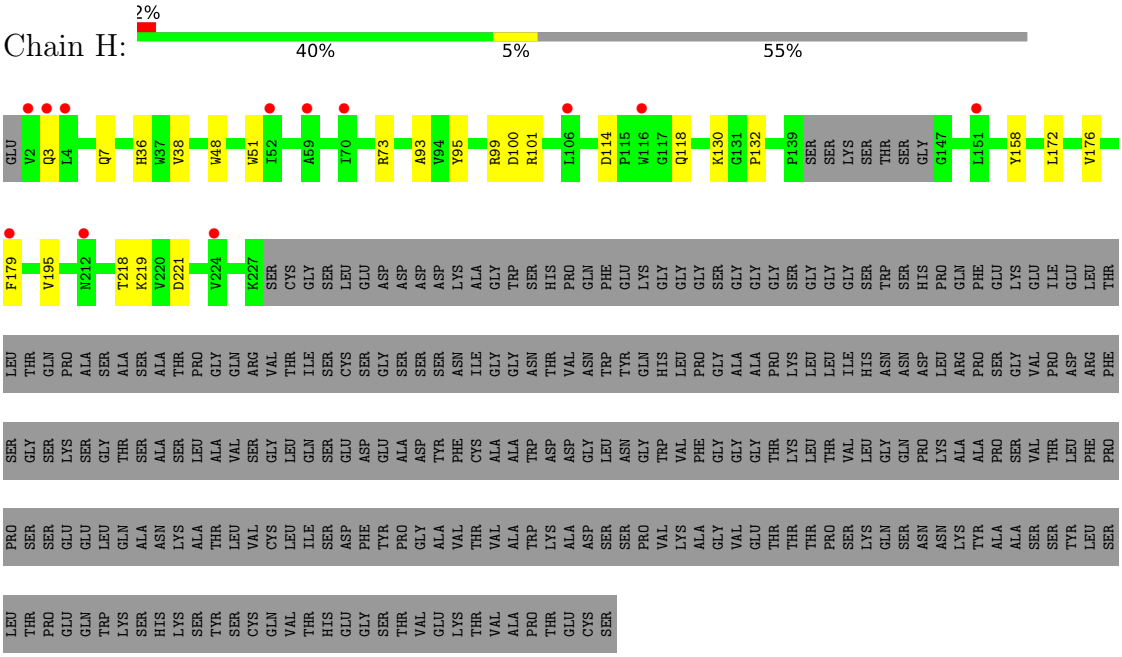






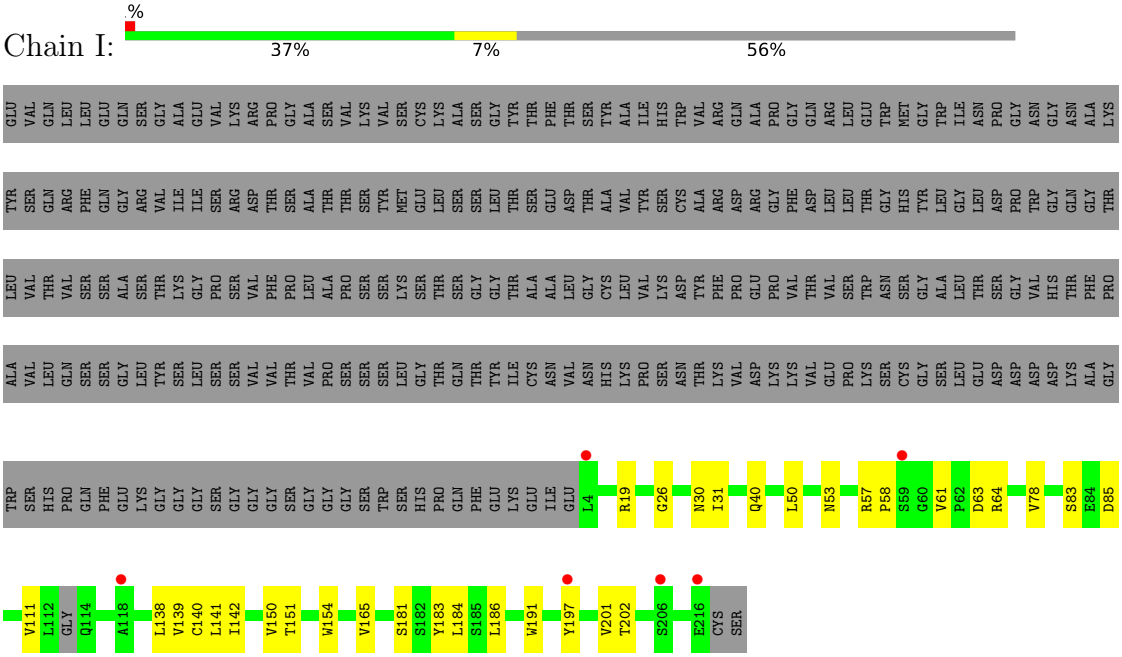
• Molecule 2: F(ab) IGH526

Chain H:



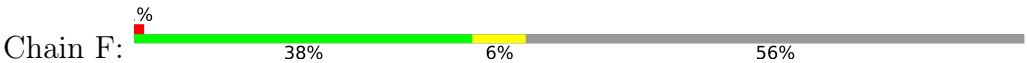
• Molecule 2: F(ab) IGH526

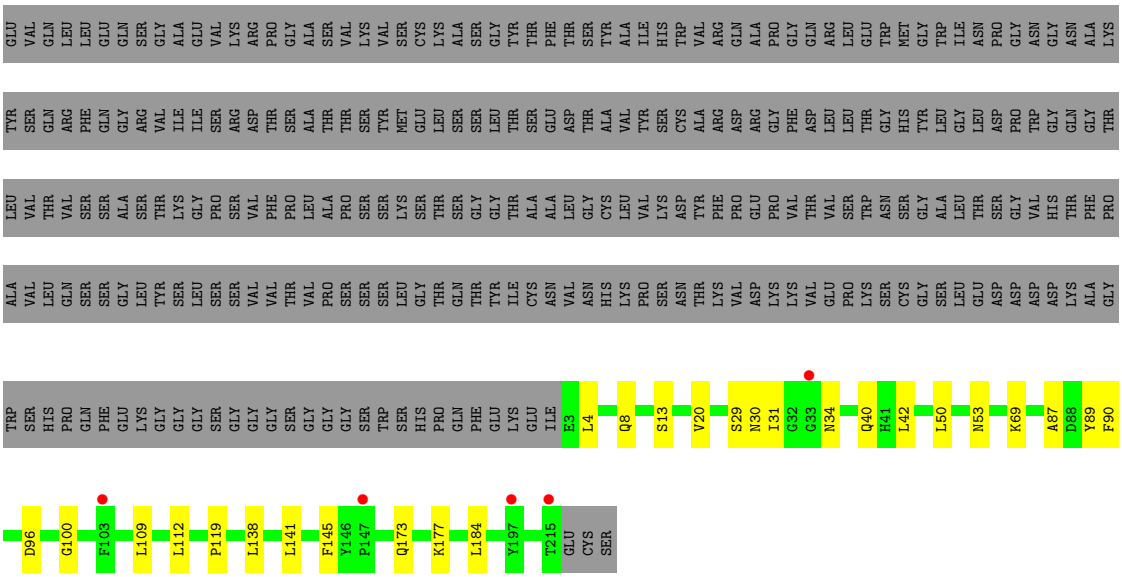
Chain I:



• Molecule 2: F(ab) IGH526

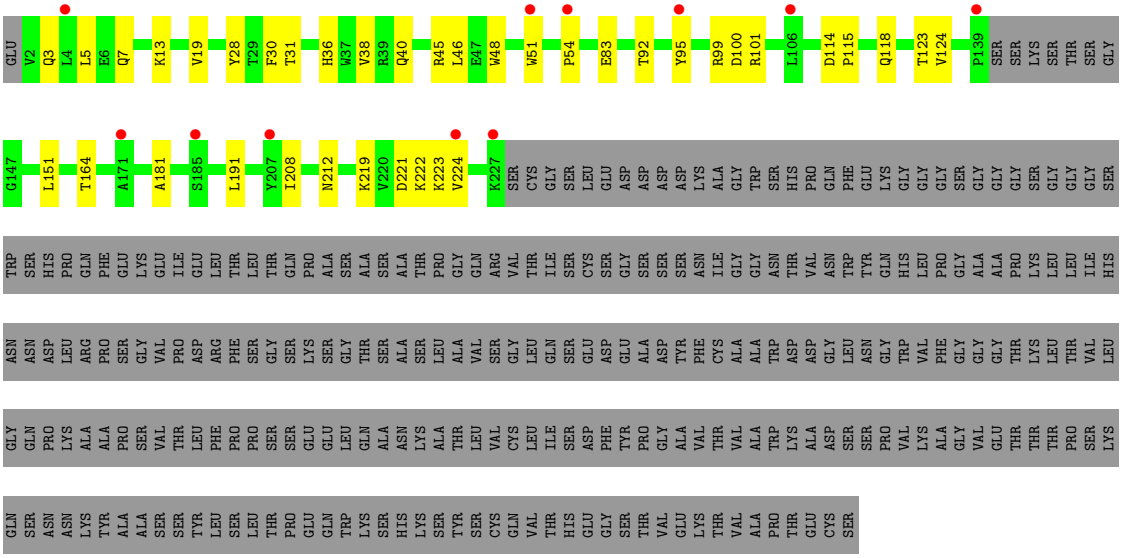
Chain F:





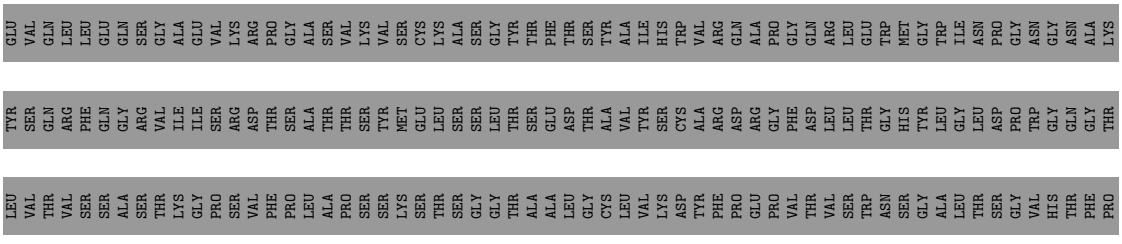
• Molecule 2: F(ab) IGH526

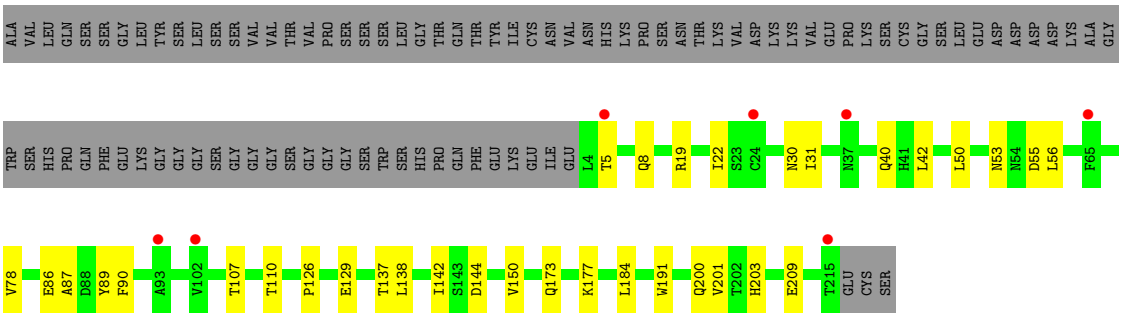
Chain K:



• Molecule 2: F(ab) IGH526

Chain L:




ALA VAL LEU GLN SER SER GLY LEU TYR SER LEU SER SER VAL VAL THR VAL PRO SER SER SER LEU GLY THR GLN THR TYR ILE CYS ASN VAL ASN HIS LYS PRO SER ASN THR LYS VAL ASP LYS LYS VAL GLU PRO LYS SER CYS GLY SER LEU GLU ASP ASP ASP LYS ALA GLY
TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY SER GLY GLY GLY SER TRP SER HIS PRO GLN PHE GLU LYS GLU ILE GLU L4 T5 Q8 R19 I22 S23 C24 N30 I31 N37 Q40 H41 L42 L50 N53 N54 D55 L56 F65
V78 E86 A87 D88 Y89 F90 A93 V102 T107 T110 P126 E129 T137 L138 I142 S143 D144 V150 Q173 K177 L184 W191 Q200 V201 T202 H203 E209 T215 GLU CYS SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.32Å 121.76Å 234.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.63 – 2.59 48.63 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.63-2.59) 99.8 (48.63-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.18_3861	Depositor
R, R_{free}	0.232 , 0.273 0.233 , 0.273	Depositor DCC
R_{free} test set	3245 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	71.1	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 48.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13211	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.22 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1811e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.21	0/207	0.38	0/279
1	D	0.22	0/131	0.42	0/178
1	G	0.21	0/115	0.39	0/156
1	J	0.21	0/216	0.37	0/291
2	B	0.25	0/1657	0.46	0/2261
2	C	0.25	0/1550	0.46	0/2131
2	E	0.25	0/1655	0.48	0/2260
2	F	0.25	0/1580	0.48	0/2169
2	H	0.25	0/1655	0.46	0/2260
2	I	0.25	0/1551	0.47	0/2131
2	K	0.25	0/1645	0.47	0/2245
2	L	0.25	0/1565	0.49	0/2150
All	All	0.25	0/13527	0.47	0/18511

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	206	0	193	2	0
1	D	128	0	123	2	0
1	G	112	0	109	0	0
1	J	215	0	204	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1617	0	1530	24	0
2	C	1511	0	1380	15	0
2	E	1615	0	1540	18	0
2	F	1541	0	1433	15	0
2	H	1615	0	1531	22	0
2	I	1513	0	1391	22	0
2	K	1605	0	1538	25	0
2	L	1526	0	1417	19	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	F	1	0	0	0	0
3	H	2	0	0	0	0
All	All	13211	0	12389	146	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 (146) 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:B:3:GLN:NE2	2:H:3:GLN:OE1	2.25	0.69
2:B:27:GLY:O	2:H:3:GLN:NE2	2.28	0.66
2:H:172:LEU:HD21	2:H:195:VAL:HG11	1.75	0.66
2:I:138:LEU:HD11	2:I:197:TYR:HD2	1.60	0.66
2:L:200:GLN:HG2	2:L:209:GLU:HB2	1.77	0.66
2:K:92:THR:HG23	2:K:123:THR:HA	1.79	0.64
2:L:173:GLN:HE21	2:L:177:LYS:HB2	1.65	0.62
2:C:40:GLN:HB2	2:C:50:LEU:HD11	1.82	0.61
2:B:38:VAL:HG12	2:B:48:TRP:HA	1.83	0.61
2:K:5:LEU:HD13	2:K:115:PRO:HG2	1.83	0.61
2:F:173:GLN:HE21	2:F:177:LYS:HB2	1.66	0.60
2:B:92:THR:HG23	2:B:123:THR:HA	1.83	0.60
2:H:48:TRP:HZ2	2:H:51:TRP:CD1	2.20	0.59
2:L:22:ILE:HD12	2:L:107:THR:HG21	1.83	0.59
2:K:38:VAL:HG12	2:K:48:TRP:HA	1.83	0.59
2:E:5:LEU:HD13	2:E:115:PRO:HG2	1.86	0.57
2:H:221:ASP:HB2	2:K:219:LYS:HB2	1.86	0.57
2:B:7:GLN:H	2:B:118:GLN:HE22	1.53	0.56
2:E:7:GLN:NE2	2:E:95:TYR:O	2.39	0.56
2:L:126:PRO:HB3	2:L:137:THR:H	1.69	0.56
2:K:3:GLN:HG2	2:K:99:ARG:HH22	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:7:GLN:H	2:H:118:GLN:HE22	1.54	0.56
2:B:7:GLN:NE2	2:B:95:TYR:O	2.38	0.55
2:H:7:GLN:NE2	2:H:95:TYR:O	2.39	0.55
2:B:206:THR:HB	2:B:223:LYS:HD2	1.89	0.55
2:H:99:ARG:NE	2:H:114:ASP:O	2.33	0.55
2:K:7:GLN:O	2:K:118:GLN:NE2	2.40	0.55
2:K:7:GLN:H	2:K:118:GLN:HE22	1.55	0.55
2:K:101:ARG:HD2	2:K:114:ASP:HB3	1.89	0.55
2:B:157:ASP:OD1	2:B:184:GLN:NE2	2.39	0.54
2:L:30:ASN:OD1	2:L:31:ILE:N	2.40	0.54
2:L:150:VAL:HG12	2:L:203:HIS:HB2	1.89	0.54
2:E:92:THR:HG23	2:E:123:THR:HA	1.91	0.53
2:H:176:VAL:HG22	2:H:195:VAL:HG22	1.90	0.53
2:L:8:GLN:NE2	2:L:89:TYR:O	2.42	0.53
2:K:151:LEU:HD13	2:K:224:VAL:HG13	1.89	0.53
2:B:7:GLN:O	2:B:118:GLN:NE2	2.42	0.53
2:I:40:GLN:HB2	2:I:50:LEU:HD11	1.91	0.52
1:A:37:VAL:HG11	1:D:18:MET:HB3	1.91	0.52
2:E:151:LEU:HD13	2:E:224:VAL:HG13	1.91	0.52
2:E:30:PHE:CE2	2:E:54:PRO:HB3	2.45	0.52
2:F:30:ASN:OD1	2:F:31:ILE:N	2.43	0.52
2:C:186:LEU:HD13	2:C:197:TYR:HE2	1.76	0.51
2:E:7:GLN:O	2:E:118:GLN:NE2	2.43	0.51
2:B:179:PHE:HD2	2:C:181:SER:HB3	1.75	0.51
2:H:101:ARG:HD2	2:H:114:ASP:HB3	1.93	0.51
2:F:138:LEU:HB2	2:F:184:LEU:HB3	1.91	0.51
2:B:68:ARG:NH1	2:B:91:ASP:OD2	2.43	0.51
2:F:40:GLN:HB2	2:F:50:LEU:HD11	1.93	0.50
2:B:3:GLN:NE2	2:H:3:GLN:H	2.08	0.50
2:E:48:TRP:HZ2	2:E:51:TRP:CD1	2.30	0.50
2:K:36:HIS:CD2	2:K:100:ASP:HB2	2.48	0.49
2:K:181:ALA:HA	2:K:191:LEU:HB3	1.94	0.49
2:L:40:GLN:HB2	2:L:50:LEU:HD11	1.94	0.49
2:B:48:TRP:HZ2	2:B:51:TRP:CD1	2.30	0.49
2:C:151:THR:HB	2:C:202:THR:HB	1.95	0.49
2:E:13:LYS:HE3	2:E:19:VAL:HA	1.95	0.49
2:F:42:LEU:HD23	2:F:87:ALA:HB2	1.95	0.49
2:K:30:PHE:CE2	2:K:54:PRO:HB3	2.48	0.49
2:F:13:SER:HB2	2:F:112:LEU:HD11	1.95	0.48
1:D:9:PRO:HA	2:F:96:ASP:OD1	2.13	0.48
2:I:138:LEU:HD21	2:I:191:TRP:CZ3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:42:LEU:HD23	2:L:87:ALA:HB2	1.95	0.48
2:H:93:ALA:HB3	2:H:95:TYR:HE1	1.78	0.48
2:I:30:ASN:OD1	2:I:31:ILE:N	2.44	0.48
2:I:138:LEU:HD11	2:I:197:TYR:CD2	2.46	0.48
2:I:165:VAL:HG22	2:I:184:LEU:HD23	1.96	0.48
2:L:8:GLN:HE22	2:L:90:PHE:HA	1.78	0.48
2:K:31:THR:HA	2:K:54:PRO:HB2	1.96	0.48
2:K:48:TRP:HZ2	2:K:51:TRP:CD1	2.31	0.47
2:K:208:ILE:HG12	2:K:223:LYS:HB2	1.96	0.47
2:B:179:PHE:CD2	2:C:181:SER:HB3	2.49	0.47
2:E:181:ALA:HA	2:E:191:LEU:HB3	1.97	0.47
2:I:150:VAL:HG13	2:I:201:VAL:HG13	1.96	0.47
2:C:30:ASN:OD1	2:C:31:ILE:N	2.44	0.47
2:E:36:HIS:CD2	2:E:100:ASP:HB2	2.50	0.47
2:H:218:THR:OG1	2:K:222:LYS:HE2	2.14	0.47
2:B:36:HIS:CD2	2:B:100:ASP:HB2	2.50	0.47
2:E:54:PRO:O	2:E:73:ARG:HD2	2.15	0.47
2:I:57:ARG:NH1	2:I:63:ASP:HA	2.30	0.46
2:H:7:GLN:O	2:H:118:GLN:NE2	2.48	0.46
2:H:179:PHE:CD2	2:I:141:LEU:HD22	2.51	0.46
2:I:186:LEU:HD13	2:I:197:TYR:HE2	1.79	0.46
2:B:132:PRO:HB3	2:B:158:TYR:HB3	1.98	0.45
2:I:139:VAL:HG13	2:I:183:TYR:HE1	1.81	0.45
2:I:142:ILE:HD13	2:I:150:VAL:HG11	1.99	0.45
2:I:151:THR:HB	2:I:202:THR:HB	1.98	0.45
2:H:130:LYS:HA	2:L:129:GLU:HG2	1.97	0.45
2:I:83:SER:HA	2:I:111:VAL:HG21	1.99	0.45
2:H:179:PHE:HD2	2:I:181:SER:HB2	1.82	0.45
2:E:19:VAL:O	2:E:83:GLU:HA	2.17	0.45
2:B:19:VAL:O	2:B:83:GLU:HA	2.18	0.44
2:E:7:GLN:H	2:E:118:GLN:HE22	1.65	0.44
2:K:3:GLN:HG3	2:K:28:TYR:HB3	1.99	0.44
1:A:19:LEU:HD22	1:A:21:ILE:HG13	2.00	0.44
2:B:93:ALA:HB3	2:B:95:TYR:HE1	1.82	0.44
2:C:114:GLN:HG3	2:C:146:TYR:CE2	2.52	0.44
2:F:119:PRO:HB3	2:F:145:PHE:HB3	2.00	0.44
2:C:8:GLN:NE2	2:C:89:TYR:O	2.50	0.44
2:F:34:ASN:O	2:F:69:LYS:NZ	2.51	0.44
2:L:19:ARG:HA	2:L:78:VAL:O	2.18	0.44
2:K:40:GLN:HB2	2:K:46:LEU:HG	2.00	0.44
2:C:26:GLY:HA3	2:C:31:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:GLN:HG2	2:B:120:THR:OG1	2.18	0.43
2:I:139:VAL:HG13	2:I:183:TYR:CE1	2.53	0.43
2:F:8:GLN:NE2	2:F:89:TYR:O	2.51	0.43
2:F:8:GLN:HE22	2:F:90:PHE:HA	1.82	0.43
2:K:45:ARG:NH1	2:L:5:THR:HB	2.33	0.43
2:H:132:PRO:HB3	2:H:158:TYR:HB3	2.00	0.43
2:L:86:GLU:HG3	2:L:110:THR:HA	2.00	0.43
2:H:219:LYS:HB2	2:K:221:ASP:HB2	2.01	0.43
2:I:19:ARG:HA	2:I:78:VAL:O	2.18	0.43
2:B:93:ALA:HB3	2:B:95:TYR:CE1	2.54	0.43
2:H:93:ALA:HB3	2:H:95:TYR:CE1	2.54	0.43
2:C:8:GLN:HE22	2:C:90:PHE:HA	1.83	0.43
2:H:36:HIS:CD2	2:H:100:ASP:HB2	2.54	0.42
2:K:7:GLN:NE2	2:K:95:TYR:O	2.47	0.42
2:L:144:ASP:OD1	2:L:173:GLN:NE2	2.52	0.42
2:C:83:SER:HA	2:C:111:VAL:HG11	2.01	0.42
2:E:13:LYS:HD2	2:E:19:VAL:HB	2.01	0.42
2:H:38:VAL:HG12	2:H:48:TRP:HA	2.01	0.42
2:C:139:VAL:HG13	2:C:183:TYR:CE1	2.55	0.42
2:B:179:PHE:CD2	2:C:141:LEU:HD22	2.54	0.42
2:I:58:PRO:HD2	2:I:61:VAL:HG21	2.01	0.42
2:I:138:LEU:HB2	2:I:184:LEU:HB3	2.01	0.42
2:F:4:LEU:HD13	2:F:29:SER:OG	2.20	0.42
2:C:119:PRO:HB3	2:C:145:PHE:HB3	2.02	0.42
2:I:140:CYS:HB2	2:I:154:TRP:CH2	2.55	0.42
2:B:62:SER:O	2:B:66:GLN:HG3	2.20	0.42
2:L:142:ILE:HG12	2:L:201:VAL:HG21	2.02	0.42
2:B:30:PHE:CE2	2:B:54:PRO:HB3	2.55	0.42
2:E:13:LYS:O	2:E:124:VAL:HA	2.20	0.42
2:E:179:PHE:CD2	2:F:141:LEU:HD22	2.55	0.41
2:K:13:LYS:O	2:K:124:VAL:HA	2.20	0.41
2:E:48:TRP:CZ3	2:F:100:GLY:HA3	2.55	0.41
2:L:55:ASP:OD1	2:L:56:LEU:HD12	2.20	0.41
2:E:99:ARG:NE	2:E:114:ASP:O	2.43	0.41
2:B:113:LEU:HB2	2:C:39:TYR:OH	2.21	0.41
2:K:13:LYS:HE3	2:K:19:VAL:HA	2.02	0.41
2:I:26:GLY:HA3	2:I:31:ILE:HD12	2.03	0.41
2:I:64:ARG:NH2	2:I:85:ASP:OD2	2.54	0.41
2:F:20:VAL:HG11	2:F:109:LEU:HD11	2.03	0.41
2:K:164:THR:OG1	2:K:212:ASN:HB3	2.21	0.41
2:K:19:VAL:O	2:K:83:GLU:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:138:LEU:HD21	2:L:191:TRP:HZ3	1.86	0.40
2:L:138:LEU:HB2	2:L:184:LEU:HB3	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	24/60 (40%)	24 (100%)	0	0	100	100
1	D	16/60 (27%)	16 (100%)	0	0	100	100
1	G	13/60 (22%)	13 (100%)	0	0	100	100
1	J	26/60 (43%)	26 (100%)	0	0	100	100
2	B	216/486 (44%)	214 (99%)	2 (1%)	0	100	100
2	C	211/486 (43%)	206 (98%)	5 (2%)	0	100	100
2	E	215/486 (44%)	212 (99%)	3 (1%)	0	100	100
2	F	211/486 (43%)	206 (98%)	5 (2%)	0	100	100
2	H	215/486 (44%)	213 (99%)	2 (1%)	0	100	100
2	I	208/486 (43%)	203 (98%)	5 (2%)	0	100	100
2	K	215/486 (44%)	212 (99%)	3 (1%)	0	100	100
2	L	210/486 (43%)	205 (98%)	5 (2%)	0	100	100
All	All	1780/4128 (43%)	1750 (98%)	30 (2%)	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	15/44 (34%)	15 (100%)	0	100 100
1	D	10/44 (23%)	10 (100%)	0	100 100
1	G	9/44 (20%)	9 (100%)	0	100 100
1	J	17/44 (39%)	17 (100%)	0	100 100
2	B	168/399 (42%)	167 (99%)	1 (1%)	84 94
2	C	152/399 (38%)	151 (99%)	1 (1%)	81 93
2	E	167/399 (42%)	167 (100%)	0	100 100
2	F	161/399 (40%)	160 (99%)	1 (1%)	84 94
2	H	168/399 (42%)	167 (99%)	1 (1%)	84 94
2	I	153/399 (38%)	152 (99%)	1 (1%)	81 93
2	K	163/399 (41%)	163 (100%)	0	100 100
2	L	159/399 (40%)	158 (99%)	1 (1%)	84 94
All	All	1342/3368 (40%)	1336 (100%)	6 (0%)	89 96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	73	ARG
2	C	53	ASN
2	H	73	ARG
2	I	53	ASN
2	F	53	ASN
2	L	53	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

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 oligosaccharides 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	30/60 (50%)	1.12	6 (20%) 3 3	55, 101, 157, 175	0
1	D	18/60 (30%)	0.64	0 100 100	52, 71, 117, 120	0
1	G	15/60 (25%)	0.55	1 (6%) 25 20	60, 78, 107, 109	0
1	J	32/60 (53%)	1.50	9 (28%) 2 1	63, 103, 155, 162	0
2	B	220/486 (45%)	0.29	8 (3%) 46 40	49, 72, 120, 151	0
2	C	213/486 (43%)	0.31	10 (4%) 37 32	57, 75, 111, 137	0
2	E	219/486 (45%)	0.29	12 (5%) 32 26	53, 71, 103, 164	0
2	F	213/486 (43%)	0.27	5 (2%) 61 55	54, 68, 98, 125	0
2	H	219/486 (45%)	0.35	12 (5%) 32 26	53, 76, 107, 121	0
2	I	212/486 (43%)	0.22	6 (2%) 55 49	58, 72, 100, 127	0
2	K	219/486 (45%)	0.48	11 (5%) 35 30	60, 84, 117, 137	0
2	L	212/486 (43%)	0.58	7 (3%) 49 43	59, 75, 105, 130	0
All	All	1822/4128 (44%)	0.38	87 (4%) 36 31	49, 74, 112, 175	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	9	PRO	5.6
2	B	2	VAL	5.1
2	H	106	LEU	5.1
2	E	227	LYS	4.8
2	K	139	PRO	4.8
1	J	8	THR	4.1
2	B	179	PHE	4.1
2	K	224	VAL	4.0
2	L	215	THR	3.5
2	L	102	VAL	3.4
1	J	12	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
2	C	4	LEU	3.3
2	E	84	LEU	3.3
2	C	124	PHE	3.3
2	H	3	GLN	3.2
2	L	93	ALA	3.1
2	E	224	VAL	3.0
2	E	172	LEU	2.9
2	C	141	LEU	2.9
1	J	26	VAL	2.9
2	H	224	VAL	2.8
2	B	51	TRP	2.8
2	F	215	THR	2.8
2	H	59	ALA	2.8
2	B	147	GLY	2.8
2	F	103	PHE	2.8
1	J	37	VAL	2.8
2	C	5	THR	2.7
1	A	21	ILE	2.7
2	K	227	LYS	2.7
2	E	3	GLN	2.7
2	I	216	GLU	2.7
2	L	65	PHE	2.7
2	K	171	ALA	2.6
2	F	33	GLY	2.6
1	J	24	SER	2.6
1	J	44	ALA	2.6
1	J	34	VAL	2.5
1	A	44	ALA	2.5
1	G	5	GLU	2.5
2	H	70	ILE	2.5
2	H	151	LEU	2.5
2	B	224	VAL	2.5
2	I	118	ALA	2.5
2	I	59	SER	2.5
1	A	17	MET	2.5
2	C	184	LEU	2.4
2	E	106	LEU	2.4
2	H	2	VAL	2.4
2	B	193	SER	2.4
2	I	197	TYR	2.4
2	C	118	ALA	2.4
2	K	207	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	25	LYS	2.4
1	A	23	ALA	2.3
2	H	4	LEU	2.3
2	C	122	THR	2.3
2	F	197	TYR	2.3
2	E	58	ASN	2.2
2	B	3	GLN	2.2
2	H	52	ILE	2.2
2	B	4	LEU	2.2
2	E	55	GLY	2.2
2	L	24	CYS	2.2
2	E	128	SER	2.2
2	L	5	THR	2.2
1	A	12	ALA	2.2
2	K	51	TRP	2.2
2	K	95	TYR	2.1
2	C	185	SER	2.1
2	C	119	PRO	2.1
2	H	212	ASN	2.1
2	L	37	ASN	2.1
2	I	4	LEU	2.1
2	I	206	SER	2.1
2	K	4	LEU	2.1
2	F	147	PRO	2.1
2	E	95	TYR	2.0
2	E	139	PRO	2.0
2	K	185	SER	2.0
2	K	106	LEU	2.0
1	J	43	TRP	2.0
2	H	116	TRP	2.0
2	E	226	PRO	2.0
2	K	54	PRO	2.0
2	C	132	GLN	2.0
2	H	179	PHE	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 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.