Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 11:26 pm BST

PDB ID	:	6FY1
Title	:	Crystal structure of a V2p-reactive RV144 vaccine-like antibody, CAP228-16H, in complex with a scaffolded autologous V1V2
Authors	:	Wibmer, C.K.; Moore, P.L.; Morris, L.
Deposited on	:	2018-03-10
Resolution	:	3.13 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:

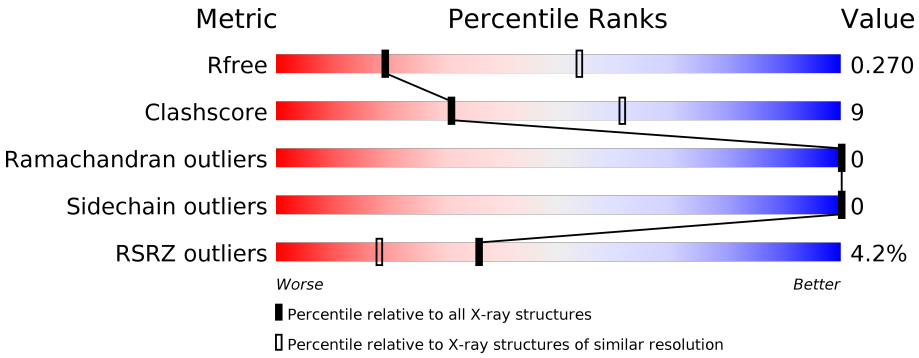
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)

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 <=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	H	235	84% 12% .
1	Y	235	4% 67% 14% 18%
2	G	117	9% 74% 15% 11%
2	X	117	3% 68% 15% 16%
3	L	213	77% 23% .
3	Z	213	9% 65% 18% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15110 atoms, of which 7457 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 CAP228-16H Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Y	192	Total	C	H	N	O	S	0	0	0
			2917	937	1450	248	275	7			
1	H	226	Total	C	H	N	O	S	0	0	0
			3361	1068	1667	289	329	8			

- Molecule 2 is a protein called CAP228 Autologous Scaffolded V1V2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	X	98	Total	C	H	N	O	S	0	0	0
			1532	498	757	118	154	5			
2	G	104	Total	C	H	N	O	S	0	0	0
			1625	524	798	131	168	4			

- Molecule 3 is a protein called CAP228-16H Light Chain.

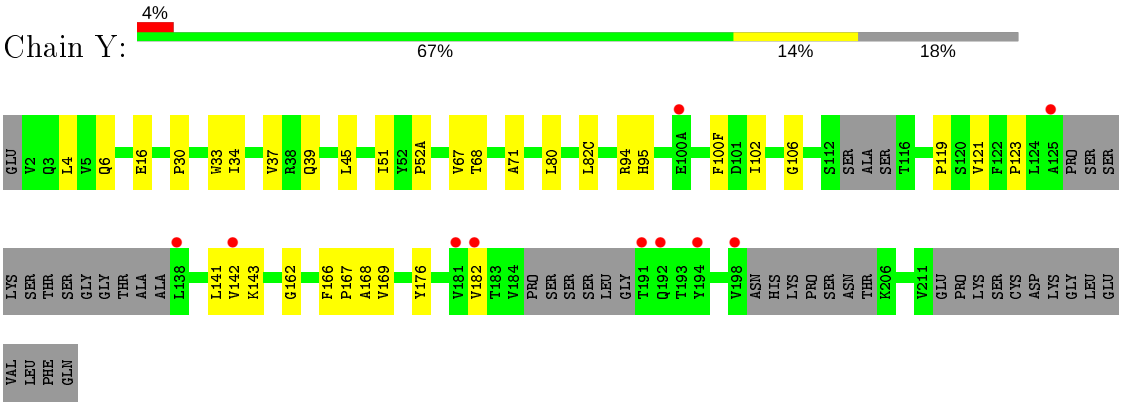
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	Z	177	Total	C	H	N	O	S	0	0	0
			2574	821	1263	216	269	5			
3	L	211	Total	C	H	N	O	S	0	0	0
			3101	989	1522	262	322	6			

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 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.

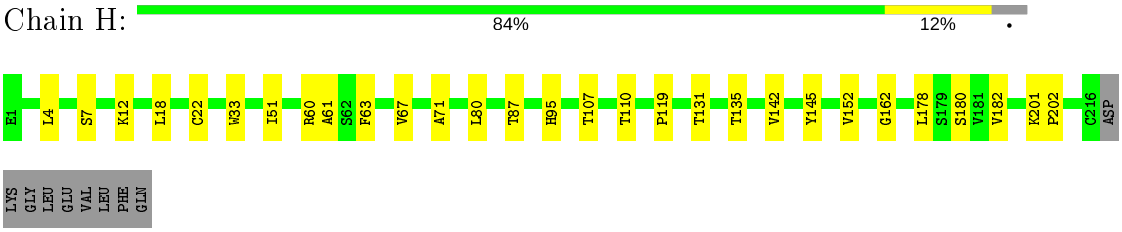
- Molecule 1: CAP228-16H Heavy Chain

Chain Y:



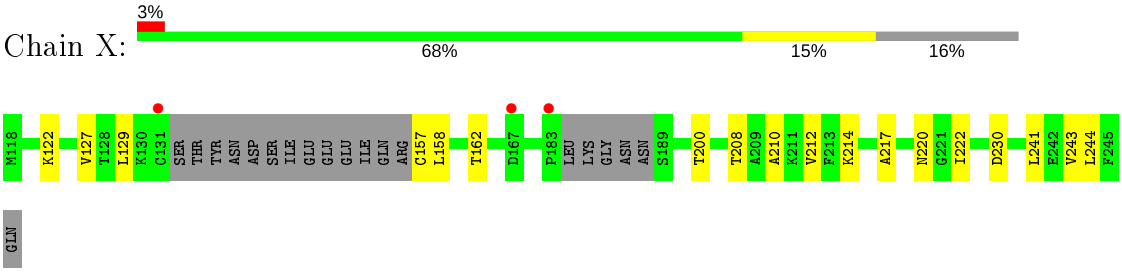
- Molecule 1: CAP228-16H Heavy Chain

Chain H:



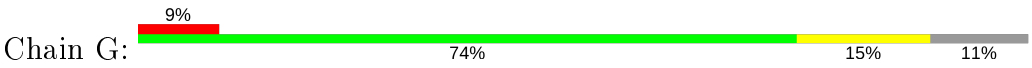
- Molecule 2: CAP228 Autologous Scaffolded V1V2

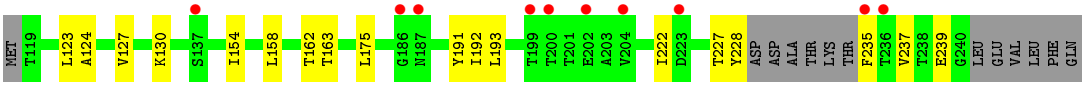
Chain X:



- Molecule 2: CAP228 Autologous Scaffolded V1V2

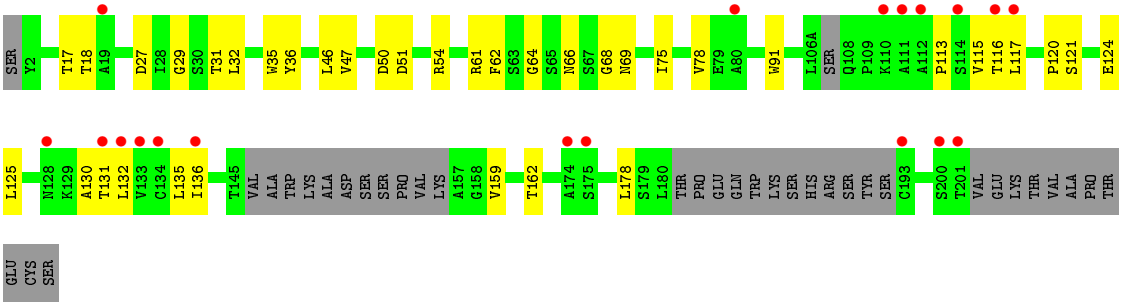
Chain G:





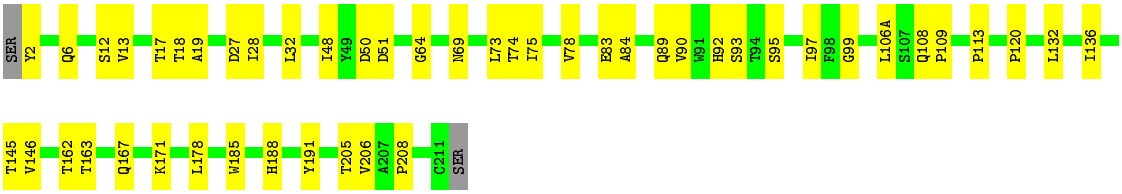
- Molecule 3: CAP228-16H Light Chain

Chain Z:



- Molecule 3: CAP228-16H Light Chain

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	81.99Å 73.99Å 191.03Å 90.00° 91.98° 90.00°	Depositor
Resolution (Å)	40.97 – 3.13 40.97 – 3.13	Depositor EDS
% Data completeness (in resolution range)	87.3 (40.97-3.13) 87.3 (40.97-3.13)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.221 , 0.271 0.221 , 0.270	Depositor DCC
R_{free} test set	1804 reflections (10.15%)	wwPDB-VP
Wilson B-factor (Å^2)	82.4	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 34.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	15110	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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	H	0.31	0/1736	0.51	0/2360
1	Y	0.29	0/1500	0.50	0/2033
2	G	0.31	0/840	0.49	0/1138
2	X	0.31	0/787	0.52	0/1066
3	L	0.40	0/1619	0.53	0/2218
3	Z	0.39	0/1339	0.52	0/1830
All	All	0.34	0/7821	0.51	0/10645

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	H	1694	1667	1667	17	0
1	Y	1467	1450	1447	32	0
2	G	827	798	798	18	0
2	X	775	757	756	15	0
3	L	1579	1522	1521	30	0
3	Z	1311	1263	1260	37	0
All	All	7653	7457	7449	137	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 9.

All (137) 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:H:60:ARG:NH1	3:L:95:SER:O	2.14	0.79
3:Z:132:LEU:HD23	3:Z:178:LEU:HD12	1.68	0.74
3:L:32:LEU:HD22	3:L:50:ASP:HA	1.72	0.71
2:G:162:THR:HG22	2:G:163:THR:H	1.55	0.71
3:L:48:ILE:HD12	3:L:73:LEU:HD13	1.76	0.68
1:Y:67:VAL:HG11	1:Y:80:LEU:HD11	1.77	0.67
3:Z:159:VAL:HG22	3:Z:178:LEU:HD22	1.77	0.67
1:Y:169:VAL:HG12	3:Z:162:THR:OG1	1.95	0.66
1:Y:4:LEU:HD13	1:Y:102:ILE:CG2	2.25	0.66
2:X:127:VAL:HG11	2:X:162:THR:HG21	1.78	0.64
3:L:2:TYR:O	3:L:97:ILE:HD13	1.98	0.64
1:Y:119:PRO:HB2	1:Y:142:VAL:HG13	1.81	0.63
3:L:113:PRO:HB2	3:L:136:ILE:HG23	1.80	0.62
2:G:175:LEU:HD21	3:L:93:SER:HA	1.81	0.62
3:Z:159:VAL:HG13	3:Z:178:LEU:HD23	1.83	0.60
2:X:122:LYS:HG2	2:X:200:THR:HG22	1.85	0.59
1:Y:16:GLU:O	1:Y:82(C):LEU:HD13	2.02	0.59
1:H:7:SER:O	1:H:107:THR:HG22	2.03	0.58
1:H:87:THR:HG23	1:H:110:THR:HA	1.84	0.58
3:Z:113:PRO:HG2	3:Z:136:ILE:HD11	1.85	0.57
1:H:119:PRO:HB2	1:H:142:VAL:HG13	1.86	0.57
2:X:158:LEU:O	2:X:158:LEU:HD12	2.03	0.57
1:Y:141:LEU:HD21	1:Y:143:LYS:HB2	1.87	0.57
3:L:162:THR:HG22	3:L:163:THR:O	2.05	0.56
3:Z:36:TYR:CE1	3:Z:46:LEU:HD13	2.41	0.56
3:L:132:LEU:HD12	3:L:178:LEU:HD23	1.87	0.56
2:X:122:LYS:CG	2:X:200:THR:HG22	2.35	0.55
3:Z:125:LEU:HD23	3:Z:130:ALA:HB2	1.86	0.55
3:Z:17:THR:HG22	3:Z:18:THR:H	1.70	0.55
3:L:120:PRO:HD3	3:L:132:LEU:HD23	1.88	0.55
1:H:67:VAL:HB	1:H:80:LEU:HD11	1.88	0.55
1:Y:166:PHE:CE2	3:Z:135:LEU:HD13	2.41	0.55
2:G:127:VAL:HG21	2:G:163:THR:HG23	1.89	0.54
1:H:51:ILE:HD13	1:H:71:ALA:HB2	1.88	0.54
1:Y:67:VAL:CG1	1:Y:80:LEU:HD11	2.38	0.54
2:X:217:ALA:HB1	2:X:222:ILE:HB	1.90	0.53
2:X:230:ASP:O	2:X:230:ASP:OD1	2.27	0.52
1:H:152:VAL:HG11	1:H:180:SER:CB	2.39	0.52
3:L:83:GLU:O	3:L:84:ALA:HB2	2.10	0.52
2:G:123:LEU:HD11	2:G:237:VAL:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:191:TYR:C	2:G:192:ILE:HD12	2.31	0.51
1:H:63:PHE:O	1:H:67:VAL:HG22	2.10	0.51
3:Z:27:ASP:N	3:Z:69:ASN:OD1	2.40	0.51
1:Y:82(C):LEU:HD12	1:Y:82(C):LEU:N	2.25	0.51
2:G:130:LYS:HB2	2:G:191:TYR:O	2.11	0.51
3:L:167:GLN:N	3:L:171:LYS:O	2.43	0.51
3:Z:35:TRP:O	3:Z:47:VAL:HG22	2.11	0.51
3:L:28:ILE:HG22	3:L:69:ASN:HA	1.93	0.50
1:Y:169:VAL:CG1	3:Z:162:THR:OG1	2.59	0.50
3:L:32:LEU:HD22	3:L:50:ASP:CA	2.41	0.50
3:Z:115:VAL:HG12	3:Z:136:ILE:CD1	2.42	0.50
1:H:131:THR:HG23	1:H:135:THR:O	2.12	0.50
1:Y:4:LEU:HD13	1:Y:102:ILE:HG21	1.92	0.50
1:Y:33:TRP:C	1:Y:34:ILE:HD12	2.33	0.49
2:X:127:VAL:HG11	2:X:162:THR:CG2	2.43	0.49
3:Z:113:PRO:CG	3:Z:136:ILE:HD11	2.42	0.48
3:L:185:TRP:O	3:L:208:PRO:HG3	2.12	0.48
3:L:108:GLN:HB2	3:L:109:PRO:HD2	1.95	0.48
3:L:2:TYR:CG	3:L:92:HIS:CD2	3.02	0.48
2:X:243:VAL:C	2:X:244:LEU:HD12	2.34	0.48
2:G:191:TYR:HE1	2:G:193:LEU:HD23	1.79	0.48
1:Y:123:PRO:O	3:Z:121:SER:OG	2.32	0.48
1:Y:95:HIS:CD2	3:Z:91:TRP:HZ3	2.32	0.48
3:Z:31:THR:HG22	3:Z:32:LEU:N	2.29	0.48
1:H:162:GLY:O	1:H:182:VAL:HA	2.14	0.48
1:H:12:LYS:HE3	1:H:18:LEU:HD13	1.95	0.48
3:L:50:ASP:O	3:L:51:ASP:HB2	2.14	0.48
2:G:193:LEU:C	2:G:193:LEU:HD12	2.35	0.47
3:Z:29:GLY:N	3:Z:68:GLY:O	2.36	0.47
1:Y:95:HIS:NE2	3:Z:91:TRP:HZ3	2.11	0.47
2:G:154:ILE:O	2:G:158:LEU:N	2.45	0.47
1:H:178:LEU:HD12	1:H:178:LEU:C	2.34	0.47
2:X:210:ALA:O	2:X:214:LYS:HG2	2.14	0.47
3:Z:32:LEU:HD22	3:Z:50:ASP:HA	1.95	0.47
3:Z:124:GLU:OE2	3:Z:131:THR:HG22	2.14	0.47
1:Y:95:HIS:NE2	3:Z:91:TRP:CZ3	2.83	0.47
3:L:2:TYR:CD2	3:L:92:HIS:HD2	2.33	0.47
1:Y:33:TRP:HB2	1:Y:95:HIS:HB3	1.97	0.47
1:H:4:LEU:HD23	1:H:22:CYS:SG	2.54	0.47
2:X:129:LEU:HD21	2:X:162:THR:HG23	1.97	0.46
3:Z:17:THR:HG22	3:Z:18:THR:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:241:LEU:O	1:H:61:ALA:HB2	2.15	0.46
1:Y:51:ILE:HD13	1:Y:71:ALA:HB2	1.97	0.46
3:Z:51:ASP:O	3:Z:64:GLY:HA3	2.15	0.45
3:L:89:GLN:NE2	3:L:90:VAL:O	2.44	0.45
3:Z:159:VAL:HG22	3:Z:178:LEU:CD2	2.45	0.45
3:L:73:LEU:HD12	3:L:74:THR:N	2.32	0.45
1:H:33:TRP:HB2	1:H:95:HIS:HB3	1.99	0.45
3:Z:115:VAL:HA	3:Z:136:ILE:HD12	1.98	0.45
1:Y:94:ARG:O	1:Y:100(F):PHE:HA	2.17	0.45
3:Z:159:VAL:HG13	3:Z:178:LEU:CD2	2.47	0.45
1:Y:166:PHE:HE2	3:Z:135:LEU:HD13	1.82	0.44
2:G:162:THR:HG22	2:G:163:THR:N	2.28	0.44
1:Y:162:GLY:O	1:Y:182:VAL:HA	2.17	0.44
2:G:123:LEU:HD12	2:G:124:ALA:H	1.83	0.43
3:L:51:ASP:O	3:L:64:GLY:HA3	2.17	0.43
1:Y:37:VAL:HG11	1:Y:45:LEU:HD22	2.00	0.43
2:G:154:ILE:HD12	2:G:154:ILE:C	2.39	0.43
2:X:220:ASN:N	2:X:220:ASN:OD1	2.51	0.43
1:H:119:PRO:HB3	1:H:145:TYR:HB3	2.00	0.43
2:X:157:CYS:SG	2:X:158:LEU:N	2.92	0.43
1:Y:121:VAL:HA	1:Y:141:LEU:O	2.18	0.43
3:Z:120:PRO:HB3	3:Z:131:THR:H	1.84	0.43
2:G:127:VAL:HG21	2:G:163:THR:CG2	2.47	0.42
2:G:227:THR:O	2:G:235:PHE:HA	2.18	0.42
1:Y:82(C):LEU:N	1:Y:82(C):LEU:CD1	2.82	0.42
1:Y:167:PRO:HG2	3:Z:162:THR:HG21	2.00	0.42
3:Z:17:THR:O	3:Z:78:VAL:HG23	2.19	0.42
3:L:205:THR:HG22	3:L:206:VAL:N	2.35	0.42
1:Y:6:GLN:OE1	1:Y:106:GLY:HA2	2.18	0.42
1:Y:37:VAL:CG1	1:Y:45:LEU:HD22	2.49	0.42
1:Y:67:VAL:HG12	1:Y:68:THR:N	2.34	0.42
3:Z:35:TRP:O	3:Z:46:LEU:HD12	2.20	0.42
2:G:191:TYR:CE1	2:G:193:LEU:HD23	2.55	0.42
1:Y:39:GLN:HB2	1:Y:45:LEU:HD23	2.00	0.42
2:X:243:VAL:HG12	2:X:244:LEU:N	2.34	0.42
2:X:208:THR:O	2:X:212:VAL:HG23	2.19	0.42
2:G:227:THR:HG22	2:G:228:TYR:N	2.35	0.42
2:G:222:ILE:HD12	2:G:239:GLU:HG2	2.00	0.42
3:L:17:THR:O	3:L:78:VAL:CG2	2.67	0.42
3:L:6:GLN:OE1	3:L:99:GLY:HA3	2.20	0.42
2:G:130:LYS:HG3	2:G:130:LYS:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:168:ALA:HB1	1:Y:176:TYR:HB3	2.01	0.41
3:L:13:VAL:HG21	3:L:19:ALA:HB2	2.01	0.41
3:L:18:THR:HA	3:L:75:ILE:O	2.20	0.41
1:Y:30:PRO:HA	1:Y:52(A):PRO:HG2	2.02	0.41
3:Z:61:ARG:O	3:Z:75:ILE:HA	2.19	0.41
3:L:188:HIS:HB2	3:L:191:TYR:CE1	2.56	0.41
3:L:27:ASP:N	3:L:69:ASN:OD1	2.48	0.41
3:Z:54:ARG:HD3	3:Z:62:PHE:O	2.19	0.41
3:L:145:THR:HG22	3:L:146:VAL:N	2.35	0.41
3:L:12:SER:HB2	3:L:106(A):LEU:HD21	2.03	0.41
1:Y:4:LEU:HD13	1:Y:102:ILE:HG22	1.99	0.41
3:Z:117:LEU:HD11	3:Z:132:LEU:HD11	2.03	0.41
3:Z:115:VAL:O	3:Z:116:THR:OG1	2.34	0.40
1:H:201:LYS:N	1:H:202:PRO:CD	2.84	0.40
3:Z:31:THR:O	3:Z:66:ASN:ND2	2.54	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	H	224/235 (95%)	211 (94%)	13 (6%)	0	100	100
1	Y	182/235 (77%)	171 (94%)	11 (6%)	0	100	100
2	G	100/117 (86%)	98 (98%)	2 (2%)	0	100	100
2	X	92/117 (79%)	87 (95%)	5 (5%)	0	100	100
3	L	209/213 (98%)	199 (95%)	10 (5%)	0	100	100
3	Z	169/213 (79%)	162 (96%)	7 (4%)	0	100	100
All	All	976/1130 (86%)	928 (95%)	48 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	H	189/197 (96%)	189 (100%)	0	100	100
1	Y	161/197 (82%)	161 (100%)	0	100	100
2	G	90/102 (88%)	90 (100%)	0	100	100
2	X	84/102 (82%)	84 (100%)	0	100	100
3	L	178/180 (99%)	178 (100%)	0	100	100
3	Z	147/180 (82%)	147 (100%)	0	100	100
All	All	849/958 (89%)	849 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

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, 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	H	226/235 (96%)	-0.18	0 100 100	39, 62, 98, 121	0
1	Y	192/235 (81%)	0.18	10 (5%) 27 12	57, 100, 148, 172	0
2	G	104/117 (88%)	0.50	10 (9%) 8 3	56, 130, 181, 236	0
2	X	98/117 (83%)	0.10	3 (3%) 49 27	57, 97, 133, 181	0
3	L	211/213 (99%)	-0.16	0 100 100	34, 58, 92, 121	0
3	Z	177/213 (83%)	0.50	19 (10%) 6 2	59, 106, 164, 208	0
All	All	1008/1130 (89%)	0.11	42 (4%) 36 18	34, 83, 155, 236	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Z	132	LEU	6.2
2	G	223	ASP	5.3
3	Z	201	THR	4.7
3	Z	117	LEU	4.0
2	G	200	THR	3.9
2	G	199	THR	3.6
1	Y	125	ALA	3.5
2	G	204	VAL	3.5
3	Z	134	CYS	3.5
2	G	187	ASN	3.4
3	Z	175	SER	3.3
3	Z	80	ALA	3.2
3	Z	174	ALA	3.1
3	Z	128	ASN	3.1
3	Z	136	ILE	3.0
3	Z	131	THR	3.0
1	Y	138	LEU	2.9
3	Z	110	LYS	2.9
1	Y	182	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	G	186	GLY	2.8
1	Y	192	GLN	2.7
3	Z	111	ALA	2.7
3	Z	114	SER	2.6
2	G	202	GLU	2.5
3	Z	133	VAL	2.4
1	Y	142	VAL	2.4
1	Y	198	VAL	2.4
3	Z	200	SER	2.4
3	Z	193	CYS	2.3
3	Z	112	ALA	2.3
1	Y	181	VAL	2.3
3	Z	19	ALA	2.3
2	G	236	THR	2.2
2	G	235	PHE	2.2
3	Z	116	THR	2.2
1	Y	191	THR	2.2
2	X	131	CYS	2.1
2	X	167	ASP	2.1
1	Y	194	TYR	2.1
2	G	137	SER	2.1
1	Y	100(A)	GLU	2.0
2	X	183	PRO	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.