wwPDB X-ray Structure Validation Summary Report (i)

Feb 2, 2022 – 12:24 am GMT

PDB ID	:	7PI3
Title	:	PfCyRPA bound to Fab fragments from monoclonal antibodies Cy.003, Cy.004 and Cy.007
Authors	:	Ragotte, R.J.; Higgins, M.K.
Deposited on	:	2021-08-19
Resolution	:	3.27 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

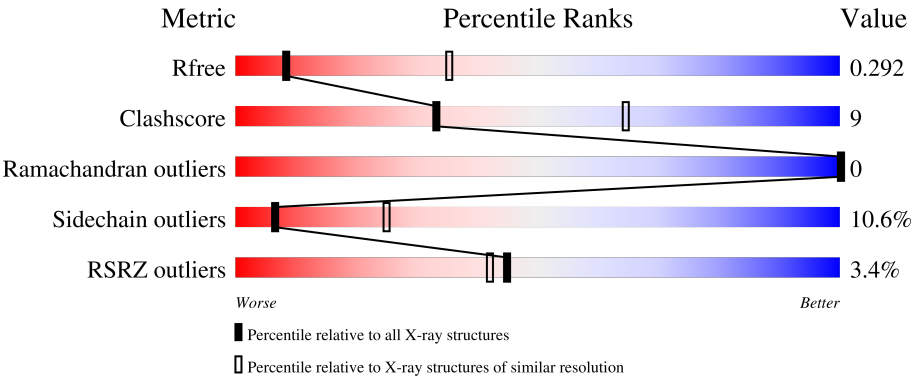
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.26
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 3.27 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	343	55% 36% 6%
1	H	343	60% 29% 6%
1	O	343	61% 32% 5%
1	V	343	60% 30% 5%
2	B	230	72% 23%

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Mol	Chain	Length	Quality of chain
2	I	230	2% 76% 18%
2	P	230	2% 80% 14%
2	W	230	3% 73% 20% 5%
3	C	210	% 77% 20%
3	J	210	2% 79% 19%
3	Q	210	5% 86% 12%
3	X	210	2% 72% 24%
4	D	230	4% 78% 15%
4	K	230	% 78% 16%
4	R	230	2% 76% 18%
4	Y	230	8% 79% 15%
5	E	209	% 85% 12%
5	L	209	3% 85% 11%
5	S	209	3% 84% 11%
5	Z	209	6% 83% 13%
6	F	321	% 60% 10% 31%
6	M	321	2% 56% 13% 31%
6	T	321	% 58% 10% 32%
6	a	321	% 64% 32%
7	G	209	% 87% 12%
7	N	209	4% 88% 11%
7	U	209	3% 85% 14%
7	b	209	3% 89% 11%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 48847 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 Cysteine-rich protective antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2730	1755	439	523	13			
1	H	321	Total	C	N	O	S	0	0	0
			2675	1723	429	510	13			
1	O	327	Total	C	N	O	S	0	0	0
			2722	1751	438	520	13			
1	V	325	Total	C	N	O	S	0	0	0
			2705	1741	435	516	13			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	ALA	SER	conflict	UNP Q8IFM8
A	324	ALA	THR	conflict	UNP Q8IFM8
A	340	ALA	THR	conflict	UNP Q8IFM8
A	363	GLY	-	expression tag	UNP Q8IFM8
A	364	GLY	-	expression tag	UNP Q8IFM8
A	365	GLY	-	expression tag	UNP Q8IFM8
A	366	GLY	-	expression tag	UNP Q8IFM8
A	367	SER	-	expression tag	UNP Q8IFM8
A	368	GLU	-	expression tag	UNP Q8IFM8
A	369	PRO	-	expression tag	UNP Q8IFM8
A	370	GLU	-	expression tag	UNP Q8IFM8
A	371	ALA	-	expression tag	UNP Q8IFM8
H	147	ALA	SER	conflict	UNP Q8IFM8
H	324	ALA	THR	conflict	UNP Q8IFM8
H	340	ALA	THR	conflict	UNP Q8IFM8
H	363	GLY	-	expression tag	UNP Q8IFM8
H	364	GLY	-	expression tag	UNP Q8IFM8
H	365	GLY	-	expression tag	UNP Q8IFM8
H	366	GLY	-	expression tag	UNP Q8IFM8
H	367	SER	-	expression tag	UNP Q8IFM8
H	368	GLU	-	expression tag	UNP Q8IFM8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	369	PRO	-	expression tag	UNP Q8IFM8
H	370	GLU	-	expression tag	UNP Q8IFM8
H	371	ALA	-	expression tag	UNP Q8IFM8
O	147	ALA	SER	conflict	UNP Q8IFM8
O	324	ALA	THR	conflict	UNP Q8IFM8
O	340	ALA	THR	conflict	UNP Q8IFM8
O	363	GLY	-	expression tag	UNP Q8IFM8
O	364	GLY	-	expression tag	UNP Q8IFM8
O	365	GLY	-	expression tag	UNP Q8IFM8
O	366	GLY	-	expression tag	UNP Q8IFM8
O	367	SER	-	expression tag	UNP Q8IFM8
O	368	GLU	-	expression tag	UNP Q8IFM8
O	369	PRO	-	expression tag	UNP Q8IFM8
O	370	GLU	-	expression tag	UNP Q8IFM8
O	371	ALA	-	expression tag	UNP Q8IFM8
V	147	ALA	SER	conflict	UNP Q8IFM8
V	324	ALA	THR	conflict	UNP Q8IFM8
V	340	ALA	THR	conflict	UNP Q8IFM8
V	363	GLY	-	expression tag	UNP Q8IFM8
V	364	GLY	-	expression tag	UNP Q8IFM8
V	365	GLY	-	expression tag	UNP Q8IFM8
V	366	GLY	-	expression tag	UNP Q8IFM8
V	367	SER	-	expression tag	UNP Q8IFM8
V	368	GLU	-	expression tag	UNP Q8IFM8
V	369	PRO	-	expression tag	UNP Q8IFM8
V	370	GLU	-	expression tag	UNP Q8IFM8
V	371	ALA	-	expression tag	UNP Q8IFM8

- Molecule 2 is a protein called Monoclonal antibody Cy.003 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	221	Total	C	N	O	S	0	0	0
			1611	1009	276	319	7			
2	I	221	Total	C	N	O	S	132	0	0
			1611	1009	276	319	7			
2	P	221	Total	C	N	O	S	442	0	0
			1611	1009	276	319	7			
2	W	218	Total	C	N	O	S	0	0	0
			1597	1002	273	315	7			

- Molecule 3 is a protein called Monoclonal antibody Cy.003 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	0
			1552	963	263	322	4			
3	J	207	Total	C	N	O	S	102	0	0
			1552	963	263	322	4			
3	Q	207	Total	C	N	O	S	580	0	0
			1552	963	263	322	4			
3	X	206	Total	C	N	O	S	0	0	0
			1547	960	262	321	4			

- Molecule 4 is a protein called Monoclonal antibody Cy.007 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	221	Total	C	N	O	S	621	0	0
			1619	1013	272	327	7			
4	K	220	Total	C	N	O	S	690	0	0
			1614	1010	271	326	7			
4	R	221	Total	C	N	O	S	690	0	0
			1619	1013	272	327	7			
4	Y	221	Total	C	N	O	S	621	0	0
			1619	1013	272	327	7			

- Molecule 5 is a protein called Monoclonal antibody Cy.007 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	204	Total	C	N	O	S	777	0	0
			1541	957	262	318	4			
5	L	203	Total	C	N	O	S	777	0	0
			1536	954	261	317	4			
5	S	200	Total	C	N	O	S	796	0	0
			1517	942	258	313	4			
5	Z	203	Total	C	N	O	S	777	0	0
			1537	955	261	317	4			

- Molecule 6 is a protein called Monoclonal antibody Cy.004 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	223	Total	C	N	O	S	685	0	0
			1634	1023	277	329	5			
6	M	223	Total	C	N	O	S	493	0	0
			1634	1023	277	329	5			
6	T	218	Total	C	N	O	S	533	0	0
			1603	1005	271	322	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	a	219	Total 1604	C 1004	N 272	O 323	S 5	660	0	0

- Molecule 7 is a protein called Monoclonal antibody Cy.004 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	209	Total 1577	C 978	N 265	O 329	S 5	834	0	0
7	N	209	Total 1577	C 978	N 265	O 329	S 5	30	0	0
7	U	208	Total 1572	C 975	N 264	O 328	S 5	359	0	0
7	b	208	Total 1571	C 975	N 264	O 328	S 4	535	0	0

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

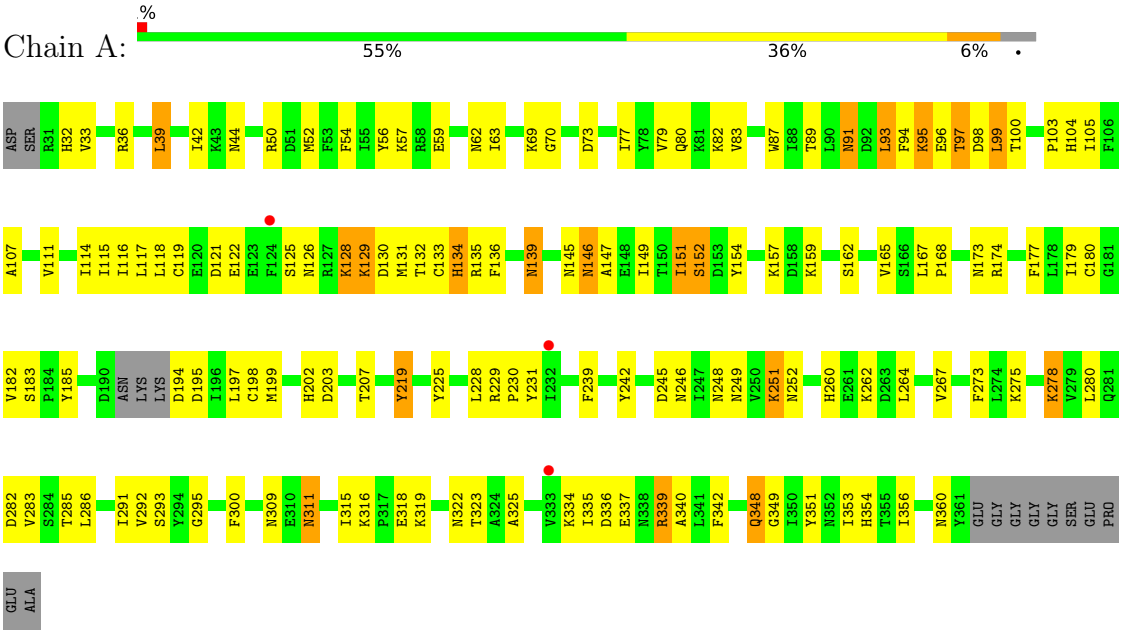
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	2	Total 2	Ca 2	2	0
8	H	1	Total 1	Ca 1	1	0
8	M	1	Total 1	Ca 1	1	0
8	T	2	Total 2	Ca 2	2	0
8	a	2	Total 2	Ca 2	2	0

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.

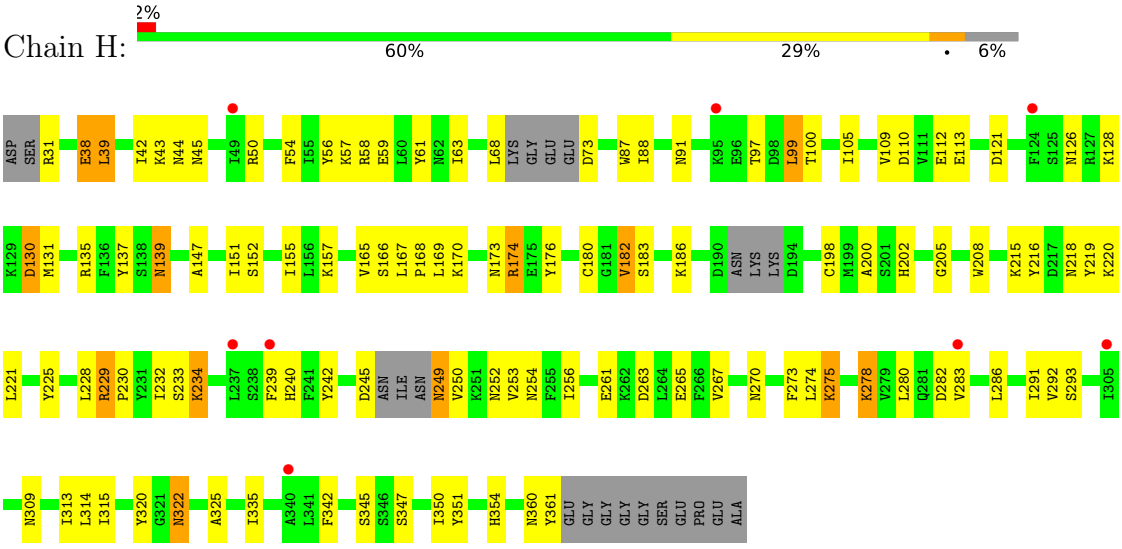
• Molecule 1: Cysteine-rich protective antigen

Chain A:



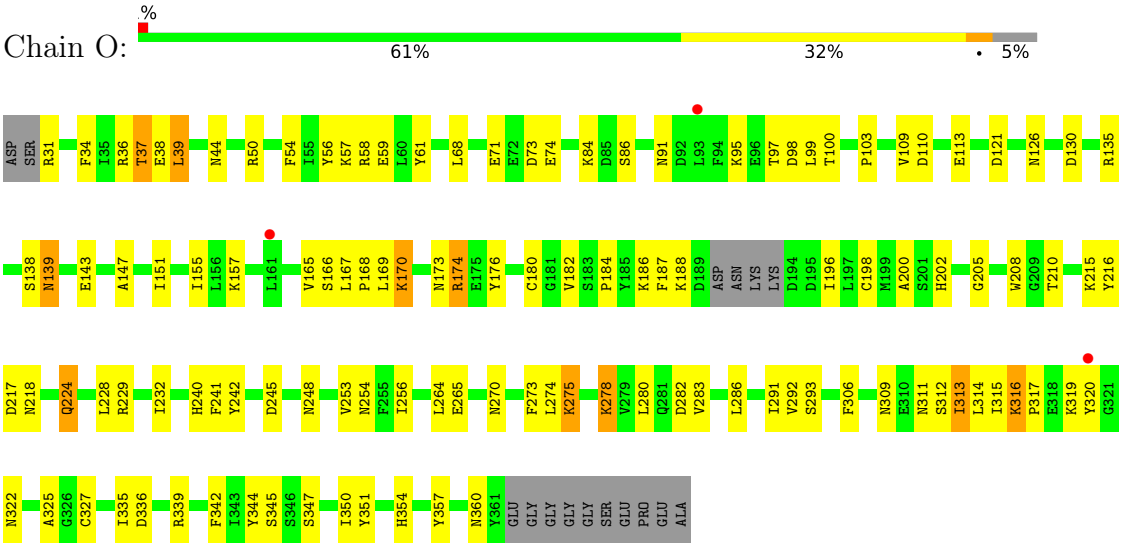
• Molecule 1: Cysteine-rich protective antigen

Chain H:



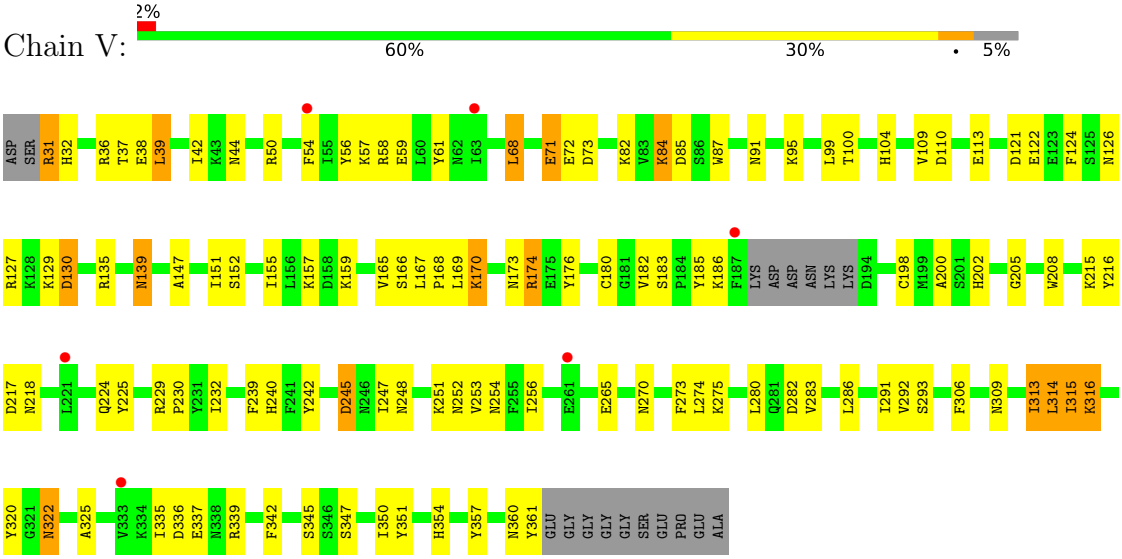
• Molecule 1: Cysteine-rich protective antigen

Chain O:



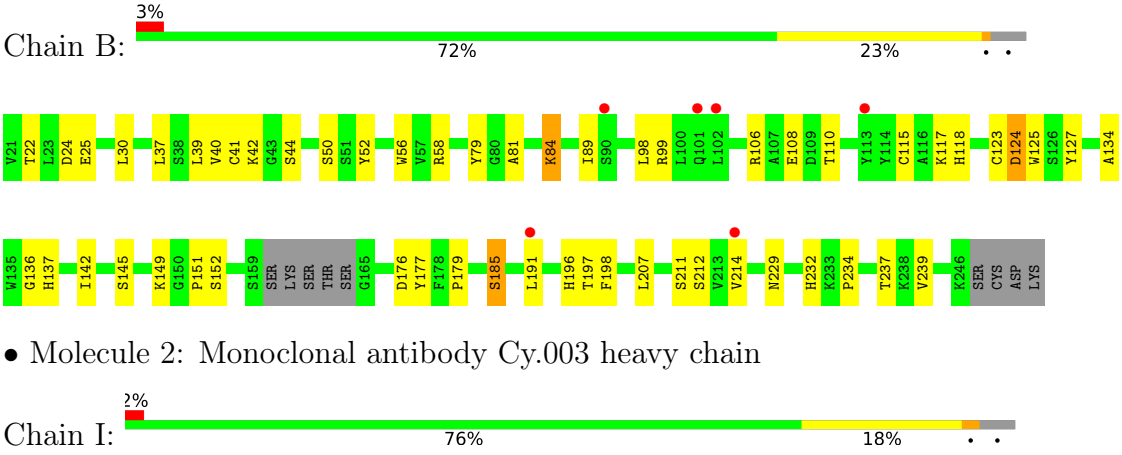
• Molecule 1: Cysteine-rich protective antigen

Chain V:



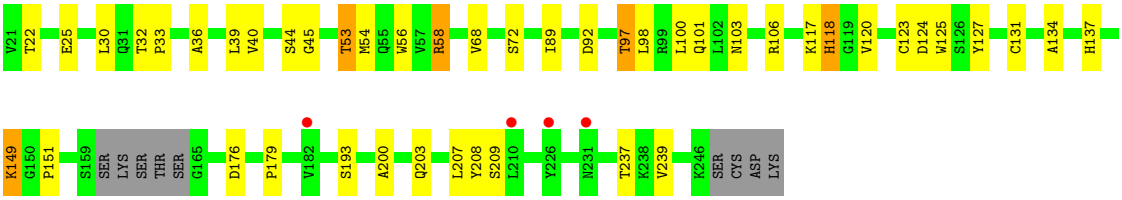
• Molecule 2: Monoclonal antibody Cy.003 heavy chain

Chain B:



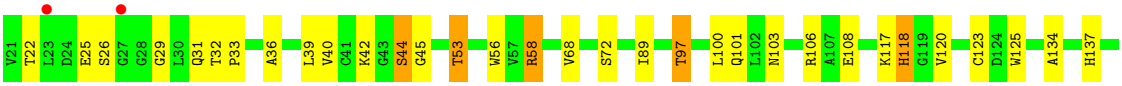
• Molecule 2: Monoclonal antibody Cy.003 heavy chain

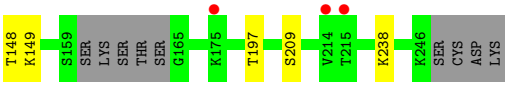
Chain I:



• Molecule 2: Monoclonal antibody Cy.003 heavy chain

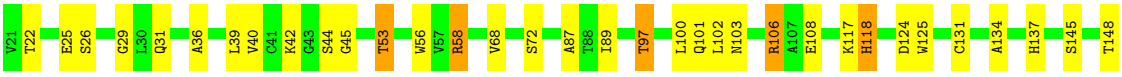
Chain P:

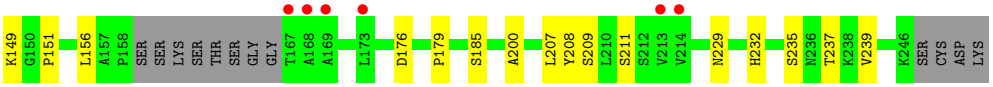




• Molecule 2: Monoclonal antibody Cy.003 heavy chain

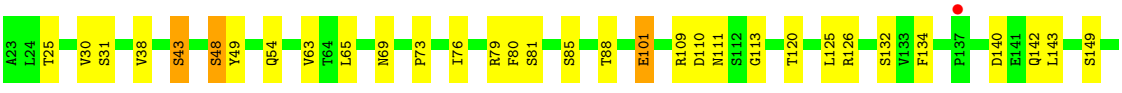
Chain W:





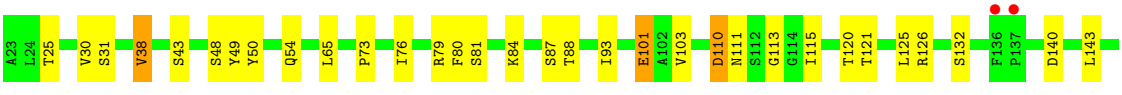
• Molecule 3: Monoclonal antibody Cy.003 light chain

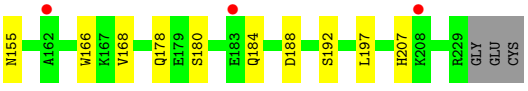
Chain C:



• Molecule 3: Monoclonal antibody Cy.003 light chain

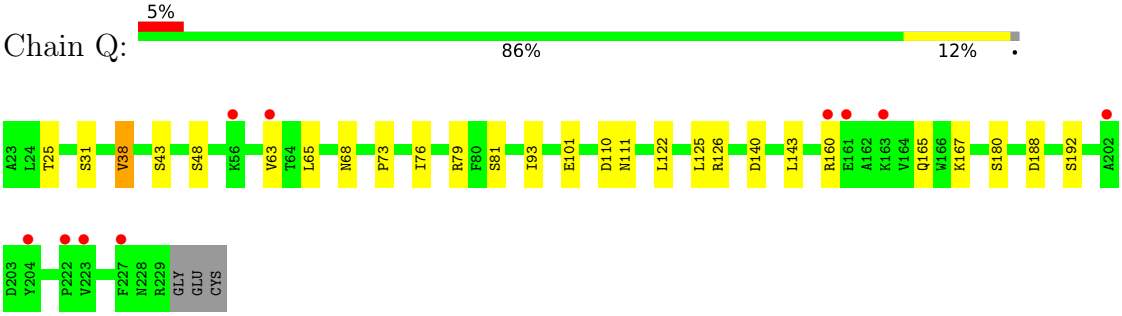
Chain J:





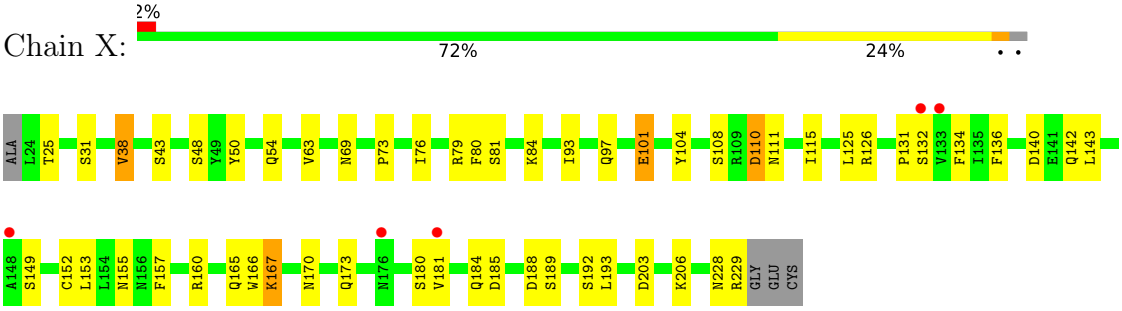
• Molecule 3: Monoclonal antibody Cy.003 light chain

Chain Q:



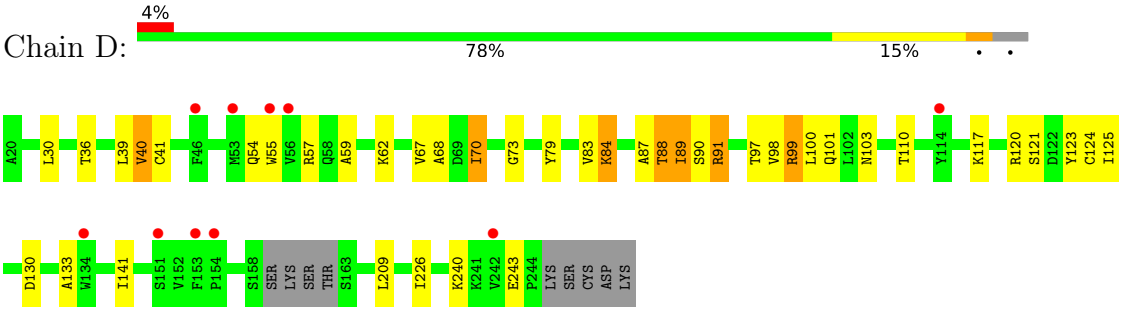
• Molecule 3: Monoclonal antibody Cy.003 light chain

Chain X:



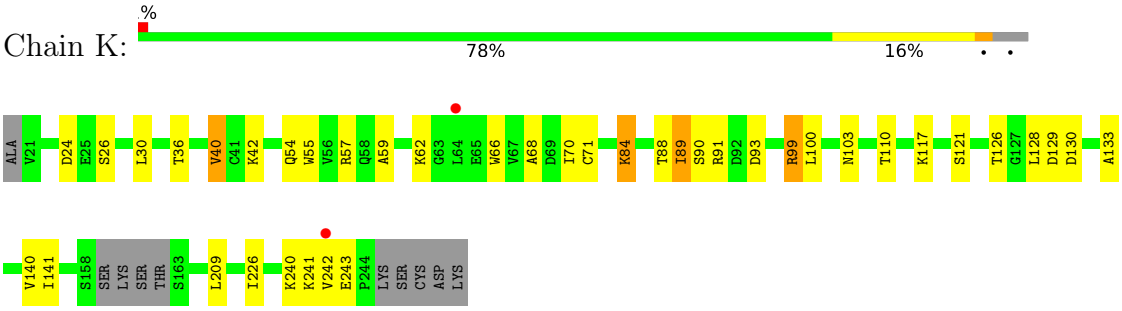
• Molecule 4: Monoclonal antibody Cy.007 heavy chain

Chain D:



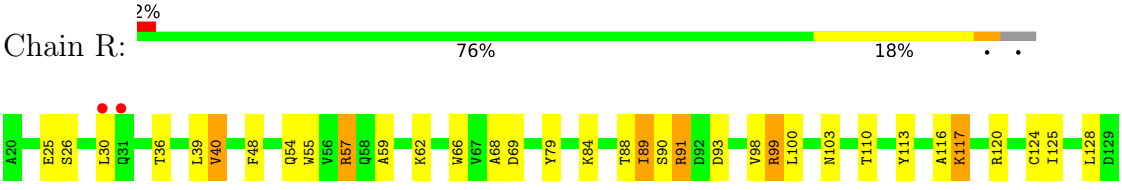
• Molecule 4: Monoclonal antibody Cy.007 heavy chain

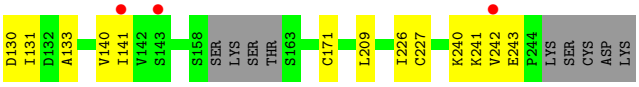
Chain K:



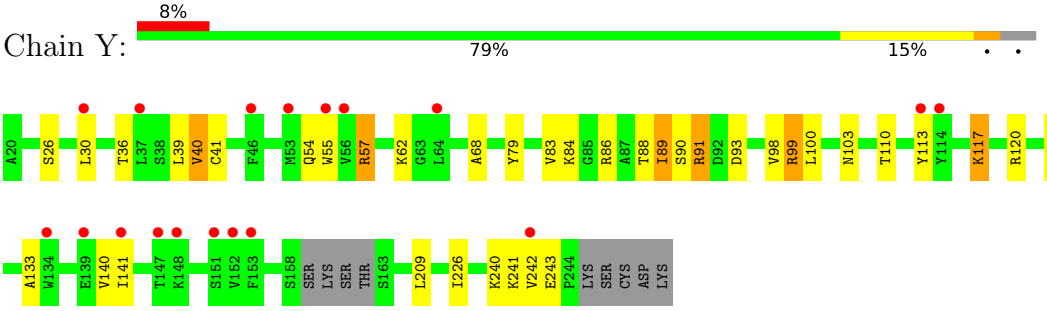
• Molecule 4: Monoclonal antibody Cy.007 heavy chain

Chain R:

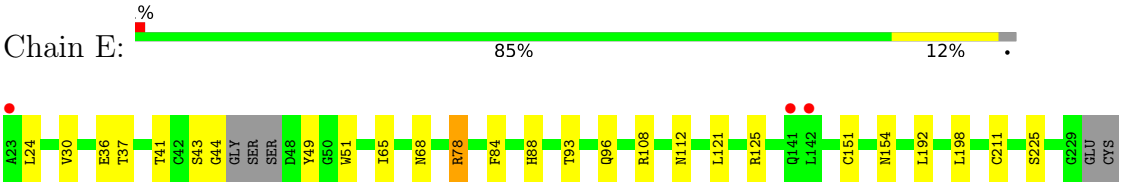




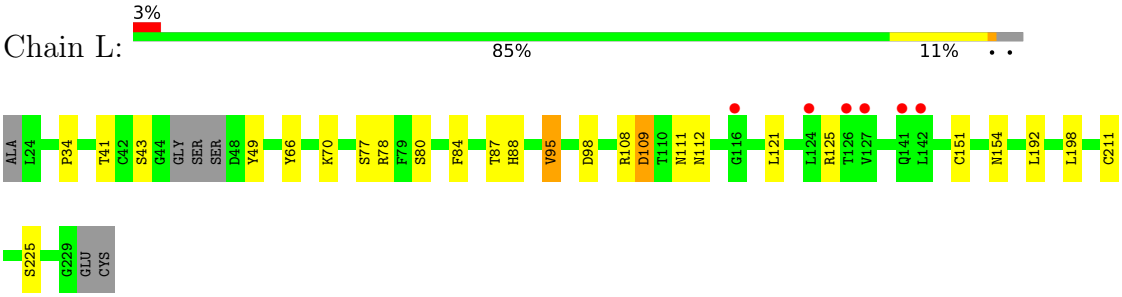
• Molecule 4: Monoclonal antibody Cy.007 heavy chain



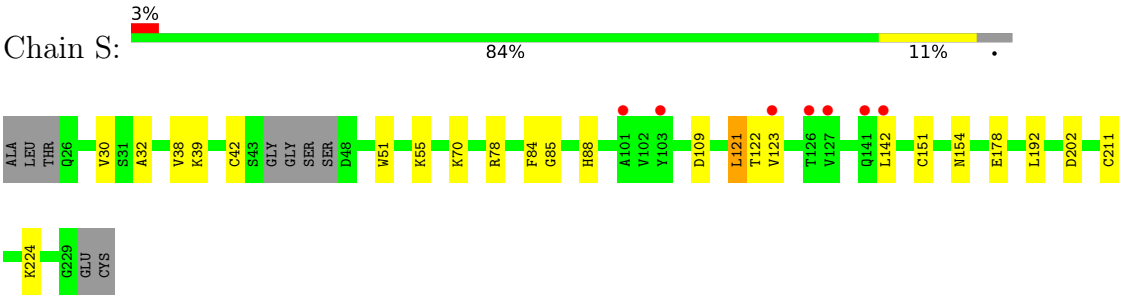
• Molecule 5: Monoclonal antibody Cy.007 light chain



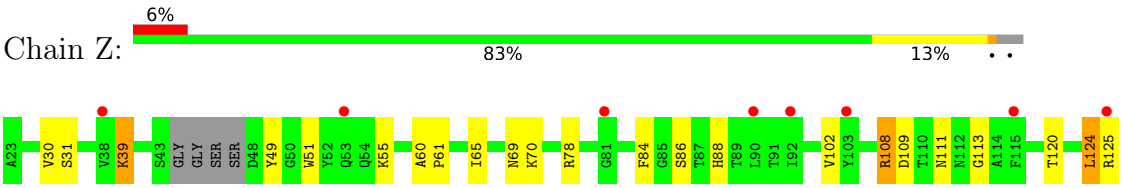
• Molecule 5: Monoclonal antibody Cy.007 light chain



• Molecule 5: Monoclonal antibody Cy.007 light chain

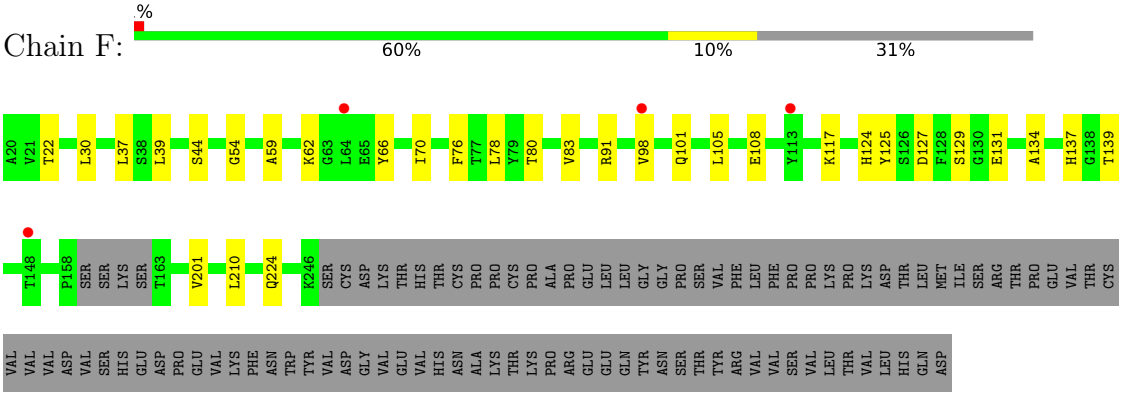


• Molecule 5: Monoclonal antibody Cy.007 light chain



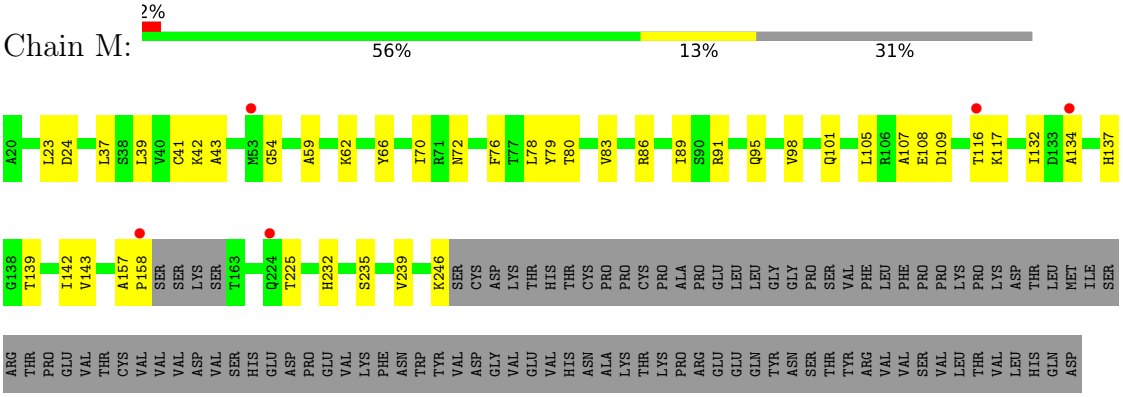
• Molecule 6: Monoclonal antibody Cy.004 heavy chain

Chain F:



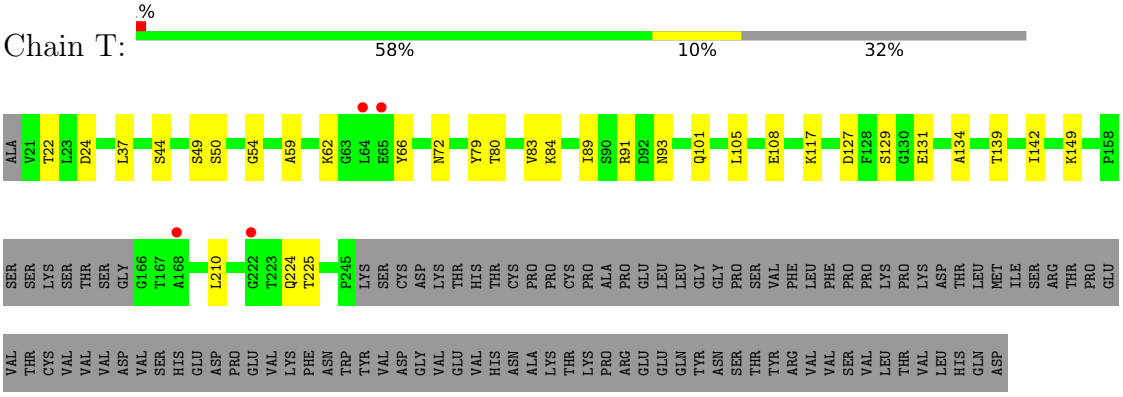
• Molecule 6: Monoclonal antibody Cy.004 heavy chain

Chain M:



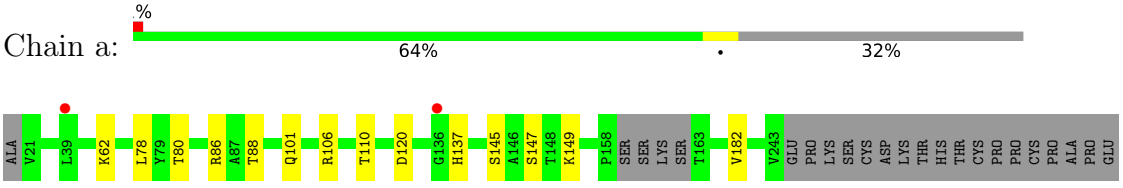
• Molecule 6: Monoclonal antibody Cy.004 heavy chain

Chain T:



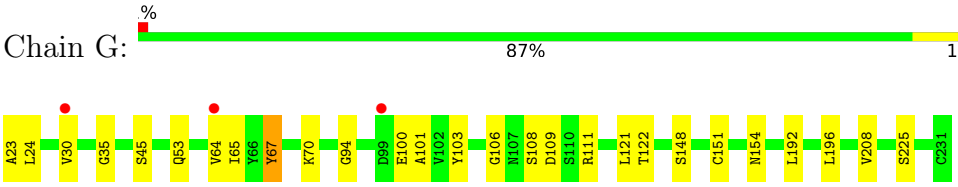
• Molecule 6: Monoclonal antibody Cy.004 heavy chain

Chain a:



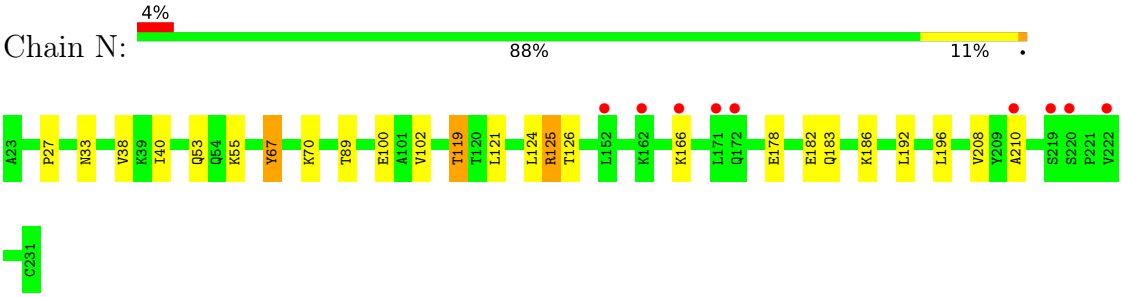
• Molecule 7: Monoclonal antibody Cy.004 light chain

Chain G:



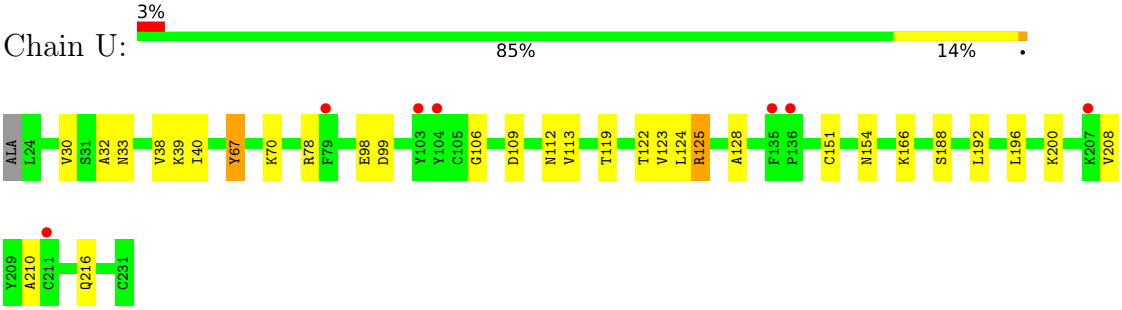
• Molecule 7: Monoclonal antibody Cy.004 light chain

Chain N:



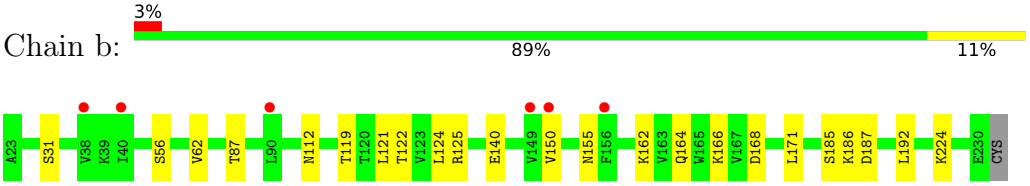
• Molecule 7: Monoclonal antibody Cy.004 light chain

Chain U:



• Molecule 7: Monoclonal antibody Cy.004 light chain

Chain b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	164.84Å 164.84Å 382.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.64 – 3.27 47.64 – 3.27	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.64-3.27) 99.9 (47.64-3.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 3.25Å)	Xtriage
Refinement program	BUSTER 2.10.4 (20-OCT-2021)	Depositor
R, R_{free}	0.285 , 0.298 0.280 , 0.292	Depositor DCC
R_{free} test set	7806 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	113.8	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.107 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	48847	wwPDB-VP
Average B, all atoms (Å^2)	187.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.54	0/2793	0.73	0/3772
1	H	0.37	0/2736	0.62	0/3693
1	O	0.37	0/2785	0.63	0/3761
1	V	0.35	0/2768	0.60	0/3739
2	B	0.35	0/1648	0.64	0/2243
2	I	0.29	0/1648	0.54	0/2243
2	P	0.28	0/1648	0.53	0/2243
2	W	0.31	0/1634	0.55	0/2225
3	C	0.32	0/1584	0.54	0/2153
3	J	0.30	0/1584	0.52	0/2153
3	Q	0.28	0/1584	0.51	0/2153
3	X	0.31	0/1579	0.53	0/2146
4	D	0.25	0/1654	0.46	0/2254
4	K	0.26	0/1649	0.46	0/2247
4	R	0.25	0/1654	0.46	0/2254
4	Y	0.25	0/1654	0.45	0/2254
5	E	0.27	0/1573	0.45	0/2139
5	L	0.26	0/1568	0.44	0/2132
5	S	0.26	0/1549	0.44	0/2106
5	Z	0.26	0/1569	0.44	0/2134
6	F	0.25	0/1670	0.46	0/2273
6	M	0.29	0/1670	0.51	0/2273
6	T	0.26	0/1639	0.46	0/2232
6	a	0.27	0/1639	0.48	0/2231
7	G	0.27	0/1610	0.49	0/2192
7	N	0.29	0/1610	0.51	0/2192
7	U	0.27	0/1605	0.49	0/2185
7	b	0.29	0/1604	0.51	0/2184
All	All	0.31	0/49908	0.53	0/67806

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 (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	2730	0	2615	101	0
1	H	2675	0	2562	65	0
1	O	2722	0	2611	67	0
1	V	2705	0	2594	71	0
2	B	1611	0	1561	43	0
2	I	1611	0	1561	28	0
2	P	1611	0	1561	21	0
2	W	1597	0	1550	29	0
3	C	1552	0	1499	26	0
3	J	1552	0	1499	22	0
3	Q	1552	0	1499	6	0
3	X	1547	0	1494	23	0
4	D	1619	0	1570	20	0
4	K	1614	0	1565	19	0
4	R	1619	0	1570	17	0
4	Y	1619	0	1570	13	0
5	E	1541	0	1479	7	0
5	L	1536	0	1474	7	0
5	S	1517	0	1453	6	0
5	Z	1537	0	1476	8	0
6	F	1634	0	1582	14	0
6	M	1634	0	1582	16	0
6	T	1603	0	1549	15	0
6	a	1604	0	1551	0	0
7	G	1577	0	1513	11	0
7	N	1577	0	1513	8	0
7	U	1572	0	1508	12	0
7	b	1571	0	1508	0	0
8	F	2	0	0	0	0
8	H	1	0	0	0	0
8	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	T	2	0	0	0	0
8	a	2	0	0	0	0
All	All	48847	0	47069	619	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.

The worst 5 of 619 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:V:130:ASP:HB3	1:V:152:SER:HA	1.19	1.15
7:U:40:ILE:HG21	7:U:119:THR:HG21	1.47	0.95
1:V:68:LEU:HB2	1:V:73:ASP:HB3	1.49	0.91
1:A:130:ASP:HB3	1:A:152:SER:HA	1.53	0.91
1:A:130:ASP:CB	1:A:152:SER:HA	2.05	0.86

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	324/343 (94%)	267 (82%)	57 (18%)	0	100	100
1	H	313/343 (91%)	283 (90%)	30 (10%)	0	100	100
1	O	323/343 (94%)	295 (91%)	28 (9%)	0	100	100
1	V	321/343 (94%)	289 (90%)	32 (10%)	0	100	100
2	B	217/230 (94%)	202 (93%)	15 (7%)	0	100	100
2	I	217/230 (94%)	198 (91%)	19 (9%)	0	100	100
2	P	217/230 (94%)	202 (93%)	15 (7%)	0	100	100
2	W	214/230 (93%)	193 (90%)	21 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	205/210 (98%)	189 (92%)	16 (8%)	0	100	100
3	J	205/210 (98%)	191 (93%)	14 (7%)	0	100	100
3	Q	205/210 (98%)	189 (92%)	16 (8%)	0	100	100
3	X	204/210 (97%)	190 (93%)	14 (7%)	0	100	100
4	D	217/230 (94%)	210 (97%)	7 (3%)	0	100	100
4	K	216/230 (94%)	207 (96%)	9 (4%)	0	100	100
4	R	217/230 (94%)	212 (98%)	5 (2%)	0	100	100
4	Y	217/230 (94%)	210 (97%)	7 (3%)	0	100	100
5	E	200/209 (96%)	190 (95%)	10 (5%)	0	100	100
5	L	199/209 (95%)	191 (96%)	8 (4%)	0	100	100
5	S	196/209 (94%)	187 (95%)	9 (5%)	0	100	100
5	Z	199/209 (95%)	190 (96%)	9 (4%)	0	100	100
6	F	219/321 (68%)	205 (94%)	14 (6%)	0	100	100
6	M	219/321 (68%)	203 (93%)	16 (7%)	0	100	100
6	T	214/321 (67%)	201 (94%)	13 (6%)	0	100	100
6	a	215/321 (67%)	195 (91%)	20 (9%)	0	100	100
7	G	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
7	N	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
7	U	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
7	b	206/209 (99%)	193 (94%)	13 (6%)	0	100	100
All	All	6319/7008 (90%)	5874 (93%)	445 (7%)	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	306/316 (97%)	254 (83%)	52 (17%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	300/316 (95%)	254 (85%)	46 (15%)	2	12
1	O	305/316 (96%)	263 (86%)	42 (14%)	3	16
1	V	303/316 (96%)	255 (84%)	48 (16%)	2	11
2	B	177/186 (95%)	161 (91%)	16 (9%)	9	32
2	I	177/186 (95%)	165 (93%)	12 (7%)	16	44
2	P	177/186 (95%)	164 (93%)	13 (7%)	14	40
2	W	176/186 (95%)	163 (93%)	13 (7%)	13	40
3	C	177/179 (99%)	159 (90%)	18 (10%)	7	27
3	J	177/179 (99%)	163 (92%)	14 (8%)	12	37
3	Q	177/179 (99%)	158 (89%)	19 (11%)	6	25
3	X	177/179 (99%)	156 (88%)	21 (12%)	5	20
4	D	179/188 (95%)	160 (89%)	19 (11%)	6	25
4	K	179/188 (95%)	161 (90%)	18 (10%)	7	27
4	R	179/188 (95%)	155 (87%)	24 (13%)	4	16
4	Y	179/188 (95%)	156 (87%)	23 (13%)	4	18
5	E	175/179 (98%)	160 (91%)	15 (9%)	10	34
5	L	175/179 (98%)	155 (89%)	20 (11%)	5	22
5	S	173/179 (97%)	156 (90%)	17 (10%)	8	29
5	Z	175/179 (98%)	155 (89%)	20 (11%)	5	22
6	F	179/272 (66%)	169 (94%)	10 (6%)	21	52
6	M	179/272 (66%)	166 (93%)	13 (7%)	14	40
6	T	176/272 (65%)	165 (94%)	11 (6%)	18	47
6	a	176/272 (65%)	162 (92%)	14 (8%)	12	37
7	G	180/180 (100%)	169 (94%)	11 (6%)	18	49
7	N	180/180 (100%)	168 (93%)	12 (7%)	16	45
7	U	180/180 (100%)	165 (92%)	15 (8%)	11	36
7	b	179/180 (99%)	156 (87%)	23 (13%)	4	18
All	All	5472/6000 (91%)	4893 (89%)	579 (11%)	6	25

5 of 579 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	345	SER

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Mol	Chain	Res	Type
7	b	171	LEU
2	W	211	SER
1	V	337	GLU
4	Y	242	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
1	V	224	GLN
5	Z	112	ASN
1	V	254	ASN
2	W	101	GLN
7	b	141	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	328/343 (95%)	-0.07	3 (0%) 84 84	76, 140, 180, 206	0
1	H	321/343 (93%)	-0.02	8 (2%) 57 53	122, 149, 182, 203	0
1	O	327/343 (95%)	-0.13	3 (0%) 84 84	125, 151, 182, 196	0
1	V	325/343 (94%)	-0.13	6 (1%) 68 65	139, 169, 200, 214	0
2	B	221/230 (96%)	-0.15	6 (2%) 54 51	123, 147, 178, 193	0
2	I	202/230 (87%)	-0.13	4 (1%) 65 63	119, 146, 248, 251	0
2	P	159/230 (69%)	-0.06	5 (3%) 49 47	141, 168, 274, 277	0
2	W	218/230 (94%)	-0.22	6 (2%) 53 50	142, 168, 219, 229	0
3	C	207/210 (98%)	-0.20	3 (1%) 75 74	118, 151, 189, 201	0
3	J	192/210 (91%)	-0.12	5 (2%) 56 52	123, 151, 258, 268	0
3	Q	129/210 (61%)	0.10	10 (7%) 13 12	134, 162, 271, 278	0
3	X	206/210 (98%)	-0.08	5 (2%) 59 55	140, 190, 222, 233	0
4	D	136/230 (59%)	0.27	10 (7%) 14 14	154, 190, 243, 257	1 (0%)
4	K	125/230 (54%)	-0.33	2 (1%) 72 69	159, 189, 212, 216	1 (0%)
4	R	126/230 (54%)	-0.22	5 (3%) 38 35	167, 203, 227, 233	1 (0%)
4	Y	136/230 (59%)	0.38	18 (13%) 3 3	181, 207, 264, 283	1 (0%)
5	E	104/209 (49%)	-0.02	3 (2%) 51 50	157, 185, 199, 283	2 (1%)
5	L	103/209 (49%)	0.01	6 (5%) 23 22	161, 188, 208, 247	2 (1%)
5	S	98/209 (46%)	0.09	7 (7%) 16 15	191, 205, 219, 279	2 (2%)
5	Z	103/209 (49%)	0.32	12 (11%) 4 4	184, 211, 230, 298	2 (1%)
6	F	129/321 (40%)	-0.08	4 (3%) 49 47	143, 181, 202, 205	0
6	M	155/321 (48%)	-0.05	5 (3%) 47 45	133, 153, 203, 252	0
6	T	146/321 (45%)	-0.22	4 (2%) 54 51	170, 194, 241, 251	0
6	a	128/321 (39%)	-0.42	2 (1%) 72 69	181, 203, 209, 212	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
7	G	101/209 (48%)	-0.18	3 (2%) 50 48	146, 162, 178, 184	0
7	N	206/209 (98%)	-0.18	9 (4%) 34 32	149, 183, 211, 219	0
7	U	160/209 (76%)	-0.08	7 (4%) 34 32	168, 194, 251, 256	0
7	b	139/209 (66%)	-0.21	6 (4%) 35 33	180, 193, 236, 242	0
All	All	4930/7008 (70%)	-0.09	167 (3%) 45 42	76, 172, 228, 298	12 (0%)

The worst 5 of 167 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	141	GLN	27.1
4	Y	242	VAL	16.7
5	S	126	THR	16.1
4	D	242	VAL	15.1
5	Z	142	LEU	12.8

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)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.