wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 05:43 AM EDT

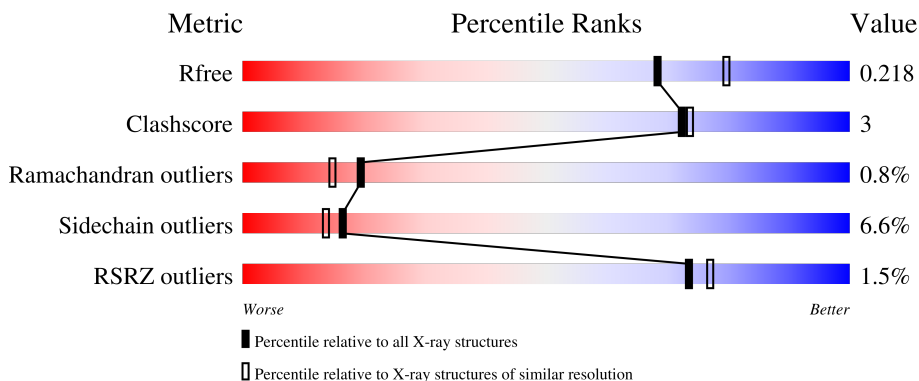|		
PDB ID	:	7T0I
Title	:	Crystal structure of S25-39 Fab Unliganded 3
Authors	:	Legg, M.S.G.; Blackler, R.J.; Evans, S.V.
Deposited on	:	2021-11-29
Resolution	:	2.10 Å(reported)

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 2.10 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	Percentile Ranks	Value
Rfree		0.218
Clashscore		3
Ramachandran outliers		0.8%
Sidechain outliers		6.6%
RSRZ outliers		1.5%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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	B	222	2% 82% 12% • •
1	D	222	2% 83% 12% • •
1	F	222	86% 8% • 5%
1	H	222	2% 83% 11% • •
2	A	219	86% 13% •

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Mol	Chain	Length	Quality of chain
2	C	219	84% ▓▓▓▓▓▓▓▓▓▓▓▓▓ 15% ·
2	E	219	2% ▓▓▓▓▓▓▓▓▓▓▓ 78% ▓▓▓ 17% · ·
2	L	219	3% ▓▓▓▓▓▓▓▓▓▓▓▓ 85% ▓ 13% ·

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 13498 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 S25-39 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	213	Total	C	N	O	S	0	0	0
			1616	1027	269	313	7			
1	B	214	Total	C	N	O	S	0	0	0
			1631	1037	271	316	7			
1	D	215	Total	C	N	O	S	0	0	0
			1632	1039	271	315	7			
1	F	210	Total	C	N	O	S	0	0	0
			1593	1012	266	308	7			

- Molecule 2 is a protein called S25-39 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	219	Total	C	N	O	S	0	0	0
			1698	1055	291	344	8			
2	A	219	Total	C	N	O	S	0	0	0
			1701	1056	291	346	8			
2	C	219	Total	C	N	O	S	0	0	0
			1697	1053	290	346	8			
2	E	219	Total	C	N	O	S	0	0	0
			1701	1056	291	346	8			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	32	Total	O	0	0
			32	32		
3	L	14	Total	O	0	0
			14	14		
3	B	48	Total	O	0	0
			48	48		
3	A	17	Total	O	0	0
			17	17		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	32	Total 32	O 32	0	0
3	C	43	Total 43	O 43	0	0
3	F	35	Total 35	O 35	0	0
3	E	8	Total 8	O 8	0	0

3 Residue-property plots ⓘ

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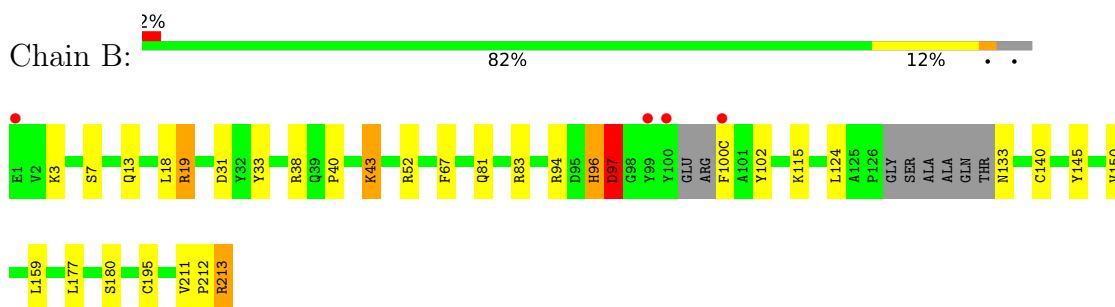 annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.
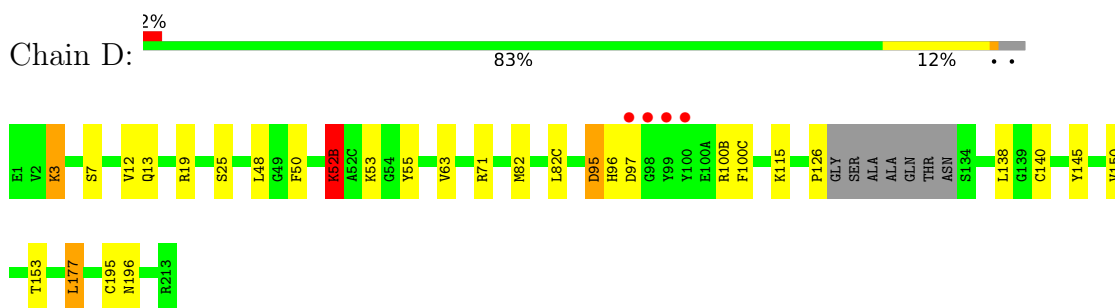
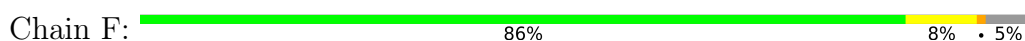- Molecule 1: S25-39 Fab heavy chain

Chain H:

- Molecule 1: S25-39 Fab heavy chain

Chain B:

- Molecule 1: S25-39 Fab heavy chain

Chain D:

- Molecule 1: S25-39 Fab heavy chain

Chain F:

E1 S7 F29 G42 K43 F50 Y55 R71 S76 S77 M82 L82C R83 H96 D97 GLY TYR TYR GLU ARG F100C P126 GLY SER ALA ALA GLN THR ASN S134 M135 Y145 V150 L177 P189 C195 P212 R213

• Molecule 2: S25-39 Fab light chain

Chain L:

3%

85%	13%

D1 S10 L11 A12 V13 G16 E17 K18 V19 S27E D60 R61 F62 S67 E81 D82 L83 Q90 R96 L104 K107 R108 A109 T126 Y140 P141 K142 D143 I150 R155 Q166 K169 L181 Y192 T193 C194 T197 T200 V206

K207 S208 E213 C214

• Molecule 2: S25-39 Fab light chain

Chain A:

86%	13%

D1 T5 Q6 S7 L11 A12 V13 E17 K18 K39 R54 E55 S56 G57 V58 S76 A80 E81 D82 L83 N93 L94 R96 K107 P120 S127 V132 F135 K142 N161 M175 L181 Y186 Y192 S203 S208 R211 N212

E213 C214

• Molecule 2: S25-39 Fab light chain

Chain C:

84%	15%

D1 T5 Q6 S7 L11 V19 T20 M21 Q37 L47 R54 V58 R61 D82 L83 Y86 Q90 R96 L104 K107 E123 T126 S127 L136 K142 V146 R155 Q156 L181 T182 K183 D184 E185 Y186 E187 R188 H189 Y192

S208 R211 C214

• Molecule 2: S25-39 Fab light chain

Chain E:

2%

78%	17%

D1 T5 L11 A12 V13 S14 A15 G16 E17 K18 V19 N27D S27E R27F T28 T53 R54 E55 S56 G57 V58 P59 D60 R61 F62 T63 S67 D70 I75 S76 S77 V78 Q79 A80 E81 D82 L83 C88 L104 E105 I106 K107 R108 A109 K142 Q156 S171

L181 H189 Y192 K199 S208 R211 C214

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	101.56Å 111.75Å 154.70Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	29.89 – 2.10	Depositor
	29.89 – 2.10	EDS
% Data completeness (in resolution range)	98.9 (29.89-2.10)	Depositor
	98.9 (29.89-2.10)	EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.87 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.180 , 0.225	Depositor
	0.174 , 0.218	DCC
R_{free} test set	4905 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	33.8	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 23.4	EDS
L-test for twinning[2]	$< |L| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.216 for -h,-k,l	Xtriage
Reported twinning fraction	0.760 for H, K, L 0.240 for h,-k,-l	Depositor
Outliers	0 of 99437 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13498	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	B	1.02	0/1674	1.05	6/2283 (0.3%)
1	D	1.00	0/1676	1.07	5/2289 (0.2%)
1	F	0.94	0/1634	0.99	1/2229 (0.0%)
1	H	1.05	1/1658 (0.1%)	1.04	5/2262 (0.2%)
2	A	0.88	0/1736	0.96	2/2351 (0.1%)
2	C	1.03	1/1732 (0.1%)	1.04	6/2347 (0.3%)
2	E	0.88	0/1736	1.00	4/2351 (0.2%)
2	L	0.78	0/1733	0.94	2/2347 (0.1%)
All	All	0.95	2/13579 (0.0%)	1.01	31/18459 (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
1	B	0	1
1	D	0	1
1	F	0	1
2	E	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	97	ASP	CB-CG	-5.44	1.40	1.51
2	C	86	TYR	CE1-CZ	-5.25	1.31	1.38

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	52(B)	LYS	O-C-N	-12.31	103.00	122.70
1	B	19	ARG	NE-CZ-NH1	8.54	124.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	19	ARG	NE-CZ-NH2	-8.18	116.21	120.30
2	C	96	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	F	177	LEU	CA-CB-CG	7.94	133.56	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	96	HIS	Peptide
1	D	52(B)	LYS	Mainchain
2	E	80	ALA	Peptide
1	F	96	HIS	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	B	1631	0	1588	12	0
1	D	1632	0	1587	9	0
1	F	1593	0	1559	8	0
1	H	1616	0	1572	10	0
2	A	1701	0	1648	10	0
2	C	1697	0	1637	11	0
2	E	1701	0	1648	22	0
2	L	1698	0	1646	9	1
3	A	17	0	0	0	0
3	B	48	0	0	2	0
3	C	43	0	0	0	0
3	D	32	0	0	0	0
3	E	8	0	0	0	0
3	F	35	0	0	1	0
3	H	32	0	0	1	0
3	L	14	0	0	0	0
All	All	13498	0	12885	90	1

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 3.

The worst 5 of 90 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:E:108:ARG:NH1	2:E:109:ALA:O	2.02	0.92
2:C:123:GLU:O	2:C:126:THR:HG22	1.89	0.72
2:C:189:HIS:O	2:C:211:ARG:NH1	2.23	0.71
2:E:77:SER:O	2:E:78:VAL:HG23	1.90	0.71
2:A:18:LYS:HG3	2:A:76:SER:HA	1.80	0.63

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:27(E):SER:OG	2:L:213:GLU:OE2[3_445]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	B	208/222 (94%)	202 (97%)	5 (2%)	1 (0%)	29	26
1	D	211/222 (95%)	207 (98%)	3 (1%)	1 (0%)	29	26
1	F	204/222 (92%)	201 (98%)	3 (2%)	0	100	100
1	H	207/222 (93%)	202 (98%)	3 (1%)	2 (1%)	15	11
2	A	217/219 (99%)	208 (96%)	9 (4%)	0	100	100
2	C	217/219 (99%)	206 (95%)	11 (5%)	0	100	100
2	E	217/219 (99%)	196 (90%)	13 (6%)	8 (4%)	3	1
2	L	217/219 (99%)	203 (94%)	13 (6%)	1 (0%)	29	26
All	All	1698/1764 (96%)	1625 (96%)	60 (4%)	13 (1%)	19	15

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	97	ASP
1	H	100	TYR
1	B	97	ASP
2	E	60	ASP
2	E	78	VAL

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	B	181/187 (97%)	168 (93%)	13 (7%)	14	11
1	D	180/187 (96%)	170 (94%)	10 (6%)	21	18
1	F	177/187 (95%)	170 (96%)	7 (4%)	31	32
1	H	178/187 (95%)	167 (94%)	11 (6%)	18	15
2	A	194/194 (100%)	182 (94%)	12 (6%)	18	15
2	C	193/194 (100%)	182 (94%)	11 (6%)	20	18
2	E	194/194 (100%)	176 (91%)	18 (9%)	9	6
2	L	193/194 (100%)	177 (92%)	16 (8%)	11	7
All	All	1490/1524 (98%)	1392 (93%)	98 (7%)	16	14

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	100(C)	PHE
2	C	181	LEU
1	D	140	CYS
2	C	19	VAL
1	F	77	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	42	GLN

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Mol	Chain	Res	Type
2	C	79	GLN
2	C	212	ASN
2	C	93	ASN
2	L	212	ASN

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 monosaccharides 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	B	214/222 (96%)	-0.33	4 (1%)	66	71	22, 36, 56, 74	0
1	D	215/222 (96%)	-0.29	4 (1%)	66	71	22, 37, 63, 80	0
1	F	210/222 (94%)	-0.25	0	100	100	24, 38, 68, 86	0
1	H	213/222 (95%)	-0.21	5 (2%)	60	65	21, 35, 73, 97	0
2	A	219/219 (100%)	-0.21	1 (0%)	91	92	26, 45, 69, 85	0
2	C	219/219 (100%)	-0.29	1 (0%)	91	92	23, 37, 57, 73	0
2	E	219/219 (100%)	0.11	5 (2%)	60	65	28, 52, 75, 97	0
2	L	219/219 (100%)	0.08	6 (2%)	54	60	29, 52, 74, 88	0
All	All	1728/1764 (97%)	-0.17	26 (1%)	73	77	21, 41, 69, 97	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	99	TYR	4.9
2	E	59	PRO	4.6
1	B	100	TYR	3.6
2	E	80	ALA	3.5
2	E	63	THR	3.4

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.