



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 9, 2023 – 09:50 pm GMT

PDB ID : 2J1K
Title : CAV-2 fibre head in complex with CAR D1
Authors : Seiradake, E.; Lortat-Jacob, H.; Billet, O.; Kremer, E.J.; Cusack, S.
Deposited on : 2006-08-14
Resolution : 2.30 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 ⓘ 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 : 2.36
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) : 2.36

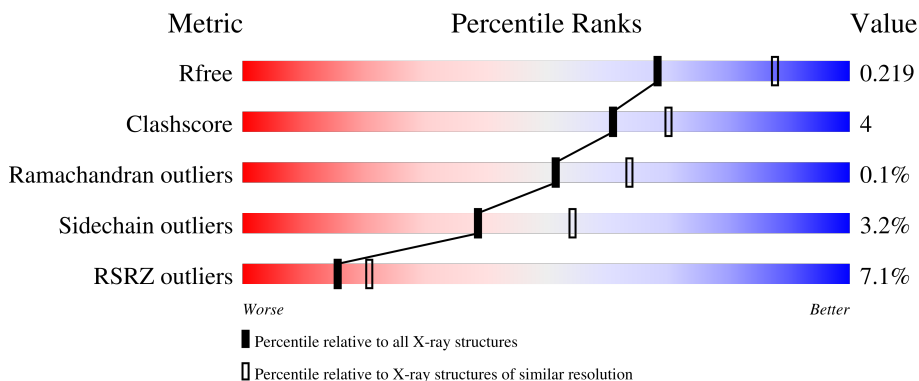
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	128	<div style="display: flex; align-items: center;"> <div style="width: 28%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div>
1	B	128	<div style="display: flex; align-items: center;"> <div style="width: 37%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 63%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div>
1	G	128	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div>
1	J	128	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div>
1	K	128	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div>

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Mol	Chain	Length	Quality of chain
1	O	128	3% 73% 18% 8%
1	P	128	9% 84% 10% 8%
1	T	128	9% 76% 14% 7%
1	V	128	23% 78% 16% 5%
1	X	128	7% 80% 16% 8%
1	Y	128	19% 75% 16% 7%
1	Z	128	34% 73% 16% 9%
2	C	197	86% 6% 8%
2	D	197	3% 85% 7% 8%
2	E	197	1% 86% 7% 8%
2	F	197	86% 6% 8%
2	H	197	85% 7% 8%
2	I	197	87% 6% 8%
2	L	197	2% 84% 8% 8%
2	M	197	2% 85% 7% 8%
2	N	197	84% 8% 8%
2	Q	197	6% 84% 8% 8%
2	R	197	88% 5% 8%
2	S	197	85% 7% 8%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 29978 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 COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	117	Total 914	C 581	N 147	O 183	S 3	0	0	0
1	B	113	Total 881	C 565	N 142	O 171	S 3	0	0	0
1	G	123	Total 959	C 611	N 156	O 189	S 3	0	0	0
1	J	123	Total 959	C 611	N 156	O 189	S 3	0	0	0
1	K	123	Total 963	C 615	N 156	O 189	S 3	0	0	0
1	O	118	Total 917	C 587	N 145	O 182	S 3	0	0	0
1	P	123	Total 959	C 611	N 156	O 189	S 3	0	0	0
1	T	119	Total 928	C 591	N 149	O 185	S 3	0	0	0
1	V	121	Total 944	C 600	N 154	O 187	S 3	0	0	0
1	X	123	Total 959	C 611	N 156	O 189	S 3	0	0	0
1	Y	119	Total 928	C 591	N 149	O 185	S 3	0	0	0
1	Z	117	Total 914	C 581	N 147	O 183	S 3	0	0	0

- Molecule 2 is a protein called FIBER PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	182	Total 1406	C 892	N 239	O 266	S 9	0	0	0
2	D	182	Total 1406	C 892	N 239	O 266	S 9	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	F	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	H	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	I	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	L	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	M	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	N	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	Q	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	R	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	S	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total	O	0	0
			24	24		
3	B	15	Total	O	0	0
			15	15		
3	C	140	Total	O	0	0
			140	140		
3	D	127	Total	O	0	0
			127	127		
3	E	121	Total	O	0	0
			121	121		
3	F	129	Total	O	0	0
			129	129		
3	G	53	Total	O	0	0
			53	53		
3	H	135	Total	O	0	0
			135	135		
3	I	148	Total	O	0	0
			148	148		

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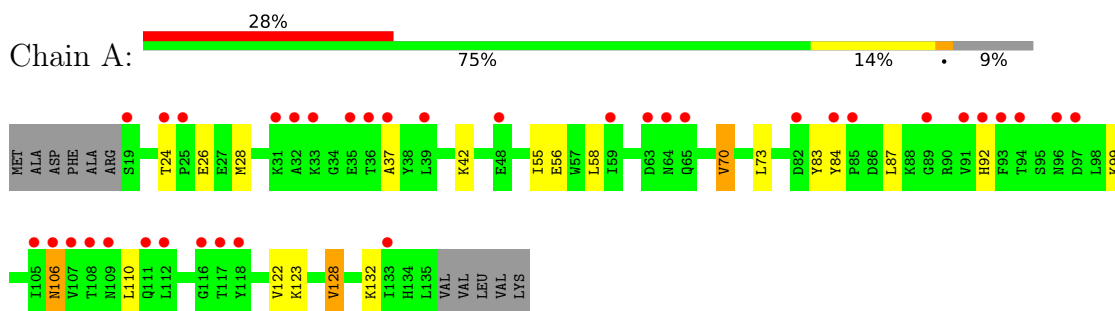
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	45	Total 45	O 45	0	0
3	K	45	Total 45	O 45	0	0
3	L	116	Total 116	O 116	0	0
3	M	134	Total 134	O 134	0	0
3	N	118	Total 118	O 118	0	0
3	O	31	Total 31	O 31	0	0
3	P	54	Total 54	O 54	0	0
3	Q	101	Total 101	O 101	0	0
3	R	111	Total 111	O 111	0	0
3	S	93	Total 93	O 93	0	0
3	T	32	Total 32	O 32	0	0
3	V	23	Total 23	O 23	0	0
3	X	50	Total 50	O 50	0	0
3	Y	23	Total 23	O 23	0	0
3	Z	13	Total 13	O 13	0	0

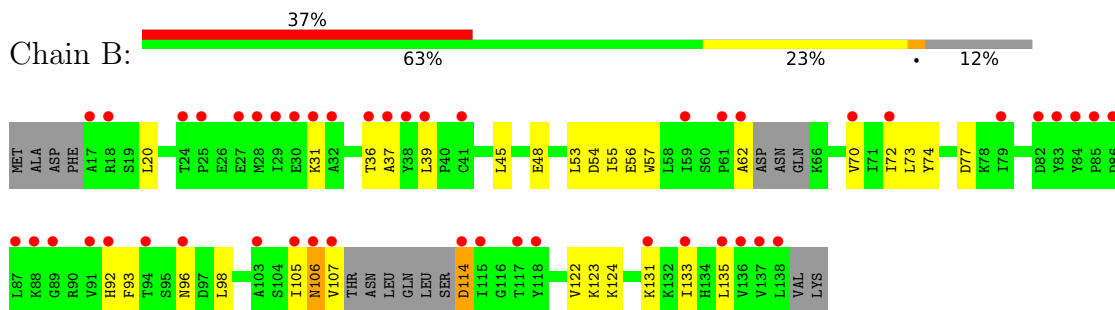
3 Residue-property plots [i](#)

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.

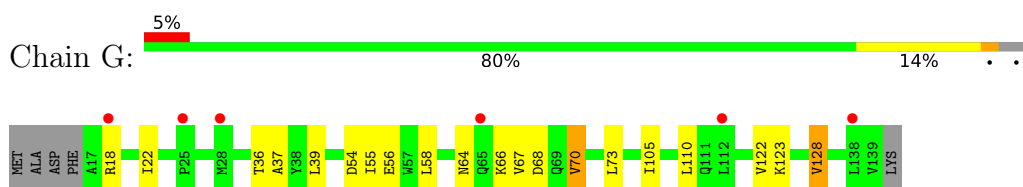
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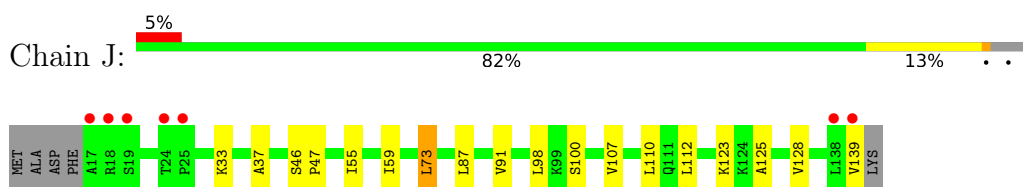
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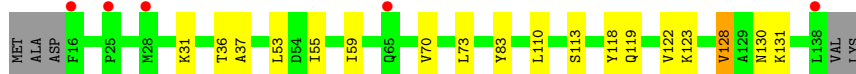
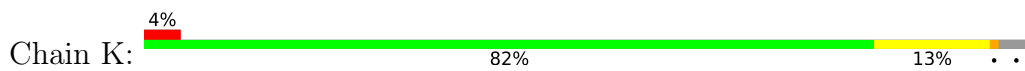
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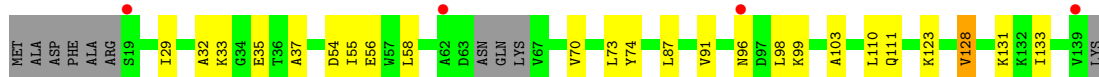
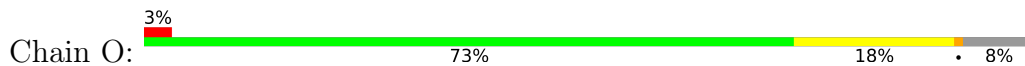
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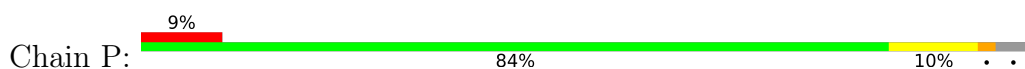
- Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



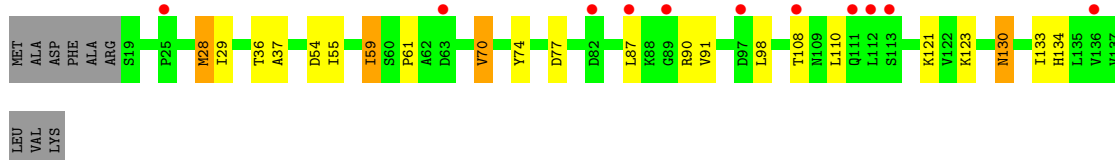
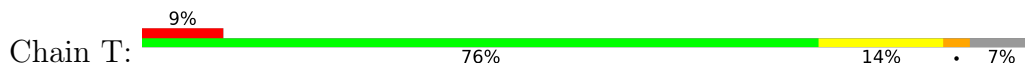
• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



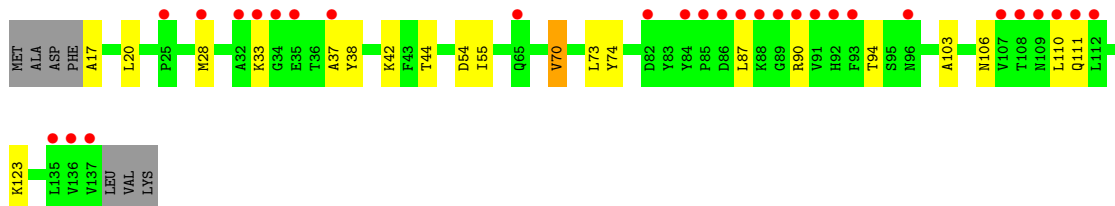
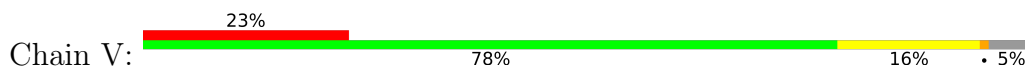
• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



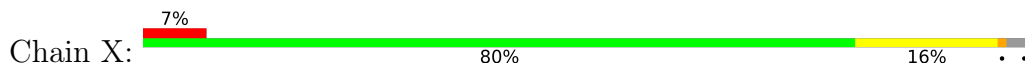
• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



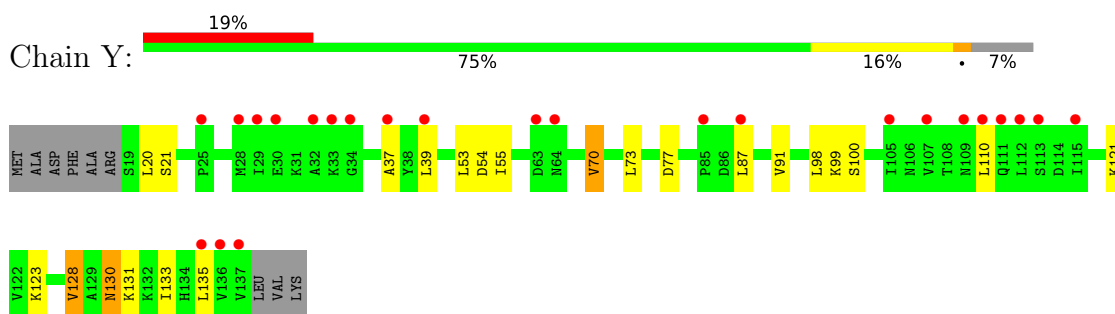
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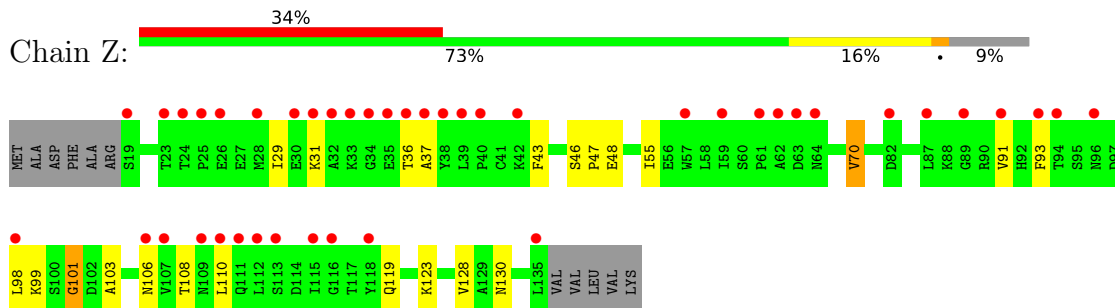
• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



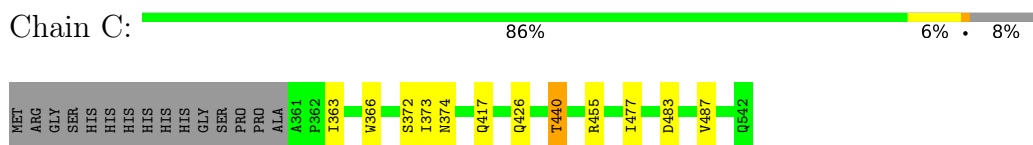
• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



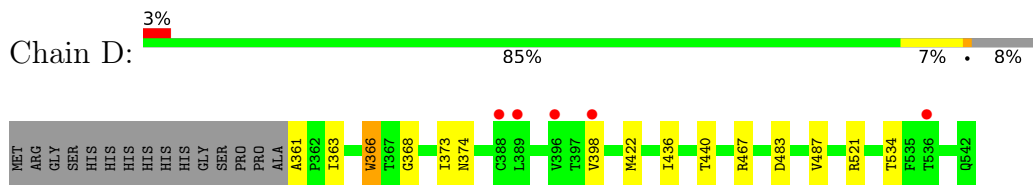
• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



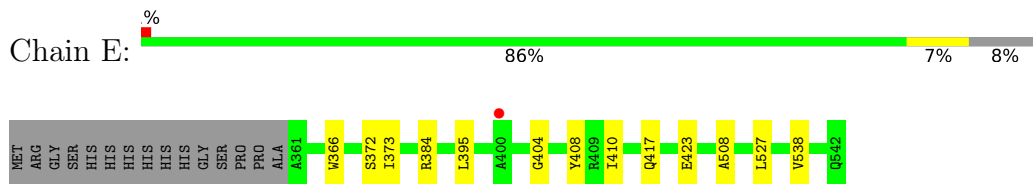
• Molecule 2: FIBER PROTEIN



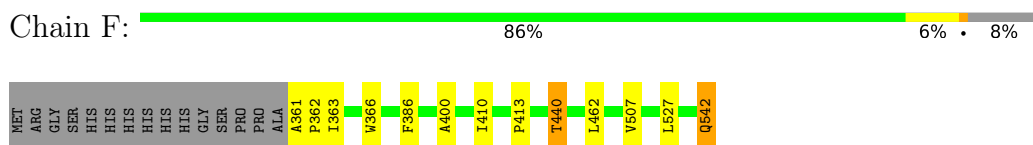
• Molecule 2: FIBER PROTEIN



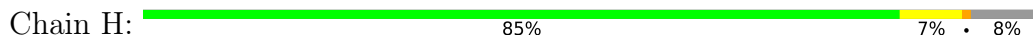
• Molecule 2: FIBER PROTEIN



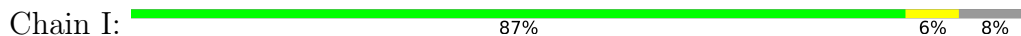
• Molecule 2: FIBER PROTEIN



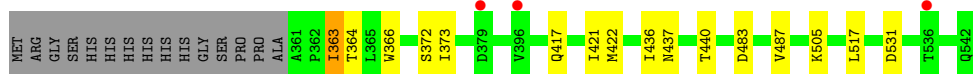
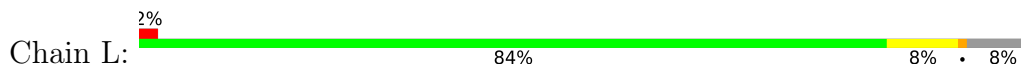
• Molecule 2: FIBER PROTEIN



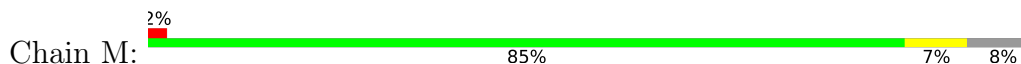
● Molecule 2: FIBER PROTEIN



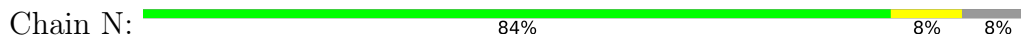
● Molecule 2: FIBER PROTEIN



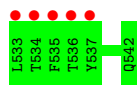
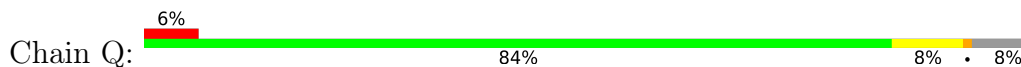
● Molecule 2: FIBER PROTEIN



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● Molecule 2: FIBER PROTEIN



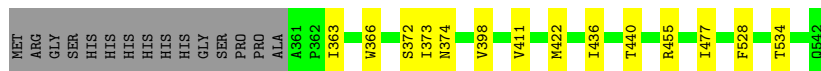
● Molecule 2: FIBER PROTEIN





- Molecule 2: FIBER PROTEIN

Chain S:
85% 7% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	219.94Å 219.94Å 387.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	192.45 – 2.30 47.67 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.0 (192.45-2.30) 92.0 (47.67-2.30)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.172 , 0.220 0.172 , 0.219	Depositor DCC
R_{free} test set	1890 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtrriage
Anisotropy	0.144	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	29978	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [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	A	0.37	0/932	0.57	0/1264
1	B	0.78	3/897 (0.3%)	0.63	1/1213 (0.1%)
1	G	0.43	0/977	0.64	0/1326
1	J	0.44	0/977	0.61	0/1326
1	K	0.43	0/982	0.61	0/1332
1	O	0.44	0/934	0.60	0/1268
1	P	0.40	0/977	0.61	0/1326
1	T	0.41	0/946	0.60	0/1284
1	V	0.38	0/962	0.55	0/1305
1	X	0.42	0/977	0.59	0/1326
1	Y	0.38	0/946	0.56	0/1284
1	Z	0.36	0/932	0.52	0/1264
2	C	0.50	0/1441	0.68	0/1964
2	D	0.51	0/1441	0.68	0/1964
2	E	0.51	0/1441	0.66	0/1964
2	F	0.52	0/1441	0.67	0/1964
2	H	0.53	0/1441	0.65	0/1964
2	I	0.50	0/1441	0.65	0/1964
2	L	0.48	0/1441	0.64	0/1964
2	M	0.51	0/1441	0.63	0/1964
2	N	0.47	0/1441	0.63	0/1964
2	Q	0.46	0/1441	0.63	0/1964
2	R	0.45	0/1441	0.65	0/1964
2	S	0.46	0/1441	0.62	0/1964
All	All	0.48	3/28731 (0.0%)	0.63	1/39086 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	62	ALA	C-O	16.91	1.55	1.23
1	B	114	ASP	CG-OD1	7.06	1.41	1.25
1	B	114	ASP	CG-OD2	6.25	1.39	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	ASP	CB-CG-OD2	-6.11	112.81	118.30

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	914	0	910	13	0
1	B	881	0	889	22	0
1	G	959	0	966	15	0
1	J	959	0	966	10	0
1	K	963	0	966	13	0
1	O	917	0	920	21	0
1	P	959	0	966	14	0
1	T	928	0	928	16	0
1	V	944	0	946	14	0
1	X	959	0	966	13	0
1	Y	928	0	928	17	0
1	Z	914	0	910	13	0
2	C	1406	0	1382	9	0
2	D	1406	0	1382	10	0
2	E	1406	0	1382	9	0
2	F	1406	0	1382	8	0
2	H	1406	0	1382	8	0
2	I	1406	0	1382	6	0
2	L	1406	0	1382	10	0
2	M	1406	0	1382	6	0
2	N	1406	0	1382	10	0
2	Q	1406	0	1382	10	0
2	R	1406	0	1382	6	0
2	S	1406	0	1382	10	0
3	A	24	0	0	0	0
3	B	15	0	0	0	0
3	C	140	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	127	0	0	2	0
3	E	121	0	0	0	0
3	F	129	0	0	1	0
3	G	53	0	0	0	0
3	H	135	0	0	2	0
3	I	148	0	0	1	0
3	J	45	0	0	0	0
3	K	45	0	0	1	0
3	L	116	0	0	0	0
3	M	134	0	0	0	0
3	N	118	0	0	1	0
3	O	31	0	0	1	0
3	P	54	0	0	2	0
3	Q	101	0	0	1	0
3	R	111	0	0	0	0
3	S	93	0	0	2	0
3	T	32	0	0	0	0
3	V	23	0	0	0	0
3	X	50	0	0	0	0
3	Y	23	0	0	0	0
3	Z	13	0	0	0	0
All	All	29978	0	27845	251	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 4.

The worst 5 of 251 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:373:ILE:HD11	1:V:70:VAL:HG21	1.30	1.07
2:C:374:ASN:HB3	2:C:440:THR:HG21	1.45	0.98
2:D:440:THR:HG23	3:D:2056:HOH:O	1.64	0.95
1:B:70:VAL:HG21	2:D:373:ILE:HD11	1.46	0.95
2:F:462:LEU:HD21	2:F:542:GLN:HG2	1.47	0.94

There are no symmetry-related clashes.

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	A	115/128 (90%)	107 (93%)	7 (6%)	1 (1%)	17	20
1	B	107/128 (84%)	96 (90%)	11 (10%)	0	100	100
1	G	121/128 (94%)	115 (95%)	6 (5%)	0	100	100
1	J	121/128 (94%)	119 (98%)	2 (2%)	0	100	100
1	K	121/128 (94%)	116 (96%)	5 (4%)	0	100	100
1	O	114/128 (89%)	107 (94%)	7 (6%)	0	100	100
1	P	121/128 (94%)	115 (95%)	6 (5%)	0	100	100
1	T	117/128 (91%)	109 (93%)	8 (7%)	0	100	100
1	V	119/128 (93%)	114 (96%)	5 (4%)	0	100	100
1	X	121/128 (94%)	117 (97%)	4 (3%)	0	100	100
1	Y	117/128 (91%)	109 (93%)	8 (7%)	0	100	100
1	Z	115/128 (90%)	106 (92%)	8 (7%)	1 (1%)	17	20
2	C	180/197 (91%)	174 (97%)	6 (3%)	0	100	100
2	D	180/197 (91%)	172 (96%)	8 (4%)	0	100	100
2	E	180/197 (91%)	172 (96%)	8 (4%)	0	100	100
2	F	180/197 (91%)	174 (97%)	6 (3%)	0	100	100
2	H	180/197 (91%)	174 (97%)	6 (3%)	0	100	100
2	I	180/197 (91%)	174 (97%)	6 (3%)	0	100	100
2	L	180/197 (91%)	174 (97%)	6 (3%)	0	100	100
2	M	180/197 (91%)	173 (96%)	7 (4%)	0	100	100
2	N	180/197 (91%)	173 (96%)	7 (4%)	0	100	100
2	Q	180/197 (91%)	174 (97%)	6 (3%)	0	100	100
2	R	180/197 (91%)	173 (96%)	7 (4%)	0	100	100
2	S	180/197 (91%)	171 (95%)	9 (5%)	0	100	100
All	All	3569/3900 (92%)	3408 (96%)	159 (4%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Z	101	GLY
1	A	24	THR

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	104/113 (92%)	98 (94%)	6 (6%)	20	27
1	B	99/113 (88%)	94 (95%)	5 (5%)	24	33
1	G	109/113 (96%)	104 (95%)	5 (5%)	27	38
1	J	109/113 (96%)	105 (96%)	4 (4%)	34	48
1	K	109/113 (96%)	106 (97%)	3 (3%)	43	60
1	O	105/113 (93%)	100 (95%)	5 (5%)	25	36
1	P	109/113 (96%)	106 (97%)	3 (3%)	43	60
1	T	106/113 (94%)	102 (96%)	4 (4%)	33	47
1	V	107/113 (95%)	103 (96%)	4 (4%)	34	48
1	X	109/113 (96%)	104 (95%)	5 (5%)	27	38
1	Y	106/113 (94%)	100 (94%)	6 (6%)	20	28
1	Z	104/113 (92%)	99 (95%)	5 (5%)	25	36
2	C	159/171 (93%)	153 (96%)	6 (4%)	33	47
2	D	159/171 (93%)	156 (98%)	3 (2%)	57	73
2	E	159/171 (93%)	156 (98%)	3 (2%)	57	73
2	F	159/171 (93%)	154 (97%)	5 (3%)	40	55
2	H	159/171 (93%)	156 (98%)	3 (2%)	57	73
2	I	159/171 (93%)	155 (98%)	4 (2%)	47	65
2	L	159/171 (93%)	156 (98%)	3 (2%)	57	73
2	M	159/171 (93%)	154 (97%)	5 (3%)	40	55
2	N	159/171 (93%)	154 (97%)	5 (3%)	40	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Q	159/171 (93%)	155 (98%)	4 (2%)	47	65
2	R	159/171 (93%)	156 (98%)	3 (2%)	57	73
2	S	159/171 (93%)	155 (98%)	4 (2%)	47	65
All	All	3184/3408 (93%)	3081 (97%)	103 (3%)	39	54

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	372	SER
2	Q	521	ARG
1	Z	70	VAL
2	N	529	LYS
1	P	70	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	109	ASN
1	Z	130	ASN
2	S	378	ASN
2	S	458	HIS
2	S	542	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](#)

There are no ligands in this entry.

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 i

6.1 Protein, DNA and RNA chains i

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	A	117/128 (91%)	1.39	36 (30%) 0 0	34, 44, 54, 57	0
1	B	113/128 (88%)	1.95	47 (41%) 0 0	32, 46, 58, 60	0
1	G	123/128 (96%)	0.08	6 (4%) 29 36	33, 44, 55, 58	0
1	J	123/128 (96%)	0.18	7 (5%) 23 30	33, 44, 55, 57	0
1	K	123/128 (96%)	0.27	5 (4%) 37 44	33, 45, 56, 57	0
1	O	118/128 (92%)	0.21	4 (3%) 45 52	33, 44, 54, 58	0
1	P	123/128 (96%)	0.47	12 (9%) 7 10	33, 44, 55, 57	0
1	T	119/128 (92%)	0.64	11 (9%) 9 12	33, 45, 55, 57	0
1	V	121/128 (94%)	1.16	29 (23%) 0 0	34, 44, 55, 57	0
1	X	123/128 (96%)	0.25	9 (7%) 15 20	33, 45, 55, 58	0
1	Y	119/128 (92%)	0.99	24 (20%) 1 1	34, 44, 54, 57	0
1	Z	117/128 (91%)	1.59	43 (36%) 0 0	34, 45, 55, 57	0
2	C	182/197 (92%)	-0.05	0 100 100	19, 24, 30, 36	0
2	D	182/197 (92%)	0.26	5 (2%) 54 62	20, 25, 33, 36	0
2	E	182/197 (92%)	-0.00	1 (0%) 91 94	20, 25, 32, 36	0
2	F	182/197 (92%)	-0.01	0 100 100	19, 23, 30, 34	0
2	H	182/197 (92%)	-0.17	0 100 100	19, 24, 30, 35	0
2	I	182/197 (92%)	0.09	0 100 100	19, 25, 30, 35	0
2	L	182/197 (92%)	0.18	3 (1%) 72 77	22, 27, 34, 36	0
2	M	182/197 (92%)	0.10	3 (1%) 72 77	21, 25, 30, 33	0
2	N	182/197 (92%)	-0.04	0 100 100	21, 26, 32, 37	0
2	Q	182/197 (92%)	0.37	12 (6%) 18 23	22, 29, 34, 39	0
2	R	182/197 (92%)	-0.03	0 100 100	22, 27, 34, 39	0
2	S	182/197 (92%)	-0.09	0 100 100	24, 31, 39, 41	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3623/3900 (92%)	0.33	257 (7%) 16 21	19, 30, 52, 60	0

The worst 5 of 257 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	ALA	8.6
1	Y	112	LEU	6.6
1	V	34	GLY	6.4
1	B	91	VAL	6.0
1	B	136	VAL	6.0

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.