



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 12:08 AM UTC

PDB ID : 8OFV / pdb_00008ofv
Title : Human adenovirus type 53 fiber-knob protein complexed with sialic acid
Authors : Rizkallah, P.J.; Parker, A.L.; Mundy, R.M.; Baker, A.T.
Deposited on : 2023-03-16
Resolution : 1.77 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

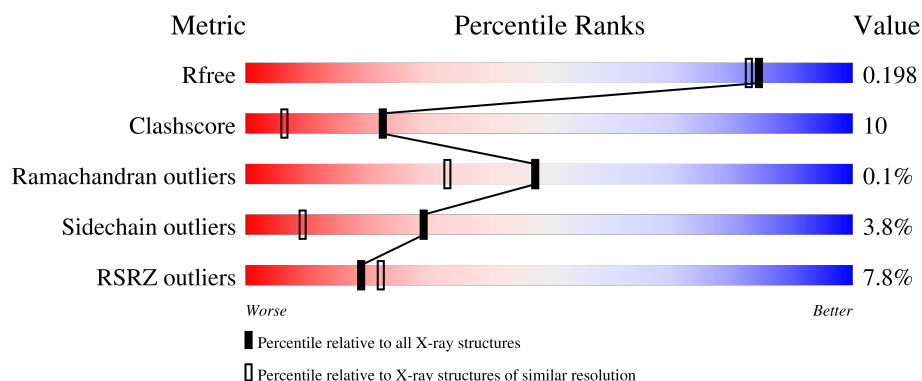
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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}	180053	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	189	5% 83% 15%
1	B	189	4% 80% 19%
1	C	189	5% 84% 16%
1	D	189	8% 84% 14%
1	E	189	3% 85% 14%

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Mol	Chain	Length	Quality of chain
1	F	189	
1	G	189	
1	H	189	
1	I	189	
1	J	189	
1	K	189	
1	L	189	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PEG	B	407	-	-	X	-
2	PEG	B	408	-	-	X	-
2	PEG	C	401	-	-	X	-
2	PEG	G	404	-	-	X	-
2	PEG	G	405	-	-	X	-
2	PEG	H	402	-	-	X	-
3	EDO	B	401	-	-	X	-
3	EDO	G	403	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19866 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 Fiber protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	5	0
			1509	968	245	289	7			
1	B	189	Total	C	N	O	S	0	5	0
			1545	988	256	294	7			
1	C	188	Total	C	N	O	S	0	6	0
			1539	984	251	297	7			
1	D	187	Total	C	N	O	S	0	2	0
			1501	960	247	287	7			
1	E	189	Total	C	N	O	S	0	4	0
			1535	980	253	295	7			
1	F	175	Total	C	N	O	S	0	3	0
			1418	911	234	268	5			
1	G	178	Total	C	N	O	S	0	2	0
			1434	925	234	270	5			
1	H	188	Total	C	N	O	S	0	5	0
			1534	980	254	292	8			
1	I	189	Total	C	N	O	S	0	9	0
			1574	1005	260	301	8			
1	J	185	Total	C	N	O	S	0	4	0
			1500	963	244	285	8			
1	K	187	Total	C	N	O	S	0	4	0
			1518	970	249	292	7			
1	L	174	Total	C	N	O	S	0	0	0
			1384	893	225	261	5			

There are 36 discrepancies between the modelled and reference sequences:

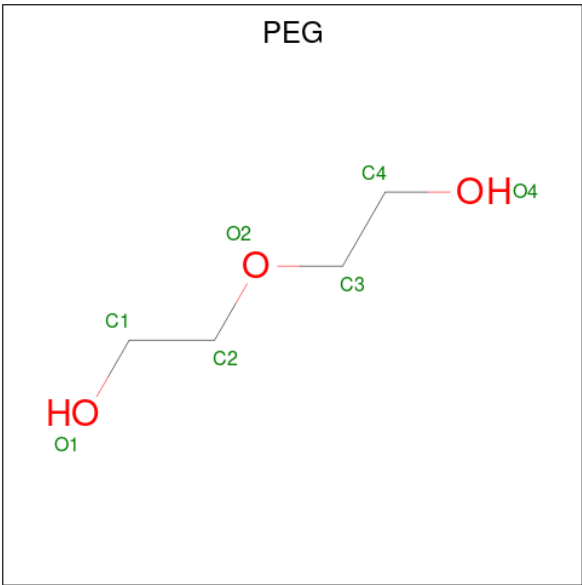
Chain	Residue	Modelled	Actual	Comment	Reference
A	180	ASN	LYS	conflict	UNP E5RWD1
A	181	ASN	GLU	conflict	UNP E5RWD1
A	184	LEU	ARG	conflict	UNP E5RWD1
B	180	ASN	LYS	conflict	UNP E5RWD1
B	181	ASN	GLU	conflict	UNP E5RWD1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	184	LEU	ARG	conflict	UNP E5RWD1
C	180	ASN	LYS	conflict	UNP E5RWD1
C	181	ASN	GLU	conflict	UNP E5RWD1
C	184	LEU	ARG	conflict	UNP E5RWD1
D	180	ASN	LYS	conflict	UNP E5RWD1
D	181	ASN	GLU	conflict	UNP E5RWD1
D	184	LEU	ARG	conflict	UNP E5RWD1
E	180	ASN	LYS	conflict	UNP E5RWD1
E	181	ASN	GLU	conflict	UNP E5RWD1
E	184	LEU	ARG	conflict	UNP E5RWD1
F	180	ASN	LYS	conflict	UNP E5RWD1
F	181	ASN	GLU	conflict	UNP E5RWD1
F	184	LEU	ARG	conflict	UNP E5RWD1
G	180	ASN	LYS	conflict	UNP E5RWD1
G	181	ASN	GLU	conflict	UNP E5RWD1
G	184	LEU	ARG	conflict	UNP E5RWD1
H	180	ASN	LYS	conflict	UNP E5RWD1
H	181	ASN	GLU	conflict	UNP E5RWD1
H	184	LEU	ARG	conflict	UNP E5RWD1
I	180	ASN	LYS	conflict	UNP E5RWD1
I	181	ASN	GLU	conflict	UNP E5RWD1
I	184	LEU	ARG	conflict	UNP E5RWD1
J	180	ASN	LYS	conflict	UNP E5RWD1
J	181	ASN	GLU	conflict	UNP E5RWD1
J	184	LEU	ARG	conflict	UNP E5RWD1
K	180	ASN	LYS	conflict	UNP E5RWD1
K	181	ASN	GLU	conflict	UNP E5RWD1
K	184	LEU	ARG	conflict	UNP E5RWD1
L	180	ASN	LYS	conflict	UNP E5RWD1
L	181	ASN	GLU	conflict	UNP E5RWD1
L	184	LEU	ARG	conflict	UNP E5RWD1

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



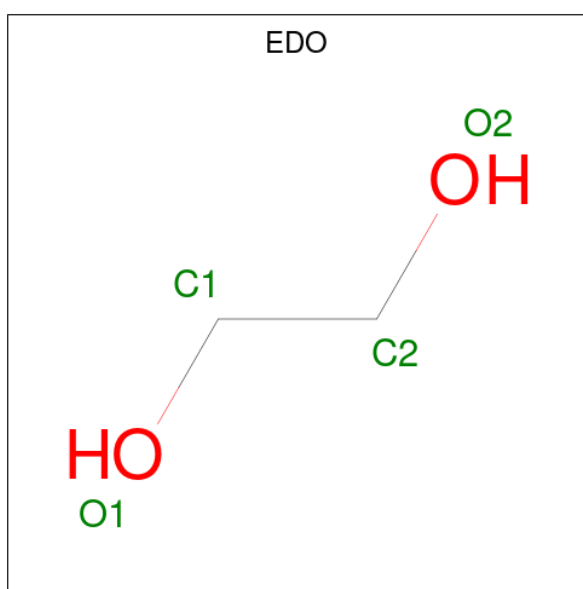
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			7	4	3		
2	F	1	Total	C	O	0	0
			7	4	3		
2	G	1	Total	C	O	0	0
			7	4	3		
2	G	1	Total	C	O	0	0
			7	4	3		
2	H	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	C	O	0	0
			7	4	3		
2	I	1	Total	C	O	0	0
			7	4	3		
2	I	1	Total	C	O	0	0
			7	4	3		
2	K	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



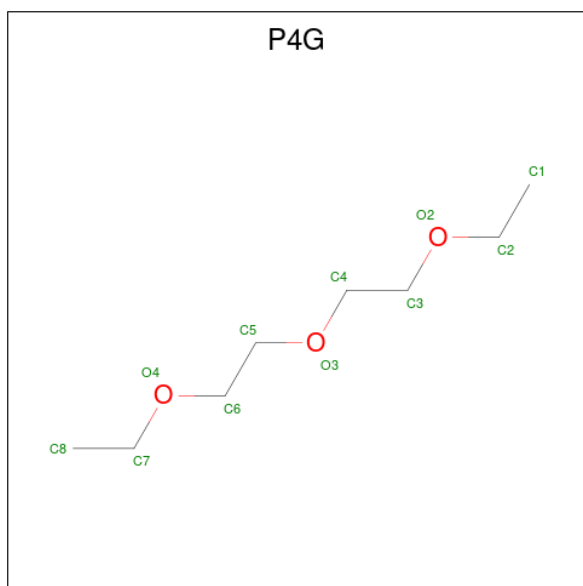
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	L	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 1-ETHOXY-2-(2-ETHOXYETHOXY)ETHANE (CCD ID: P4G) (formula: $C_8H_{18}O_3$).



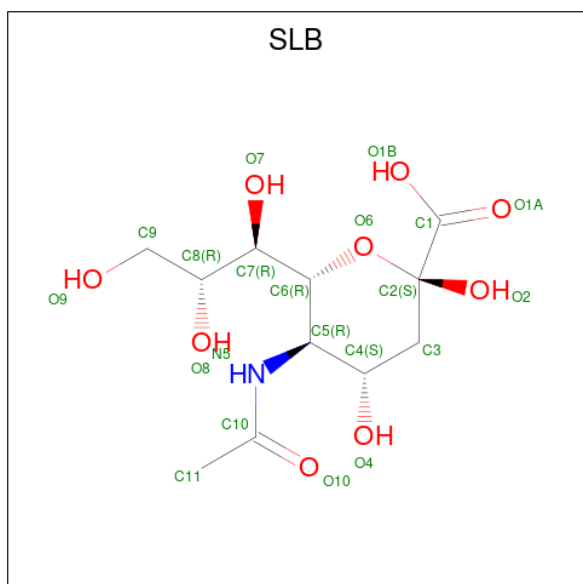
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			11	8	3		
4	B	1	Total	C	O	0	0
			11	8	3		
4	C	1	Total	C	O	0	0
			11	8	3		
4	C	1	Total	C	O	0	0
			11	8	3		
4	F	1	Total	C	O	0	0
			11	8	3		
4	G	1	Total	C	O	0	0
			11	8	3		
4	G	1	Total	C	O	0	0
			11	8	3		

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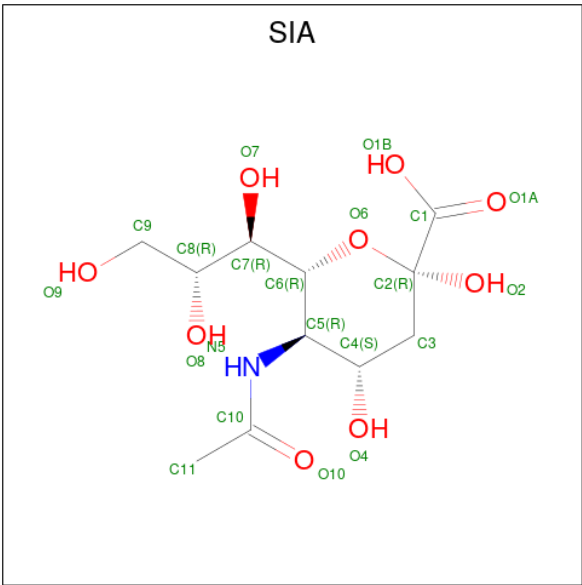
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	I	1	Total	C	O	0	0
			11	8	3		
4	K	1	Total	C	O	0	0
			11	8	3		
4	L	1	Total	C	O	0	0
			11	8	3		
4	L	1	Total	C	O	0	0
			11	8	3		

- Molecule 5 is N-acetyl-beta-neuraminic acid (CCD ID: SLB) (formula: $C_{11}H_{19}NO_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	F	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 6 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	165	Total	O	0	0
			165	165		
7	B	161	Total	O	0	0
			161	161		
7	C	159	Total	O	0	0
			159	159		
7	D	124	Total	O	0	0
			124	124		
7	E	138	Total	O	0	0
			138	138		
7	F	111	Total	O	0	0
			111	111		
7	G	94	Total	O	0	0
			94	94		
7	H	149	Total	O	0	0
			149	149		
7	I	156	Total	O	0	0
			156	156		
7	J	111	Total	O	0	0
			111	111		
7	K	122	Total	O	0	0
			122	122		

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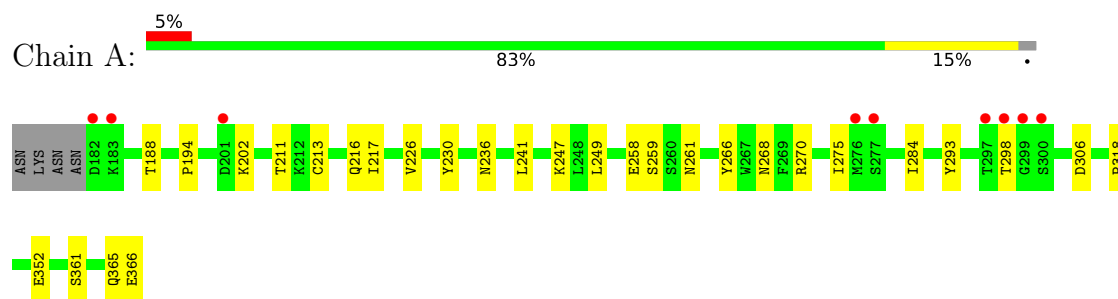
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	52	Total	O	0	0
			52	52		

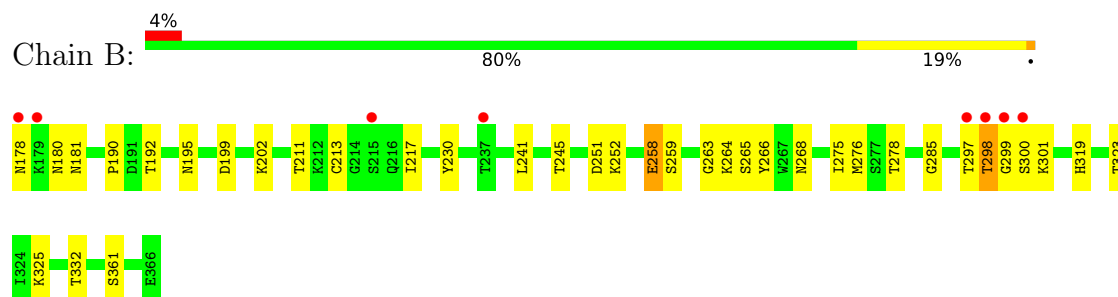
3 Residue-property plots [i](#)

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.

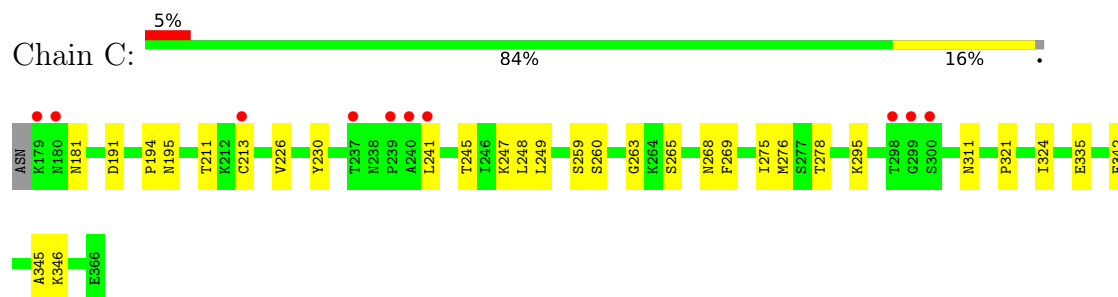
- Molecule 1: Fiber protein



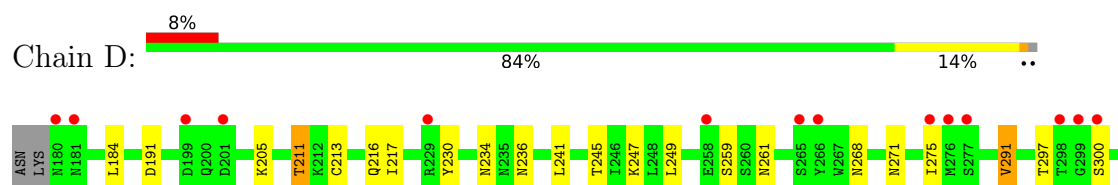
- Molecule 1: Fiber protein



- Molecule 1: Fiber protein

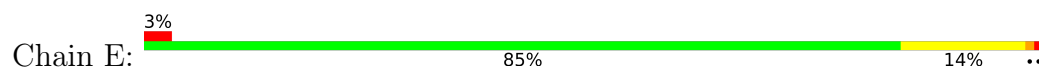


- Molecule 1: Fiber protein

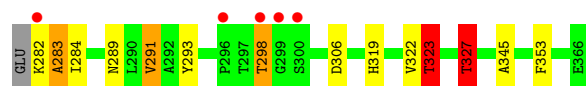
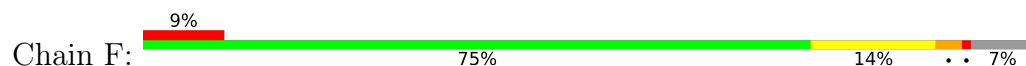




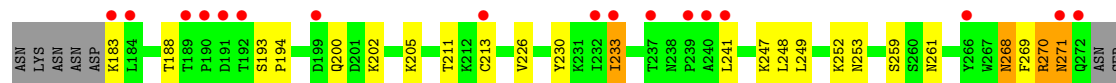
- Molecule 1: Fiber protein



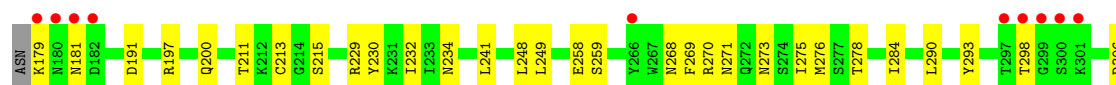
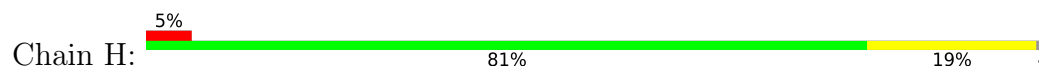
- Molecule 1: Fiber protein



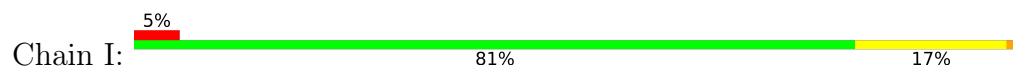
- Molecule 1: Fiber protein



- Molecule 1: Fiber protein

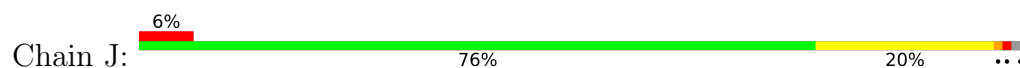


- Molecule 1: Fiber protein

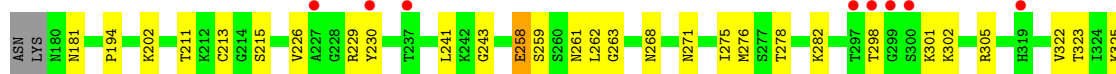
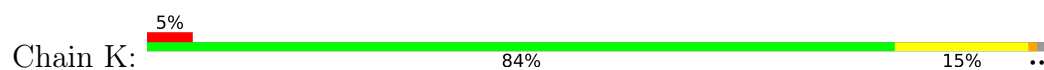




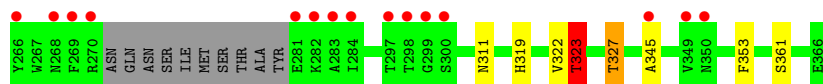
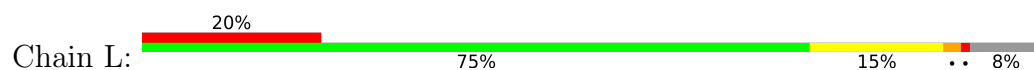
- Molecule 1: Fiber protein



- Molecule 1: Fiber protein



- Molecule 1: Fiber protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	93.56Å 60.41Å 243.69Å 90.00° 99.88° 90.00°	Depositor
Resolution (Å)	92.17 – 1.77 92.17 – 1.77	Depositor EDS
% Data completeness (in resolution range)	98.7 (92.17-1.77) 98.7 (92.17-1.77)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.208 , 0.228 (Not available) , 0.198	Depositor DCC
R_{free} test set	12951 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19866	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P4G, EDO, SIA, PEG, SLB

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	1.05	2/1543 (0.1%)	1.18	2/2093 (0.1%)
1	B	1.02	4/1580 (0.3%)	1.17	3/2140 (0.1%)
1	C	0.97	1/1573 (0.1%)	1.15	1/2134 (0.0%)
1	D	0.94	0/1536	1.16	1/2084 (0.0%)
1	E	0.94	0/1570	1.19	5/2128 (0.2%)
1	F	0.95	0/1450	1.21	5/1965 (0.3%)
1	G	0.94	0/1467	1.20	3/1988 (0.2%)
1	H	1.01	0/1568	1.16	3/2125 (0.1%)
1	I	1.01	3/1608 (0.2%)	1.20	3/2178 (0.1%)
1	J	0.95	1/1534 (0.1%)	1.22	7/2079 (0.3%)
1	K	0.95	0/1553	1.10	2/2106 (0.1%)
1	L	0.91	0/1416	1.19	4/1919 (0.2%)
All	All	0.97	11/18398 (0.1%)	1.18	39/24939 (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	C	0	1
1	F	0	1
1	G	0	1
1	L	0	1
All	All	0	4

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	ARG	NE-CZ	6.72	1.40	1.33
1	I	190	PRO	C-O	-5.75	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	299	GLY	C-O	5.75	1.30	1.24
1	I	296	PRO	C-O	-5.54	1.16	1.24
1	I	201	ASP	CG-OD2	5.44	1.35	1.25

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	201	ASP	CA-CB-CG	-9.80	102.80	112.60
1	F	271	ASN	CA-CB-CG	6.93	119.53	112.60
1	F	323	THR	CB-CA-C	6.92	121.12	109.84
1	B	297	THR	CA-C-O	-6.74	113.23	121.11
1	L	323	THR	CB-CA-C	6.61	120.61	109.84

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	345	ALA	Mainchain
1	F	345	ALA	Mainchain
1	G	345	ALA	Mainchain
1	L	345	ALA	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1509	0	1502	25	0
1	B	1545	0	1536	45	0
1	C	1539	0	1527	29	0
1	D	1501	0	1482	31	0
1	E	1535	0	1515	33	0
1	F	1418	0	1413	44	0
1	G	1434	0	1432	53	0
1	H	1534	0	1522	39	0
1	I	1574	0	1565	41	0
1	J	1500	0	1494	37	0
1	K	1518	0	1496	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1384	0	1384	29	0
2	A	7	0	10	0	0
2	B	35	0	50	19	0
2	C	7	0	10	5	0
2	E	21	0	30	2	0
2	F	7	0	10	1	0
2	G	14	0	20	11	0
2	H	14	0	20	7	0
2	I	14	0	20	2	0
2	K	7	0	10	3	0
3	B	12	0	18	9	0
3	E	4	0	6	0	0
3	F	4	0	6	3	0
3	G	12	0	18	4	0
3	H	4	0	6	0	0
3	I	4	0	6	0	0
3	L	4	0	6	3	0
4	B	22	0	36	0	0
4	C	22	0	36	2	0
4	F	11	0	18	0	0
4	G	22	0	36	5	0
4	I	11	0	18	1	0
4	K	11	0	18	4	0
4	L	22	0	36	3	0
5	F	21	0	18	0	0
6	L	21	0	18	1	0
7	A	165	0	0	2	0
7	B	161	0	0	5	0
7	C	159	0	0	3	0
7	D	124	0	0	2	0
7	E	138	0	0	5	0
7	F	111	0	0	8	0
7	G	94	0	0	5	0
7	H	149	0	0	3	0
7	I	156	0	0	3	0
7	J	111	0	0	7	0
7	K	122	0	0	3	0
7	L	52	0	0	4	0
All	All	19866	0	18348	385	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 10.

The worst 5 of 385 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:G:211:THR:HG21	1:H:213[A]:CYS:O	1.47	1.13
1:D:211:THR:HG23	1:E:216:GLN:HE21	1.12	1.09
1:L:233:ILE:HD11	1:L:353:PHE:HD2	1.15	1.09
1:G:211:THR:HG21	1:H:213[B]:CYS:O	1.49	1.06
1:K:258[A]:GLU:CD	1:K:258[A]:GLU:H	1.63	1.02

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	188/189 (100%)	183 (97%)	5 (3%)	0	100	100
1	B	192/189 (102%)	187 (97%)	5 (3%)	0	100	100
1	C	192/189 (102%)	184 (96%)	8 (4%)	0	100	100
1	D	187/189 (99%)	181 (97%)	6 (3%)	0	100	100
1	E	191/189 (101%)	185 (97%)	6 (3%)	0	100	100
1	F	174/189 (92%)	172 (99%)	1 (1%)	1 (1%)	21	9
1	G	176/189 (93%)	171 (97%)	5 (3%)	0	100	100
1	H	191/189 (101%)	185 (97%)	6 (3%)	0	100	100
1	I	196/189 (104%)	190 (97%)	6 (3%)	0	100	100
1	J	187/189 (99%)	179 (96%)	8 (4%)	0	100	100
1	K	189/189 (100%)	180 (95%)	9 (5%)	0	100	100
1	L	170/189 (90%)	166 (98%)	3 (2%)	1 (1%)	21	9
All	All	2233/2268 (98%)	2163 (97%)	68 (3%)	2 (0%)	48	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	191	ASP
1	F	189	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	10/169 (6%)	10 (100%)	0	100	100
1	D	132/169 (78%)	129 (98%)	3 (2%)	44	25
1	E	173/169 (102%)	168 (97%)	5 (3%)	37	16
1	F	159/169 (94%)	149 (94%)	10 (6%)	16	3
1	G	160/169 (95%)	150 (94%)	10 (6%)	16	3
1	H	173/169 (102%)	169 (98%)	4 (2%)	44	25
1	I	178/169 (105%)	172 (97%)	6 (3%)	32	12
1	J	169/169 (100%)	162 (96%)	7 (4%)	27	8
1	K	171/169 (101%)	166 (97%)	5 (3%)	37	16
1	L	155/169 (92%)	147 (95%)	8 (5%)	21	4
All	All	1480/1690 (88%)	1422 (96%)	58 (4%)	29	8

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	179	LYS
1	L	322	VAL
1	I	322	VAL
1	L	252	LYS
1	K	322	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	271	ASN
1	L	311	ASN

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Mol	Chain	Res	Type
1	I	271	ASN
1	K	320	GLN
1	I	178	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

42 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PEG	E	404	-	6,6,6	0.30	0	5,5,5	0.18	0
3	EDO	F	401	-	3,3,3	0.15	0	2,2,2	0.31	0
3	EDO	H	401	-	3,3,3	0.27	0	2,2,2	0.25	0
2	PEG	K	401	-	6,6,6	0.25	0	5,5,5	0.14	0
3	EDO	E	401	-	3,3,3	0.35	0	2,2,2	0.30	0
2	PEG	B	407	-	6,6,6	0.19	0	5,5,5	0.25	0
4	P4G	K	402	-	10,10,10	0.37	0	9,9,9	0.20	0
4	P4G	B	409	-	10,10,10	0.19	0	9,9,9	0.13	0
2	PEG	B	404	-	6,6,6	0.26	0	5,5,5	0.14	0
2	PEG	G	404	-	6,6,6	0.16	0	5,5,5	0.10	0
2	PEG	H	402	-	6,6,6	0.18	0	5,5,5	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	G	402	-	3,3,3	0.11	0	2,2,2	0.16	0
2	PEG	A	401	-	6,6,6	0.16	0	5,5,5	0.04	0
2	PEG	B	408	-	6,6,6	0.42	0	5,5,5	0.31	0
3	EDO	L	401	-	3,3,3	0.11	0	2,2,2	0.23	0
2	PEG	F	402	-	6,6,6	0.17	0	5,5,5	0.20	0
2	PEG	C	401	-	6,6,6	0.21	0	5,5,5	0.26	0
3	EDO	G	403	-	3,3,3	0.17	0	2,2,2	0.30	0
3	EDO	I	401	-	3,3,3	0.12	0	2,2,2	0.14	0
4	P4G	B	410	-	10,10,10	0.29	0	9,9,9	0.09	0
4	P4G	F	403	-	10,10,10	0.33	0	9,9,9	0.19	0
5	SLB	F	404	-	21,21,21	0.86	1 (4%)	24,31,31	0.94	1 (4%)
3	EDO	B	402	-	3,3,3	0.13	0	2,2,2	0.23	0
4	P4G	C	402	-	10,10,10	0.30	0	9,9,9	0.10	0
4	P4G	G	407	-	10,10,10	0.32	0	9,9,9	0.25	0
6	SIA	L	404	-	21,21,21	0.88	1 (4%)	24,31,31	0.99	1 (4%)
2	PEG	I	402	-	6,6,6	0.30	0	5,5,5	0.13	0
4	P4G	C	403	-	10,10,10	0.23	0	9,9,9	0.09	0
2	PEG	G	405	-	6,6,6	0.63	0	5,5,5	0.35	0
3	EDO	B	403	-	3,3,3	0.21	0	2,2,2	0.43	0
4	P4G	G	406	-	10,10,10	0.22	0	9,9,9	0.21	0
2	PEG	H	403	-	6,6,6	0.38	0	5,5,5	0.25	0
4	P4G	L	402	-	10,10,10	0.23	0	9,9,9	0.13	0
2	PEG	B	405	-	6,6,6	0.20	0	5,5,5	0.09	0
2	PEG	I	403	-	6,6,6	0.26	0	5,5,5	0.09	0
3	EDO	G	401	-	3,3,3	0.14	0	2,2,2	0.02	0
2	PEG	E	402	-	6,6,6	0.26	0	5,5,5	0.11	0
2	PEG	E	403	-	6,6,6	0.17	0	5,5,5	0.11	0
4	P4G	I	404	-	10,10,10	0.44	0	9,9,9	0.21	0
2	PEG	B	406	-	6,6,6	0.25	0	5,5,5	0.18	0
3	EDO	B	401	-	3,3,3	0.35	0	2,2,2	0.18	0
4	P4G	L	403	-	10,10,10	0.31	0	9,9,9	0.14	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	E	404	-	-	1/4/4/4	-
3	EDO	F	401	-	-	0/1/1/1	-
3	EDO	H	401	-	-	1/1/1/1	-
2	PEG	K	401	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	E	401	-	-	1/1/1/1	-
2	PEG	B	407	-	-	3/4/4/4	-
4	P4G	K	402	-	-	6/8/8/8	-
4	P4G	B	409	-	-	4/8/8/8	-
2	PEG	B	404	-	-	3/4/4/4	-
2	PEG	G	404	-	-	3/4/4/4	-
2	PEG	H	402	-	-	2/4/4/4	-
3	EDO	G	402	-	-	0/1/1/1	-
2	PEG	A	401	-	-	2/4/4/4	-
2	PEG	B	408	-	-	4/4/4/4	-
3	EDO	L	401	-	-	1/1/1/1	-
2	PEG	F	402	-	-	1/4/4/4	-
2	PEG	C	401	-	-	2/4/4/4	-
3	EDO	G	403	-	-	1/1/1/1	-
3	EDO	I	401	-	-	1/1/1/1	-
4	P4G	B	410	-	-	0/8/8/8	-
4	P4G	F	403	-	-	5/8/8/8	-
5	SLB	F	404	-	-	9/20/38/38	0/1/1/1
3	EDO	B	402	-	-	0/1/1/1	-
4	P4G	C	402	-	-	3/8/8/8	-
4	P4G	G	407	-	-	6/8/8/8	-
6	SIA	L	404	-	-	5/20/38/38	0/1/1/1
2	PEG	I	402	-	-	3/4/4/4	-
4	P4G	C	403	-	-	2/8/8/8	-
2	PEG	G	405	-	-	2/4/4/4	-
3	EDO	B	403	-	-	1/1/1/1	-
4	P4G	G	406	-	-	2/8/8/8	-
2	PEG	H	403	-	-	3/4/4/4	-
4	P4G	L	402	-	-	2/8/8/8	-
2	PEG	B	405	-	-	3/4/4/4	-
2	PEG	I	403	-	-	2/4/4/4	-
3	EDO	G	401	-	-	1/1/1/1	-
2	PEG	E	402	-	-	2/4/4/4	-
2	PEG	E	403	-	-	3/4/4/4	-
4	P4G	I	404	-	-	4/8/8/8	-
2	PEG	B	406	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	401	-	-	1/1/1/1	-
4	P4G	L	403	-	-	0/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	404	SLB	O1B-C1	-2.50	1.21	1.30
6	L	404	SIA	O1B-C1	-2.28	1.22	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	404	SIA	O1A-C1-C2	-2.70	119.34	123.85
5	F	404	SLB	O2-C2-C1	-2.31	105.84	110.73

There are no chirality outliers.

5 of 100 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	404	SLB	C5-C6-C7-C8
5	F	404	SLB	C5-C6-C7-O7
5	F	404	SLB	O6-C6-C7-C8
5	F	404	SLB	O6-C6-C7-O7
5	F	404	SLB	C7-C8-C9-O9

There are no ring outliers.

27 monomers are involved in 83 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	404	PEG	2	0
3	F	401	EDO	3	0
2	K	401	PEG	3	0
2	B	407	PEG	6	0
4	K	402	P4G	4	0
2	B	404	PEG	1	0
2	G	404	PEG	7	0
2	H	402	PEG	4	0
2	B	408	PEG	12	0
3	L	401	EDO	3	0
2	F	402	PEG	1	0
2	C	401	PEG	5	0

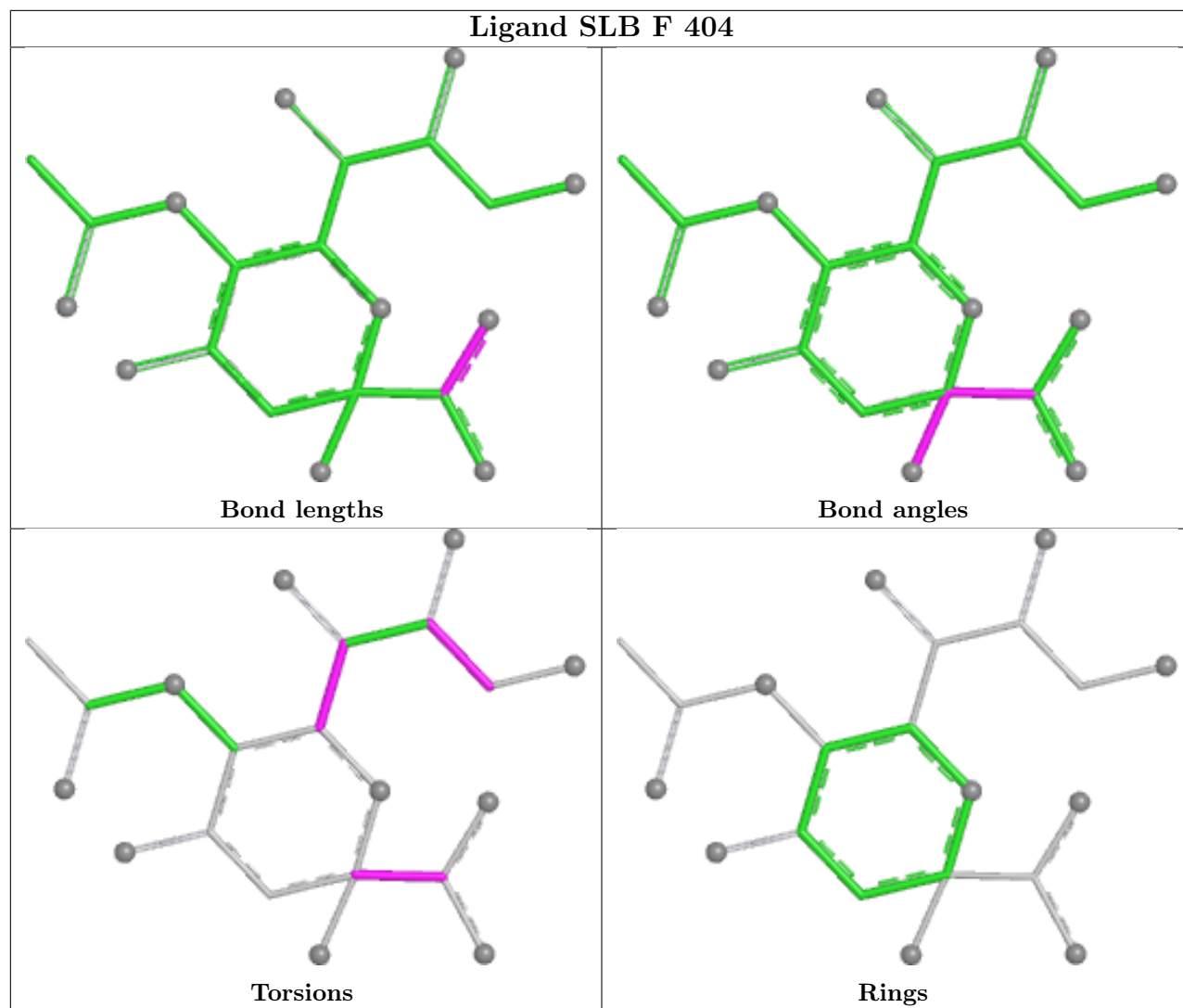
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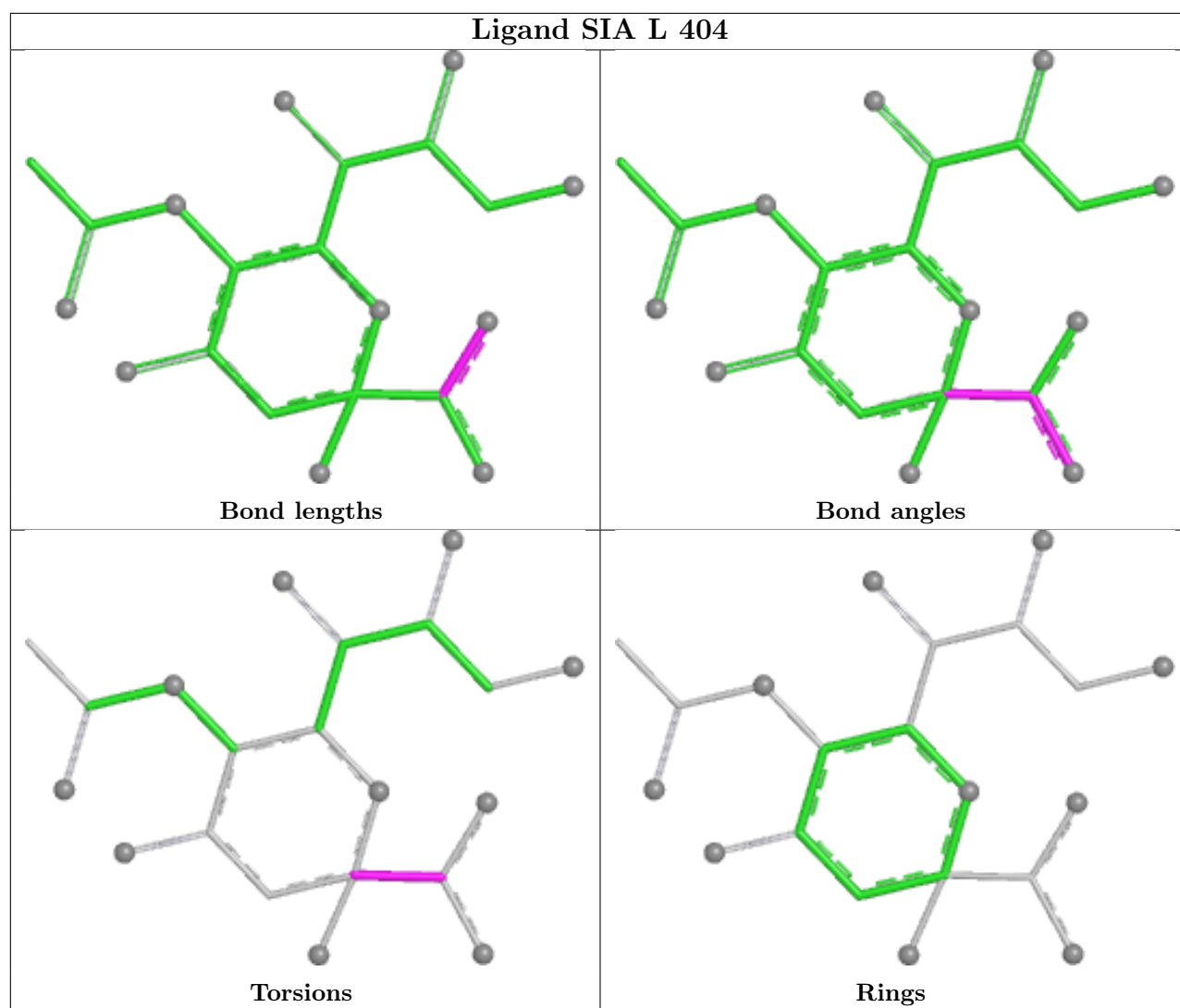
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	403	EDO	4	0
3	B	402	EDO	2	0
4	C	402	P4G	1	0
4	G	407	P4G	2	0
6	L	404	SIA	1	0
2	I	402	PEG	2	0
4	C	403	P4G	1	0
2	G	405	PEG	4	0
3	B	403	EDO	1	0
4	G	406	P4G	3	0
2	H	403	PEG	3	0
4	L	402	P4G	3	0
2	B	405	PEG	1	0
4	I	404	P4G	1	0
3	B	401	EDO	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SLB F 404





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	185/189 (97%)	0.05	9 (4%) 35 41	8, 19, 34, 75	5 (2%)
1	B	189/189 (100%)	-0.00	8 (4%) 40 47	11, 19, 34, 75	5 (2%)
1	C	188/189 (99%)	0.20	10 (5%) 32 38	8, 22, 50, 70	6 (3%)
1	D	187/189 (98%)	0.50	15 (8%) 18 21	13, 28, 47, 73	2 (1%)
1	E	189/189 (100%)	0.21	6 (3%) 50 57	14, 26, 41, 68	4 (2%)
1	F	175/189 (92%)	0.60	17 (9%) 13 15	15, 30, 48, 76	3 (1%)
1	G	178/189 (94%)	0.92	30 (16%) 4 4	9, 31, 61, 85	2 (1%)
1	H	188/189 (99%)	0.14	10 (5%) 32 38	8, 22, 44, 93	5 (2%)
1	I	189/189 (100%)	-0.03	9 (4%) 35 41	7, 20, 36, 66	9 (4%)
1	J	185/189 (97%)	0.52	12 (6%) 25 30	13, 29, 44, 78	4 (2%)
1	K	187/189 (98%)	0.39	9 (4%) 35 41	16, 28, 43, 59	4 (2%)
1	L	174/189 (92%)	1.28	38 (21%) 2 2	25, 41, 68, 83	0
All	All	2214/2268 (97%)	0.39	173 (7%) 19 22	7, 26, 52, 93	49 (2%)

The worst 5 of 173 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	280	TYR	5.9
1	G	279	ALA	5.3
1	L	298	THR	5.1
1	H	297	THR	4.8
1	A	299	GLY	4.6

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	G	402	4/4	0.52	0.30	67,70,71,74	0
4	P4G	L	402	11/11	0.66	0.31	56,66,76,77	0
4	P4G	B	409	11/11	0.69	0.33	66,73,78,79	0
4	P4G	K	402	11/11	0.69	0.26	38,52,60,60	0
2	PEG	B	404	7/7	0.69	0.23	15,16,19,19	7
4	P4G	F	403	11/11	0.70	0.21	38,41,43,44	0
2	PEG	K	401	7/7	0.71	0.26	63,69,74,75	0
4	P4G	I	404	11/11	0.73	0.22	43,47,54,56	0
2	PEG	I	403	7/7	0.73	0.20	42,54,60,61	0
3	EDO	I	401	4/4	0.73	0.26	59,60,61,64	0
2	PEG	B	406	7/7	0.74	0.21	45,49,54,54	0
5	SLB	F	404	21/21	0.74	0.18	59,64,68,70	0
3	EDO	E	401	4/4	0.76	0.22	48,52,52,56	0
4	P4G	G	407	11/11	0.76	0.20	36,41,47,49	0
2	PEG	H	402	7/7	0.76	0.24	47,48,53,56	0
4	P4G	L	403	11/11	0.77	0.20	46,48,54,55	0
4	P4G	G	406	11/11	0.78	0.20	45,51,53,55	0
6	SIA	L	404	21/21	0.78	0.15	55,65,68,69	0
2	PEG	E	403	7/7	0.80	0.19	45,49,59,66	0
2	PEG	I	402	7/7	0.80	0.17	34,37,49,50	0
4	P4G	B	410	11/11	0.80	0.20	47,50,53,53	0
2	PEG	G	405	7/7	0.80	0.15	5,5,7,8	7
2	PEG	F	402	7/7	0.81	0.20	47,49,56,56	0
2	PEG	B	405	7/7	0.81	0.21	54,57,59,59	0
2	PEG	E	402	7/7	0.83	0.17	50,56,56,56	0
3	EDO	H	401	4/4	0.83	0.17	44,50,50,55	0
4	P4G	C	403	11/11	0.84	0.14	28,32,38,38	0
2	PEG	H	403	7/7	0.85	0.15	36,39,40,44	0
4	P4G	C	402	11/11	0.85	0.19	41,54,66,68	0
2	PEG	B	407	7/7	0.85	0.15	32,32,40,46	0
2	PEG	G	404	7/7	0.85	0.17	18,20,20,21	7
3	EDO	G	401	4/4	0.86	0.17	39,41,41,43	0

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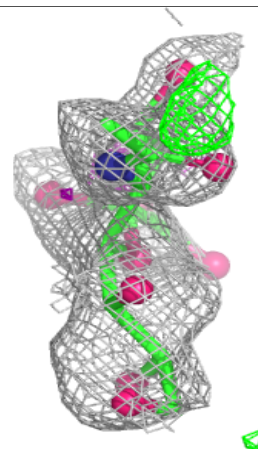
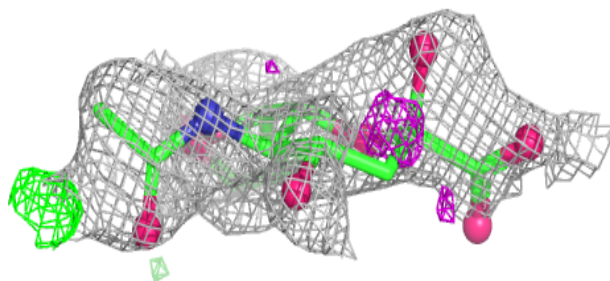
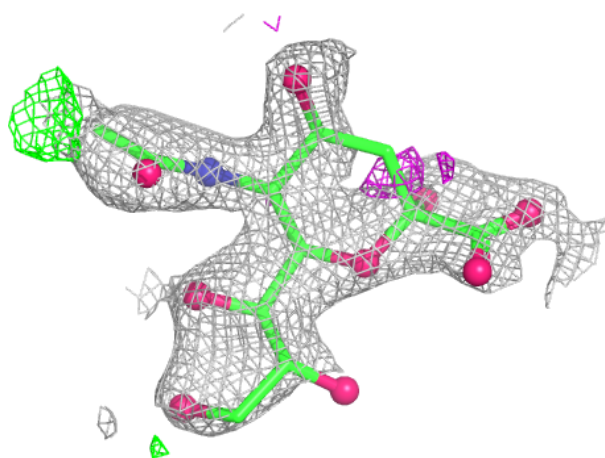
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PEG	E	404	7/7	0.87	0.13	37,38,41,43	0
2	PEG	B	408	7/7	0.88	0.12	26,29,33,36	0
3	EDO	L	401	4/4	0.89	0.17	34,42,44,47	0
2	PEG	A	401	7/7	0.90	0.13	44,46,49,52	0
2	PEG	C	401	7/7	0.90	0.12	25,29,36,44	0
3	EDO	F	401	4/4	0.90	0.16	28,32,37,43	0
3	EDO	B	402	4/4	0.91	0.13	44,45,47,48	0
3	EDO	G	403	4/4	0.93	0.15	24,31,35,40	0
3	EDO	B	401	4/4	0.94	0.16	21,22,22,23	0
3	EDO	B	403	4/4	0.95	0.09	20,21,23,24	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

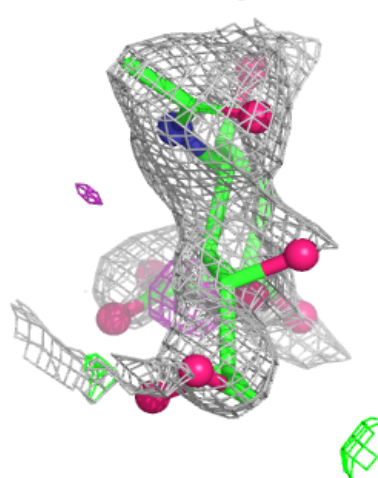
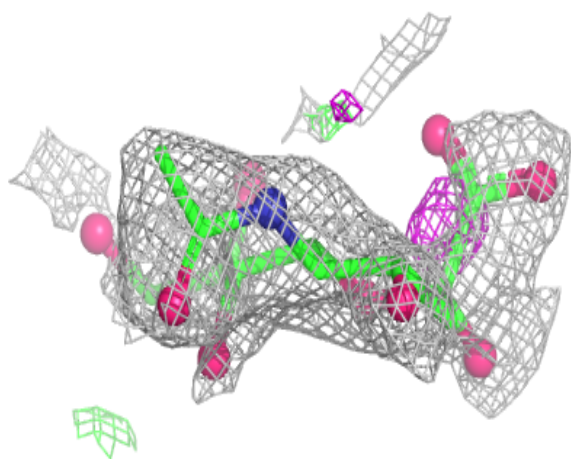
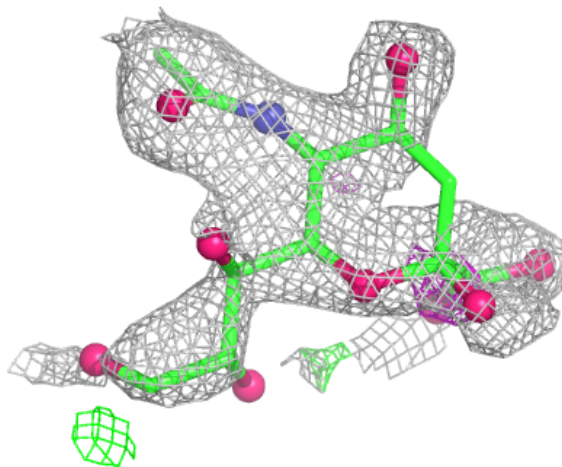
Electron density around SLB F 404:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SIA L 404:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.