



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 22, 2026 – 03:58 PM UTC

PDB ID : 9BIF / pdb_00009bif
Title : Fab B11-OspCA complex
Authors : Rudolph, M.J.; Mantis, N.
Deposited on : 2024-04-23
Resolution : 3.09 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
Xtriage (Phenix) : 2.0
EDS : 3.0
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

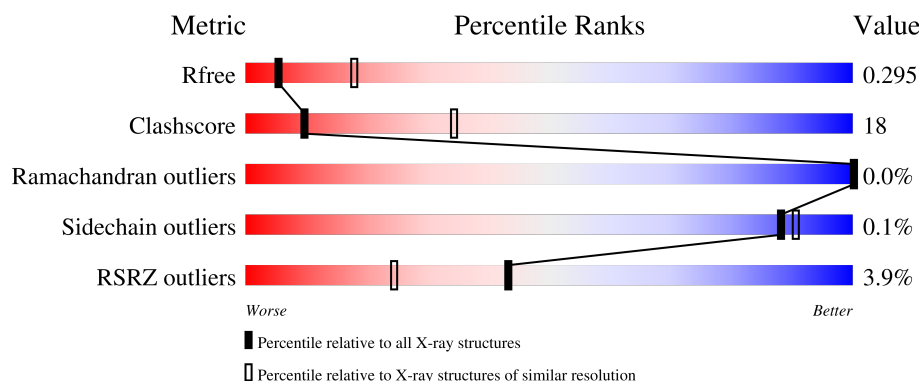
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	C	228	2% 61% 32% • 6%
1	G	228	3% 56% 37% • 5%
1	H	228	4% 55% 37% • 6%
1	J	228	4% 54% 38% • 6%
1	O	228	8% 57% 36% • 6%

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Mol	Chain	Length	Quality of chain
1	Q	228	
1	U	228	
1	W	228	
2	D	215	
2	I	215	
2	K	215	
2	L	215	
2	P	215	
2	R	215	
2	V	215	
2	X	215	
3	A	164	
3	B	164	
3	E	164	
3	F	164	
3	M	164	
3	N	164	
3	S	164	
3	T	164	

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
5	CL	S	302	-	-	X	-
5	CL	W	301	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 35581 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 VH-CH1 domain of B11 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	214	Total	C	N	O	S	0	0	0
			1592	1005	266	315	6			
1	C	215	Total	C	N	O	S	0	0	0
			1604	1014	267	317	6			
1	G	216	Total	C	N	O	S	0	0	0
			1613	1020	269	318	6			
1	J	215	Total	C	N	O	S	0	0	0
			1604	1014	267	317	6			
1	O	215	Total	C	N	O	S	0	0	0
			1604	1014	267	317	6			
1	Q	215	Total	C	N	O	S	0	0	0
			1604	1014	267	317	6			
1	U	213	Total	C	N	O	S	0	0	0
			1586	1002	265	313	6			
1	W	215	Total	C	N	O	S	0	0	0
			1604	1014	267	317	6			

- Molecule 2 is a protein called VH-VL domain of B11 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1656	1034	285	332	5			
2	D	215	Total	C	N	O	S	0	0	0
			1662	1037	286	333	6			
2	I	212	Total	C	N	O	S	0	0	0
			1638	1024	283	326	5			
2	K	214	Total	C	N	O	S	0	0	0
			1656	1034	285	332	5			
2	P	210	Total	C	N	O	S	0	0	0
			1623	1016	278	324	5			
2	R	214	Total	C	N	O	S	0	0	0
			1656	1034	285	332	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	V	211	Total	C	N	O	S	0	0	0
			1634	1022	282	325	5			
2	X	214	Total	C	N	O	S	0	0	0
			1656	1034	285	332	5			

- Molecule 3 is a protein called Outer surface protein C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	155	Total	C	N	O	S	0	0	0
			1161	724	198	237	2			
3	B	157	Total	C	N	O	S	0	0	0
			1174	732	200	240	2			
3	E	158	Total	C	N	O	S	0	0	0
			1182	737	201	242	2			
3	F	154	Total	C	N	O	S	0	0	0
			1154	720	197	235	2			
3	M	154	Total	C	N	O	S	0	0	0
			1154	720	197	235	2			
3	N	158	Total	C	N	O	S	0	0	0
			1183	737	201	243	2			
3	S	157	Total	C	N	O	S	0	0	0
			1177	733	200	242	2			
3	T	156	Total	C	N	O	S	0	0	0
			1170	729	199	240	2			

- Molecule 4 is PRASEODYMIUM ION (CCD ID: PR) (formula: Pr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	1	Total	Pr	0	0
			1	1		
4	D	1	Total	Pr	0	0
			1	1		
4	I	1	Total	Pr	0	0
			1	1		
4	K	1	Total	Pr	0	0
			1	1		
4	P	1	Total	Pr	0	0
			1	1		
4	R	1	Total	Pr	0	0
			1	1		
4	S	1	Total	Pr	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	1	Total 1	Pr 1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Cl 1	0	0
5	O	1	Total 1	Cl 1	0	0
5	S	1	Total 1	Cl 1	0	0
5	T	1	Total 1	Cl 1	0	0
5	W	1	Total 1	Cl 1	0	0
5	X	1	Total 1	Cl 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	10	Total 10	O 10	0	0
6	L	7	Total 7	O 7	0	0
6	A	7	Total 7	O 7	0	0
6	B	10	Total 10	O 10	0	0
6	C	10	Total 10	O 10	0	0
6	D	15	Total 15	O 15	0	0
6	G	11	Total 11	O 11	0	0
6	I	13	Total 13	O 13	0	0
6	E	4	Total 4	O 4	0	0
6	F	6	Total 6	O 6	0	0

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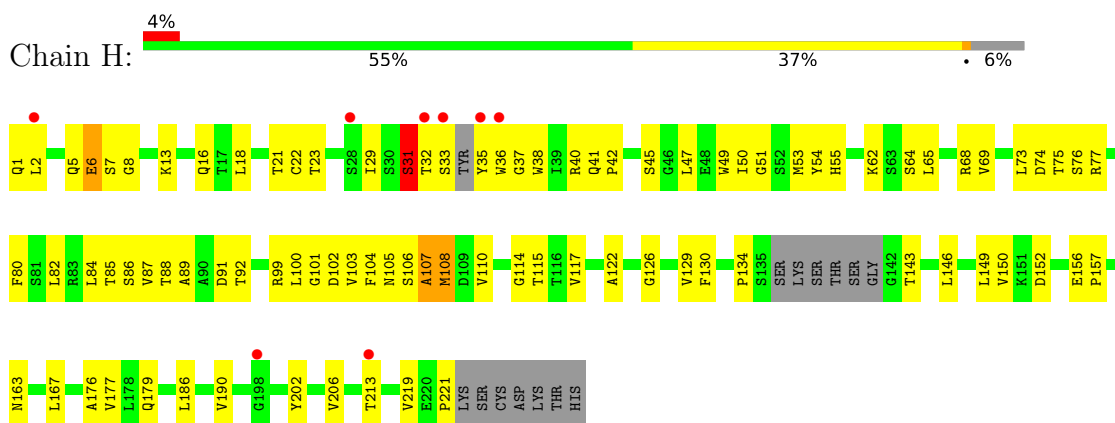
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	8	Total 8	O 8	0	0
6	K	7	Total 7	O 7	0	0
6	O	4	Total 4	O 4	0	0
6	P	2	Total 2	O 2	0	0
6	M	3	Total 3	O 3	0	0
6	N	4	Total 4	O 4	0	0
6	Q	19	Total 19	O 19	0	0
6	R	14	Total 14	O 14	0	0
6	U	4	Total 4	O 4	0	0
6	V	6	Total 6	O 6	0	0
6	S	11	Total 11	O 11	0	0
6	T	7	Total 7	O 7	0	0
6	W	22	Total 22	O 22	0	0
6	X	16	Total 16	O 16	0	0

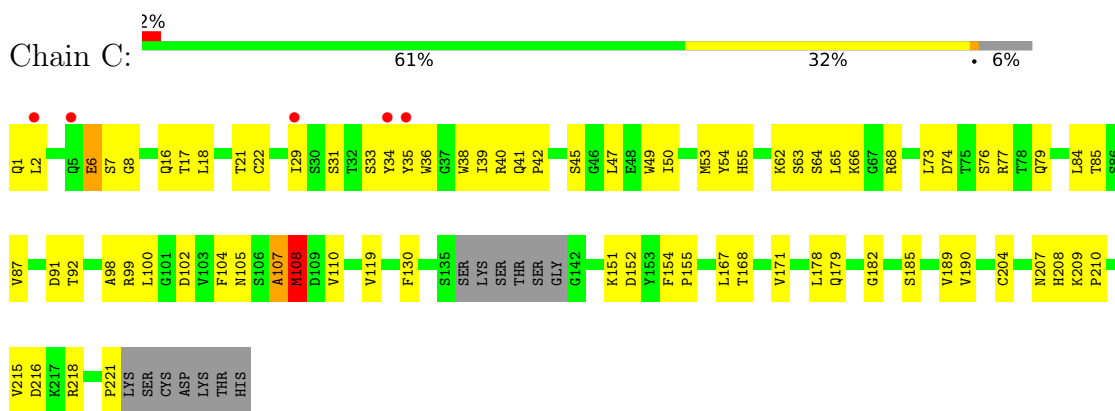
3 Residue-property plots [i](#)

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.

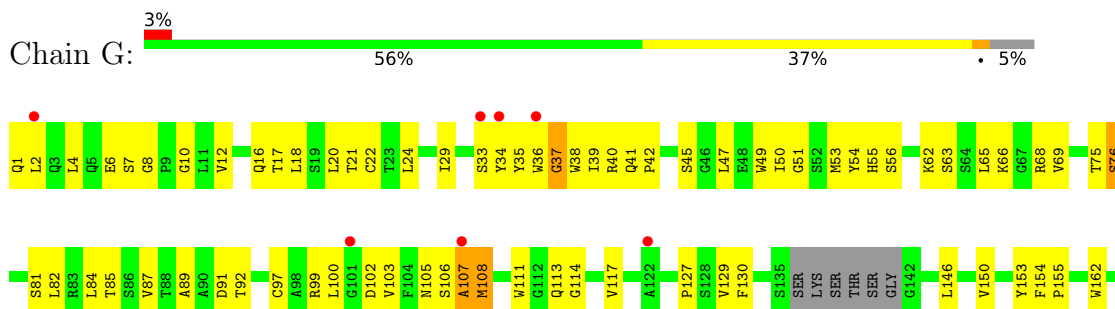
- Molecule 1: VH-CH1 domain of B11 Fab



- Molecule 1: VH-CH1 domain of B11 Fab

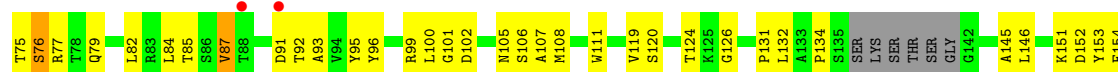
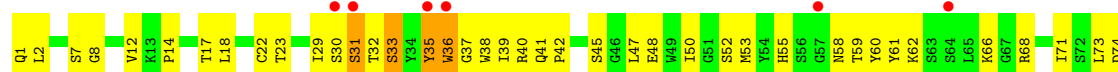


- Molecule 1: VH-CH1 domain of B11 Fab

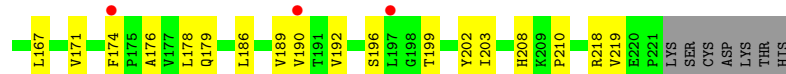
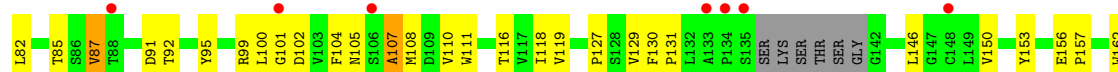
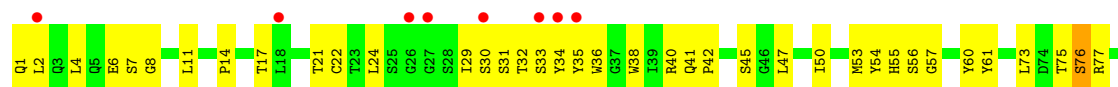




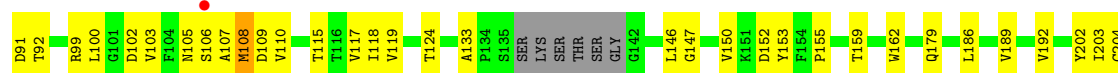
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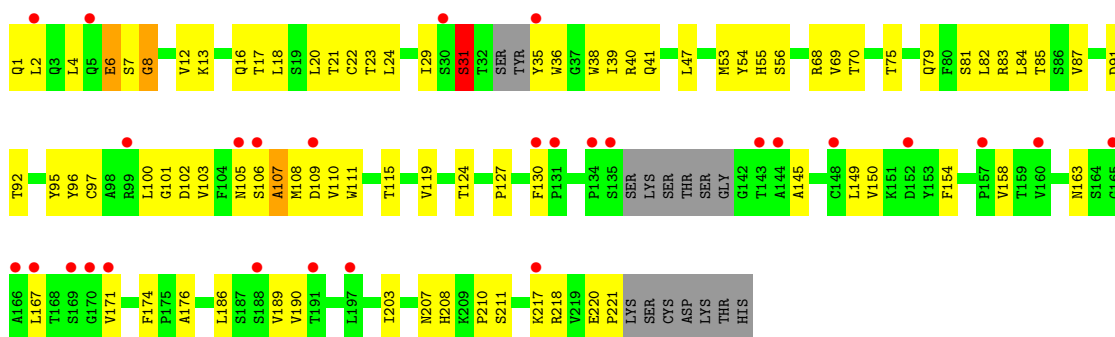


• Molecule 1: VH-CH1 domain of B11 Fab

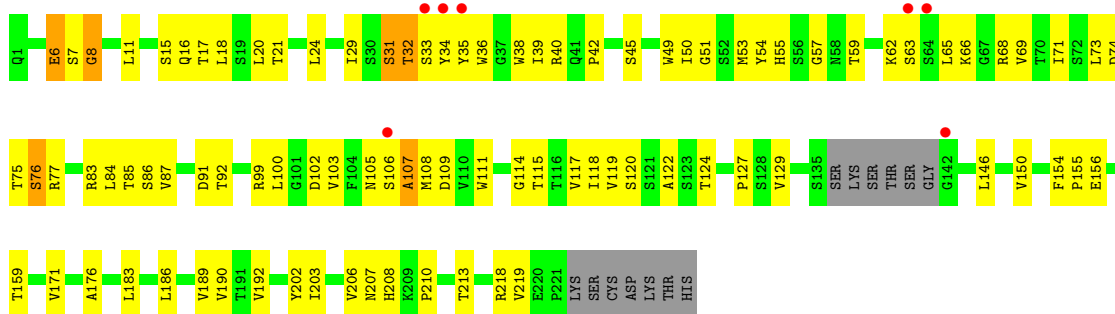


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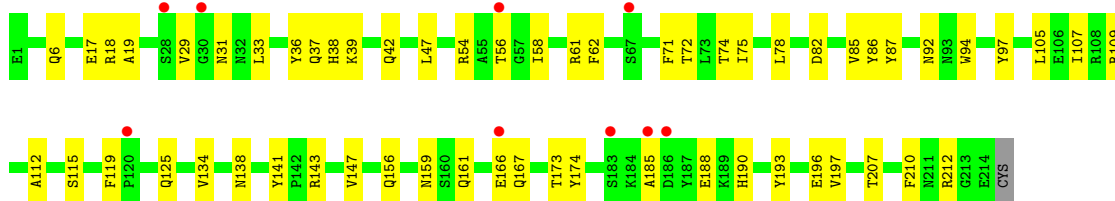
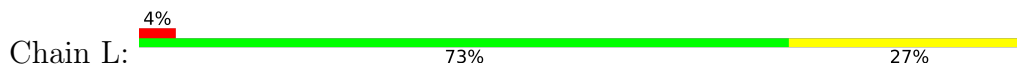




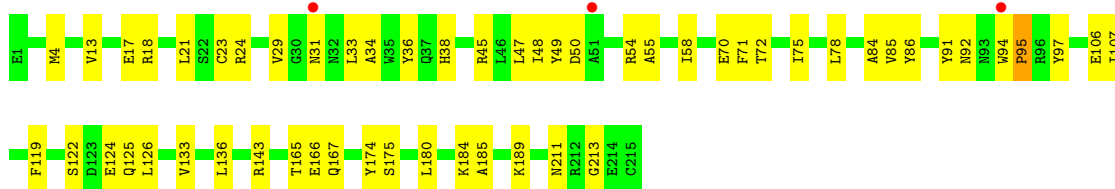
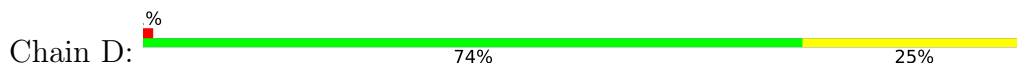
- Molecule 1: VH-CH1 domain of B11 Fab



- Molecule 2: VH-VL domain of B11 Fab

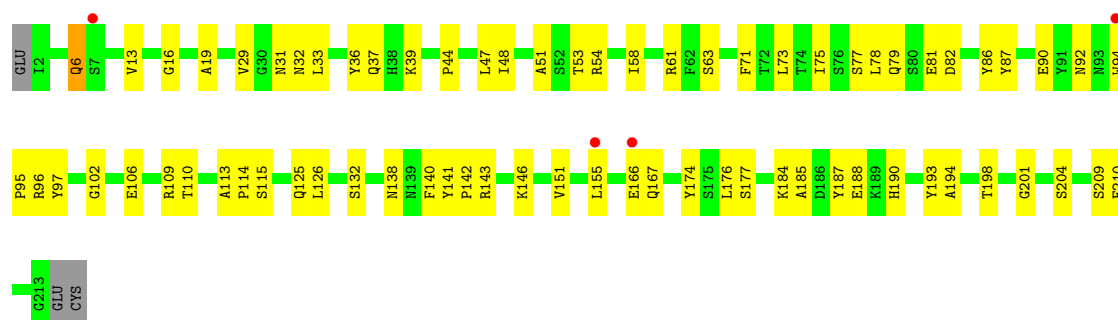


- Molecule 2: VH-VL domain of B11 Fab

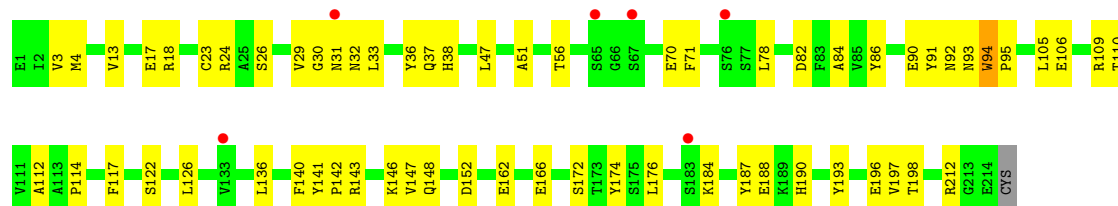


- Molecule 2: VH-VL domain of B11 Fab

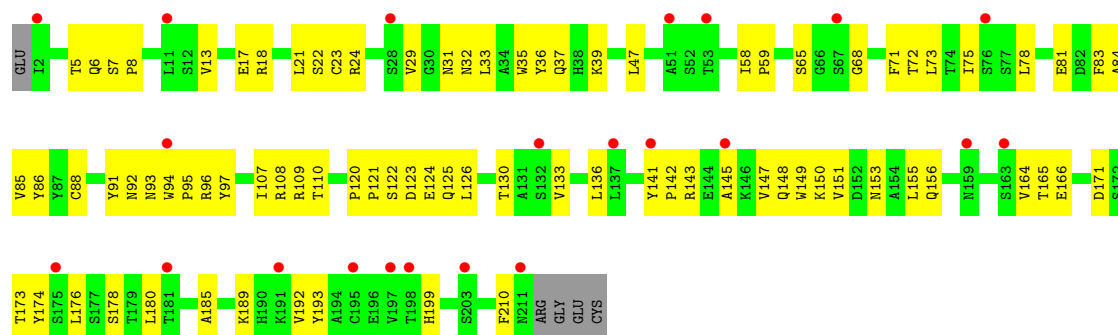




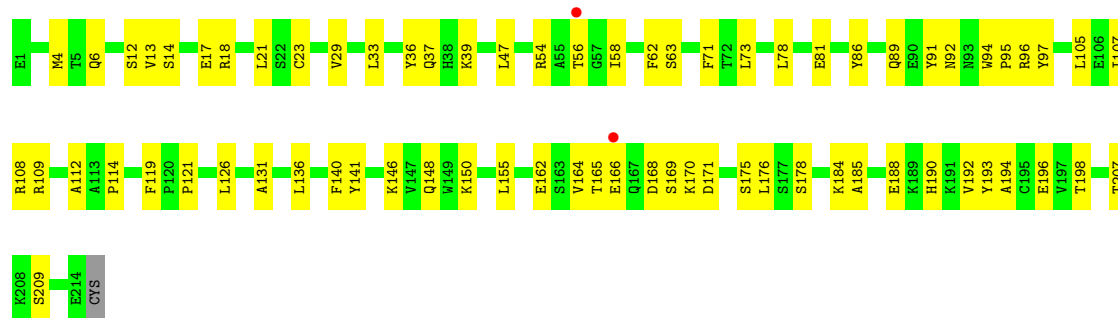
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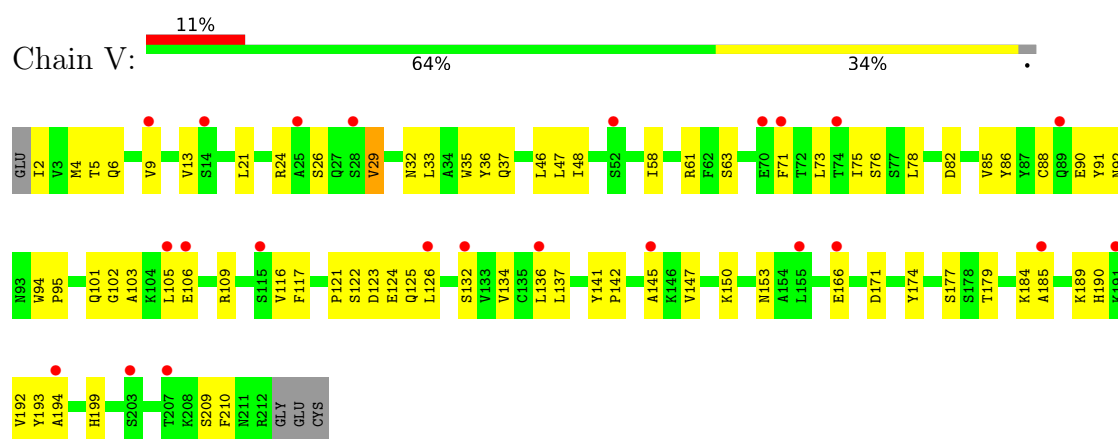
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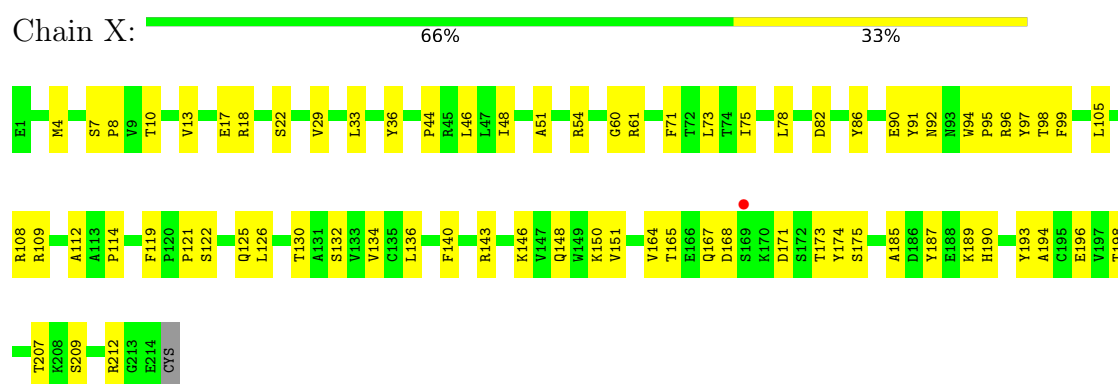
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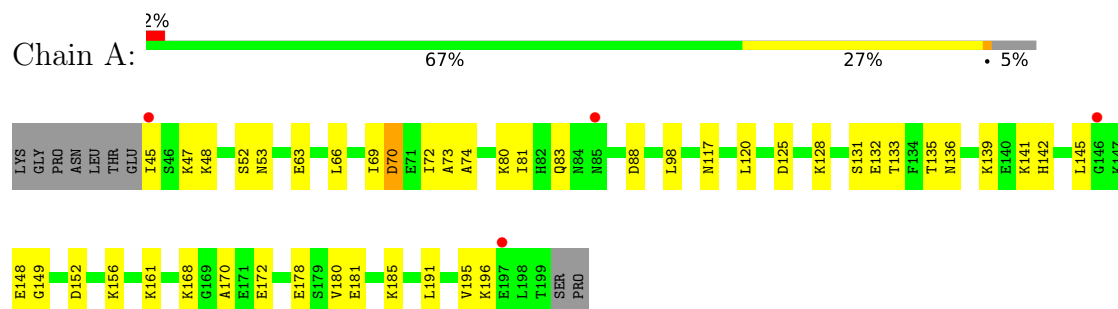
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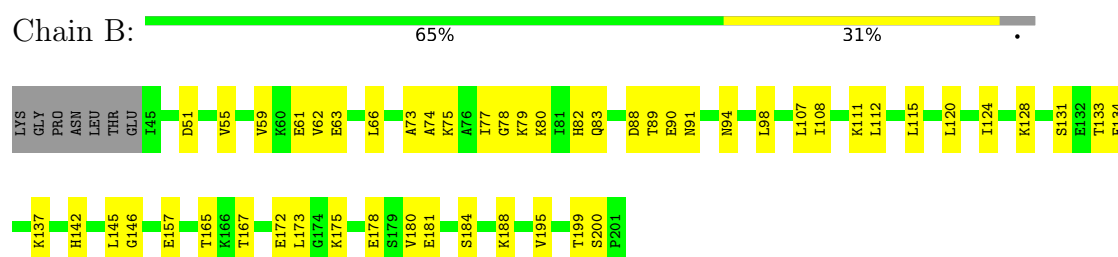
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• Molecule 3: Outer surface protein C

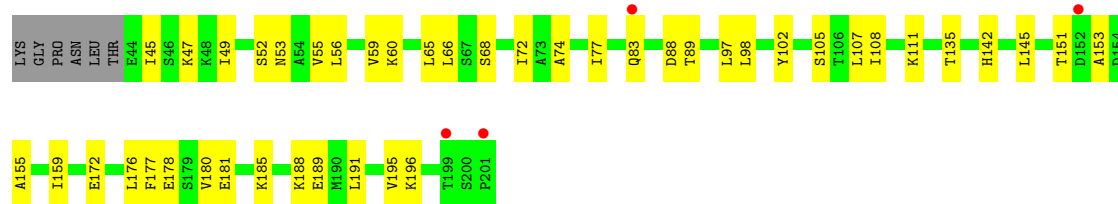


• Molecule 3: Outer surface protein C

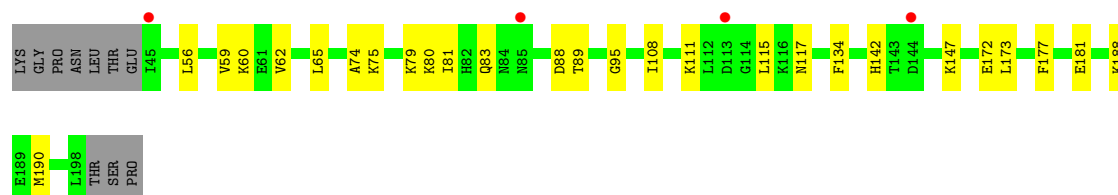
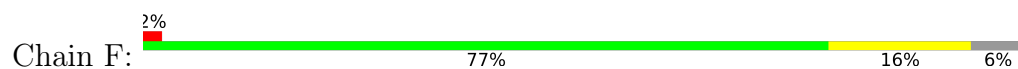


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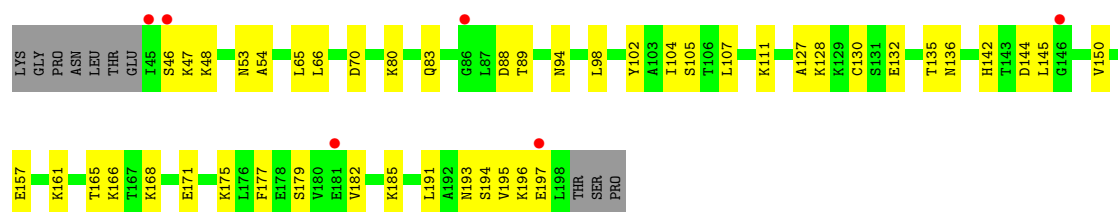




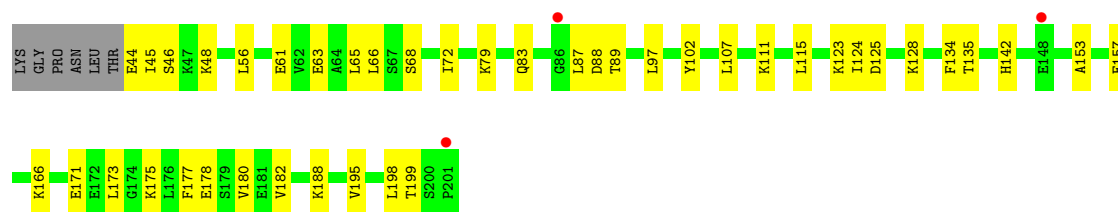
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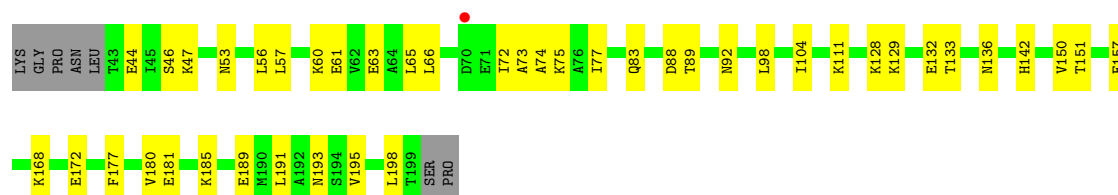
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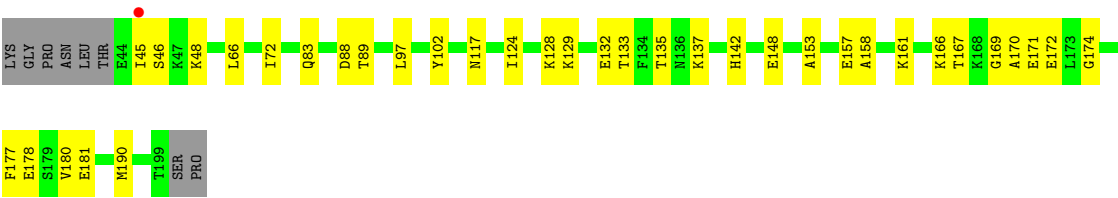
• Molecule 3: Outer surface protein C



• Molecule 3: Outer surface protein C



● Molecule 3: Outer surface protein C



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	96.74Å 97.29Å 168.34Å 97.60° 90.27° 106.21°	Depositor
Resolution (Å)	48.62 – 3.09 48.62 – 3.09	Depositor EDS
% Data completeness (in resolution range)	90.0 (48.62-3.09) 90.0 (48.62-3.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.07Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.240 , 0.295 0.240 , 0.295	Depositor DCC
R_{free} test set	4728 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.672	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	35581	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.12% 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: PR, CL

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	C	0.20	0/1643	0.74	5/2245 (0.2%)
1	G	0.19	0/1652	0.67	3/2256 (0.1%)
1	H	0.18	0/1629	0.68	4/2224 (0.2%)
1	J	0.22	0/1643	0.69	2/2245 (0.1%)
1	O	0.17	0/1643	0.66	4/2245 (0.2%)
1	Q	0.21	0/1643	0.75	4/2245 (0.2%)
1	U	0.18	0/1623	0.63	4/2216 (0.2%)
1	W	0.20	0/1643	0.72	4/2245 (0.2%)
2	D	0.28	1/1699 (0.1%)	0.53	0/2308
2	I	0.21	0/1675	0.54	0/2276
2	K	0.22	0/1693	0.54	0/2300
2	L	0.19	0/1693	0.47	0/2300
2	P	0.20	0/1660	0.50	0/2257
2	R	0.19	0/1693	0.54	0/2300
2	V	0.21	0/1671	0.53	1/2271 (0.0%)
2	X	0.20	0/1693	0.51	0/2300
3	A	0.13	0/1166	0.44	0/1559
3	B	0.14	0/1180	0.43	0/1579
3	E	0.16	0/1188	0.46	0/1590
3	F	0.11	0/1159	0.38	0/1549
3	M	0.12	0/1159	0.41	0/1549
3	N	0.12	0/1189	0.43	0/1591
3	S	0.11	0/1182	0.38	0/1581
3	T	0.14	0/1175	0.39	0/1571
All	All	0.19	1/35994 (0.0%)	0.57	31/48802 (0.1%)

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	5
1	G	0	2
1	H	0	4
1	J	0	6
1	O	0	3
1	Q	0	6
1	U	0	3
1	W	0	4
2	I	0	2
2	K	0	2
2	P	0	1
All	All	0	38

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	95	PRO	N-CD	-8.21	1.36	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	107	ALA	CA-C-N	10.06	139.80	121.70
1	Q	107	ALA	C-N-CA	10.06	139.80	121.70
1	H	107	ALA	CA-C-N	10.01	139.71	121.70
1	H	107	ALA	C-N-CA	10.01	139.71	121.70
1	G	107	ALA	CA-C-N	10.01	139.71	121.70

There are no chirality outliers.

5 of 38 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	6	GLU	Peptide
1	H	108	MET	Peptide
1	H	31	SER	Peptide
1	H	6	GLU	Peptide
1	H	76	SER	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	C	1604	0	1580	63	1
1	G	1613	0	1593	89	0
1	H	1592	0	1570	81	0
1	J	1604	0	1580	87	0
1	O	1604	0	1580	75	0
1	Q	1604	0	1580	78	0
1	U	1586	0	1565	81	0
1	W	1604	0	1580	84	0
2	D	1662	0	1603	47	0
2	I	1638	0	1584	61	0
2	K	1656	0	1599	57	0
2	L	1656	0	1599	48	0
2	P	1623	0	1568	76	0
2	R	1656	0	1599	54	0
2	V	1634	0	1581	62	0
2	X	1656	0	1599	59	1
3	A	1161	0	1222	34	0
3	B	1174	0	1234	38	0
3	E	1182	0	1237	38	0
3	F	1154	0	1215	20	0
3	M	1154	0	1215	42	0
3	N	1183	0	1240	38	0
3	S	1177	0	1235	33	0
3	T	1170	0	1228	27	0
4	D	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	P	1	0	0	0	0
4	R	1	0	0	0	0
4	S	1	0	0	0	0
4	X	1	0	0	0	0
5	A	1	0	0	0	0
5	O	1	0	0	1	0
5	S	1	0	0	3	0
5	T	1	0	0	0	0
5	W	1	0	0	4	0
5	X	1	0	0	0	0
6	A	7	0	0	2	0
6	B	10	0	0	5	0
6	C	10	0	0	7	0
6	D	15	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	4	0	0	0	0
6	F	6	0	0	0	0
6	G	11	0	0	4	0
6	H	10	0	0	1	0
6	I	13	0	0	6	0
6	J	8	0	0	1	0
6	K	7	0	0	4	0
6	L	7	0	0	3	0
6	M	3	0	0	4	0
6	N	4	0	0	1	0
6	O	4	0	0	2	0
6	P	2	0	0	3	0
6	Q	19	0	0	11	0
6	R	14	0	0	3	0
6	S	11	0	0	4	0
6	T	7	0	0	5	0
6	U	4	0	0	4	0
6	V	6	0	0	1	0
6	W	22	0	0	5	0
6	X	16	0	0	3	0
All	All	35581	0	35186	1248	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 18.

The worst 5 of 1248 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:I:141:TYR:HD1	2:I:142:PRO:HA	1.11	1.12
2:X:54:ARG:HH12	2:X:60:GLY:HA2	1.23	1.00
2:P:148:GLN:HG3	2:P:155:LEU:HD11	1.43	0.99
2:I:141:TYR:CD1	2:I:142:PRO:HA	1.98	0.98
1:O:101:GLY:O	6:O:401:HOH:O	1.83	0.97

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)
1:C:168:THR:OG1	2:X:18:ARG:NH2[1_565]	2.15	0.05

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	C	211/228 (92%)	207 (98%)	4 (2%)	0	100	100
1	G	212/228 (93%)	209 (99%)	3 (1%)	0	100	100
1	H	208/228 (91%)	204 (98%)	4 (2%)	0	100	100
1	J	211/228 (92%)	207 (98%)	4 (2%)	0	100	100
1	O	211/228 (92%)	207 (98%)	4 (2%)	0	100	100
1	Q	211/228 (92%)	205 (97%)	6 (3%)	0	100	100
1	U	207/228 (91%)	203 (98%)	4 (2%)	0	100	100
1	W	211/228 (92%)	205 (97%)	6 (3%)	0	100	100
2	D	213/215 (99%)	212 (100%)	1 (0%)	0	100	100
2	I	210/215 (98%)	210 (100%)	0	0	100	100
2	K	212/215 (99%)	210 (99%)	2 (1%)	0	100	100
2	L	212/215 (99%)	211 (100%)	1 (0%)	0	100	100
2	P	208/215 (97%)	207 (100%)	1 (0%)	0	100	100
2	R	212/215 (99%)	210 (99%)	2 (1%)	0	100	100
2	V	209/215 (97%)	208 (100%)	1 (0%)	0	100	100
2	X	212/215 (99%)	211 (100%)	1 (0%)	0	100	100
3	A	153/164 (93%)	152 (99%)	0	1 (1%)	18	49
3	B	155/164 (94%)	153 (99%)	2 (1%)	0	100	100
3	E	156/164 (95%)	155 (99%)	1 (1%)	0	100	100
3	F	152/164 (93%)	151 (99%)	1 (1%)	0	100	100
3	M	152/164 (93%)	152 (100%)	0	0	100	100
3	N	156/164 (95%)	156 (100%)	0	0	100	100
3	S	155/164 (94%)	154 (99%)	1 (1%)	0	100	100
3	T	154/164 (94%)	154 (100%)	0	0	100	100
All	All	4603/4856 (95%)	4553 (99%)	49 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	70	ASP

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	C	184/196 (94%)	184 (100%)	0	100	100
1	G	185/196 (94%)	185 (100%)	0	100	100
1	H	183/196 (93%)	183 (100%)	0	100	100
1	J	184/196 (94%)	183 (100%)	1 (0%)	81	85
1	O	184/196 (94%)	184 (100%)	0	100	100
1	Q	184/196 (94%)	184 (100%)	0	100	100
1	U	182/196 (93%)	181 (100%)	1 (0%)	81	85
1	W	184/196 (94%)	184 (100%)	0	100	100
2	D	186/186 (100%)	186 (100%)	0	100	100
2	I	183/186 (98%)	183 (100%)	0	100	100
2	K	185/186 (100%)	185 (100%)	0	100	100
2	L	185/186 (100%)	185 (100%)	0	100	100
2	P	182/186 (98%)	182 (100%)	0	100	100
2	R	185/186 (100%)	185 (100%)	0	100	100
2	V	183/186 (98%)	183 (100%)	0	100	100
2	X	185/186 (100%)	185 (100%)	0	100	100
3	A	126/134 (94%)	126 (100%)	0	100	100
3	B	128/134 (96%)	128 (100%)	0	100	100
3	E	128/134 (96%)	128 (100%)	0	100	100
3	F	125/134 (93%)	125 (100%)	0	100	100
3	M	125/134 (93%)	125 (100%)	0	100	100
3	N	129/134 (96%)	129 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	S	128/134 (96%)	128 (100%)	0	100	100
3	T	127/134 (95%)	127 (100%)	0	100	100
All	All	3960/4128 (96%)	3958 (100%)	2 (0%)	88	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	22	CYS
1	U	22	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	84	ASN
1	Q	200	GLN
1	W	172	HIS
1	U	163	ASN
3	M	91	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 14 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

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	C	215/228 (94%)	0.41	5 (2%) 61 39	40, 59, 84, 94	0
1	G	216/228 (94%)	0.38	7 (3%) 50 30	35, 63, 91, 102	0
1	H	214/228 (93%)	0.46	8 (3%) 45 25	47, 67, 88, 111	0
1	J	215/228 (94%)	0.55	9 (4%) 40 22	50, 68, 91, 107	0
1	O	215/228 (94%)	0.80	18 (8%) 17 9	52, 89, 135, 152	0
1	Q	215/228 (94%)	0.26	6 (2%) 55 34	16, 43, 75, 92	0
1	U	213/228 (93%)	0.99	28 (13%) 7 4	41, 88, 169, 180	0
1	W	215/228 (94%)	0.18	7 (3%) 49 29	17, 41, 75, 94	0
2	D	215/215 (100%)	0.08	3 (1%) 73 53	34, 52, 77, 101	0
2	I	212/215 (98%)	0.13	4 (1%) 66 45	30, 48, 78, 89	0
2	K	214/215 (99%)	0.38	6 (2%) 55 34	39, 65, 103, 115	0
2	L	214/215 (99%)	0.42	9 (4%) 40 22	38, 66, 103, 116	0
2	P	210/215 (97%)	1.06	22 (10%) 11 6	73, 110, 137, 144	0
2	R	214/215 (99%)	0.08	2 (0%) 81 63	18, 39, 70, 90	0
2	V	211/215 (98%)	1.20	23 (10%) 10 5	73, 132, 162, 176	0
2	X	214/215 (99%)	0.03	1 (0%) 87 73	17, 43, 79, 98	0
3	A	155/164 (94%)	0.43	4 (2%) 57 36	47, 67, 90, 104	0
3	B	157/164 (95%)	0.19	0 100 100	47, 66, 92, 132	0
3	E	158/164 (96%)	0.28	4 (2%) 58 37	44, 67, 93, 121	0
3	F	154/164 (93%)	0.24	4 (2%) 57 36	47, 63, 82, 91	0
3	M	154/164 (93%)	0.26	6 (3%) 43 24	37, 57, 82, 104	0
3	N	158/164 (96%)	0.01	3 (1%) 66 45	25, 44, 72, 102	0
3	S	157/164 (95%)	0.08	1 (0%) 85 70	28, 47, 70, 97	0
3	T	156/164 (95%)	0.03	1 (0%) 85 70	26, 43, 73, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4671/4856 (96%)	0.39	181 (3%) 43 24	16, 61, 127, 180	0

The worst 5 of 181 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	35	TYR	5.4
1	U	106	SER	5.4
1	W	34	TYR	5.1
1	W	33	SER	4.6
1	U	35	TYR	4.4

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 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
5	CL	A	301	1/1	0.86	0.11	38,38,38,38	0
5	CL	S	302	1/1	0.86	0.13	52,52,52,52	0
5	CL	O	301	1/1	0.87	0.09	37,37,37,37	0
4	PR	P	301	1/1	0.87	0.11	164,164,164,164	1
4	PR	S	301	1/1	0.90	0.14	237,237,237,237	0
5	CL	W	301	1/1	0.94	0.07	49,49,49,49	0
4	PR	I	301	1/1	0.97	0.05	67,67,67,67	1
5	CL	T	301	1/1	0.97	0.12	42,42,42,42	0
4	PR	X	301	1/1	0.97	0.09	111,111,111,111	0
5	CL	X	302	1/1	0.97	0.06	36,36,36,36	0
4	PR	D	301	1/1	0.98	0.07	109,109,109,109	0
4	PR	R	301	1/1	0.98	0.06	75,75,75,75	0
4	PR	L	301	1/1	0.99	0.05	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PR	K	301	1/1	0.99	0.02	81,81,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.