



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2024 – 07:24 AM EDT

PDB ID : 3JQO
Title : Crystal structure of the outer membrane complex of a type IV secretion system
Authors : Chandran, V.; Fronzes, R.; Duquerroy, S.; Cronin, N.; Navaza, J.; Waksman, G.
Deposited on : 2009-09-07
Resolution : 2.60 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

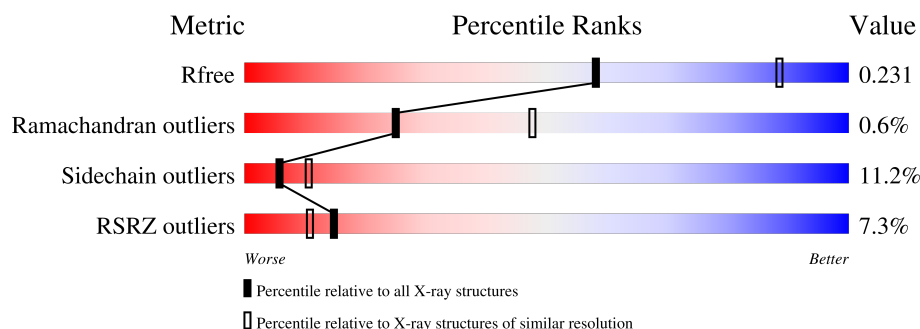
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	227	<div> <div>8%</div> <div> <div></div> <div>75%</div> <div>9%</div> <div>•</div> <div>14%</div> </div> </div>
1	D	227	<div> <div>9%</div> <div> <div></div> <div>74%</div> <div>10%</div> <div>•</div> <div>14%</div> </div> </div>
1	G	227	<div> <div>8%</div> <div> <div></div> <div>76%</div> <div>7%</div> <div>•</div> <div>15%</div> </div> </div>
1	J	227	<div> <div>11%</div> <div> <div></div> <div>75%</div> <div>10%</div> <div>•</div> <div>13%</div> </div> </div>
1	M	227	<div> <div>10%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>•</div> <div>13%</div> </div> </div>
1	P	227	<div> <div>11%</div> <div> <div></div> <div>76%</div> <div>8%</div> <div>•</div> <div>13%</div> </div> </div>
1	S	227	<div> <div>10%</div> <div> <div></div> <div>75%</div> <div>8%</div> <div>•</div> <div>13%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	V	227	<div> <div>9%</div> <div>75%</div> <div>9%</div> <div>14%</div> </div>
1	Y	227	<div> <div>9%</div> <div>76%</div> <div>8%</div> <div>14%</div> </div>
1	b	227	<div> <div>9%</div> <div>74%</div> <div>9%</div> <div>14%</div> </div>
1	e	227	<div> <div>10%</div> <div>74%</div> <div>11%</div> <div>14%</div> </div>
1	h	227	<div> <div>7%</div> <div>76%</div> <div>8%</div> <div>14%</div> </div>
1	k	227	<div> <div>9%</div> <div>76%</div> <div>9%</div> <div>14%</div> </div>
1	n	227	<div> <div>10%</div> <div>75%</div> <div>9%</div> <div>14%</div> </div>
2	B	135	<div> <div>2%</div> <div>85%</div> <div>10%</div> <div>3%</div> </div>
2	E	135	<div> <div>1%</div> <div>83%</div> <div>12%</div> <div>3%</div> </div>
2	H	135	<div> <div>1%</div> <div>84%</div> <div>10%</div> <div>3%</div> </div>
2	K	135	<div> <div>1%</div> <div>86%</div> <div>10%</div> <div>3%</div> </div>
2	N	135	<div> <div>1%</div> <div>84%</div> <div>11%</div> <div>3%</div> </div>
2	Q	135	<div> <div>2%</div> <div>81%</div> <div>13%</div> <div>3%</div> </div>
2	T	135	<div> <div>2%</div> <div>84%</div> <div>12%</div> <div>3%</div> </div>
2	W	135	<div> <div>2%</div> <div>85%</div> <div>10%</div> <div>3%</div> </div>
2	Z	135	<div> <div>1%</div> <div>84%</div> <div>11%</div> <div>3%</div> </div>
2	c	135	<div> <div>1%</div> <div>84%</div> <div>10%</div> <div>3%</div> </div>
2	f	135	<div> <div>1%</div> <div>84%</div> <div>11%</div> <div>3%</div> </div>
2	i	135	<div> <div>1%</div> <div>84%</div> <div>10%</div> <div>3%</div> </div>
2	l	135	<div> <div>2%</div> <div>83%</div> <div>11%</div> <div>3%</div> </div>
2	o	135	<div> <div>1%</div> <div>84%</div> <div>10%</div> <div>3%</div> </div>
3	C	34	<div> <div>6%</div> <div>68%</div> <div>9%</div> <div>24%</div> </div>
3	F	34	<div> <div>6%</div> <div>68%</div> <div>6%</div> <div>26%</div> </div>
3	I	34	<div> <div>65%</div> <div>9%</div> <div>26%</div> </div>
3	L	34	<div> <div>12%</div> <div>74%</div> <div>9%</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
3	O	34	
3	R	34	
3	U	34	
3	X	34	
3	a	34	
3	d	34	
3	g	34	
3	j	34	
3	m	34	
3	p	34	

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	LDA	J	1	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 38842 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 TraF protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	Se	0	0	0
			1448	898	253	290	2	5			
1	D	195	Total	C	N	O	S	Se	0	0	0
			1448	898	253	290	2	5			
1	G	193	Total	C	N	O	S	Se	0	0	0
			1437	890	252	288	2	5			
1	J	197	Total	C	N	O	S	Se	0	0	0
			1457	903	256	291	2	5			
1	M	197	Total	C	N	O	S	Se	0	0	0
			1461	905	256	293	2	5			
1	P	197	Total	C	N	O	S	Se	0	0	0
			1461	905	256	293	2	5			
1	S	197	Total	C	N	O	S	Se	0	0	0
			1461	905	256	293	2	5			
1	V	196	Total	C	N	O	S	Se	0	0	0
			1457	903	255	292	2	5			
1	Y	195	Total	C	N	O	S	Se	0	0	0
			1448	898	253	290	2	5			
1	b	195	Total	C	N	O	S	Se	0	0	0
			1449	898	254	290	2	5			
1	e	196	Total	C	N	O	S	Se	0	0	0
			1457	903	255	292	2	5			
1	h	195	Total	C	N	O	S	Se	0	0	0
			1439	893	250	289	2	5			
1	k	196	Total	C	N	O	S	Se	0	0	0
			1457	903	255	292	2	5			
1	n	196	Total	C	N	O	S	Se	0	0	0
			1457	900	256	294	2	5			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	308	ARG	ALA	SEE REMARK 999	UNP Q46705

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Chain	Residue	Modelled	Actual	Comment	Reference
D	308	ARG	ALA	SEE REMARK 999	UNP Q46705
G	308	ARG	ALA	SEE REMARK 999	UNP Q46705
J	308	ARG	ALA	SEE REMARK 999	UNP Q46705
M	308	ARG	ALA	SEE REMARK 999	UNP Q46705
P	308	ARG	ALA	SEE REMARK 999	UNP Q46705
S	308	ARG	ALA	SEE REMARK 999	UNP Q46705
V	308	ARG	ALA	SEE REMARK 999	UNP Q46705
Y	308	ARG	ALA	SEE REMARK 999	UNP Q46705
b	308	ARG	ALA	SEE REMARK 999	UNP Q46705
e	308	ARG	ALA	SEE REMARK 999	UNP Q46705
h	308	ARG	ALA	SEE REMARK 999	UNP Q46705
k	308	ARG	ALA	SEE REMARK 999	UNP Q46705
n	308	ARG	ALA	SEE REMARK 999	UNP Q46705

- Molecule 2 is a protein called TraO protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			
2	E	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			
2	H	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			
2	K	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			
2	N	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			
2	Q	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			
2	T	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			
2	W	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			
2	Z	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			
2	c	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			
2	f	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			
2	i	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			
2	l	130	Total	C	N	O	Se	0	0	0
			1033	648	193	189	3			

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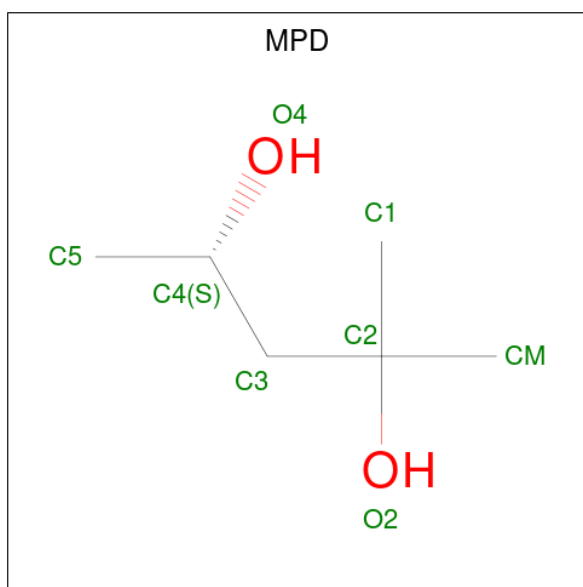
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	o	130	Total	C	N	O	Se	0	0	0
			1032	647	193	189	3			

- Molecule 3 is a protein called TraN protein.

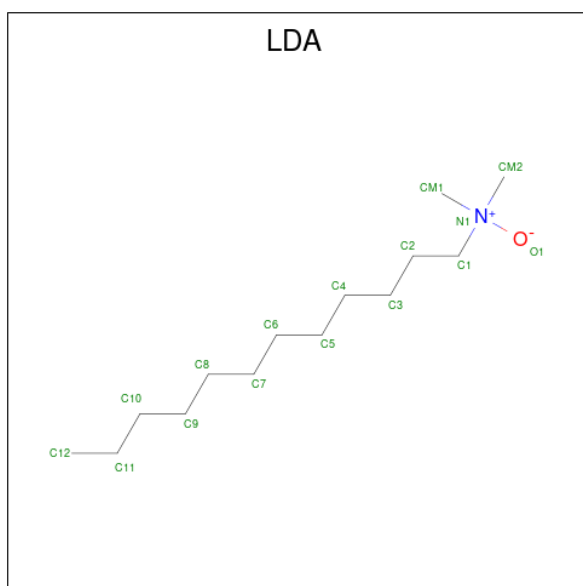
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	26	Total	C	N	O		0	0	0
			200	126	34	40				
3	F	25	Total	C	N	O		0	0	0
			194	123	33	38				
3	I	25	Total	C	N	O		0	0	0
			194	123	33	38				
3	L	28	Total	C	N	O	S	0	0	0
			212	132	36	43	1			
3	O	24	Total	C	N	O		0	0	0
			190	121	32	37				
3	R	24	Total	C	N	O		0	0	0
			185	118	31	36				
3	U	27	Total	C	N	O		0	0	0
			206	129	35	42				
3	X	24	Total	C	N	O		0	0	0
			190	121	32	37				
3	a	24	Total	C	N	O		0	0	0
			190	121	32	37				
3	d	24	Total	C	N	O		0	0	0
			190	121	32	37				
3	g	25	Total	C	N	O		0	0	0
			194	123	33	38				
3	j	25	Total	C	N	O		0	0	0
			194	123	33	38				
3	m	25	Total	C	N	O		0	0	0
			194	123	33	38				
3	p	23	Total	C	N	O		0	0	0
			181	116	30	35				

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			8	6	2		
4	h	1	Total	C	O	0	0
			8	6	2		
4	k	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	J	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	65	Total	O			0	0
			65	65				
6	B	31	Total	O			0	0
			31	31				
6	C	7	Total	O			0	0
			7	7				
6	D	65	Total	O			0	0
			65	65				
6	E	28	Total	O			0	0
			28	28				
6	F	9	Total	O			0	0
			9	9				
6	G	50	Total	O			0	0
			50	50				
6	H	22	Total	O			0	0
			22	22				
6	I	9	Total	O			0	0
			9	9				
6	J	49	Total	O			0	0
			49	49				
6	K	30	Total	O			0	0
			30	30				
6	L	12	Total	O			0	0
			12	12				
6	M	48	Total	O			0	0
			48	48				
6	N	35	Total	O			0	0
			35	35				
6	O	11	Total	O			0	0
			11	11				
6	P	58	Total	O			0	0
			58	58				
6	Q	27	Total	O			0	0
			27	27				
6	R	7	Total	O			0	0
			7	7				
6	S	57	Total	O			0	0
			57	57				

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	T	21	Total O 21 21	0	0
6	U	10	Total O 10 10	0	0
6	V	63	Total O 63 63	0	0
6	W	26	Total O 26 26	0	0
6	X	7	Total O 7 7	0	0
6	Y	57	Total O 57 57	0	0
6	Z	21	Total O 21 21	0	0
6	a	8	Total O 8 8	0	0
6	b	59	Total O 59 59	0	0
6	c	31	Total O 31 31	0	0
6	d	3	Total O 3 3	0	0
6	e	52	Total O 52 52	0	0
6	f	28	Total O 28 28	0	0
6	g	4	Total O 4 4	0	0
6	h	50	Total O 50 50	0	0
6	i	21	Total O 21 21	0	0
6	j	11	Total O 11 11	0	0
6	k	56	Total O 56 56	0	0
6	l	37	Total O 37 37	0	0
6	m	8	Total O 8 8	0	0
6	n	50	Total O 50 50	0	0

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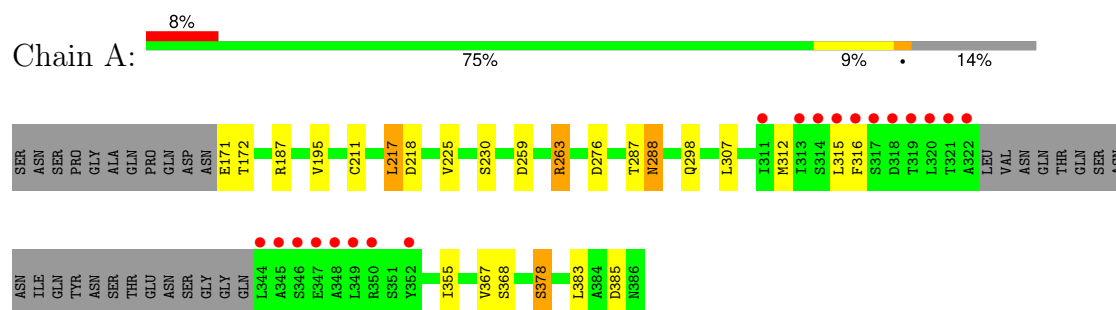
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	o	35	Total 35	O 35	0	0
6	p	12	Total 12	O 12	0	0

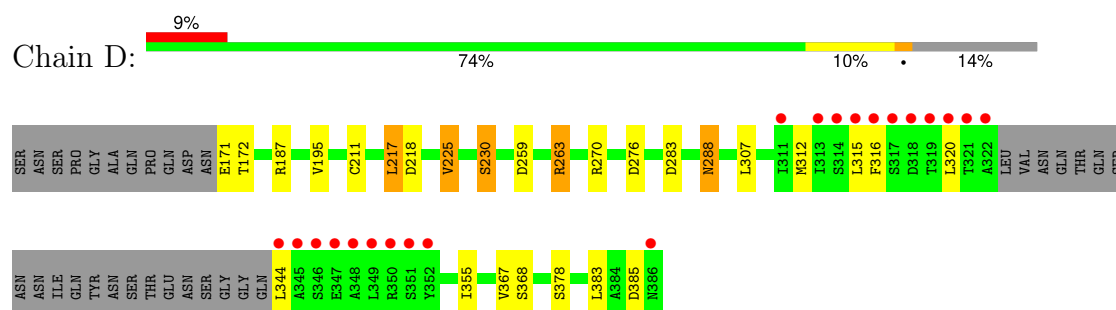
3 Residue-property plots

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.

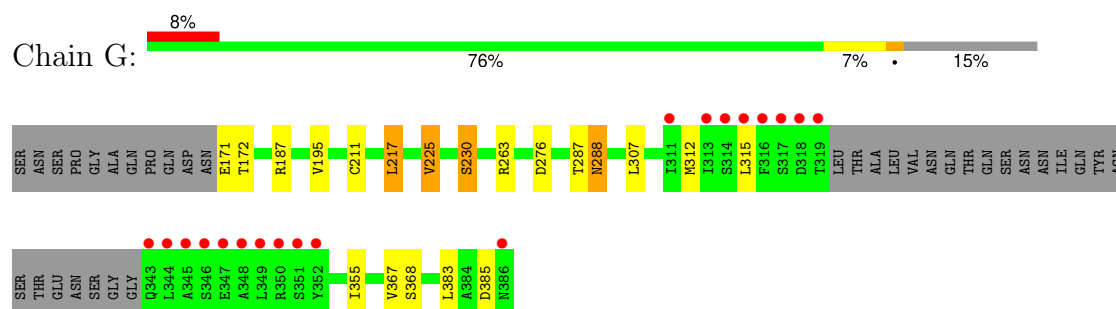
• Molecule 1: TraF protein



• Molecule 1: TraF protein

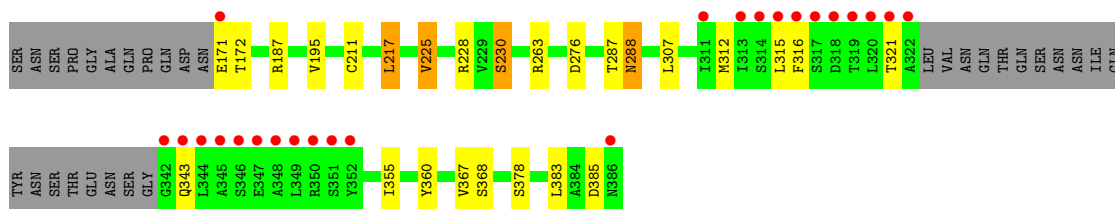


• Molecule 1: TraF protein

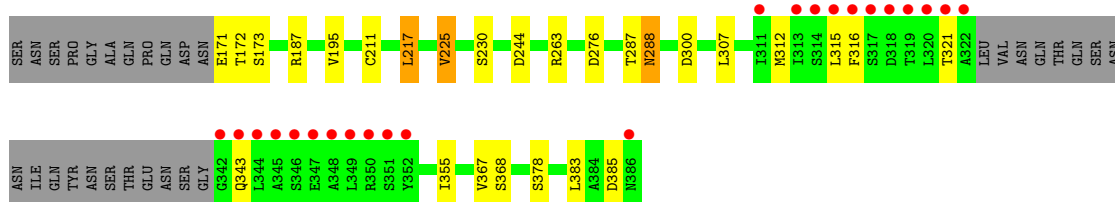
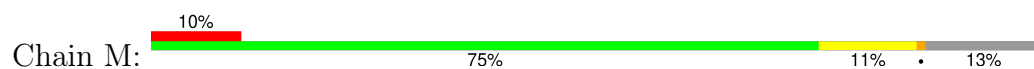


• Molecule 1: TraF protein

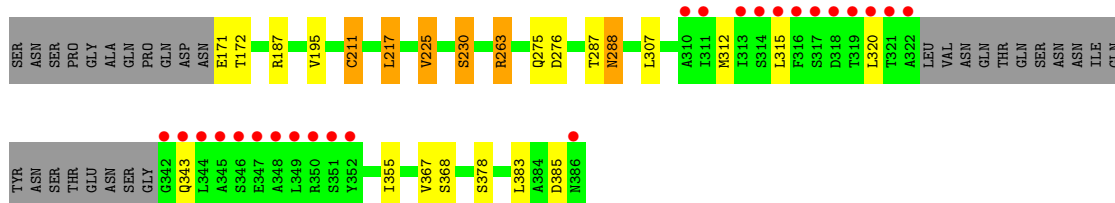
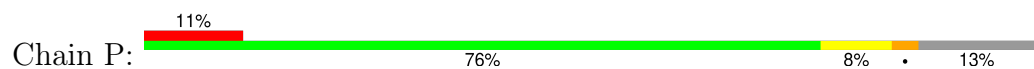




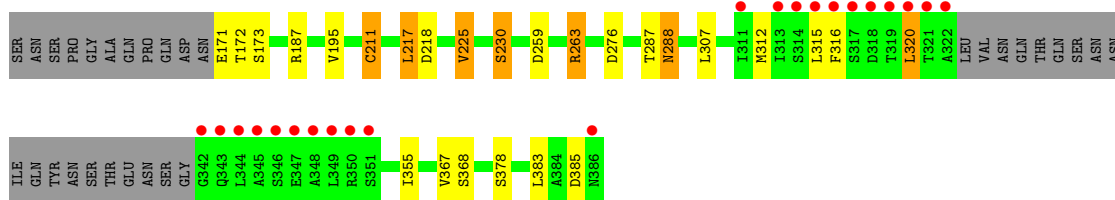
• Molecule 1: TraF protein



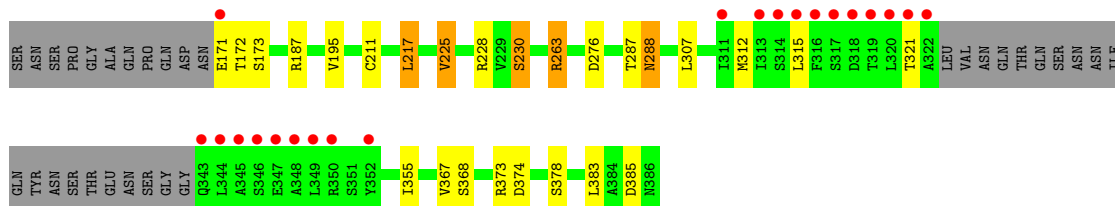
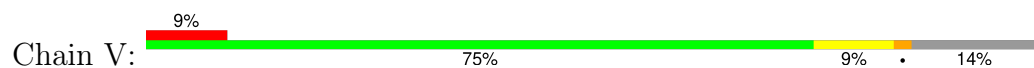
• Molecule 1: TraF protein



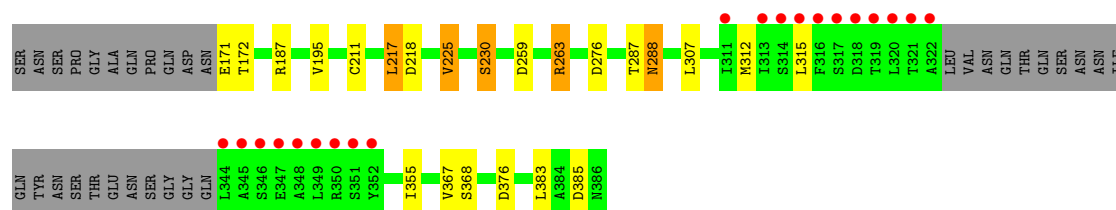
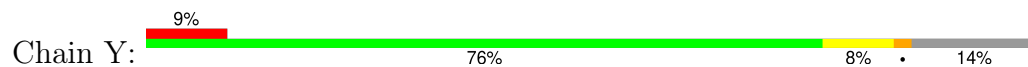
• Molecule 1: TraF protein



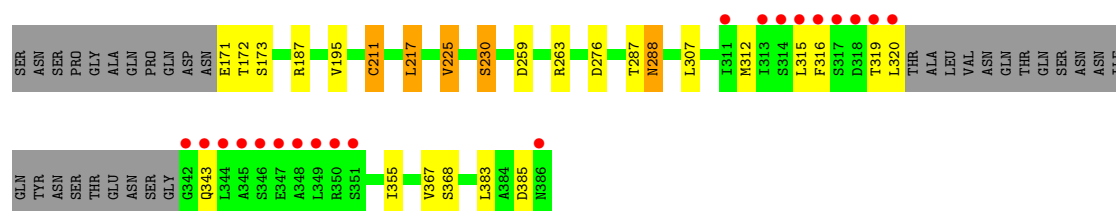
• Molecule 1: TraF protein



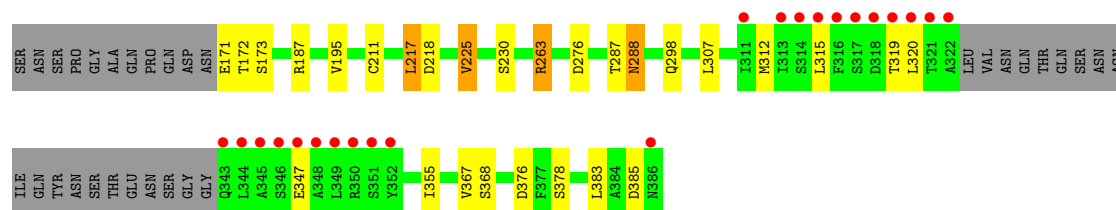
- Molecule 1: TraF protein



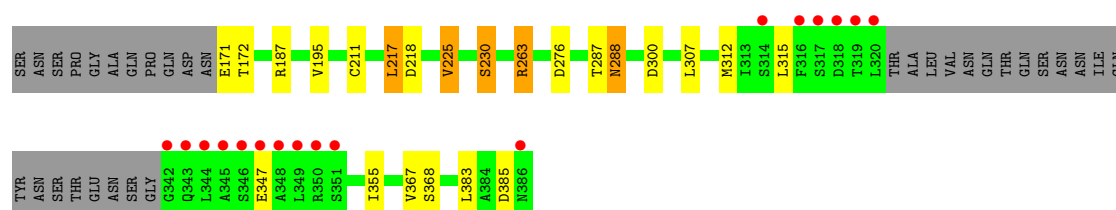
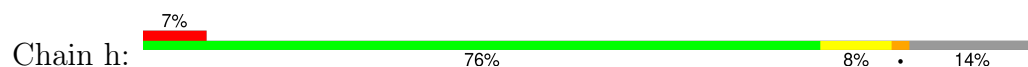
- Molecule 1: TraF protein



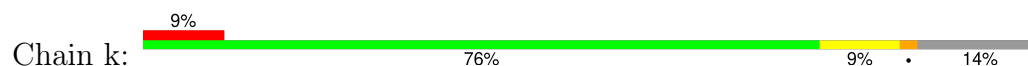
- Molecule 1: TraF protein

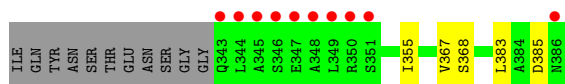


- Molecule 1: TraF protein

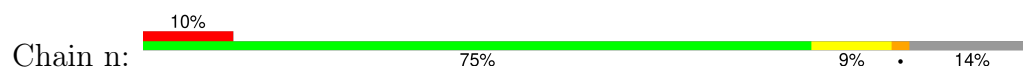


- Molecule 1: TraF protein

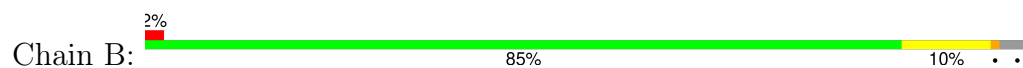




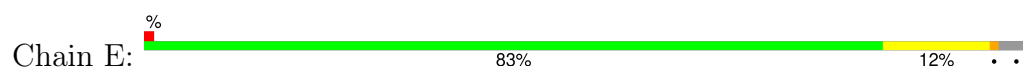
• Molecule 1: TraF protein



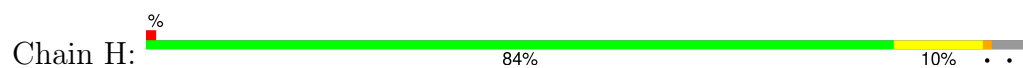
• Molecule 2: TraO protein



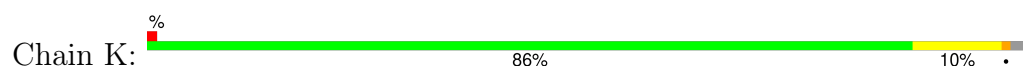
• Molecule 2: TraO protein



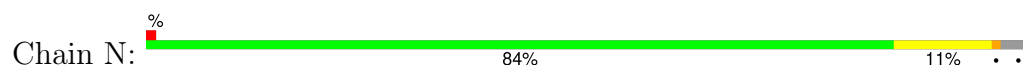
• Molecule 2: TraO protein



• Molecule 2: TraO protein

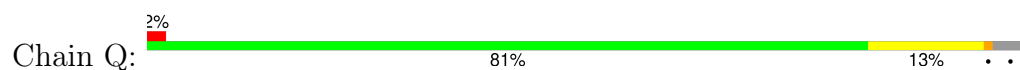


• Molecule 2: TraO protein

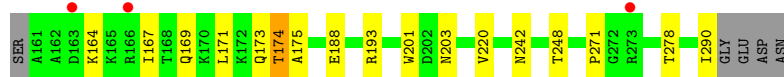
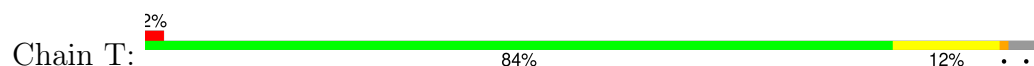




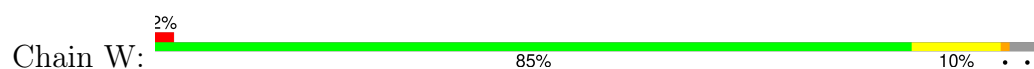
- Molecule 2: TraO protein



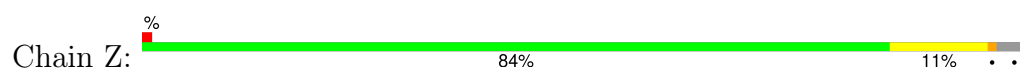
- Molecule 2: TraO protein



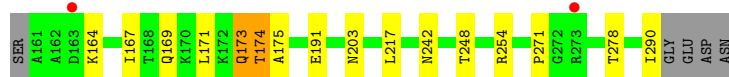
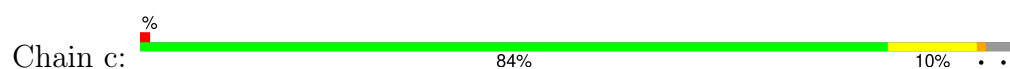
- Molecule 2: TraO protein



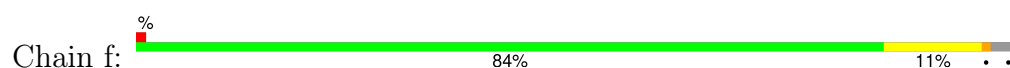
- Molecule 2: TraO protein



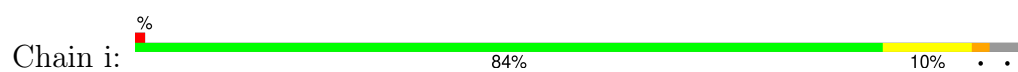
- Molecule 2: TraO protein



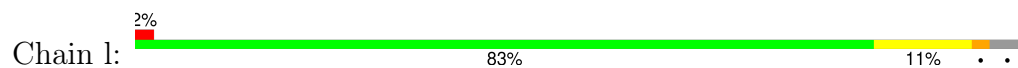
- Molecule 2: TraO protein



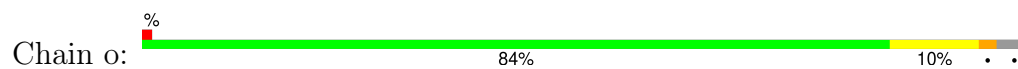
- Molecule 2: TraO protein



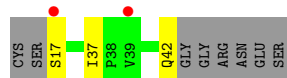
• Molecule 2: TraO protein



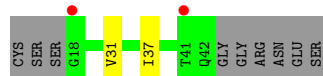
• Molecule 2: TraO protein



• Molecule 3: TraN protein



• Molecule 3: TraN protein



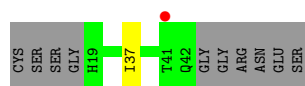
• Molecule 3: TraN protein



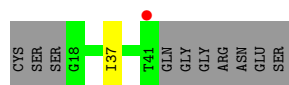
• Molecule 3: TraN protein



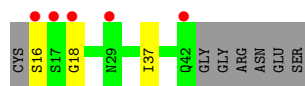
- Molecule 3: TraN protein



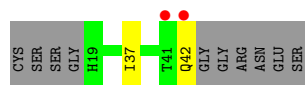
- Molecule 3: TraN protein



- Molecule 3: TraN protein



- Molecule 3: TraN protein



- Molecule 3: TraN protein

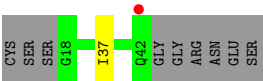


- Molecule 3: TraN protein

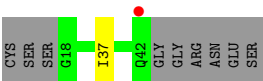


- Molecule 3: TraN protein

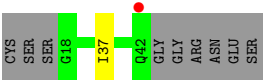




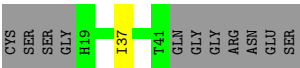
● Molecule 3: TraN protein



● Molecule 3: TraN protein



● Molecule 3: TraN protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	202.40Å 211.63Å 203.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.91 – 2.60 52.91 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.5 (52.91-2.60) 97.2 (52.91-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.227 , 0.259 0.206 , 0.231	Depositor DCC
R_{free} test set	12939 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k 0.010 for -k,-h,l 0.011 for l,-k,h 0.003 for l,h,k 0.003 for k,l,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	38842	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: LDA, MPD

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	0.95	2/1464 (0.1%)	1.04	9/1978 (0.5%)
1	D	0.99	2/1464 (0.1%)	1.11	16/1978 (0.8%)
1	G	0.96	2/1453 (0.1%)	1.01	7/1962 (0.4%)
1	J	0.97	1/1473 (0.1%)	1.03	10/1990 (0.5%)
1	M	0.98	1/1477 (0.1%)	1.05	13/1995 (0.7%)
1	P	0.95	3/1477 (0.2%)	1.03	9/1995 (0.5%)
1	S	0.96	2/1477 (0.1%)	1.04	13/1995 (0.7%)
1	V	0.94	1/1473 (0.1%)	1.03	12/1990 (0.6%)
1	Y	0.97	2/1464 (0.1%)	1.07	13/1978 (0.7%)
1	b	0.95	3/1465 (0.2%)	1.01	10/1978 (0.5%)
1	e	0.99	3/1473 (0.2%)	1.03	10/1990 (0.5%)
1	h	0.99	3/1455 (0.2%)	1.07	13/1966 (0.7%)
1	k	0.96	2/1473 (0.1%)	1.06	12/1990 (0.6%)
1	n	0.98	2/1472 (0.1%)	1.02	11/1986 (0.6%)
2	B	0.96	0/1051	0.97	2/1417 (0.1%)
2	E	0.96	1/1051 (0.1%)	0.97	4/1417 (0.3%)
2	H	1.07	0/1051	0.99	3/1417 (0.2%)
2	K	0.91	0/1051	0.99	3/1417 (0.2%)
2	N	0.88	0/1051	0.95	1/1417 (0.1%)
2	Q	0.93	0/1051	0.97	7/1417 (0.5%)
2	T	0.95	0/1051	0.97	2/1417 (0.1%)
2	W	0.96	0/1051	0.93	2/1417 (0.1%)
2	Z	0.92	0/1051	0.99	4/1417 (0.3%)
2	c	0.93	0/1051	0.98	4/1417 (0.3%)
2	f	0.97	0/1051	0.98	4/1417 (0.3%)
2	i	1.00	1/1051 (0.1%)	0.95	2/1417 (0.1%)
2	l	0.93	0/1051	0.98	6/1417 (0.4%)
2	o	1.01	0/1050	0.94	2/1415 (0.1%)
3	C	0.93	0/208	0.80	0/289
3	F	0.79	0/202	0.75	0/281
3	I	0.86	0/202	0.75	0/281
3	L	0.80	0/220	0.88	0/305

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	O	0.68	0/198	0.76	0/276
3	R	0.77	0/193	0.75	0/269
3	U	0.90	0/214	0.93	0/297
3	X	0.71	0/198	0.73	0/276
3	a	0.68	0/198	0.72	0/276
3	d	0.76	0/198	0.77	0/276
3	g	0.86	0/202	0.82	0/281
3	j	0.82	0/202	0.75	0/281
3	m	0.82	0/202	0.75	0/281
3	p	0.78	0/189	0.79	0/264
All	All	0.95	31/38099 (0.1%)	1.00	204/51540 (0.4%)

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	A	0	1
1	G	0	1
1	J	0	1
1	M	0	1
1	P	0	2
1	S	0	1
1	V	0	1
1	Y	0	1
1	b	0	1
1	e	0	1
1	h	0	1
1	k	0	1
1	n	0	1
2	B	0	2
2	E	0	2
2	H	0	2
2	K	0	2
2	N	0	2
2	Q	0	2
2	T	0	2
2	W	0	2
2	Z	0	2
2	c	0	2
2	f	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	i	0	2
2	l	0	2
2	o	0	2
3	U	0	1
All	All	0	43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	298	GLN	CD-NE2	-8.19	1.12	1.32
1	e	298	GLN	CD-OE1	-8.10	1.06	1.24
1	A	298	GLN	CD-OE1	-8.09	1.06	1.24
1	n	211	CYS	CB-SG	-7.71	1.69	1.82
1	J	276	ASP	CB-CG	-7.16	1.36	1.51

The worst 5 of 204 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	217	LEU	CA-CB-CG	10.11	138.54	115.30
1	h	276	ASP	CB-CG-OD1	-9.75	109.53	118.30
1	k	217	LEU	CA-CB-CG	9.54	137.23	115.30
1	S	217	LEU	CA-CB-CG	9.39	136.90	115.30
1	A	217	LEU	CA-CB-CG	9.39	136.89	115.30

There are no chirality outliers.

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	287	THR	Peptide
2	B	174	THR	Peptide
2	B	175	ALA	Peptide
2	E	174	THR	Peptide
2	E	175	ALA	Peptide

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	191/227 (84%)	179 (94%)	10 (5%)	2 (1%)	15	32
1	D	191/227 (84%)	177 (93%)	13 (7%)	1 (0%)	29	52
1	G	189/227 (83%)	176 (93%)	12 (6%)	1 (0%)	29	52
1	J	193/227 (85%)	178 (92%)	14 (7%)	1 (0%)	29	52
1	M	193/227 (85%)	178 (92%)	13 (7%)	2 (1%)	15	32
1	P	193/227 (85%)	179 (93%)	13 (7%)	1 (0%)	29	52
1	S	193/227 (85%)	179 (93%)	13 (7%)	1 (0%)	29	52
1	V	192/227 (85%)	179 (93%)	12 (6%)	1 (0%)	29	52
1	Y	191/227 (84%)	179 (94%)	11 (6%)	1 (0%)	29	52
1	b	191/227 (84%)	176 (92%)	13 (7%)	2 (1%)	15	32
1	e	192/227 (85%)	180 (94%)	10 (5%)	2 (1%)	15	32
1	h	191/227 (84%)	179 (94%)	11 (6%)	1 (0%)	29	52
1	k	192/227 (85%)	180 (94%)	11 (6%)	1 (0%)	29	52
1	n	191/227 (84%)	178 (93%)	12 (6%)	1 (0%)	29	52
2	B	128/135 (95%)	118 (92%)	10 (8%)	0	100	100
2	E	128/135 (95%)	120 (94%)	7 (6%)	1 (1%)	19	39
2	H	128/135 (95%)	118 (92%)	9 (7%)	1 (1%)	19	39
2	K	128/135 (95%)	119 (93%)	9 (7%)	0	100	100
2	N	128/135 (95%)	121 (94%)	7 (6%)	0	100	100
2	Q	128/135 (95%)	120 (94%)	7 (6%)	1 (1%)	19	39
2	T	128/135 (95%)	120 (94%)	8 (6%)	0	100	100
2	W	128/135 (95%)	122 (95%)	5 (4%)	1 (1%)	19	39
2	Z	128/135 (95%)	118 (92%)	9 (7%)	1 (1%)	19	39
2	c	128/135 (95%)	119 (93%)	8 (6%)	1 (1%)	19	39
2	f	128/135 (95%)	120 (94%)	7 (6%)	1 (1%)	19	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	i	128/135 (95%)	120 (94%)	7 (6%)	1 (1%)	19	39
2	l	128/135 (95%)	120 (94%)	7 (6%)	1 (1%)	19	39
2	o	128/135 (95%)	120 (94%)	7 (6%)	1 (1%)	19	39
3	C	24/34 (71%)	23 (96%)	1 (4%)	0	100	100
3	F	23/34 (68%)	22 (96%)	1 (4%)	0	100	100
3	I	23/34 (68%)	22 (96%)	1 (4%)	0	100	100
3	L	26/34 (76%)	24 (92%)	1 (4%)	1 (4%)	3	4
3	O	22/34 (65%)	21 (96%)	1 (4%)	0	100	100
3	R	22/34 (65%)	21 (96%)	1 (4%)	0	100	100
3	U	25/34 (74%)	24 (96%)	1 (4%)	0	100	100
3	X	22/34 (65%)	21 (96%)	1 (4%)	0	100	100
3	a	22/34 (65%)	20 (91%)	2 (9%)	0	100	100
3	d	22/34 (65%)	20 (91%)	2 (9%)	0	100	100
3	g	23/34 (68%)	21 (91%)	2 (9%)	0	100	100
3	j	23/34 (68%)	21 (91%)	2 (9%)	0	100	100
3	m	23/34 (68%)	22 (96%)	1 (4%)	0	100	100
3	p	21/34 (62%)	21 (100%)	0	0	100	100
All	All	4796/5544 (86%)	4475 (93%)	292 (6%)	29 (1%)	25	47

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	ASN
1	D	288	ASN
1	G	288	ASN
3	L	17	SER
1	M	288	ASN

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	A	157/180 (87%)	139 (88%)	18 (12%)	5	10
1	D	157/180 (87%)	138 (88%)	19 (12%)	5	9
1	G	156/180 (87%)	141 (90%)	15 (10%)	8	16
1	J	157/180 (87%)	137 (87%)	20 (13%)	4	8
1	M	158/180 (88%)	139 (88%)	19 (12%)	5	9
1	P	158/180 (88%)	140 (89%)	18 (11%)	5	10
1	S	158/180 (88%)	138 (87%)	20 (13%)	4	8
1	V	158/180 (88%)	139 (88%)	19 (12%)	5	9
1	Y	157/180 (87%)	141 (90%)	16 (10%)	7	14
1	b	157/180 (87%)	138 (88%)	19 (12%)	5	9
1	e	158/180 (88%)	138 (87%)	20 (13%)	4	8
1	h	155/180 (86%)	138 (89%)	17 (11%)	6	11
1	k	158/180 (88%)	141 (89%)	17 (11%)	6	12
1	n	158/180 (88%)	138 (87%)	20 (13%)	4	8
2	B	109/110 (99%)	97 (89%)	12 (11%)	6	11
2	E	109/110 (99%)	96 (88%)	13 (12%)	5	9
2	H	109/110 (99%)	97 (89%)	12 (11%)	6	11
2	K	109/110 (99%)	99 (91%)	10 (9%)	9	17
2	N	109/110 (99%)	95 (87%)	14 (13%)	4	8
2	Q	109/110 (99%)	96 (88%)	13 (12%)	5	9
2	T	109/110 (99%)	96 (88%)	13 (12%)	5	9
2	W	109/110 (99%)	97 (89%)	12 (11%)	6	11
2	Z	109/110 (99%)	96 (88%)	13 (12%)	5	9
2	c	109/110 (99%)	97 (89%)	12 (11%)	6	11
2	f	109/110 (99%)	97 (89%)	12 (11%)	6	11
2	i	109/110 (99%)	96 (88%)	13 (12%)	5	9
2	l	109/110 (99%)	96 (88%)	13 (12%)	5	9
2	o	108/110 (98%)	94 (87%)	14 (13%)	4	7
3	C	25/31 (81%)	22 (88%)	3 (12%)	5	9
3	F	24/31 (77%)	22 (92%)	2 (8%)	11	22
3	I	24/31 (77%)	22 (92%)	2 (8%)	11	22
3	L	27/31 (87%)	25 (93%)	2 (7%)	13	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	O	24/31 (77%)	23 (96%)	1 (4%)	30	55
3	R	23/31 (74%)	22 (96%)	1 (4%)	29	54
3	U	26/31 (84%)	24 (92%)	2 (8%)	13	25
3	X	24/31 (77%)	22 (92%)	2 (8%)	11	22
3	a	24/31 (77%)	22 (92%)	2 (8%)	11	22
3	d	24/31 (77%)	23 (96%)	1 (4%)	30	55
3	g	24/31 (77%)	23 (96%)	1 (4%)	30	55
3	j	24/31 (77%)	23 (96%)	1 (4%)	30	55
3	m	24/31 (77%)	23 (96%)	1 (4%)	30	55
3	p	23/31 (74%)	22 (96%)	1 (4%)	29	54
All	All	4067/4494 (90%)	3612 (89%)	455 (11%)	6	10

5 of 455 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	173	SER
2	o	171	LEU
2	Z	220	VAL
1	n	383	LEU
1	k	315	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 110 such sidechains are listed below:

Mol	Chain	Res	Type
2	W	268	ASN
2	c	169	GLN
3	p	19	HIS
2	l	242	ASN
3	X	42	GLN

5.3.3 RNA ⓘ

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](#)

4 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	$\# Z > 2$
4	MPD	h	2	-	7,7,7	0.20	0	9,10,10	0.81	0
4	MPD	D	1	-	7,7,7	0.25	0	9,10,10	0.57	0
5	LDA	J	1	-	13,15,15	2.50	2 (15%)	14,17,17	1.17	2 (14%)
4	MPD	k	3	-	7,7,7	0.32	0	9,10,10	0.95	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
4	MPD	h	2	-	-	3/5/5/5	-
4	MPD	D	1	-	-	5/5/5/5	-
5	LDA	J	1	-	-	11/13/13/13	-
4	MPD	k	3	-	-	0/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	1	LDA	O1-N1	-7.70	1.23	1.42
5	J	1	LDA	C1-N1	-4.24	1.47	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	1	LDA	CM2-N1-C1	3.17	116.89	110.23
5	J	1	LDA	C12-C11-C10	2.17	128.01	113.36

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	MPD	C2-C3-C4-O4
4	D	1	MPD	C2-C3-C4-C5
5	J	1	LDA	C2-C1-N1-O1
5	J	1	LDA	C2-C1-N1-CM1
5	J	1	LDA	C2-C1-N1-CM2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	190/227 (83%)	0.08	19 (10%) 7 4	19, 27, 76, 95	0
1	D	190/227 (83%)	0.12	21 (11%) 5 3	19, 27, 76, 96	0
1	G	188/227 (82%)	-0.05	19 (10%) 7 4	19, 27, 74, 87	0
1	J	192/227 (84%)	0.10	24 (12%) 3 2	19, 27, 76, 97	0
1	M	192/227 (84%)	0.07	23 (11%) 4 2	19, 27, 77, 93	0
1	P	192/227 (84%)	0.09	24 (12%) 3 2	19, 27, 77, 97	0
1	S	192/227 (84%)	0.04	22 (11%) 4 3	19, 27, 77, 95	0
1	V	191/227 (84%)	0.03	21 (10%) 5 3	19, 27, 77, 95	0
1	Y	190/227 (83%)	0.01	20 (10%) 6 4	19, 27, 76, 95	0
1	b	190/227 (83%)	0.03	20 (10%) 6 4	19, 27, 76, 90	0
1	e	191/227 (84%)	0.14	22 (11%) 4 3	19, 27, 76, 97	0
1	h	190/227 (83%)	0.13	17 (8%) 9 6	19, 27, 76, 89	0
1	k	191/227 (84%)	0.14	21 (10%) 5 3	19, 27, 77, 98	0
1	n	191/227 (84%)	0.09	22 (11%) 4 3	19, 27, 75, 126	0
2	B	127/135 (94%)	-0.29	3 (2%) 59 53	24, 33, 68, 93	0
2	E	127/135 (94%)	-0.33	2 (1%) 72 68	24, 33, 68, 93	0
2	H	127/135 (94%)	-0.34	2 (1%) 72 68	24, 33, 68, 93	0
2	K	127/135 (94%)	-0.30	2 (1%) 72 68	24, 33, 68, 93	0
2	N	127/135 (94%)	-0.38	2 (1%) 72 68	24, 33, 68, 93	0
2	Q	127/135 (94%)	-0.41	3 (2%) 59 53	24, 33, 68, 93	0
2	T	127/135 (94%)	-0.29	3 (2%) 59 53	24, 33, 68, 93	0
2	W	127/135 (94%)	-0.38	3 (2%) 59 53	24, 33, 68, 93	0
2	Z	127/135 (94%)	-0.43	2 (1%) 72 68	24, 33, 68, 93	0
2	c	127/135 (94%)	-0.42	2 (1%) 72 68	24, 33, 68, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	f	127/135 (94%)	-0.21	2 (1%) 72 68	24, 33, 68, 93	0
2	i	127/135 (94%)	-0.38	1 (0%) 86 84	24, 33, 68, 93	0
2	l	127/135 (94%)	-0.43	3 (2%) 59 53	24, 33, 68, 93	0
2	o	127/135 (94%)	-0.27	2 (1%) 72 68	24, 33, 68, 93	0
3	C	26/34 (76%)	0.22	2 (7%) 13 10	30, 40, 76, 83	0
3	F	25/34 (73%)	0.11	2 (8%) 12 9	31, 37, 76, 84	0
3	I	25/34 (73%)	-0.10	0 100 100	30, 37, 76, 82	0
3	L	28/34 (82%)	0.12	4 (14%) 2 1	30, 41, 79, 82	0
3	O	24/34 (70%)	-0.12	1 (4%) 36 29	30, 37, 76, 85	0
3	R	24/34 (70%)	-0.38	1 (4%) 36 29	30, 37, 69, 81	0
3	U	27/34 (79%)	0.53	5 (18%) 1 0	30, 40, 76, 84	0
3	X	24/34 (70%)	-0.17	2 (8%) 11 8	30, 37, 76, 84	0
3	a	24/34 (70%)	-0.26	0 100 100	31, 37, 76, 83	0
3	d	24/34 (70%)	0.17	3 (12%) 3 2	30, 37, 76, 85	0
3	g	25/34 (73%)	-0.16	1 (4%) 38 31	30, 37, 76, 86	0
3	j	25/34 (73%)	-0.03	1 (4%) 38 31	30, 37, 76, 84	0
3	m	25/34 (73%)	-0.18	1 (4%) 38 31	30, 37, 76, 84	0
3	p	23/34 (67%)	-0.36	0 100 100	30, 37, 69, 81	0
All	All	4797/5544 (86%)	-0.09	350 (7%) 15 11	19, 31, 77, 126	0

The worst 5 of 350 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	342	GLY	12.5
1	h	349	LEU	9.2
1	n	345	ALA	9.2
1	G	349	LEU	9.1
1	A	345	ALA	8.8

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 [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
5	LDA	J	1	16/16	0.75	0.50	11,42,48,52	0
4	MPD	D	1	8/8	0.91	0.25	62,63,64,67	0
4	MPD	h	2	8/8	0.92	0.19	50,52,56,59	0
4	MPD	k	3	8/8	0.94	0.19	44,45,48,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.