



# Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

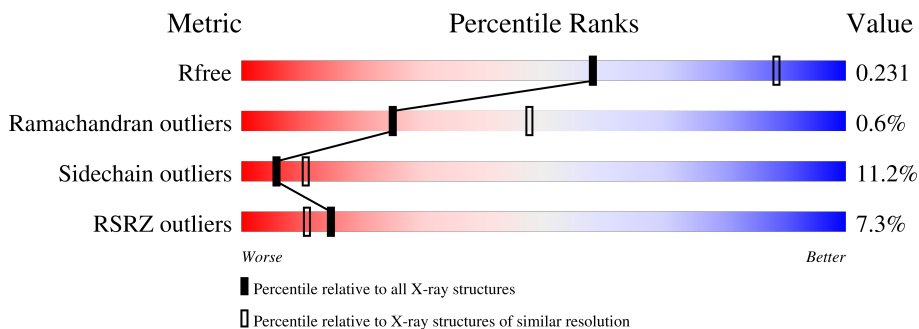
# 1 Overall quality at a glance i

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  $\geq 3$ , 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	
1	D	227	
1	G	227	
1	J	227	
1	M	227	
1	P	227	
1	S	227	

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

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Mol	Chain	Length	Quality of chain
3	O	34	 3% 68% 29%
3	R	34	 3% 68% 29%
3	U	34	 15% 71% 9% 21%
3	X	34	 6% 65% 6% 29%
3	a	34	 65% 6% 29%
3	d	34	 9% 68% 29%
3	g	34	 3% 71% 26%
3	j	34	 3% 71% 26%
3	m	34	 3% 71% 26%
3	p	34	 65% 32%

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 [i](#)

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

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
			Total	C	N	O	Se			
2	B	130	1033	648	193	189	3	0	0	0
2	E	130	1033	648	193	189	3	0	0	0
2	H	130	1033	648	193	189	3	0	0	0
2	K	130	1033	648	193	189	3	0	0	0
2	N	130	1033	648	193	189	3	0	0	0
2	Q	130	1033	648	193	189	3	0	0	0
2	T	130	1033	648	193	189	3	0	0	0
2	W	130	1033	648	193	189	3	0	0	0
2	Z	130	1033	648	193	189	3	0	0	0
2	c	130	1033	648	193	189	3	0	0	0
2	f	130	1033	648	193	189	3	0	0	0
2	i	130	1033	648	193	189	3	0	0	0
2	l	130	1033	648	193	189	3	0	0	0

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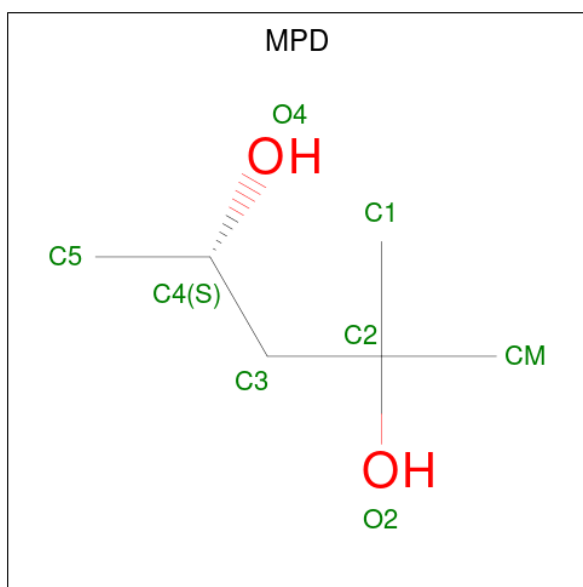
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	o	130	Total	C	N	O	Se	0	0	0
			1032	647	193	189	3			

- Molecule 3 is a protein called TraN protein.

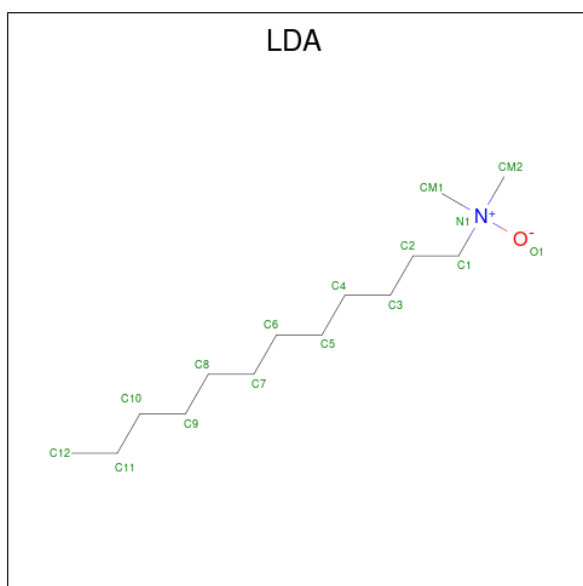
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	26	Total	C	N	O	0	0	0	
			200	126	34	40				
3	F	25	Total	C	N	O	0	0	0	
			194	123	33	38				
3	I	25	Total	C	N	O	0	0	0	
			194	123	33	38				
3	L	28	Total	C	N	O	S	0	0	0
			212	132	36	43	1			
3	O	24	Total	C	N	O	0	0	0	
			190	121	32	37				
3	R	24	Total	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: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



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

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





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

- Molecule 6 is water.

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

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

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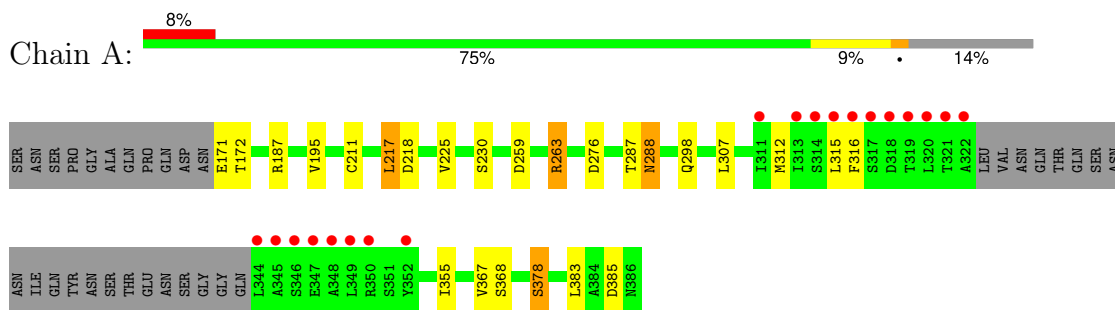
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	o	35	Total	O	0	0
			35	35		
6	p	12	Total	O	0	0
			12	12		

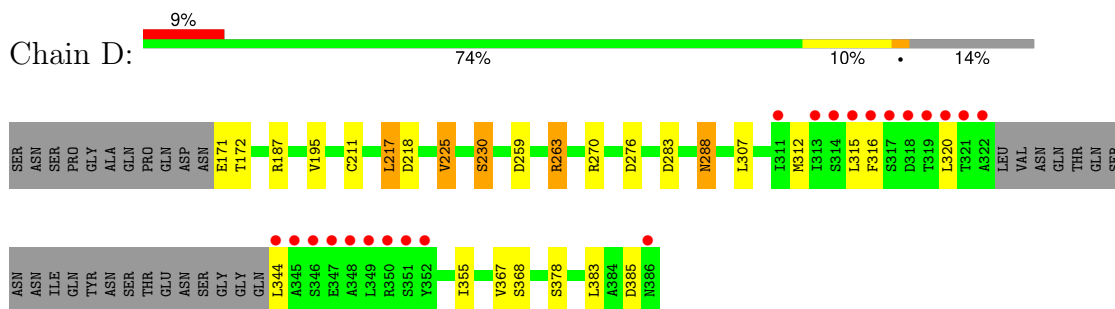
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

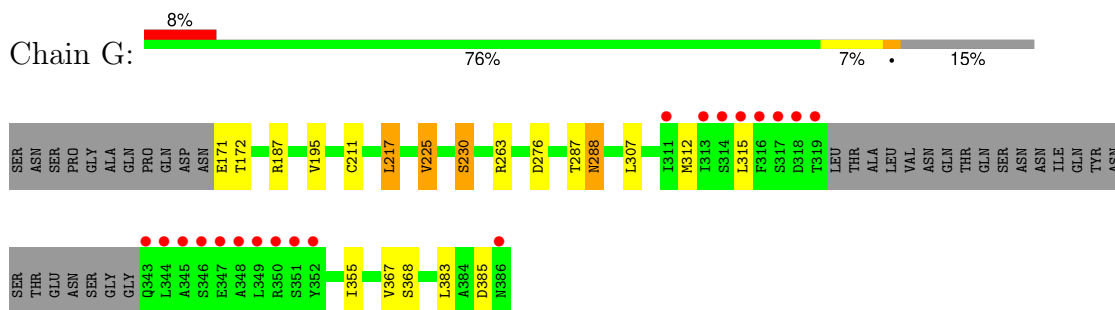
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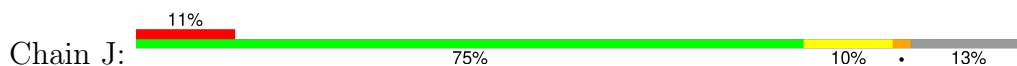
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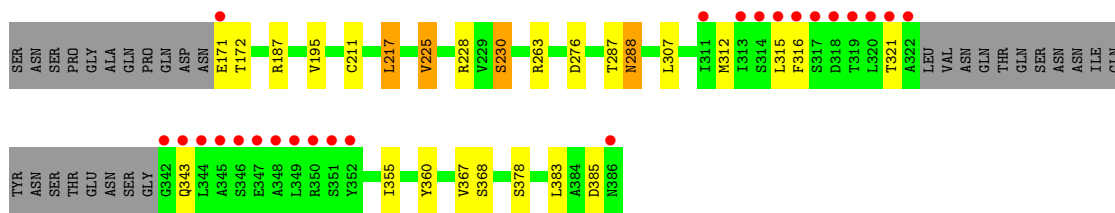


- Molecule 1: TraF protein

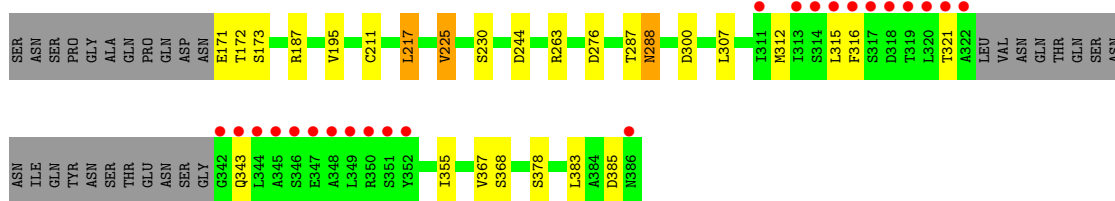
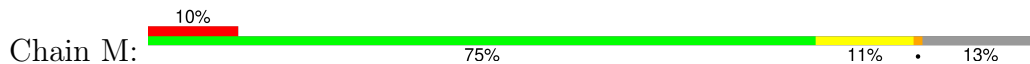


- Molecule 1: TraF protein

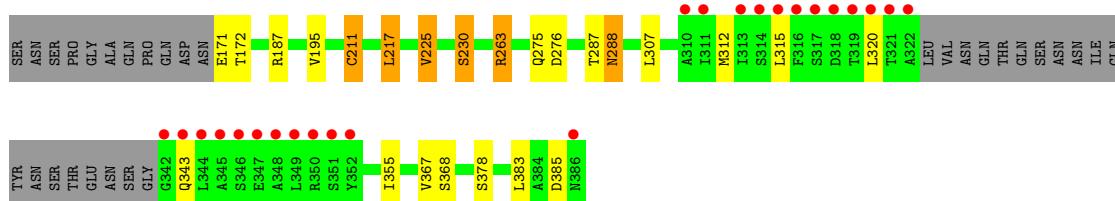
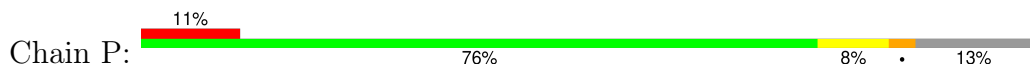




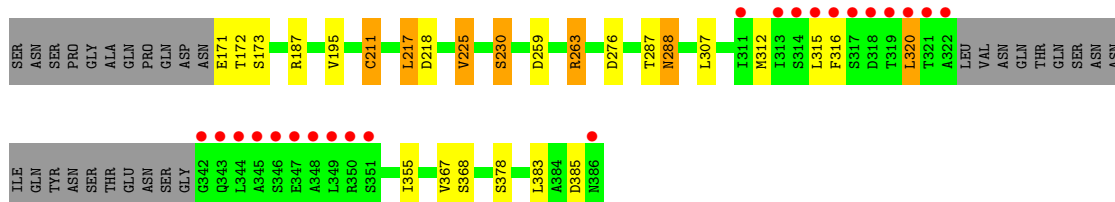
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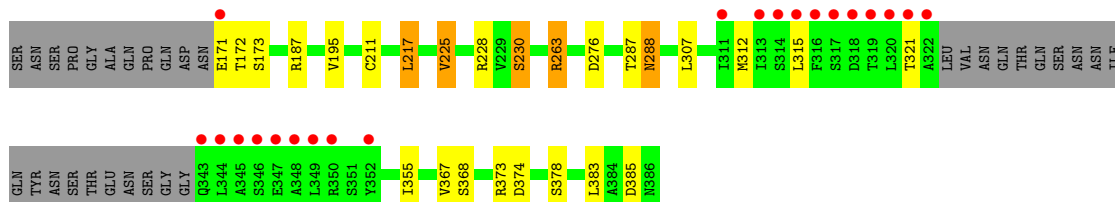
● Molecule 1: TraF protein



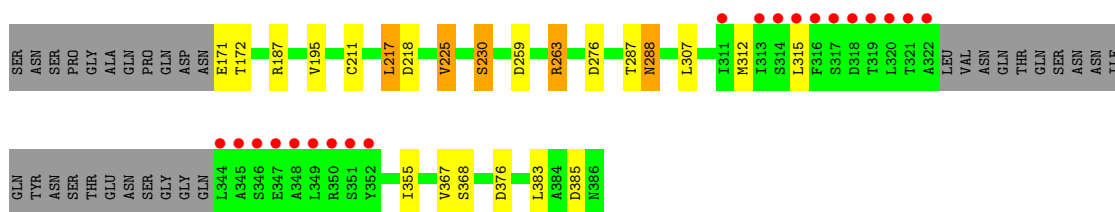
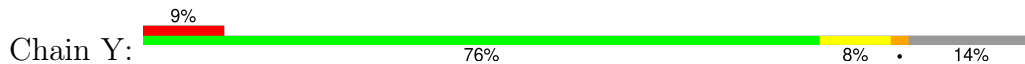
● Molecule 1: TraF protein



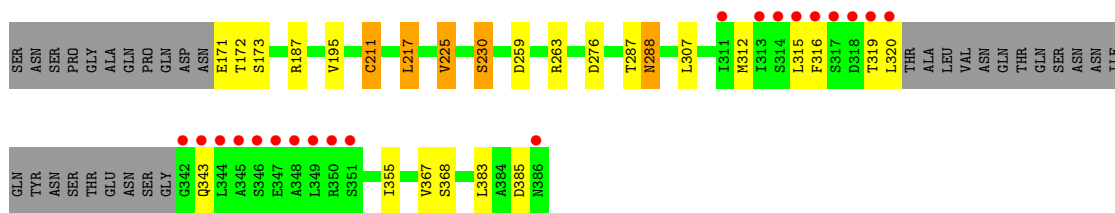
● Molecule 1: TraF protein



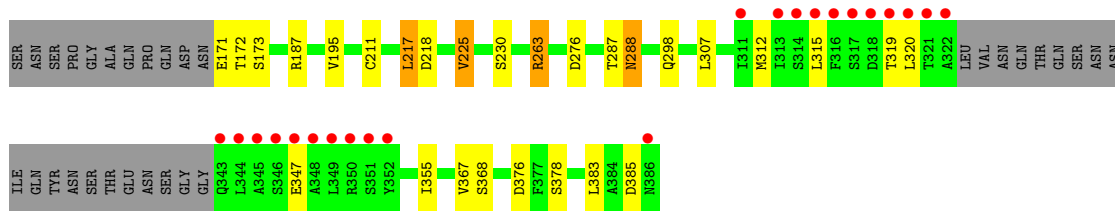
• Molecule 1: TraF protein



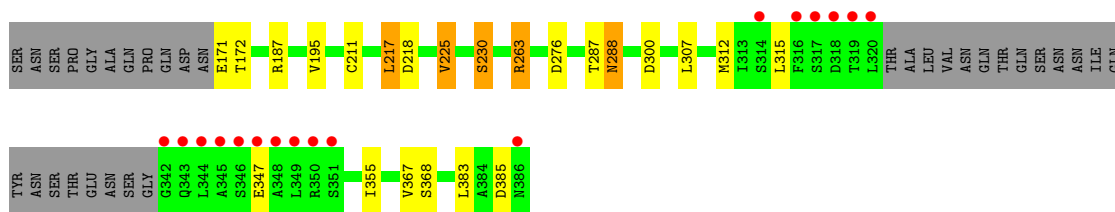
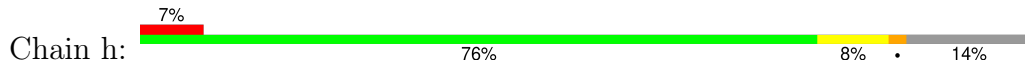
• Molecule 1: TraF protein



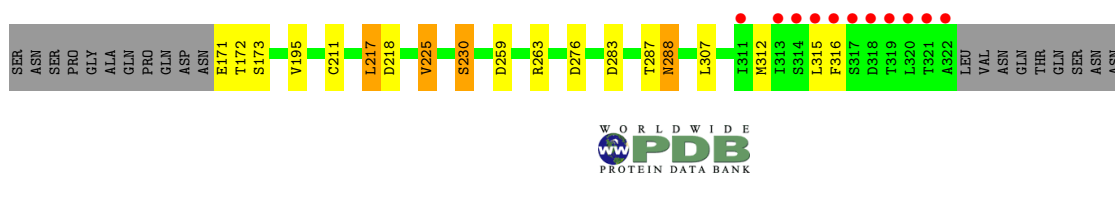
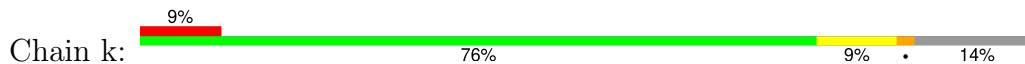
• Molecule 1: TraF protein

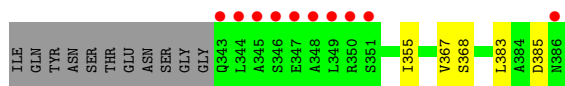


• Molecule 1: TraF protein

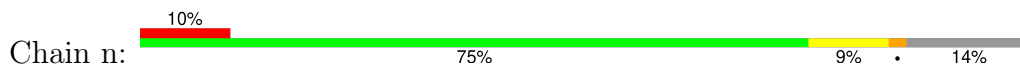


• Molecule 1: TraF protein

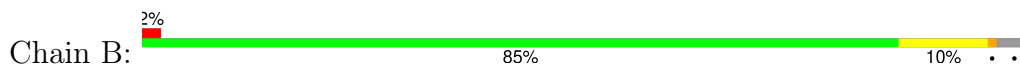




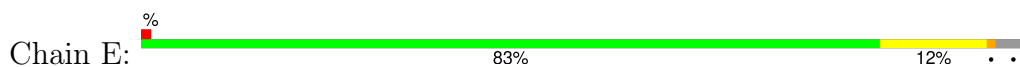
- Molecule 1: TraF protein



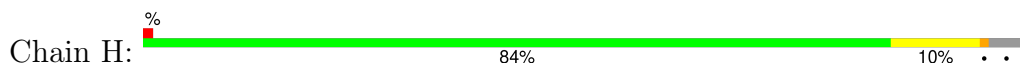
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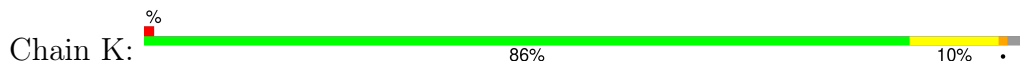
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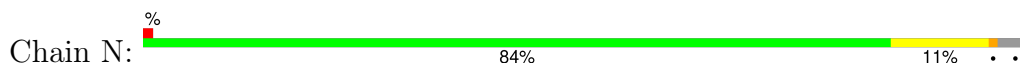
- Molecule 2: TraO protein



- Molecule 2: TraO protein

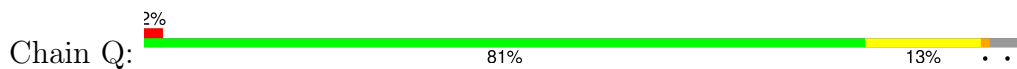


- Molecule 2: TraO protein

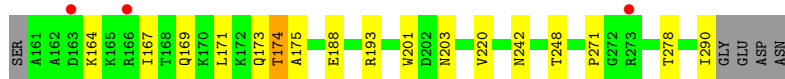
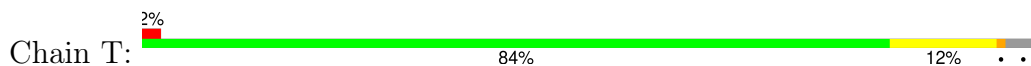




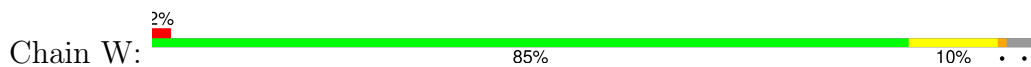
● Molecule 2: TraO protein



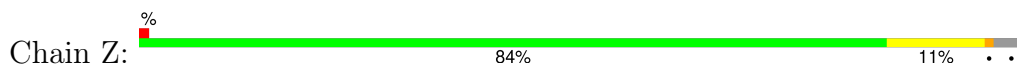
● Molecule 2: TraO protein



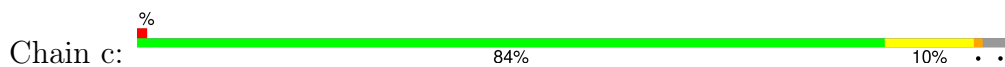
● Molecule 2: TraO protein



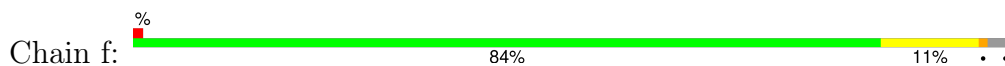
● Molecule 2: TraO protein



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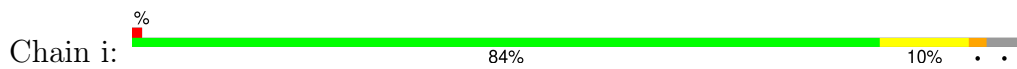


● Molecule 2: TraO protein

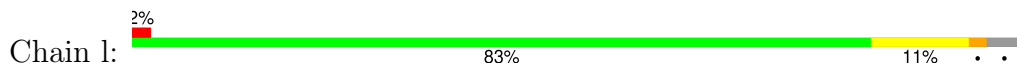


● Molecule 2: TraO protein

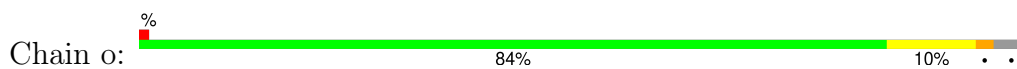




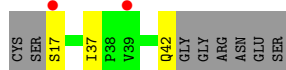
• Molecule 2: TraO protein



• Molecule 2: TraO protein



• Molecule 3: TraN protein



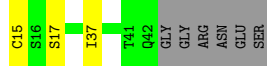
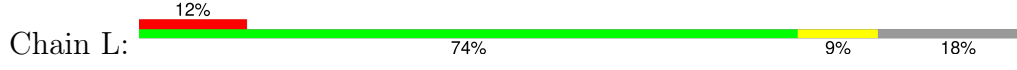
• Molecule 3: TraN protein



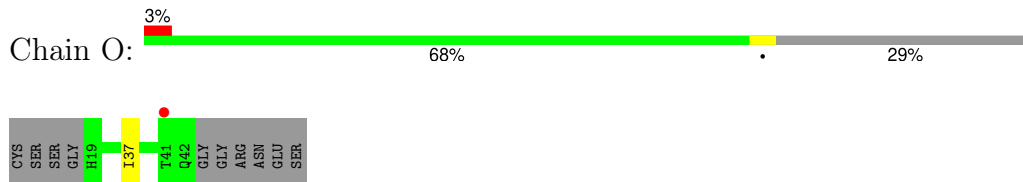
• Molecule 3: TraN protein



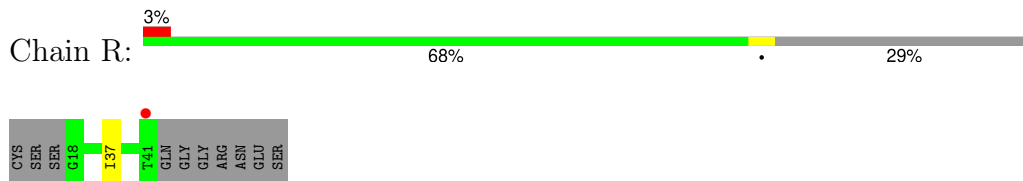
• Molecule 3: TraN protein



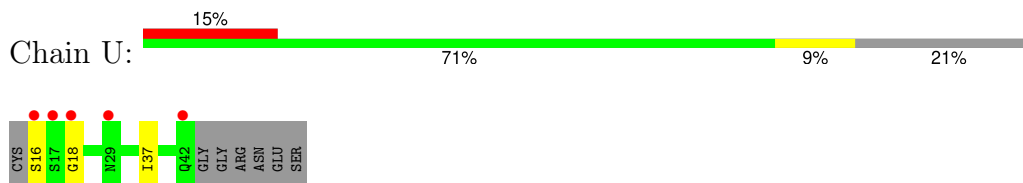
- Molecule 3: TraN protein



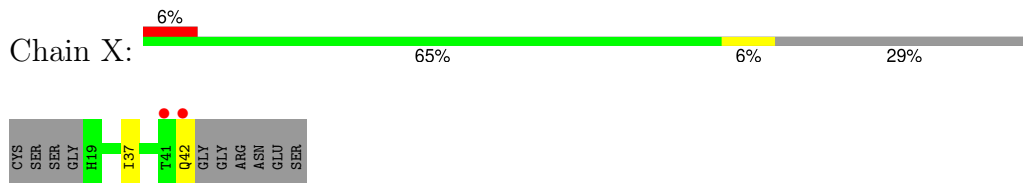
- Molecule 3: TraN protein



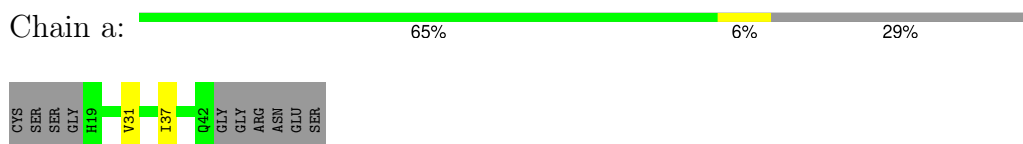
- Molecule 3: TraN protein



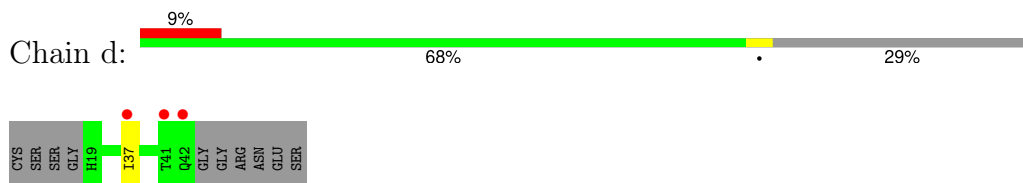
- Molecule 3: TraN protein



- Molecule 3: TraN protein

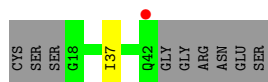


- Molecule 3: TraN protein

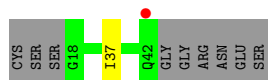


- Molecule 3: TraN protein





- Molecule 3: TraN protein



- Molecule 3: TraN protein



- Molecule 3: TraN protein



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.10 (at 2.61Å)	Xtrriage
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 <sup>2</sup> )	34.8	Xtrriage
Anisotropy	0.096	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
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	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	38842	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

All (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
1	k	276	ASP	CB-CG	-7.06	1.36	1.51
1	M	276	ASP	CB-CG	-6.86	1.37	1.51
1	V	230	SER	CB-OG	-6.80	1.33	1.42
1	h	288	ASN	CB-CG	-6.44	1.36	1.51
1	A	298	GLN	CD-NE2	-6.37	1.17	1.32
2	i	191	GLU	CB-CG	-6.35	1.40	1.52
1	D	276	ASP	CB-CG	-6.32	1.38	1.51
1	P	230	SER	CB-OG	-6.17	1.34	1.42
1	h	276	ASP	CB-CG	-6.16	1.38	1.51
1	S	211	CYS	CB-SG	-6.03	1.72	1.82
1	Y	276	ASP	CB-CG	-5.99	1.39	1.51
1	G	276	ASP	CB-CG	-5.86	1.39	1.51
1	e	276	ASP	CB-CG	-5.84	1.39	1.51
1	P	211	CYS	CB-SG	-5.83	1.72	1.81
1	G	230	SER	CB-OG	-5.80	1.34	1.42
1	b	230	SER	CB-OG	-5.57	1.35	1.42
1	Y	230	SER	CB-OG	-5.50	1.35	1.42
1	n	276	ASP	CB-CG	-5.44	1.40	1.51
1	D	230	SER	CB-OG	-5.43	1.35	1.42
1	b	276	ASP	CB-CG	-5.43	1.40	1.51
1	k	230	SER	CB-OG	-5.38	1.35	1.42
1	P	288	ASN	CB-CG	-5.36	1.38	1.51
1	b	211	CYS	CB-SG	-5.29	1.73	1.81
2	E	246	VAL	CB-CG1	-5.26	1.41	1.52
1	h	230	SER	CB-OG	-5.18	1.35	1.42
1	S	230	SER	CB-OG	-5.03	1.35	1.42

All (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
1	e	217	LEU	CA-CB-CG	9.37	136.85	115.30
1	M	217	LEU	CA-CB-CG	9.24	136.55	115.30
1	e	276	ASP	CB-CG-OD1	-9.20	110.02	118.30
1	n	217	LEU	CA-CB-CG	9.18	136.42	115.30
1	D	217	LEU	CA-CB-CG	9.13	136.31	115.30
1	e	263	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	M	263	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	D	276	ASP	CB-CG-OD1	-9.00	110.20	118.30
1	J	276	ASP	CB-CG-OD1	-8.84	110.34	118.30
1	J	217	LEU	CA-CB-CG	8.79	135.53	115.30
1	P	217	LEU	CA-CB-CG	8.73	135.37	115.30
1	Y	218	ASP	CB-CG-OD1	8.60	126.04	118.30
1	V	217	LEU	CA-CB-CG	8.60	135.08	115.30
1	h	263	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	b	217	LEU	CA-CB-CG	8.44	134.72	115.30
1	A	276	ASP	CB-CG-OD1	-8.40	110.74	118.30
1	S	263	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	h	217	LEU	CA-CB-CG	8.29	134.37	115.30
1	h	263	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	P	263	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	V	263	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	Y	217	LEU	CA-CB-CG	8.14	134.03	115.30
1	k	263	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	M	263	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	S	288	ASN	CB-CA-C	-7.83	94.74	110.40
1	k	259	ASP	CB-CG-OD1	7.73	125.26	118.30
1	S	259	ASP	CB-CG-OD1	7.65	125.19	118.30
1	J	263	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	Y	276	ASP	CB-CG-OD1	-7.47	111.58	118.30
1	A	218	ASP	CB-CG-OD2	-7.44	111.60	118.30
1	k	263	ARG	NE-CZ-NH1	7.35	123.98	120.30
2	f	265	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	A	263	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	218	ASP	CB-CG-OD1	7.20	124.78	118.30
1	G	276	ASP	CB-CG-OD1	-7.19	111.83	118.30
1	S	259	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	M	276	ASP	CB-CG-OD1	-7.12	111.89	118.30
1	n	288	ASN	CB-CA-C	-7.09	96.22	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	187	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	S	263	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	h	187	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	D	288	ASN	CB-CA-C	-6.99	96.41	110.40
1	Y	288	ASN	CB-CA-C	-6.92	96.56	110.40
1	e	187	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	A	288	ASN	CB-CA-C	-6.79	96.82	110.40
1	V	276	ASP	CB-CG-OD1	-6.79	112.19	118.30
2	Z	241	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	Y	259	ASP	CB-CG-OD1	6.78	124.40	118.30
1	k	288	ASN	CB-CA-C	-6.76	96.88	110.40
1	h	288	ASN	CB-CA-C	-6.75	96.89	110.40
2	B	271	PRO	C-N-CA	-6.73	108.16	122.30
1	V	288	ASN	CB-CA-C	-6.73	96.94	110.40
1	J	225	VAL	CB-CA-C	-6.69	98.69	111.40
1	n	263	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	Y	218	ASP	CB-CG-OD2	-6.66	112.30	118.30
1	n	187	ARG	CG-CD-NE	-6.64	97.85	111.80
1	k	218	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	P	263	ARG	NE-CZ-NH1	6.59	123.59	120.30
2	c	254	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	P	276	ASP	CB-CG-OD1	-6.55	112.41	118.30
1	J	288	ASN	CB-CA-C	-6.54	97.32	110.40
1	P	288	ASN	CB-CA-C	-6.49	97.42	110.40
1	G	288	ASN	CB-CA-C	-6.48	97.44	110.40
1	b	276	ASP	CB-CG-OD1	-6.47	112.48	118.30
1	n	263	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	b	288	ASN	CB-CA-C	-6.47	97.46	110.40
1	M	225	VAL	CB-CA-C	-6.47	99.11	111.40
1	D	225	VAL	CB-CA-C	-6.44	99.16	111.40
1	D	187	ARG	CG-CD-NE	-6.41	98.34	111.80
2	K	205	ARG	NE-CZ-NH1	-6.38	117.11	120.30
2	c	271	PRO	C-N-CA	-6.38	108.91	122.30
1	k	276	ASP	CB-CG-OD1	-6.38	112.56	118.30
1	M	288	ASN	CB-CA-C	-6.34	97.73	110.40
1	V	225	VAL	CB-CA-C	-6.33	99.38	111.40
2	N	271	PRO	C-N-CA	-6.31	109.05	122.30
1	D	217	LEU	CB-CG-CD1	-6.24	100.39	111.00
1	Y	376	ASP	CB-CG-OD1	6.24	123.92	118.30
1	D	218	ASP	CB-CG-OD1	6.21	123.89	118.30
2	W	271	PRO	C-N-CA	-6.21	109.26	122.30
1	G	225	VAL	CB-CA-C	-6.17	99.67	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	ASP	CB-CG-OD1	6.17	123.85	118.30
2	K	271	PRO	C-N-CA	-6.17	109.35	122.30
2	Q	271	PRO	C-N-CA	-6.16	109.36	122.30
1	h	218	ASP	CB-CG-OD1	6.15	123.83	118.30
1	V	187	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	b	276	ASP	CB-CA-C	-6.14	98.13	110.40
1	A	187	ARG	CG-CD-NE	-6.13	98.94	111.80
2	E	271	PRO	C-N-CA	-6.11	109.46	122.30
1	M	276	ASP	CB-CA-C	-6.09	98.21	110.40
2	T	203	ASN	N-CA-CB	-6.04	99.73	110.60
1	D	283	ASP	CB-CG-OD1	6.02	123.72	118.30
1	h	225	VAL	CB-CA-C	-6.02	99.97	111.40
2	T	271	PRO	C-N-CA	-6.01	109.68	122.30
1	b	187	ARG	CG-CD-NE	-5.97	99.27	111.80
1	n	225	VAL	CB-CA-C	-5.96	100.07	111.40
1	k	225	VAL	CB-CA-C	-5.95	100.09	111.40
1	e	288	ASN	CB-CA-C	-5.94	98.53	110.40
2	H	203	ASN	CB-CA-C	-5.90	98.59	110.40
2	W	203	ASN	CB-CA-C	-5.89	98.63	110.40
2	H	271	PRO	C-N-CA	-5.88	109.95	122.30
1	S	320	LEU	CA-CB-CG	5.88	128.82	115.30
1	Y	263	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	n	276	ASP	CB-CA-C	-5.86	98.69	110.40
1	n	373	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	Y	225	VAL	CB-CA-C	-5.82	100.34	111.40
2	l	271	PRO	C-N-CA	-5.82	110.09	122.30
1	D	187	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	D	230	SER	N-CA-CB	-5.77	101.85	110.50
2	E	241	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	G	263	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	b	217	LEU	CB-CG-CD1	-5.74	101.24	111.00
1	P	225	VAL	CB-CA-C	-5.74	100.50	111.40
1	n	217	LEU	CB-CG-CD1	-5.74	101.25	111.00
1	S	276	ASP	CB-CA-C	-5.73	98.93	110.40
1	D	320	LEU	CA-CB-CG	5.73	128.48	115.30
2	i	254	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	k	276	ASP	CB-CA-C	-5.71	98.97	110.40
1	G	263	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	Y	187	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	P	320	LEU	CA-CB-CG	5.66	128.32	115.30
2	Z	203	ASN	CB-CA-C	-5.66	99.08	110.40
1	D	263	ARG	NE-CZ-NH1	5.65	123.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	187	ARG	CG-CD-NE	-5.65	99.94	111.80
1	J	187	ARG	CG-CD-NE	-5.64	99.94	111.80
1	Y	263	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	J	276	ASP	CB-CA-C	-5.61	99.18	110.40
1	h	276	ASP	N-CA-CB	-5.59	100.54	110.60
1	e	263	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	S	218	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	J	228	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	M	244	ASP	CB-CG-OD1	5.57	123.31	118.30
1	b	263	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	M	217	LEU	CB-CG-CD2	5.55	120.44	111.00
2	c	203	ASN	CB-CA-C	-5.55	99.30	110.40
1	Y	217	LEU	CB-CG-CD1	-5.54	101.58	111.00
2	i	271	PRO	C-N-CA	-5.54	110.67	122.30
1	b	259	ASP	CB-CG-OD1	5.54	123.28	118.30
2	l	203	ASN	CB-CA-C	-5.53	99.33	110.40
2	Z	241	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	M	217	LEU	CB-CG-CD1	-5.53	101.60	111.00
2	l	254	ARG	NE-CZ-NH2	-5.53	117.53	120.30
2	l	241	ARG	CG-CD-NE	-5.50	100.24	111.80
1	S	225	VAL	CB-CA-C	-5.50	100.95	111.40
1	S	218	ASP	CB-CG-OD1	5.49	123.24	118.30
2	l	203	ASN	N-CA-CB	-5.49	100.72	110.60
2	E	203	ASN	N-CA-CB	-5.48	100.74	110.60
1	V	228	ARG	NE-CZ-NH1	5.48	123.04	120.30
2	f	271	PRO	C-N-CA	-5.47	110.81	122.30
2	f	203	ASN	CB-CA-C	-5.44	99.52	110.40
1	D	276	ASP	CB-CA-C	-5.44	99.53	110.40
2	B	203	ASN	CB-CA-C	-5.43	99.53	110.40
1	D	259	ASP	CB-CG-OD1	5.43	123.19	118.30
2	E	203	ASN	CB-CA-C	-5.42	99.56	110.40
1	b	225	VAL	CB-CA-C	-5.41	101.12	111.40
1	k	218	ASP	CB-CG-OD1	5.40	123.16	118.30
2	Q	205	ARG	NE-CZ-NH2	5.40	123.00	120.30
2	l	217	LEU	CA-CB-CG	5.37	127.64	115.30
1	P	276	ASP	CB-CA-C	-5.36	99.68	110.40
1	e	225	VAL	CB-CA-C	-5.36	101.22	111.40
1	S	187	ARG	CG-CD-NE	-5.34	100.58	111.80
1	h	217	LEU	CB-CG-CD1	-5.34	101.93	111.00
1	V	276	ASP	CB-CA-C	-5.32	99.77	110.40
1	V	373	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	Q	203	ASN	CB-CA-C	-5.29	99.83	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	270	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	M	187	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	k	283	ASP	CB-CG-OD1	5.26	123.03	118.30
1	h	300	ASP	CB-CG-OD1	5.26	123.03	118.30
1	V	263	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	V	374	ASP	CB-CG-OD1	5.25	123.03	118.30
1	n	376	ASP	CB-CG-OD1	5.24	123.02	118.30
2	c	203	ASN	N-CA-CB	-5.22	101.20	110.60
2	Z	271	PRO	C-N-CA	-5.22	111.34	122.30
2	K	203	ASN	CB-CA-C	-5.21	99.97	110.40
2	H	208	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	h	218	ASP	CB-CG-OD2	-5.19	113.63	118.30
2	Q	217	LEU	CA-CB-CG	5.18	127.22	115.30
2	o	271	PRO	C-N-CA	-5.15	111.48	122.30
2	Q	205	ARG	NE-CZ-NH1	-5.15	117.73	120.30
1	S	187	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	M	187	ARG	CG-CD-NE	-5.13	101.02	111.80
1	D	263	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	V	187	ARG	CG-CD-NE	-5.13	101.03	111.80
1	P	187	ARG	CG-CD-NE	-5.12	101.04	111.80
1	e	218	ASP	CB-CG-OD1	5.12	122.91	118.30
2	o	217	LEU	CA-CB-CG	5.11	127.06	115.30
1	b	230	SER	N-CA-CB	-5.11	102.84	110.50
1	e	376	ASP	CB-CG-OD1	5.09	122.88	118.30
1	J	230	SER	N-CA-CB	-5.09	102.86	110.50
2	Q	254	ARG	NE-CZ-NH2	-5.09	117.75	120.30
2	f	239	GLU	CB-CA-C	-5.09	100.22	110.40
1	e	276	ASP	CB-CA-C	-5.09	100.22	110.40
1	G	187	ARG	CG-CD-NE	-5.07	101.14	111.80
1	h	230	SER	N-CA-CB	-5.03	102.96	110.50
1	k	230	SER	N-CA-CB	-5.02	102.97	110.50
1	M	300	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	276	ASP	CB-CA-C	-5.02	100.36	110.40
2	Q	239	GLU	CB-CA-C	-5.01	100.37	110.40
1	n	276	ASP	CB-CG-OD1	-5.00	113.80	118.30

There are no chirality outliers.

All (43) planarity outliers are listed below:

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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
2	B	175	ALA	Peptide
2	E	174	THR	Peptide
2	E	175	ALA	Peptide
1	G	287	THR	Peptide
2	H	174	THR	Peptide
2	H	175	ALA	Peptide
1	J	287	THR	Peptide
2	K	174	THR	Peptide
2	K	175	ALA	Peptide
1	M	287	THR	Peptide
2	N	174	THR	Peptide
2	N	175	ALA	Peptide
1	P	275	GLN	Peptide
1	P	287	THR	Peptide
2	Q	174	THR	Peptide
2	Q	175	ALA	Peptide
1	S	287	THR	Peptide
2	T	174	THR	Peptide
2	T	175	ALA	Peptide
3	U	18	GLY	Peptide
1	V	287	THR	Peptide
2	W	174	THR	Peptide
2	W	175	ALA	Peptide
1	Y	287	THR	Peptide
2	Z	174	THR	Peptide
2	Z	175	ALA	Peptide
1	b	287	THR	Peptide
2	c	174	THR	Peptide
2	c	175	ALA	Peptide
1	e	287	THR	Peptide
2	f	174	THR	Peptide
2	f	175	ALA	Peptide
1	h	287	THR	Peptide
2	i	174	THR	Peptide
2	i	175	ALA	Peptide
1	k	287	THR	Peptide
2	l	174	THR	Peptide
2	l	175	ALA	Peptide
1	n	287	THR	Peptide
2	o	174	THR	Peptide
2	o	175	ALA	Peptide

## 5.2 Too-close contacts [i](#)

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

## 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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

All (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
1	P	288	ASN
1	V	288	ASN
1	b	288	ASN
1	b	319	THR

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Mol	Chain	Res	Type
1	e	288	ASN
1	h	288	ASN
1	k	288	ASN
1	n	288	ASN
1	J	288	ASN
1	M	321	THR
1	S	288	ASN
1	Y	288	ASN
2	E	173	GLN
2	H	173	GLN
2	W	173	GLN
1	A	378	SER
2	i	173	GLN
2	l	173	GLN
2	o	173	GLN
2	Q	173	GLN
2	Z	173	GLN
1	e	319	THR
2	f	173	GLN
2	c	173	GLN

### 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	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (455) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	GLU
1	A	172	THR
1	A	195	VAL
1	A	211	CYS
1	A	217	LEU
1	A	225	VAL
1	A	230	SER
1	A	263	ARG
1	A	307	LEU
1	A	312	MSE
1	A	315	LEU
1	A	316	PHE
1	A	355	ILE
1	A	367	VAL
1	A	368	SER
1	A	378	SER
1	A	383	LEU
1	A	385	ASP
2	B	164	LYS
2	B	167	ILE
2	B	169	GLN
2	B	171	LEU
2	B	173	GLN
2	B	174	THR
2	B	191	GLU
2	B	217	LEU
2	B	242	ASN
2	B	248	THR
2	B	278	THR
2	B	290	ILE
3	C	17	SER
3	C	37	ILE
3	C	42	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	171	GLU
1	D	172	THR
1	D	195	VAL
1	D	211	CYS
1	D	217	LEU
1	D	225	VAL
1	D	230	SER
1	D	263	ARG
1	D	307	LEU
1	D	312	MSE
1	D	315	LEU
1	D	316	PHE
1	D	344	LEU
1	D	355	ILE
1	D	367	VAL
1	D	368	SER
1	D	378	SER
1	D	383	LEU
1	D	385	ASP
2	E	164	LYS
2	E	167	ILE
2	E	169	GLN
2	E	171	LEU
2	E	173	GLN
2	E	174	THR
2	E	191	GLU
2	E	217	LEU
2	E	242	ASN
2	E	248	THR
2	E	249	VAL
2	E	278	THR
2	E	290	ILE
3	F	31	VAL
3	F	37	ILE
1	G	171	GLU
1	G	172	THR
1	G	195	VAL
1	G	211	CYS
1	G	217	LEU
1	G	225	VAL
1	G	230	SER
1	G	307	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	312	MSE
1	G	315	LEU
1	G	355	ILE
1	G	367	VAL
1	G	368	SER
1	G	383	LEU
1	G	385	ASP
2	H	164	LYS
2	H	167	ILE
2	H	169	GLN
2	H	173	GLN
2	H	174	THR
2	H	191	GLU
2	H	217	LEU
2	H	220	VAL
2	H	242	ASN
2	H	248	THR
2	H	278	THR
2	H	290	ILE
3	I	31	VAL
3	I	37	ILE
1	J	171	GLU
1	J	172	THR
1	J	195	VAL
1	J	211	CYS
1	J	217	LEU
1	J	225	VAL
1	J	230	SER
1	J	307	LEU
1	J	312	MSE
1	J	315	LEU
1	J	316	PHE
1	J	321	THR
1	J	343	GLN
1	J	355	ILE
1	J	360	TYR
1	J	367	VAL
1	J	368	SER
1	J	378	SER
1	J	383	LEU
1	J	385	ASP
2	K	164	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	K	167	ILE
2	K	169	GLN
2	K	173	GLN
2	K	174	THR
2	K	217	LEU
2	K	242	ASN
2	K	248	THR
2	K	278	THR
2	K	290	ILE
3	L	15	CYS
3	L	37	ILE
1	M	171	GLU
1	M	172	THR
1	M	173	SER
1	M	195	VAL
1	M	211	CYS
1	M	217	LEU
1	M	225	VAL
1	M	230	SER
1	M	307	LEU
1	M	312	MSE
1	M	315	LEU
1	M	316	PHE
1	M	343	GLN
1	M	355	ILE
1	M	367	VAL
1	M	368	SER
1	M	378	SER
1	M	383	LEU
1	M	385	ASP
2	N	164	LYS
2	N	167	ILE
2	N	169	GLN
2	N	171	LEU
2	N	173	GLN
2	N	174	THR
2	N	191	GLU
2	N	217	LEU
2	N	232	PRO
2	N	242	ASN
2	N	248	THR
2	N	249	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	N	278	THR
2	N	290	ILE
3	O	37	ILE
1	P	171	GLU
1	P	172	THR
1	P	195	VAL
1	P	211	CYS
1	P	217	LEU
1	P	225	VAL
1	P	230	SER
1	P	263	ARG
1	P	307	LEU
1	P	312	MSE
1	P	315	LEU
1	P	343	GLN
1	P	355	ILE
1	P	367	VAL
1	P	368	SER
1	P	378	SER
1	P	383	LEU
1	P	385	ASP
2	Q	164	LYS
2	Q	167	ILE
2	Q	169	GLN
2	Q	171	LEU
2	Q	173	GLN
2	Q	174	THR
2	Q	191	GLU
2	Q	220	VAL
2	Q	242	ASN
2	Q	248	THR
2	Q	249	VAL
2	Q	278	THR
2	Q	290	ILE
3	R	37	ILE
1	S	171	GLU
1	S	172	THR
1	S	173	SER
1	S	195	VAL
1	S	211	CYS
1	S	217	LEU
1	S	225	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	S	230	SER
1	S	263	ARG
1	S	307	LEU
1	S	312	MSE
1	S	315	LEU
1	S	316	PHE
1	S	320	LEU
1	S	355	ILE
1	S	367	VAL
1	S	368	SER
1	S	378	SER
1	S	383	LEU
1	S	385	ASP
2	T	164	LYS
2	T	167	ILE
2	T	169	GLN
2	T	171	LEU
2	T	173	GLN
2	T	174	THR
2	T	188	GLU
2	T	201	TRP
2	T	220	VAL
2	T	242	ASN
2	T	248	THR
2	T	278	THR
2	T	290	ILE
3	U	16	SER
3	U	37	ILE
1	V	171	GLU
1	V	172	THR
1	V	173	SER
1	V	195	VAL
1	V	211	CYS
1	V	217	LEU
1	V	225	VAL
1	V	230	SER
1	V	263	ARG
1	V	307	LEU
1	V	312	MSE
1	V	315	LEU
1	V	321	THR
1	V	355	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	V	367	VAL
1	V	368	SER
1	V	378	SER
1	V	383	LEU
1	V	385	ASP
2	W	164	LYS
2	W	167	ILE
2	W	169	GLN
2	W	171	LEU
2	W	173	GLN
2	W	174	THR
2	W	191	GLU
2	W	217	LEU
2	W	242	ASN
2	W	248	THR
2	W	278	THR
2	W	290	ILE
3	X	37	ILE
3	X	42	GLN
1	Y	171	GLU
1	Y	172	THR
1	Y	195	VAL
1	Y	211	CYS
1	Y	217	LEU
1	Y	225	VAL
1	Y	230	SER
1	Y	263	ARG
1	Y	307	LEU
1	Y	312	MSE
1	Y	315	LEU
1	Y	355	ILE
1	Y	367	VAL
1	Y	368	SER
1	Y	383	LEU
1	Y	385	ASP
2	Z	164	LYS
2	Z	167	ILE
2	Z	169	GLN
2	Z	171	LEU
2	Z	173	GLN
2	Z	174	THR
2	Z	191	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	Z	217	LEU
2	Z	220	VAL
2	Z	242	ASN
2	Z	248	THR
2	Z	278	THR
2	Z	290	ILE
3	a	31	VAL
3	a	37	ILE
1	b	171	GLU
1	b	172	THR
1	b	173	SER
1	b	195	VAL
1	b	211	CYS
1	b	217	LEU
1	b	225	VAL
1	b	230	SER
1	b	307	LEU
1	b	312	MSE
1	b	315	LEU
1	b	316	PHE
1	b	320	LEU
1	b	343	GLN
1	b	355	ILE
1	b	367	VAL
1	b	368	SER
1	b	383	LEU
1	b	385	ASP
2	c	164	LYS
2	c	167	ILE
2	c	169	GLN
2	c	171	LEU
2	c	173	GLN
2	c	174	THR
2	c	191	GLU
2	c	217	LEU
2	c	242	ASN
2	c	248	THR
2	c	278	THR
2	c	290	ILE
3	d	37	ILE
1	e	171	GLU
1	e	172	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	e	173	SER
1	e	195	VAL
1	e	211	CYS
1	e	217	LEU
1	e	225	VAL
1	e	230	SER
1	e	263	ARG
1	e	307	LEU
1	e	312	MSE
1	e	315	LEU
1	e	320	LEU
1	e	347	GLU
1	e	355	ILE
1	e	367	VAL
1	e	368	SER
1	e	378	SER
1	e	383	LEU
1	e	385	ASP
2	f	164	LYS
2	f	167	ILE
2	f	169	GLN
2	f	171	LEU
2	f	173	GLN
2	f	174	THR
2	f	191	GLU
2	f	217	LEU
2	f	242	ASN
2	f	248	THR
2	f	278	THR
2	f	290	ILE
3	g	37	ILE
1	h	171	GLU
1	h	172	THR
1	h	195	VAL
1	h	211	CYS
1	h	217	LEU
1	h	225	VAL
1	h	230	SER
1	h	263	ARG
1	h	307	LEU
1	h	312	MSE
1	h	315	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	h	347	GLU
1	h	355	ILE
1	h	367	VAL
1	h	368	SER
1	h	383	LEU
1	h	385	ASP
2	i	164	LYS
2	i	167	ILE
2	i	169	GLN
2	i	171	LEU
2	i	173	GLN
2	i	174	THR
2	i	191	GLU
2	i	201	TRP
2	i	217	LEU
2	i	220	VAL
2	i	242	ASN
2	i	278	THR
2	i	290	ILE
3	j	37	ILE
1	k	171	GLU
1	k	172	THR
1	k	173	SER
1	k	195	VAL
1	k	211	CYS
1	k	217	LEU
1	k	225	VAL
1	k	230	SER
1	k	307	LEU
1	k	312	MSE
1	k	315	LEU
1	k	316	PHE
1	k	355	ILE
1	k	367	VAL
1	k	368	SER
1	k	383	LEU
1	k	385	ASP
2	l	164	LYS
2	l	167	ILE
2	l	169	GLN
2	l	171	LEU
2	l	173	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	l	174	THR
2	l	188	GLU
2	l	191	GLU
2	l	217	LEU
2	l	242	ASN
2	l	248	THR
2	l	278	THR
2	l	290	ILE
3	m	37	ILE
1	n	168	GLN
1	n	169	ASP
1	n	172	THR
1	n	173	SER
1	n	195	VAL
1	n	211	CYS
1	n	217	LEU
1	n	225	VAL
1	n	230	SER
1	n	258	LYS
1	n	263	ARG
1	n	307	LEU
1	n	312	MSE
1	n	315	LEU
1	n	355	ILE
1	n	367	VAL
1	n	368	SER
1	n	378	SER
1	n	383	LEU
1	n	385	ASP
2	o	164	LYS
2	o	167	ILE
2	o	169	GLN
2	o	171	LEU
2	o	173	GLN
2	o	174	THR
2	o	191	GLU
2	o	201	TRP
2	o	217	LEU
2	o	220	VAL
2	o	242	ASN
2	o	248	THR
2	o	278	THR

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Mol	Chain	Res	Type
2	o	290	ILE
3	p	37	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	302	HIS
2	B	169	GLN
2	B	199	HIS
2	B	242	ASN
2	B	268	ASN
1	D	182	ASN
1	D	298	GLN
1	D	302	HIS
2	E	169	GLN
2	E	219	GLN
2	E	242	ASN
2	E	268	ASN
1	G	182	ASN
1	G	298	GLN
1	G	302	HIS
2	H	219	GLN
2	H	242	ASN
2	H	268	ASN
1	J	298	GLN
1	J	302	HIS
2	K	169	GLN
2	K	219	GLN
2	K	242	ASN
2	K	268	ASN
1	M	182	ASN
1	M	298	GLN
1	M	302	HIS
2	N	169	GLN
2	N	219	GLN
2	N	242	ASN
2	N	268	ASN
3	O	19	HIS
1	P	182	ASN
1	P	298	GLN
1	P	302	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	Q	169	GLN
2	Q	199	HIS
2	Q	219	GLN
2	Q	242	ASN
2	Q	268	ASN
3	R	19	HIS
1	S	182	ASN
1	S	298	GLN
1	S	302	HIS
2	T	169	GLN
2	T	199	HIS
2	T	219	GLN
2	T	242	ASN
2	T	268	ASN
3	U	34	ASN
1	V	182	ASN
1	V	298	GLN
1	V	302	HIS
2	W	169	GLN
2	W	219	GLN
2	W	242	ASN
2	W	268	ASN
3	X	19	HIS
3	X	42	GLN
1	Y	182	ASN
1	Y	298	GLN
1	Y	302	HIS
2	Z	169	GLN
2	Z	219	GLN
2	Z	242	ASN
2	Z	268	ASN
3	a	19	HIS
1	b	182	ASN
1	b	298	GLN
1	b	302	HIS
2	c	169	GLN
2	c	219	GLN
2	c	242	ASN
2	c	268	ASN
3	d	19	HIS
1	e	182	ASN
1	e	302	HIS

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Mol	Chain	Res	Type
1	e	343	GLN
2	f	169	GLN
2	f	199	HIS
2	f	242	ASN
2	f	268	ASN
3	g	19	HIS
1	h	182	ASN
1	h	298	GLN
1	h	302	HIS
2	i	169	GLN
2	i	199	HIS
2	i	219	GLN
2	i	242	ASN
2	i	268	ASN
3	j	34	ASN
1	k	182	ASN
1	k	298	GLN
1	k	302	HIS
1	k	343	GLN
2	l	169	GLN
2	l	219	GLN
2	l	242	ASN
2	l	268	ASN
1	n	170	ASN
1	n	182	ASN
1	n	298	GLN
1	n	302	HIS
2	o	169	GLN
2	o	219	GLN
2	o	242	ASN
2	o	268	ASN
3	p	19	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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. '2' 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.

All (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
5	J	1	LDA	C5-C6-C7-C8
5	J	1	LDA	C2-C3-C4-C5
5	J	1	LDA	C11-C10-C9-C8
5	J	1	LDA	C4-C5-C6-C7
5	J	1	LDA	C9-C10-C11-C12
5	J	1	LDA	C6-C7-C8-C9
5	J	1	LDA	C3-C4-C5-C6
4	D	1	MPD	O2-C2-C3-C4
4	D	1	MPD	C1-C2-C3-C4
4	D	1	MPD	CM-C2-C3-C4
5	J	1	LDA	C7-C8-C9-C10
4	h	2	MPD	O2-C2-C3-C4
4	h	2	MPD	C1-C2-C3-C4
4	h	2	MPD	CM-C2-C3-C4

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	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 <sup>2</sup> )	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

All (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
1	D	345	ALA	8.4
1	b	316	PHE	8.4
1	b	343	GLN	8.4
1	J	343	GLN	8.3
1	k	345	ALA	8.3
1	e	316	PHE	8.3
1	h	342	GLY	8.2
1	b	317	SER	8.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	V	316	PHE	8.2
1	e	317	SER	8.2
1	b	342	GLY	8.1
1	P	316	PHE	8.1
1	M	316	PHE	8.1
1	e	344	LEU	8.0
1	e	343	GLN	8.0
1	h	318	ASP	8.0
1	h	344	LEU	8.0
1	k	349	LEU	8.0
1	D	344	LEU	8.0
1	P	349	LEU	7.8
1	M	320	LEU	7.8
1	D	321	THR	7.8
1	J	349	LEU	7.7
1	Y	318	ASP	7.7
1	M	343	GLN	7.6
1	A	316	PHE	7.6
1	b	345	ALA	7.5
1	k	318	ASP	7.4
1	e	318	ASP	7.3
1	k	321	THR	7.3
1	S	345	ALA	7.3
1	n	319	THR	7.3
1	n	316	PHE	7.3
1	Y	316	PHE	7.3
1	D	316	PHE	7.2
1	h	316	PHE	7.2
1	h	345	ALA	7.1
1	P	313	ILE	7.1
1	S	316	PHE	7.1
1	G	344	LEU	7.1
1	k	320	LEU	7.1
1	k	316	PHE	7.0
1	G	317	SER	7.0
1	b	320	LEU	7.0
1	P	342	GLY	7.0
1	M	344	LEU	6.9
1	P	345	ALA	6.8
1	A	318	ASP	6.8
1	e	346	SER	6.8
1	J	321	THR	6.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	M	318	ASP	6.7
1	b	318	ASP	6.6
1	A	320	LEU	6.6
1	P	348	ALA	6.6
1	Y	321	THR	6.6
1	n	168	GLN	6.5
1	D	320	LEU	6.5
1	k	344	LEU	6.5
1	V	317	SER	6.5
1	J	318	ASP	6.5
1	h	317	SER	6.4
1	V	349	LEU	6.4
1	V	318	ASP	6.4
1	D	348	ALA	6.3
1	h	343	GLN	6.3
1	n	169	ASP	6.1
1	Y	320	LEU	6.1
1	J	344	LEU	6.1
1	P	318	ASP	6.1
1	k	348	ALA	6.0
1	M	342	GLY	6.0
1	P	320	LEU	6.0
1	S	321	THR	6.0
1	e	349	LEU	6.0
1	Y	317	SER	6.0
1	k	346	SER	6.0
1	e	347	GLU	6.0
1	k	315	LEU	5.9
1	G	316	PHE	5.9
1	S	348	ALA	5.8
1	Y	344	LEU	5.8
1	e	348	ALA	5.8
1	P	314	SER	5.8
1	G	318	ASP	5.8
1	V	319	THR	5.8
1	h	346	SER	5.8
1	S	344	LEU	5.7
1	M	321	THR	5.7
1	P	321	THR	5.7
1	S	314	SER	5.7
1	S	342	GLY	5.7
1	J	345	ALA	5.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	b	319	THR	5.7
1	P	344	LEU	5.6
1	h	320	LEU	5.6
1	D	317	SER	5.6
1	n	349	LEU	5.6
1	M	349	LEU	5.6
1	h	319	THR	5.6
1	V	320	LEU	5.5
1	V	344	LEU	5.5
1	G	345	ALA	5.5
1	J	316	PHE	5.5
1	e	321	THR	5.4
1	S	349	LEU	5.4
1	V	321	THR	5.4
1	M	317	SER	5.4
1	D	349	LEU	5.4
1	n	314	SER	5.3
1	k	317	SER	5.3
1	J	346	SER	5.3
1	Y	345	ALA	5.3
1	b	349	LEU	5.3
1	M	319	THR	5.2
1	S	318	ASP	5.2
1	S	317	SER	5.2
1	V	345	ALA	5.2
1	G	346	SER	5.1
1	V	347	GLU	5.1
1	M	315	LEU	5.1
3	U	16	SER	5.1
1	b	344	LEU	5.1
1	n	318	ASP	5.1
1	J	320	LEU	5.0
1	V	348	ALA	5.0
1	A	344	LEU	5.0
1	S	320	LEU	5.0
1	G	314	SER	5.0
1	D	315	LEU	4.9
1	M	348	ALA	4.9
1	J	317	SER	4.9
1	S	343	GLN	4.9
1	e	320	LEU	4.9
1	P	343	GLN	4.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	e	322	ALA	4.8
1	e	345	ALA	4.8
1	G	343	GLN	4.8
1	M	346	SER	4.8
1	n	170	ASN	4.8
1	P	315	LEU	4.8
1	V	315	LEU	4.7
1	n	348	ALA	4.7
1	Y	315	LEU	4.7
1	G	319	THR	4.7
1	D	347	GLU	4.7
2	W	163	ASP	4.7
1	Y	349	LEU	4.7
1	h	348	ALA	4.7
1	D	318	ASP	4.6
1	Y	350	ARG	4.6
2	o	273	ARG	4.6
1	P	317	SER	4.6
1	Y	319	THR	4.6
1	A	317	SER	4.6
1	P	322	ALA	4.5
1	J	348	ALA	4.5
1	M	313	ILE	4.5
1	n	317	SER	4.4
1	n	344	LEU	4.4
1	Y	313	ILE	4.4
1	A	348	ALA	4.4
1	A	346	SER	4.3
1	b	348	ALA	4.3
1	k	347	GLU	4.3
1	h	347	GLU	4.3
1	A	314	SER	4.3
1	D	351	SER	4.3
1	S	351	SER	4.3
1	b	346	SER	4.3
1	D	322	ALA	4.2
1	P	351	SER	4.2
1	J	314	SER	4.2
2	f	273	ARG	4.2
1	P	347	GLU	4.2
1	J	350	ARG	4.1
1	n	351	SER	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	V	313	ILE	4.1
2	Z	273	ARG	4.1
1	k	314	SER	4.0
1	k	343	GLN	4.0
1	S	315	LEU	4.0
1	G	313	ILE	4.0
1	A	349	LEU	4.0
1	G	348	ALA	4.0
1	k	322	ALA	4.0
3	C	17	SER	4.0
1	b	311	ILE	4.0
1	A	319	THR	3.9
1	G	315	LEU	3.9
1	D	319	THR	3.9
1	P	319	THR	3.9
1	S	347	GLU	3.9
1	Y	314	SER	3.9
1	J	351	SER	3.9
1	k	351	SER	3.9
1	G	347	GLU	3.9
1	e	319	THR	3.9
1	S	311	ILE	3.9
1	S	350	ARG	3.8
1	M	314	SER	3.8
1	J	319	THR	3.8
1	S	322	ALA	3.8
2	i	273	ARG	3.8
1	M	345	ALA	3.7
2	T	273	ARG	3.7
1	J	315	LEU	3.7
1	D	311	ILE	3.7
1	M	311	ILE	3.7
2	N	273	ARG	3.7
1	G	386	ASN	3.7
3	U	18	GLY	3.7
3	U	17	SER	3.7
1	S	319	THR	3.7
2	Q	273	ARG	3.6
1	G	350	ARG	3.6
1	b	350	ARG	3.6
1	e	313	ILE	3.6
1	Y	347	GLU	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	P	346	SER	3.5
3	L	17	SER	3.5
1	V	311	ILE	3.5
1	b	347	GLU	3.5
1	A	347	GLU	3.5
1	P	352	TYR	3.5
1	n	347	GLU	3.5
3	O	41	THR	3.5
3	d	42	GLN	3.5
1	e	315	LEU	3.5
1	J	313	ILE	3.4
1	M	351	SER	3.4
1	M	347	GLU	3.4
2	N	163	ASP	3.3
2	H	166	ARG	3.3
3	X	42	GLN	3.3
1	b	314	SER	3.3
2	l	166	ARG	3.3
1	n	346	SER	3.3
1	D	313	ILE	3.3
1	k	319	THR	3.2
2	W	273	ARG	3.2
1	Y	348	ALA	3.2
1	h	351	SER	3.2
1	S	346	SER	3.2
1	J	347	GLU	3.2
1	Y	346	SER	3.2
1	e	386	ASN	3.2
3	d	41	THR	3.2
2	H	273	ARG	3.2
1	b	313	ILE	3.2
2	K	273	ARG	3.2
1	A	311	ILE	3.1
3	g	42	GLN	3.1
1	Y	351	SER	3.1
3	L	15	CYS	3.1
1	e	314	SER	3.1
1	A	321	THR	3.1
3	F	41	THR	3.1
1	A	322	ALA	3.0
1	k	313	ILE	3.0
1	D	386	ASN	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	c	273	ARG	3.0
1	k	350	ARG	3.0
2	f	166	ARG	3.0
1	D	346	SER	3.0
1	J	322	ALA	3.0
1	Y	352	TYR	2.9
2	B	273	ARG	2.9
3	j	42	GLN	2.9
3	X	41	THR	2.9
3	U	42	GLN	2.9
3	L	41	THR	2.9
3	d	37	ILE	2.9
1	G	351	SER	2.9
2	E	273	ARG	2.9
1	M	350	ARG	2.9
1	e	351	SER	2.9
1	Y	311	ILE	2.8
2	l	273	ARG	2.8
1	J	352	TYR	2.8
2	c	163	ASP	2.8
1	D	350	ARG	2.8
1	h	314	SER	2.8
1	J	311	ILE	2.8
1	b	315	LEU	2.8
1	k	311	ILE	2.8
1	S	386	ASN	2.8
1	M	322	ALA	2.7
2	K	163	ASP	2.7
1	V	352	TYR	2.7
1	h	386	ASN	2.7
1	V	350	ARG	2.7
1	M	386	ASN	2.7
1	V	322	ALA	2.7
1	G	352	TYR	2.7
1	n	386	ASN	2.6
1	A	315	LEU	2.6
1	G	311	ILE	2.6
1	b	386	ASN	2.6
1	n	313	ILE	2.6
3	R	41	THR	2.6
1	V	346	SER	2.6
1	A	313	ILE	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	Z	163	ASP	2.6
1	P	386	ASN	2.5
2	Q	163	ASP	2.5
1	V	314	SER	2.5
1	h	350	ARG	2.5
1	e	311	ILE	2.4
1	n	315	LEU	2.4
1	n	350	ARG	2.4
1	Y	322	ALA	2.4
2	B	166	ARG	2.4
3	F	18	GLY	2.4
2	Q	166	ARG	2.4
1	b	351	SER	2.4
2	B	163	ASP	2.4
1	k	386	ASN	2.4
3	m	42	GLN	2.4
2	T	163	ASP	2.3
2	W	171	LEU	2.3
1	V	171	GLU	2.3
1	V	343	GLN	2.3
1	M	352	TYR	2.3
1	P	311	ILE	2.3
2	T	166	ARG	2.3
3	L	16	SER	2.3
2	o	166	ARG	2.3
3	C	39	VAL	2.3
1	n	311	ILE	2.2
1	J	386	ASN	2.2
1	n	342	GLY	2.2
1	J	171	GLU	2.2
1	A	350	ARG	2.2
1	P	350	ARG	2.2
1	e	352	TYR	2.2
2	l	163	ASP	2.2
1	e	350	ARG	2.1
1	S	313	ILE	2.1
2	E	166	ARG	2.1
1	n	352	TYR	2.1
1	D	352	TYR	2.1
1	A	352	TYR	2.1
3	U	29	ASN	2.0
1	D	314	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	P	310	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	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.