



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2014 – 06:13 PM BST

PDB ID : 4F77  
Title : The 8S snRNP Assembly Intermediate  
Authors : Grimm, C.; Pelz, J.P.; Schindelin, H.; Diederichs, K.; Kuper, J.; Kisker, C.  
Deposited on : 2012-05-15  
Resolution : 3.10 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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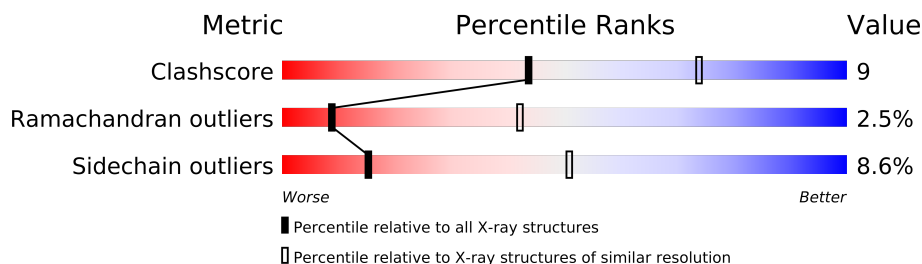
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23004

# 1 Overall quality at a glance

The reported resolution of this entry is 3.10 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))
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	119	
1	I	119	
1	Q	119	
1	Y	119	
1	g	119	
1	o	119	
1	w	119	
2	B	118	
2	J	118	
2	R	118	
2	Z	118	
2	h	118	
2	p	118	
2	x	118	
3	C	92	
3	K	92	
3	S	92	

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Mol	Chain	Length	Quality of chain
3	a	92	
3	i	92	
3	q	92	
3	y	92	
4	D	86	
4	L	86	
4	T	86	
4	b	86	
4	j	86	
4	r	86	
4	z	86	
5	1	124	
5	E	124	
5	M	124	
5	U	124	
5	c	124	
5	k	124	
5	s	124	
6	2	247	
6	F	247	
6	N	247	
6	V	247	
6	d	247	
6	l	247	
6	t	247	
7	3	186	
7	G	186	
7	O	186	
7	W	186	
7	e	186	
7	m	186	
7	u	186	
8	4	76	
8	H	76	
8	P	76	
8	X	76	
8	f	76	
8	n	76	
8	v	76	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 42689 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	A	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	Q	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	Y	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	g	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	o	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	w	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			

- Molecule 2 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	B	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	R	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	Z	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	h	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	p	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	x	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			

- Molecule 3 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	C	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	S	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	a	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	i	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	q	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	y	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			

- Molecule 4 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	71	Total	C	N	O	S	0	0	0
			556	358	92	101	5			
4	D	71	Total	C	N	O	S	0	0	0
			556	358	92	101	5			
4	T	71	Total	C	N	O	S	0	0	0
			556	358	92	101	5			
4	b	71	Total	C	N	O	S	0	0	0
			556	358	92	101	5			
4	j	71	Total	C	N	O	S	0	0	0
			556	358	92	101	5			
4	r	71	Total	C	N	O	S	0	0	0
			556	358	92	101	5			
4	z	71	Total	C	N	O	S	0	0	0
			556	358	92	101	5			

- Molecule 5 is a protein called LD23602p.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	M	17	Total	C	N	O	0	0	0
			133	85	19	29			
5	E	17	Total	C	N	O	0	0	0
			133	85	19	29			
5	U	17	Total	C	N	O	0	0	0
			133	85	19	29			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	c	17	Total	C	N	O	0	0	0
			133	85	19	29			
5	k	17	Total	C	N	O	0	0	0
			133	85	19	29			
5	s	17	Total	C	N	O	0	0	0
			133	85	19	29			
5	1	17	Total	C	N	O	0	0	0
			133	85	19	29			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
M	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
E	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
E	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
U	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
U	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
c	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
c	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
k	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
k	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
s	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
s	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
1	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
1	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74

- Molecule 6 is a protein called CG10419.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	N	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	F	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	V	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	d	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	l	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	t	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	2	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
N	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
F	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
F	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
V	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
V	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
d	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
d	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
l	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
l	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
t	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
t	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
2	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
2	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0

- Molecule 7 is a protein called Icln.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	O	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	G	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	W	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	e	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	m	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	u	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	3	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			

There are 42 discrepancies between the modelled and reference sequences:

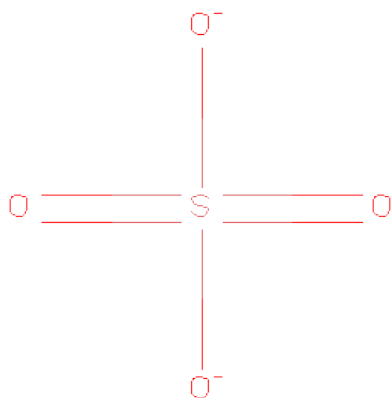
Chain	Residue	Modelled	Actual	Comment	Reference
O	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1
O	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
O	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
O	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
O	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
O	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
G	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1
G	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
G	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
G	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
G	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
G	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
W	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1
W	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
W	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
W	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
W	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
W	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
e	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1
e	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
e	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
e	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
e	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
e	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
m	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1
m	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
m	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
m	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
m	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
m	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
u	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1
u	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
u	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
u	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
u	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
u	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
3	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1
3	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
3	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
3	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
3	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
3	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1

- Molecule 8 is a protein called Small nuclear ribonucleoprotein G.



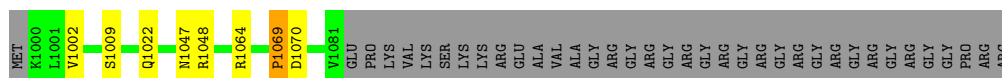
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	P	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	H	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	X	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	f	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	n	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	v	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	4	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



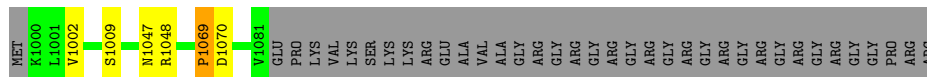
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	t	1	Total	O	S	0	0
			5	4	1		
9	2	1	Total	O	S	0	0
			5	4	1		





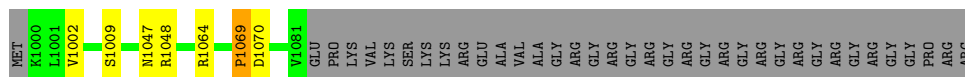
- Molecule 1: Small nuclear ribonucleoprotein Sm D1

Chain 0: 



- Molecule 1: Small nuclear ribonucleoprotein Sm D1

Chain w:



- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain J:



- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain B:



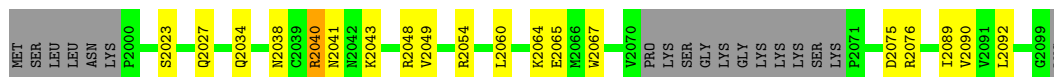
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Chain R:



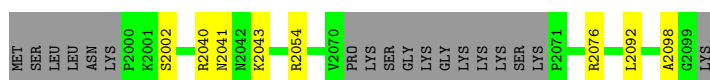
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain Z:



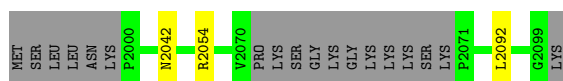
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain h:



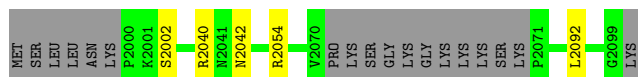
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain p:



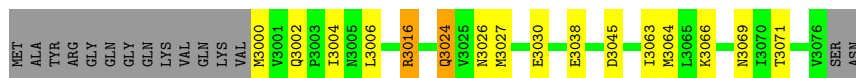
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain x:



- Molecule 3: Small nuclear ribonucleoprotein E

Chain K:



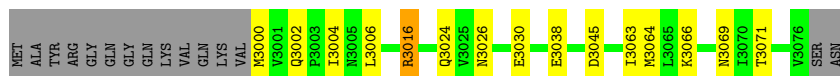
- Molecule 3: Small nuclear ribonucleoprotein E

Chain C:



- Molecule 3: Small nuclear ribonucleoprotein E

Chain S:



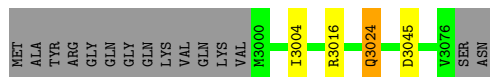
- Molecule 3: Small nuclear ribonucleoprotein E

Chain a:



- Molecule 3: Small nuclear ribonucleoprotein E

Chain i:



- Molecule 3: Small nuclear ribonucleoprotein E

Chain q: 

MET	ALA	TYR	ARG	GLY	GLN	GLY	GLN	LYS	VAL	GLN	LYS	VAL	K3000	I3004	R3016	Q3024	Y3025	N3026	D3045	V3076	SER	ASN
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- Molecule 3: Small nuclear ribonucleoprotein E

Chain y: 

MET	ALA	TYR	ARG	GLY	GLN	GLY	GLN	LYS	VAL	GLN	LYS	VAL	K3000	R3016	Q3024	V3025	N3026	D3045	V3076	SER	ASN
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- Molecule 4: Small nuclear ribonucleoprotein F

Chain L: 

MET	SER	LEU	PRO	LEU	N4000	P4001	K4002	P4003	F4004	K4016	L4017	K4018	W4019	G4020	M4021	V4030	D4031	D4046	L4053	V4056	R4059	C4060	N4061	N4062	V4063	L4064	R4067	E4070	GLU	GLU	GLU	GLU	ASP	GLY	GLY	MET	ARG	GLU
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- Molecule 4: Small nuclear ribonucleoprotein F

Chain D: 

MET	SER	LEU	PRO	LEU	N4000	P4001	K4002	P4003	F4004	K4016	L4017	K4018	W4019	G4020	M4021	V4030	D4031	D4046	L4053	V4056	R4059	C4060	N4061	N4062	V4063	L4064	R4067	E4070	GLU	GLU	GLU	GLU	ASP	GLY	GLY	MET	ARG	GLU
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- Molecule 4: Small nuclear ribonucleoprotein F

Chain T: 

MET	SER	LEU	PRO	LEU	N4000	P4001	K4002	P4003	F4004	L4005	K4016	L4017	K4018	W4019	G4020	M4021	V4030	D4031	D4046	L4053	V4056	R4059	C4060	N4061	N4062	V4063	L4064	R4067	E4070	GLU	GLU	GLU	GLU	ASP	GLY	GLY	MET	ARG	GLU
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- Molecule 4: Small nuclear ribonucleoprotein F

Chain b: 

MET	SER	LEU	PRO	LEU	N4000	P4001	K4002	M4021	D4046	L4053	E4070	GLU	GLU	GLU	GLU	ASP	GLY	GLY	MET	ARG	GLU
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- Molecule 4: Small nuclear ribonucleoprotein F

Chain j: 

MET	SER	LEU	PRO	LEU	N4000	P4001	K4002	M4021	D4046	L4053	E4070	GLU	GLU	GLU	GLU	ASP	GLY	GLY	MET	ARG	GLU
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- Molecule 4: Small nuclear ribonucleoprotein F

Chain r: 

MET	SER	LEU	PRO	LEU	N4000	P4001	K4002	M4021	D4046	L4053	E4070	GLU	GLU	GLU	GLU	ASP	GLY	GLY	MET	ARG	GLU
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- Molecule 4: Small nuclear ribonucleoprotein F

Chain z: 

MET	SER	LEU	PRO	LEU	N4000	M4021	D4046	L4053	E4070	GLU	GLU	GLU	GLU	ASP	GLY	MET	ARG	GLU
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- Molecule 5: LD23602p

Chain M: 

GLY	ALA	MET	SER	ASP	GLU	THR	ASN	LYS	A7000	V7001	W7002	S7005	L7006	L7007	T7010	S7014	V7015	G7016	LEU	ALA	ARG	GLU	ALA	ALA	VAL	ALA	ALA	ARG	ASP	LEU	ALA	GLY	ASP	THR	ASN	LYS	CYS	VAL	LEU	ARG	GLU	GLU	ASN	ALA	ALA	GLY	LEU	ASN	GLN	GLU	VAL	ALA	GLY	LEU	THR	ASP	LEU	PRO	GLY	THR	ALA	TRP
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THR	SER	PRO	GLU	VAL	THR	SER	PHE	LYS	VAL	ASP	THR	ALA	ARG	ALA	THR	VAL	ASP	GLY	VAL	ASP	GLY	VAL	ALA	ALA	VAL	VAL	VAL	ILE	ASN	GLU	ASP	LYS	THR	GLY	THR	ASN	CYS	VAL	LEU	ARG	GLU	ASN	ALA	ALA	GLY	THR	ASN	GLN	GLU	VAL	LEU	VAL	LEU	THR	ASP	LEU	PRO	GLY	THR	ALA	TRP
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- Molecule 5: LD23602p

Chain E: 

GLY	ALA	MET	SER	ASP	GLU	THR	ASN	ALA	A7000	V7001	W7002	D7003	S7005	L7007	G7016	LEU	ALA	ARG	GLU	GLU	ALA	ALA	LEU	ALA	ALA	ARG	ILE	ASN	GLU	ASP	LYS	THR	ASN	LYS	THR	ARG	GLU	GLU	ASN	ALA	ALA	ALA	GLU	GLN	GLU	GLU	ALA	GLY	VAL	LEU	LEU	VAL	LEU	ASP	LEU	THR	GLY	ALA	THR	PRO
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GLU	PRO	VAL	SER	PHE	LYS	VAL	GLY	ASP	TYR	ALA	ALA	ARG	ALA	THR	VAL	ASP	GLY	VAL	ASP	TYR	GLU	GLY	ALA	VAL	VAL	ILE	ASN	GLU	ASP	LYS	GLY	THR	ASN	CYS	VAL	LEU	ARG	TYR	LEU	ASN	GLY	ALA	ALA	GLU	GLN	GLU	VAL	LEU	VAL	LEU	VAL	ASP	LEU	THR	GLY	ALA	THR	TRP
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- Molecule 5: LD23602p

Chain U: 

GLY	ALA	MET	SER	ASP	GLU	THR	ASN	ALA	A7000	V7001	W7002	D7003	S7005	L7007	V7008	G7016	LEU	ALA	ARG	GLU	GLU	ALA	ALA	LEU	ALA	ALA	ARG	ILE	ASN	GLU	ASP	LYS	THR	ASN	LYS	THR	ARG	GLU	GLU	ASN	ALA	ALA	GLU	GLN	GLU	GLU	VAL	ALA	GLY	LEU	VAL	LEU	THR	GLY	ALA	THR	SER
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PRO	GLU	PRO	VAL	SER	PHE	LYS	VAL	GLY	ASP	TYR	ALA	ARG	ALA	THR	VAL	ASP	GLY	VAL	ASP	VAL	ASP	GLY	VAL	ALA	LEU	VAL	VAL	ILE	ASN	GLU	ASP	LYS	THR	ASN	LYS	THR	ARG	GLU	GLU	ASN	ALA	ALA	GLU	GLN	GLU	VAL	LEU	VAL	LEU	VAL	ASP	LEU	THR	GLY	ALA	THR	SER	TRP
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- Molecule 5: LD23602p

Chain c: 

GLY	ALA	MET	SER	ASP	GLU	THR	ASN	ALA	A7000	V7001	W7002	L7006	L7007	G7016	LEU	ALA	ARG	GLU	GLU	ALA	ALA	LEU	ALA	ALA	ARG	ARG	ILE	ASN	GLU	ASP	LYS	THR	ASN	LYS	THR	ARG	GLU	GLU	ASN	ALA	ALA	GLU	GLU	GLN	GLU	VAL	LEU	VAL	LEU	THR	GLY	ALA	THR	SER	PRO	GLU	PRO
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VAL	SER	PHE	LYS	VAL	GLY	ASP	TYR	ALA	ARG	ALA	THR	VAL	ASP	GLY	VAL	ASP	TYR	GLU	GLY	ALA	ALA	VAL	VAL	ARG	ILE	ASN	GLU	ASP	LYS	THR	ASN	LYS	THR	ARG	VAL	LEU	TYR	LEU	GLY	ALA	ALA	ASN	GLU	GLN	GLU	VAL	LEU	LEU	ASP	LEU	THR	GLY	ALA	THR	SER	PRO	GLU	PRO
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- Molecule 5: LD23602p

Chain k: 

GLY	ALA	MET	SER	ASP	GLU	THR	ASN	ALA	A7000	V7001	W7002	L7006	G7016	LEU	ALA	ARG	GLU	GLU	ALA	ALA	LEU	ALA	ALA	ARG	ARG	ILE	ASN	GLU	ASP	LYS	THR	ASN	LYS	THR	ARG	GLU	GLU	ASN	ALA	ALA	ALA	GLU	GLU	GLN	GLU	VAL	LEU	LEU	ILE	SER	ALA	THR	GLY	GLY	ALA	THR	SER	PRO	GLU	PRO	VAL
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SER PHE LYS VAL SER GLY ASP TYR ALA ARG ALA THR TYR VAL ASP GLY VAL ASP TYR GLY ALA VAL VAL SER ILE ASN GLU GLY LYS SER THR CYS VAL VAL LEU ARG LEU TYR LEU GLY TYR ASN GLU GLN GLU VAL LEU LEU VAL ASP LEU LEU PRO SER TRP

• Molecule 5: LD23602p

Chain s:

GLY ALA MET SER ASP GLU THR ALA A7000 V7001 W7002 L7006 L7007 G7016 LEU ALA ARG ALA ALA VAL VAL ALA ALA ARG ARG LEU LEU ASP ASP LYS SER THR ASN LYS VAL ARG LEU TYR LEU GLY ASN ALA ALA ALA ALA GLN GLU VAL LEU LEU VAL ILE ASP LEU LEU PRO SER TRP

• Molecule 5: LD23602p

Chain 1:

GLY ALA MET SER ASP GLU THR ASN ALA A7000 V7001 W7002 L7006 L7007 S7014 V7015 G7016 LEU ALA ARG ALA ALA VAL VAL ALA ALA ARG ARG LEU LEU ASN GLU ALA ALA ALA ALA GLN GLU VAL LEU LEU VAL ILE ASP LEU LEU PRO SER TRP

• Molecule 6: CG10419

Chain N:

GLY ALA MET GLN HIS PRO ASP GLN THR PHE GLN LEU GLN ALA ALA LEU LEU ILE CYS VAL ASP GLY THR VAL ASP GLU VAL ALA VAL VAL PHE ASP PRO GLN LYS PRO P8000 E8001 E8001 S8002 G8003 G8004 E8004 E8005 Y8006 L8007 H8008 H8009 H8010 F8011 Y8012 Y8016 Y8020 Y8024 S8025 S8026 R8027 L8028 T8032 L8037 E8038 M8039

E8044 L8045 P8046 P8047 T8054 T8057 Q8066 L8073 L8079 N8083 Q8086 E8089 T8093 S8094 D8095 Q8096 Q8097 R8098 R8099 R8100 R8104 R8105 Q8106 L8109 L8113 L8117 L8124 F8127 W8131 L8132 Q8133 P8135 N8136 T8137 W8139 L8140 L8141 L8142 W8146 L8147

A8148 R8149 W8150 T8154 H8159 L8160 P8161 F8167 L8170 R8171 A8174 T8176 C8177 L8178 L8180 R8181 L8184 R8185 E8186 D8187 E8188 R8189 Q8190 R8191 A8192 Y8195 N8196 L8197 L8198 L8199 T8200 Y8011 Y8012 Y8013 Y8014 R8015 R8016 Y8020 Y8024 S8025 S8026 R8027 L8028 L8037 E8038 M8039 E8044

• Molecule 6: CG10419

Chain F:

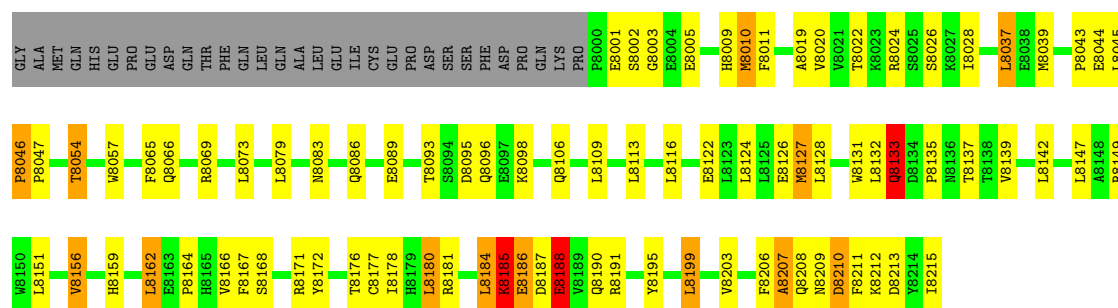
GLY ALA MET GLN HIS PRO ASP GLN THR PHE GLN LEU GLN ALA ALA LEU LEU ILE CYS VAL ASP GLY THR VAL ASP GLU VAL ALA VAL VAL PHE ASP PRO GLN LYS PRO P8000 E8001 E8001 S8002 G8003 G8004 E8004 E8005 Y8006 L8007 H8008 H8009 H8010 F8011 Y8012 Y8013 Y8014 R8015 R8016 Y8020 Y8024 S8025 S8026 R8027 L8028 L8037 E8038 M8039 E8044

L8045 P8046 P8047 T8054 T8057 Q8071 V8072 L8073 V8074 L8075 R8076 R8077 N8083 T8176 C8177 L8178 L8180 R8181 L8184 R8185 E8186 D8187 E8188 R8189 Q8190 R8191 A8192 Y8195 N8196 L8197 L8198 L8199 T8200 Y8011 Y8012 Y8013 Y8014 R8015 R8016 Y8020 Y8024 S8025 S8026 R8027 L8028 L8037 E8038 M8039 E8044

T8138 W8139 L8142 W8145 R8149 W8150 L8151 Y8152 A8153 T8154 L8155 W8156 L8159 R8160 P8161 L8162 F8167 L8170 T8176 L8180 R8181 L8184 R8185 E8186 D8187 E8188 R8189 Q8190 R8191 A8192 Y8195 N8196 L8197 L8198 L8199 T8200 Y8011 Y8012 Y8013 Y8014 R8015 R8016 Y8020 Y8024 S8025 S8026 R8027 L8028 L8037 E8038 M8039 E8044

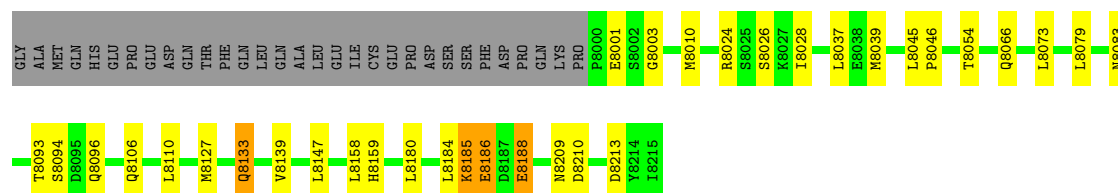
• Molecule 6: CG10419

Chain V:



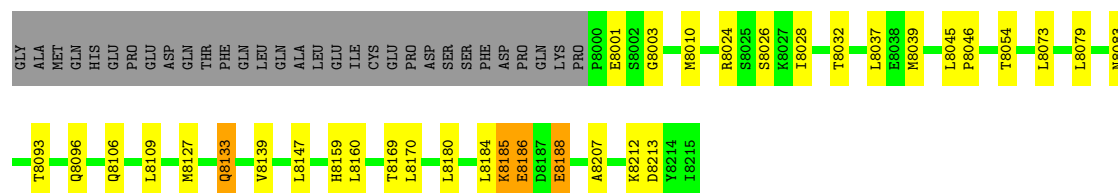
• Molecule 6: CG10419

Chain d:



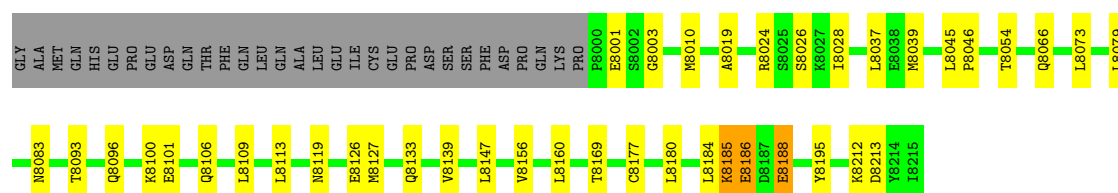
• Molecule 6: CG10419

Chain l:



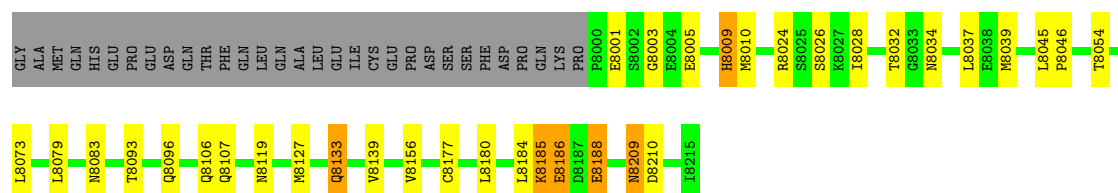
• Molecule 6: CG10419

Chain t:



• Molecule 6: CG10419

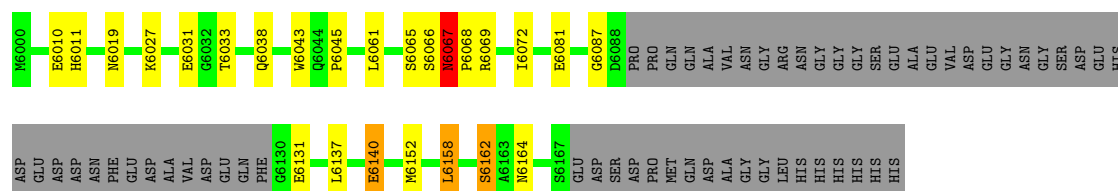
Chain 2:



• Molecule 7: Ichn

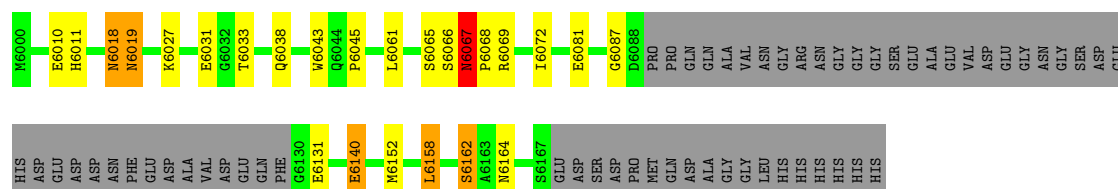
Chain O:





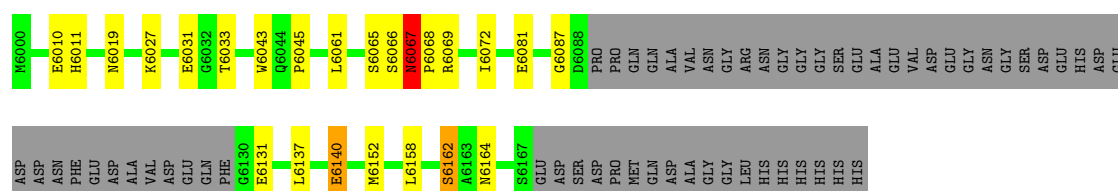
- Molecule 7: Ichn

Chain G:



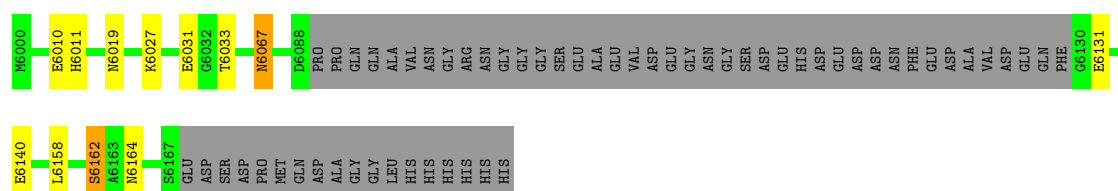
- Molecule 7: Ichn

Chain W:



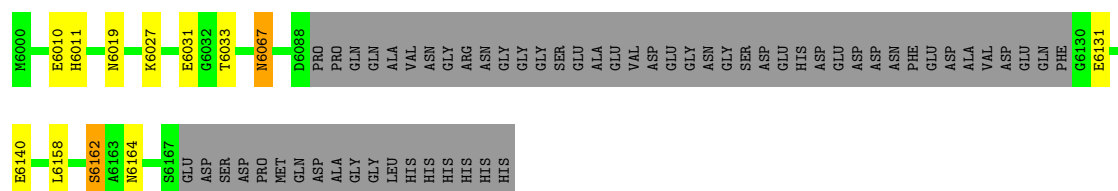
- Molecule 7: Ichn

Chain e:



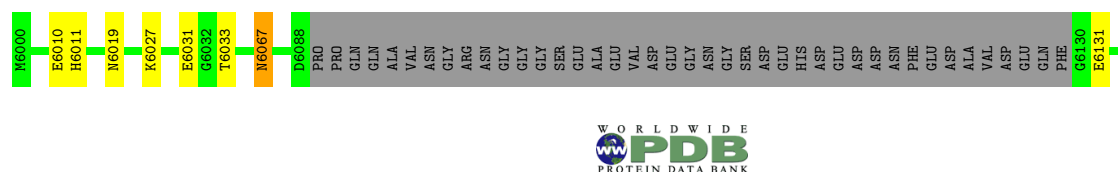
- Molecule 7: Ichn

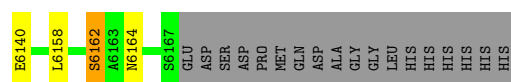
Chain m:



- Molecule 7: Ichn

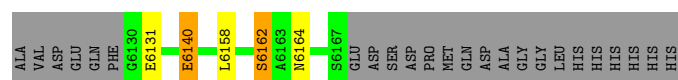
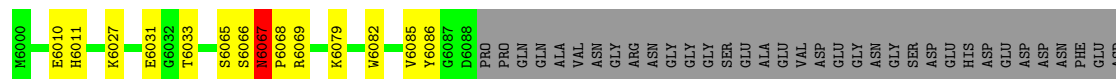
Chain u:





- Molecule 7: Ichn

Chain 3:



- Molecule 8: Small nuclear ribonucleoprotein G

Chain P:



- Molecule 8: Small nuclear ribonucleoprotein G

Chain H:



- Molecule 8: Small nuclear ribonucleoprotein G

Chain X:



- Molecule 8: Small nuclear ribonucleoprotein G

Chain f:



- Molecule 8: Small nuclear ribonucleoprotein G

Chain n:



- Molecule 8: Small nuclear ribonucleoprotein G

Chain v:



- Molecule 8: Small nuclear ribonucleoprotein G

Chain 4: 

MET	SER	LYS	ALA	HE000	HE008	LE026	RE068	FE069	ARG	VAL
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## 4 Data and refinement statistics

EDS was not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.93Å 356.81Å 230.75Å 90.00° 97.31° 90.00°	Depositor
Resolution (Å)	59.47 – 3.10	Depositor
% Data completeness (in resolution range)	64.6 (59.47-3.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 3.13Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.232 , 0.256	Depositor
Wilson B-factor (Å <sup>2</sup> )	49.1	Xtriage
Anisotropy	0.038	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	39 of 281573 reflections (0.014%)	Xtriage
Total number of atoms	42689	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 77.30 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.7504e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.51	0/656	0.75	1/888 (0.1%)
1	I	0.51	0/656	0.74	1/888 (0.1%)
1	Q	0.49	0/656	0.76	1/888 (0.1%)
1	Y	0.49	0/656	0.75	1/888 (0.1%)
1	g	0.49	0/656	0.74	1/888 (0.1%)
1	o	0.51	0/656	0.75	1/888 (0.1%)
1	w	0.46	0/656	0.74	1/888 (0.1%)
2	B	0.52	0/817	0.70	0/1096
2	J	0.50	0/817	0.70	0/1096
2	R	0.48	0/817	0.69	0/1096
2	Z	0.47	0/817	0.68	0/1096
2	h	0.47	0/817	0.68	0/1096
2	p	0.47	0/817	0.67	0/1096
2	x	0.48	0/817	0.69	0/1096
3	C	0.43	0/646	0.75	1/867 (0.1%)
3	K	0.46	0/646	0.76	1/867 (0.1%)
3	S	0.44	0/646	0.75	1/867 (0.1%)
3	a	0.40	0/646	0.74	1/867 (0.1%)
3	i	0.41	0/646	0.74	1/867 (0.1%)
3	q	0.43	0/646	0.74	1/867 (0.1%)
3	y	0.42	0/646	0.74	1/867 (0.1%)
4	D	0.39	0/567	0.65	0/765
4	L	0.39	0/567	0.65	0/765
4	T	0.40	0/567	0.64	0/765
4	b	0.40	0/567	0.64	0/765
4	j	0.39	0/567	0.64	0/765
4	r	0.39	0/567	0.67	0/765
4	z	0.38	0/567	0.64	0/765
5	l	0.65	0/135	0.90	0/184
5	E	0.57	0/135	0.88	0/184
5	M	0.63	0/135	0.89	0/184
5	U	0.56	0/135	0.83	0/184

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
5	c	0.64	0/135	0.94	0/184
5	k	0.64	0/135	0.91	0/184
5	s	0.55	0/135	0.87	0/184
6	2	0.56	0/1830	0.88	2/2489 (0.1%)
6	F	0.58	0/1830	0.89	2/2489 (0.1%)
6	N	0.60	0/1830	0.91	2/2489 (0.1%)
6	V	0.56	0/1830	0.87	2/2489 (0.1%)
6	d	0.53	0/1830	0.86	2/2489 (0.1%)
6	l	0.58	0/1830	0.89	2/2489 (0.1%)
6	t	0.60	0/1830	0.89	2/2489 (0.1%)
7	3	0.46	0/1008	0.74	0/1373
7	G	0.57	0/1008	0.76	0/1373
7	O	0.55	0/1008	0.75	0/1373
7	W	0.53	0/1008	0.75	0/1373
7	e	0.47	0/1008	0.72	0/1373
7	m	0.57	0/1008	0.75	0/1373
7	u	0.55	0/1008	0.75	0/1373
8	4	0.40	0/551	0.72	0/737
8	H	0.42	0/551	0.73	0/737
8	P	0.42	0/551	0.73	0/737
8	X	0.42	0/551	0.73	0/737
8	f	0.39	0/551	0.72	0/737
8	n	0.42	0/551	0.73	0/737
8	v	0.41	0/551	0.73	0/737
All	All	0.51	0/43470	0.78	28/58793 (0.0%)

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
7	3	0	1
7	G	0	1
7	O	0	1
7	W	0	1
7	e	0	1
7	m	0	1
7	u	0	1
All	All	0	7

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	8185	LYS	C-N-CA	7.12	139.50	121.70
6	F	8185	LYS	C-N-CA	7.10	139.44	121.70
6	2	8185	LYS	C-N-CA	7.08	139.40	121.70
6	l	8185	LYS	C-N-CA	7.01	139.21	121.70
6	t	8185	LYS	C-N-CA	7.01	139.22	121.70
6	V	8185	LYS	C-N-CA	6.98	139.16	121.70
6	d	8185	LYS	C-N-CA	6.98	139.15	121.70
6	N	8045	LEU	N-CA-C	6.54	128.66	111.00
1	o	1069	PRO	N-CA-C	6.24	128.32	112.10
1	A	1069	PRO	N-CA-C	6.17	128.14	112.10
1	I	1069	PRO	N-CA-C	6.06	127.86	112.10
1	Q	1069	PRO	N-CA-C	6.05	127.84	112.10
1	Y	1069	PRO	N-CA-C	6.01	127.72	112.10
1	g	1069	PRO	N-CA-C	6.00	127.69	112.10
6	2	8045	LEU	N-CA-C	5.98	127.14	111.00
6	V	8045	LEU	N-CA-C	5.96	127.08	111.00
6	l	8045	LEU	N-CA-C	5.95	127.06	111.00
6	t	8045	LEU	N-CA-C	5.92	126.97	111.00
3	y	3024	GLN	N-CA-C	5.85	126.79	111.00
3	i	3024	GLN	N-CA-C	5.84	126.77	111.00
3	K	3024	GLN	N-CA-C	5.84	126.76	111.00
1	w	1069	PRO	N-CA-C	5.84	127.28	112.10
6	d	8045	LEU	N-CA-C	5.82	126.72	111.00
3	S	3024	GLN	N-CA-C	5.80	126.66	111.00
3	a	3024	GLN	N-CA-C	5.79	126.64	111.00
3	q	3024	GLN	N-CA-C	5.79	126.64	111.00
6	F	8045	LEU	N-CA-C	5.78	126.61	111.00
3	C	3024	GLN	N-CA-C	5.64	126.24	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	3	6067	ASN	Mainchain
7	G	6067	ASN	Mainchain
7	O	6067	ASN	Mainchain
7	W	6067	ASN	Mainchain
7	e	6067	ASN	Mainchain
7	m	6067	ASN	Mainchain
7	u	6067	ASN	Mainchain

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	648	0	690	6	0
1	I	648	0	690	10	0
1	Q	648	0	690	10	0
1	Y	648	0	690	7	0
1	g	648	0	690	0	0
1	o	648	0	690	0	0
1	w	648	0	690	0	0
2	B	807	0	833	13	0
2	J	807	0	833	18	0
2	R	807	0	833	19	0
2	Z	807	0	833	9	0
2	h	807	0	833	0	0
2	p	807	0	833	0	0
2	x	807	0	833	0	0
3	C	638	0	657	13	0
3	K	638	0	657	15	0
3	S	638	0	657	13	0
3	a	638	0	657	0	0
3	i	638	0	657	0	0
3	q	638	0	657	0	0
3	y	638	0	657	0	0
4	D	556	0	561	16	0
4	L	556	0	561	17	0
4	T	556	0	561	17	0
4	b	556	0	561	0	0
4	j	556	0	561	0	0
4	r	556	0	561	0	0
4	z	556	0	561	0	0
5	l	133	0	0	0	0
5	E	133	0	123	2	0
5	M	133	0	123	2	0
5	U	133	0	123	2	0
5	c	133	0	123	0	0
5	k	133	0	123	0	0
5	s	133	0	123	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	2	1787	0	0	1	0
6	F	1787	0	1779	50	0
6	N	1787	0	1779	57	0
6	V	1787	0	1779	54	0
6	d	1787	0	1779	0	0
6	l	1787	0	1779	0	0
6	t	1787	0	1779	0	0
7	3	984	0	0	6	0
7	G	984	0	943	21	0
7	O	984	0	943	19	0
7	W	984	0	943	19	0
7	e	984	0	943	0	0
7	m	984	0	943	0	0
7	u	984	0	943	0	0
8	4	544	0	0	1	0
8	H	544	0	563	7	0
8	P	544	0	563	7	0
8	X	544	0	563	8	0
8	f	544	0	563	0	0
8	n	544	0	563	0	0
8	v	544	0	563	0	0
9	2	5	0	0	0	0
9	t	5	0	0	0	0
All	All	42689	0	39635	370	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (370) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:R:2043:LYS:HG2	2:R:2067:TRP:HB3	1.49	0.94
7:O:6067:ASN:HB2	7:O:6068:PRO:HD3	1.49	0.92
2:R:2092:LEU:HD23	4:T:4056:VAL:HG22	1.51	0.91
2:B:2092:LEU:HD23	4:D:4056:VAL:HG22	1.51	0.91
2:J:2092:LEU:HD23	4:L:4056:VAL:HG22	1.52	0.90
7:G:6067:ASN:HB2	7:G:6068:PRO:HD3	1.50	0.90
7:W:6067:ASN:HB2	7:W:6068:PRO:HD3	1.51	0.89
7:O:6067:ASN:HB2	7:O:6068:PRO:CD	2.07	0.84
7:G:6067:ASN:HB2	7:G:6068:PRO:CD	2.08	0.83
6:F:8185:LYS:H	6:F:8187:ASP:HB2	1.44	0.83
6:V:8185:LYS:H	6:V:8187:ASP:HB2	1.44	0.82
7:W:6067:ASN:HB2	7:W:6068:PRO:CD	2.09	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:N:8185:LYS:H	6:N:8187:ASP:HB2	1.45	0.81
2:B:2077:TYR:CE2	6:F:8209:ASN:HB2	2.16	0.80
7:G:6067:ASN:CB	7:G:6068:PRO:HD3	2.12	0.79
7:O:6067:ASN:CB	7:O:6068:PRO:HD3	2.12	0.78
7:W:6067:ASN:CB	7:W:6068:PRO:HD3	2.12	0.78
4:T:4060:CYS:O	4:T:4063:VAL:HG12	1.89	0.72
2:Z:2043:LYS:HG2	2:Z:2067:TRP:HB3	1.72	0.72
6:V:8203:VAL:HG13	6:V:8209:ASN:HA	1.72	0.71
1:Q:1050:PRO:HG3	6:V:8159:HIS:HB2	1.72	0.71
6:V:8167:PHE:O	6:V:8171:ARG:HG3	1.90	0.71
7:G:6068:PRO:HD2	7:G:6069:ARG:H	1.57	0.70
1:Q:1056:LEU:HD11	7:W:6061:LEU:HD13	1.73	0.70
1:A:1056:LEU:HD11	7:G:6061:LEU:HD13	1.74	0.70
1:I:1050:PRO:HG3	6:N:8159:HIS:CB	2.22	0.69
1:I:1056:LEU:HD11	7:O:6061:LEU:HD13	1.73	0.69
6:N:8142:LEU:HG	6:N:8191:ARG:HA	1.75	0.69
7:O:6068:PRO:HD2	7:O:6069:ARG:H	1.56	0.68
6:F:8160:LEU:HD12	6:F:8160:LEU:H	1.58	0.68
7:W:6068:PRO:HD2	7:W:6069:ARG:H	1.57	0.67
3:C:3016:ARG:HE	3:C:3030:GLU:HG2	1.59	0.67
4:D:4060:CYS:O	4:D:4063:VAL:HG12	1.94	0.67
6:F:8145:VAL:HG22	6:F:8149:ARG:HD2	1.77	0.67
6:F:8142:LEU:HG	6:F:8191:ARG:HA	1.76	0.66
6:N:8178:ILE:HG13	6:N:8199:LEU:HD21	1.77	0.66
3:K:3016:ARG:HE	3:K:3030:GLU:HG2	1.58	0.66
6:N:8209:ASN:C	6:N:8211:PHE:H	1.99	0.66
1:Y:1064:ARG:HD3	2:Z:2041:ASN:HB3	1.77	0.66
3:C:3016:ARG:NE	3:C:3030:GLU:HG2	2.10	0.66
3:K:3016:ARG:NE	3:K:3030:GLU:HG2	2.10	0.65
1:A:1050:PRO:HG3	6:F:8159:HIS:HB2	1.78	0.65
7:O:6067:ASN:CB	7:O:6068:PRO:CD	2.73	0.65
3:S:3066:LYS:HG3	4:T:4063:VAL:HG13	1.79	0.64
3:S:3016:ARG:HE	3:S:3030:GLU:HG2	1.61	0.64
7:G:6069:ARG:NH2	7:G:6140:GLU:O	2.31	0.64
7:W:6067:ASN:CB	7:W:6068:PRO:CD	2.73	0.64
3:S:3016:ARG:NE	3:S:3030:GLU:HG2	2.11	0.64
4:L:4060:CYS:O	4:L:4063:VAL:HG12	1.97	0.64
1:A:1064:ARG:HD3	2:B:2041:ASN:HB3	1.79	0.64
2:J:2043:LYS:HG2	2:J:2067:TRP:HB3	1.80	0.64
7:G:6067:ASN:CB	7:G:6068:PRO:CD	2.72	0.64
7:3:6067:ASN:CB	7:3:6068:PRO:CD	2.76	0.63
4:T:4031:ASP:HA	6:V:8020:VAL:HG22	1.79	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:V:8142:LEU:HG	6:V:8191:ARG:HA	1.80	0.63
6:V:8164:PRO:HA	6:V:8167:PHE:HD1	1.63	0.63
7:W:6069:ARG:NH2	7:W:6140:GLU:O	2.31	0.63
6:F:8203:VAL:O	6:F:8207:ALA:HA	1.99	0.62
1:I:1050:PRO:HG3	6:N:8159:HIS:HB3	1.79	0.62
6:N:8177:CYS:HB2	6:N:8195:TYR:HB3	1.80	0.62
1:I:1064:ARG:HD3	2:J:2041:ASN:HB3	1.81	0.62
3:K:3000:MET:CE	3:K:3002:GLN:HE22	2.13	0.61
8:H:5030:ASP:HB2	8:H:5031:PRO:CD	2.30	0.61
3:C:3000:MET:CE	3:C:3002:GLN:HE22	2.13	0.61
8:P:5030:ASP:HB2	8:P:5031:PRO:CD	2.30	0.61
1:Q:1050:PRO:HG3	6:V:8159:HIS:CB	2.30	0.61
6:V:8128:LEU:HD22	6:V:8151:LEU:HG	1.82	0.61
8:X:5030:ASP:HB2	8:X:5031:PRO:CD	2.30	0.61
7:O:6069:ARG:NH2	7:O:6140:GLU:O	2.34	0.60
7:3:6069:ARG:NH2	7:3:6140:GLU:O	2.34	0.60
7:G:6018:ASN:HD22	7:G:6019:ASN:HB2	1.66	0.60
3:S:3000:MET:CE	3:S:3002:GLN:HE22	2.14	0.60
7:W:6072:ILE:HD12	7:W:6152:MET:HE2	1.82	0.60
6:N:8146:TRP:O	6:N:8150:TRP:HD1	1.85	0.60
6:V:8124:LEU:HA	6:V:8127:MET:HE2	1.84	0.60
6:F:8152:TYR:O	6:F:8156:VAL:HG12	2.01	0.60
2:R:2043:LYS:HG2	2:R:2067:TRP:CB	2.28	0.60
6:N:8167:PHE:O	6:N:8171:ARG:HG3	2.03	0.59
1:Y:1069:PRO:O	1:Y:1071:SER:N	2.33	0.59
1:I:1024:HIS:HB3	6:N:8161:PRO:HD3	1.85	0.58
6:V:8177:CYS:HA	6:V:8180:LEU:HB2	1.85	0.58
6:N:8124:LEU:HA	6:N:8127:MET:HE2	1.86	0.58
7:O:6068:PRO:CD	7:O:6069:ARG:H	2.14	0.58
7:G:6072:ILE:HD12	7:G:6152:MET:HE2	1.85	0.58
6:N:8095:ASP:HB3	6:N:8098:LYS:HB2	1.86	0.58
6:N:8133:GLN:HG3	6:N:8176:THR:HG21	1.85	0.58
7:W:6068:PRO:CD	7:W:6069:ARG:H	2.14	0.57
6:N:8100:LYS:HD3	6:N:8104:ARG:CZ	2.34	0.57
6:F:8095:ASP:HB3	6:F:8098:LYS:HB2	1.87	0.57
1:I:1069:PRO:O	1:I:1071:SER:N	2.36	0.57
1:Q:1069:PRO:O	1:Q:1071:SER:N	2.36	0.57
6:V:8203:VAL:O	6:V:8207:ALA:HA	2.05	0.57
3:K:3066:LYS:HG3	4:L:4063:VAL:HG13	1.86	0.57
3:C:3066:LYS:HG3	4:D:4063:VAL:HG13	1.87	0.56
7:3:6082:TRP:N	7:3:6086:TYR:O	2.38	0.56
6:F:8199:LEU:O	6:F:8203:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:O:6066:SER:HA	7:O:6069:ARG:O	2.06	0.56
6:V:8095:ASP:HB3	6:V:8098:LYS:HB2	1.88	0.56
1:Q:1048:ARG:HG3	1:Q:1048:ARG:HH11	1.70	0.56
2:Z:2064:LYS:HE3	2:Z:2075:ASP:OD2	2.06	0.56
7:G:6066:SER:HA	7:G:6069:ARG:O	2.06	0.55
6:F:8181:ARG:O	6:F:8184:LEU:HB2	2.06	0.55
2:R:2097:ILE:HG22	6:V:8037:LEU:HB3	1.88	0.55
7:O:6072:ILE:HD12	7:O:6152:MET:HE2	1.88	0.55
1:Q:1064:ARG:HD3	2:R:2041:ASN:HB3	1.89	0.55
7:G:6068:PRO:CD	7:G:6069:ARG:H	2.14	0.55
6:N:8160:LEU:HD23	6:N:8161:PRO:HA	1.89	0.54
1:A:1069:PRO:O	1:A:1071:SER:N	2.37	0.54
6:N:8181:ARG:HA	6:N:8184:LEU:CD1	2.37	0.54
6:V:8209:ASN:C	6:V:8211:PHE:H	2.11	0.54
6:V:8113:LEU:HD13	6:V:8116:LEU:HD12	1.90	0.54
6:N:8054:THR:HG23	6:N:8057:TRP:HB2	1.90	0.54
6:V:8168:SER:O	6:V:8172:TYR:HD2	1.91	0.54
2:J:2097:ILE:HG22	6:N:8037:LEU:HB3	1.90	0.54
2:B:2040:ARG:C	2:B:2042:ASN:H	2.11	0.53
7:W:6066:SER:HA	7:W:6069:ARG:O	2.08	0.53
8:X:5008:MET:O	8:X:5026:LEU:HB3	2.08	0.53
6:V:8046:PRO:HB2	6:V:8047:PRO:HD2	1.90	0.53
2:R:2040:ARG:HE	4:T:4019:TRP:HZ2	1.56	0.53
6:F:8046:PRO:HB2	6:F:8047:PRO:HD2	1.89	0.53
2:J:2077:TYR:CD1	6:N:8210:ASP:HB3	2.43	0.53
6:V:8054:THR:HG23	6:V:8057:TRP:HB2	1.90	0.53
6:F:8184:LEU:HD22	6:F:8192:ALA:HB2	1.90	0.53
6:V:8171:ARG:NH1	6:V:8208:GLN:OE1	2.40	0.53
4:T:4019:TRP:HB2	4:T:4021:MET:SD	2.49	0.53
2:J:2023:SER:O	2:J:2027:GLN:HG3	2.09	0.53
3:K:3000:MET:HE2	3:K:3002:GLN:HE22	1.73	0.52
2:Z:2023:SER:O	2:Z:2027:GLN:HG3	2.09	0.52
5:U:7005:SER:O	5:U:7008:VAL:HG22	2.10	0.52
8:P:5008:MET:O	8:P:5026:LEU:HB3	2.09	0.52
6:F:8054:THR:HG23	6:F:8057:TRP:HB2	1.89	0.52
8:H:5008:MET:O	8:H:5026:LEU:HB3	2.09	0.52
4:L:4019:TRP:HB2	4:L:4021:MET:SD	2.50	0.52
6:N:8181:ARG:O	6:N:8184:LEU:HB2	2.09	0.52
6:N:8046:PRO:HB2	6:N:8047:PRO:HD2	1.92	0.52
2:J:2034:GLN:HG2	2:J:2048:ARG:HG3	1.92	0.52
2:B:2023:SER:O	2:B:2027:GLN:HG3	2.09	0.52
6:F:8135:PRO:C	6:F:8137:THR:H	2.13	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:N:8135:PRO:C	6:N:8137:THR:H	2.12	0.51
5:E:7005:SER:O	5:E:7007:LEU:N	2.43	0.51
6:V:8135:PRO:C	6:V:8137:THR:H	2.13	0.51
6:N:8131:TRP:O	6:N:8135:PRO:HG3	2.10	0.51
2:R:2023:SER:O	2:R:2027:GLN:HG3	2.10	0.51
6:F:8072:VAL:HG13	6:F:8114:LEU:HD21	1.91	0.51
2:B:2034:GLN:HG2	2:B:2048:ARG:HG3	1.92	0.51
7:O:6043:TRP:CZ3	7:O:6045:PRO:HG3	2.46	0.51
6:V:8188:GLU:CD	6:V:8190:GLN:HB2	2.31	0.51
2:B:2043:LYS:HD3	2:B:2067:TRP:CE3	2.46	0.51
2:R:2077:TYR:CD1	6:V:8210:ASP:HB3	2.46	0.50
7:G:6043:TRP:CZ3	7:G:6045:PRO:HG3	2.46	0.50
2:R:2092:LEU:HD22	4:T:4053:LEU:HG	1.93	0.50
2:Z:2065:GLU:O	2:Z:2075:ASP:HA	2.11	0.50
6:N:8184:LEU:HD22	6:N:8192:ALA:HB2	1.91	0.50
3:S:3063:ILE:HG22	4:T:4067:ARG:HB3	1.93	0.50
1:Y:1048:ARG:HH11	1:Y:1048:ARG:HG3	1.76	0.50
2:Z:2040:ARG:HA	2:Z:2089:ILE:HD11	1.93	0.50
3:S:3000:MET:HE2	3:S:3002:GLN:HE22	1.75	0.50
4:D:4019:TRP:HB2	4:D:4021:MET:SD	2.50	0.50
4:L:4002:LYS:HB2	4:L:4003:PRO:HD3	1.93	0.50
6:V:8177:CYS:HB2	6:V:8195:TYR:HB3	1.94	0.50
3:C:3063:ILE:HG22	4:D:4067:ARG:HB3	1.94	0.50
2:R:2074:LYS:HD3	6:V:8168:SER:OG	2.11	0.50
3:C:3000:MET:HE2	3:C:3002:GLN:HE22	1.75	0.50
1:A:1053:LEU:CD2	7:G:6065:SER:HB2	2.42	0.49
2:J:2040:ARG:HA	2:J:2089:ILE:HD11	1.93	0.49
2:J:2065:GLU:O	2:J:2075:ASP:HA	2.12	0.49
6:V:8065:PHE:CE1	6:V:8156:VAL:HG12	2.47	0.49
2:Z:2034:GLN:HG2	2:Z:2048:ARG:HG3	1.94	0.49
6:N:8181:ARG:HA	6:N:8184:LEU:HD12	1.95	0.49
6:V:8131:TRP:O	6:V:8135:PRO:HG3	2.13	0.49
3:S:3038:GLU:HB3	6:V:8011:PHE:HE1	1.78	0.49
6:V:8181:ARG:O	6:V:8184:LEU:HB2	2.13	0.49
6:N:8044:GLU:OE1	6:N:8044:GLU:HA	2.13	0.49
3:K:3063:ILE:HG22	4:L:4067:ARG:HB3	1.94	0.49
2:B:2065:GLU:O	2:B:2075:ASP:HA	2.11	0.49
6:V:8209:ASN:HB3	6:V:8212:LYS:HE3	1.95	0.49
1:I:1050:PRO:HG3	6:N:8159:HIS:HB2	1.93	0.49
7:O:6081:GLU:HA	7:O:6087:GLY:HA3	1.95	0.49
7:W:6081:GLU:HA	7:W:6087:GLY:HA3	1.95	0.49
6:F:8188:GLU:CD	6:F:8190:GLN:HB2	2.33	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:R:2034:GLN:HG2	2:R:2048:ARG:HG3	1.95	0.48
6:F:8131:TRP:O	6:F:8135:PRO:HG3	2.13	0.48
7:W:6043:TRP:CZ3	7:W:6045:PRO:HG3	2.48	0.48
2:R:2065:GLU:O	2:R:2075:ASP:HA	2.12	0.48
6:F:8108:PRO:HB2	6:F:8153:ALA:CB	2.43	0.48
6:V:8199:LEU:HB2	6:V:8215:ILE:HD13	1.95	0.48
1:I:1053:LEU:CD2	7:O:6065:SER:HB2	2.44	0.48
6:V:8188:GLU:OE2	6:V:8190:GLN:HB2	2.11	0.48
6:F:8132:LEU:O	6:F:8135:PRO:HD3	2.14	0.48
5:E:7003:ASP:O	5:E:7006:LEU:HB2	2.13	0.48
6:F:8185:LYS:N	6:F:8187:ASP:HB2	2.21	0.48
6:V:8133:GLN:HG3	6:V:8176:THR:HG21	1.96	0.48
6:F:8044:GLU:HA	6:F:8044:GLU:OE1	2.13	0.48
4:L:4016:LYS:HG2	4:L:4064:LEU:HD23	1.96	0.48
6:F:8160:LEU:HA	6:F:8162:LEU:HD13	1.96	0.48
1:Q:1048:ARG:HG3	1:Q:1048:ARG:NH1	2.27	0.47
4:T:4016:LYS:HG2	4:T:4064:LEU:HD23	1.96	0.47
6:N:8201:LEU:HD22	6:N:8205:VAL:HG21	1.95	0.47
4:D:4016:LYS:HG2	4:D:4064:LEU:HD23	1.97	0.47
7:O:6068:PRO:CD	7:O:6069:ARG:N	2.78	0.47
1:Q:1053:LEU:CD2	7:W:6065:SER:HB2	2.45	0.47
6:F:8181:ARG:HA	6:F:8184:LEU:CD1	2.45	0.47
8:P:5030:ASP:HB2	8:P:5031:PRO:HD2	1.97	0.47
6:F:8194:PRO:O	6:F:8197:LEU:HB3	2.14	0.47
3:K:3064:MET:HB2	4:L:4004:PHE:CD2	2.50	0.47
6:N:8132:LEU:O	6:N:8135:PRO:HD3	2.15	0.47
7:G:6081:GLU:HA	7:G:6087:GLY:HA3	1.97	0.47
7:3:6066:SER:O	7:3:6067:ASN:O	2.33	0.47
1:I:1064:ARG:NH2	2:J:2040:ARG:HB3	2.29	0.47
7:W:6066:SER:O	7:W:6067:ASN:O	2.33	0.47
6:V:8185:LYS:N	6:V:8187:ASP:HB2	2.22	0.47
3:C:3064:MET:HB2	4:D:4004:PHE:CD2	2.50	0.47
6:V:8066:GLN:HE22	6:V:8069:ARG:HH11	1.63	0.47
2:R:2077:TYR:CE2	6:V:8209:ASN:HB2	2.50	0.46
6:N:8141:LEU:HD22	6:N:8148:ALA:HB2	1.96	0.46
6:N:8188:GLU:CD	6:N:8190:GLN:HB2	2.36	0.46
6:F:8002:SER:H	6:F:8005:GLU:HB2	1.80	0.46
6:N:8002:SER:H	6:N:8005:GLU:HB2	1.80	0.46
4:T:4059:ARG:HD3	4:T:4061:ASN:OD1	2.16	0.46
6:V:8044:GLU:HA	6:V:8044:GLU:OE1	2.15	0.46
2:J:2092:LEU:HD22	4:L:4053:LEU:HG	1.97	0.46
8:X:5030:ASP:HB2	8:X:5031:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:8127:MET:HG2	6:F:8131:TRP:CZ2	2.51	0.46
7:G:6068:PRO:CD	7:G:6069:ARG:N	2.78	0.46
7:W:6068:PRO:CD	7:W:6069:ARG:N	2.79	0.46
2:J:2043:LYS:HD3	2:J:2067:TRP:CE3	2.51	0.46
2:B:2092:LEU:HD22	4:D:4053:LEU:HG	1.98	0.46
6:N:8203:VAL:HG22	6:N:8211:PHE:HB2	1.97	0.46
8:H:5030:ASP:HB2	8:H:5031:PRO:HD2	1.97	0.46
3:S:3064:MET:HB2	4:T:4004:PHE:CD2	2.51	0.46
6:V:8002:SER:H	6:V:8005:GLU:HB2	1.81	0.46
6:F:8184:LEU:HD23	6:F:8187:ASP:HB3	1.98	0.45
6:N:8185:LYS:N	6:N:8187:ASP:HB2	2.22	0.45
6:V:8132:LEU:O	6:V:8135:PRO:HD3	2.16	0.45
6:N:8184:LEU:HD23	6:N:8187:ASP:HB3	1.98	0.45
3:C:3024:GLN:HB2	3:C:3024:GLN:HE21	1.56	0.45
6:N:8146:TRP:O	6:N:8150:TRP:CD1	2.67	0.45
3:K:3000:MET:CE	3:K:3002:GLN:NE2	2.80	0.45
4:L:4059:ARG:HD3	4:L:4061:ASN:OD1	2.16	0.45
7:G:6066:SER:O	7:G:6067:ASN:O	2.35	0.45
6:F:8133:GLN:HG3	6:F:8176:THR:HG21	1.97	0.45
4:T:4000:ASN:ND2	6:V:8010:MET:HB2	2.32	0.45
7:O:6066:SER:O	7:O:6067:ASN:O	2.35	0.45
6:N:8174:ALA:HB2	6:N:8202:THR:HG21	1.97	0.45
6:F:8181:ARG:HA	6:F:8184:LEU:HD12	1.99	0.44
6:N:8211:PHE:O	6:N:8213:ASP:N	2.50	0.44
6:V:8178:ILE:HG13	6:V:8199:LEU:HD21	1.99	0.44
7:O:6065:SER:OG	7:O:6066:SER:N	2.50	0.44
2:B:2092:LEU:CD2	4:D:4056:VAL:HG22	2.36	0.44
7:G:6065:SER:OG	7:G:6066:SER:N	2.50	0.44
7:3:6068:PRO:CD	7:3:6069:ARG:N	2.81	0.44
6:F:8124:LEU:HA	6:F:8127:MET:HE2	1.99	0.44
3:S:3069:ASN:OD1	4:T:4018:LYS:HG2	2.18	0.44
6:F:8155:LEU:HD21	6:F:8170:LEU:HD13	1.99	0.44
7:3:6065:SER:OG	7:3:6066:SER:N	2.50	0.44
6:V:8122:GLU:O	6:V:8126:GLU:HG2	2.17	0.44
6:N:8167:PHE:O	6:N:8170:LEU:HB3	2.18	0.44
6:F:8086:GLN:O	6:F:8089:GLU:HB2	2.17	0.44
6:N:8086:GLN:O	6:N:8089:GLU:HB2	2.17	0.44
3:S:3006:LEU:HD11	8:X:5054:MET:HG2	2.00	0.44
6:V:8184:LEU:HD21	6:V:8191:ARG:HB3	2.00	0.44
7:G:6018:ASN:C	7:G:6018:ASN:HD22	2.21	0.44
6:F:8108:PRO:HB3	6:F:8150:TRP:CD2	2.53	0.44
4:D:4000:ASN:ND2	6:F:8010:MET:HB2	2.33	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:8118:GLN:HA	6:F:8121:LEU:HD12	1.99	0.44
6:N:8209:ASN:HB3	6:N:8212:LYS:HE3	1.99	0.43
3:S:3000:MET:CE	3:S:3002:GLN:NE2	2.81	0.43
4:D:4002:LYS:HG3	6:F:8014:ARG:CB	2.48	0.43
3:K:3071:THR:HG23	8:P:5061:SER:HB3	2.00	0.43
2:R:2049:VAL:HA	2:R:2060:LEU:HD23	2.01	0.43
2:Z:2049:VAL:HA	2:Z:2060:LEU:HD23	2.00	0.43
6:V:8184:LEU:HD23	6:V:8187:ASP:HB3	1.99	0.43
6:F:8203:VAL:HG13	6:F:8209:ASN:HA	2.00	0.43
2:B:2077:TYR:HE2	6:F:8209:ASN:HB2	1.71	0.43
4:T:4030:VAL:HG12	4:T:4031:ASP:N	2.34	0.43
6:F:8046:PRO:HB2	6:F:8047:PRO:CD	2.48	0.43
8:X:5025:ILE:HG21	8:X:5027:ARG:CZ	2.49	0.43
1:Y:1018:LYS:HE2	1:Y:1061:ASN:O	2.18	0.43
4:D:4059:ARG:HD3	4:D:4061:ASN:OD1	2.17	0.43
4:L:4031:ASP:HA	6:N:8020:VAL:HG22	2.01	0.43
6:N:8127:MET:HG2	6:N:8131:TRP:CZ2	2.53	0.43
8:P:5025:ILE:HG21	8:P:5027:ARG:CZ	2.49	0.43
6:V:8206:PHE:O	6:V:8208:GLN:HG2	2.19	0.43
3:C:3006:LEU:HD11	8:H:5054:MET:HG2	2.00	0.43
7:W:6152:MET:HE3	7:W:6152:MET:HB2	1.91	0.43
3:S:3038:GLU:HB3	6:V:8011:PHE:CE1	2.53	0.43
6:V:8086:GLN:O	6:V:8089:GLU:HB2	2.18	0.43
6:V:8127:MET:HG2	6:V:8131:TRP:CZ2	2.53	0.43
8:P:5008:MET:O	8:P:5026:LEU:O	2.37	0.43
1:Y:1048:ARG:HG3	1:Y:1048:ARG:NH1	2.32	0.43
6:V:8005:GLU:O	6:V:8009:HIS:ND1	2.52	0.43
8:H:5008:MET:O	8:H:5026:LEU:O	2.37	0.43
6:F:8188:GLU:OE2	6:F:8190:GLN:HB2	2.18	0.43
3:K:3038:GLU:HB3	6:N:8011:PHE:HE1	1.84	0.43
8:H:5025:ILE:HG21	8:H:5027:ARG:CZ	2.49	0.43
6:2:8005:GLU:O	6:2:8009:HIS:ND1	2.52	0.43
2:R:2019:THR:O	6:V:8022:THR:HG21	2.19	0.43
3:K:3069:ASN:OD1	4:L:4018:LYS:HG2	2.19	0.43
4:D:4030:VAL:HG12	4:D:4031:ASP:N	2.33	0.43
8:4:5008:MET:O	8:4:5026:LEU:O	2.37	0.42
6:N:8209:ASN:C	6:N:8211:PHE:N	2.69	0.42
4:T:4000:ASN:O	4:T:4003:PRO:HD2	2.19	0.42
7:G:6068:PRO:HD2	7:G:6069:ARG:N	2.29	0.42
4:L:4030:VAL:HG12	4:L:4031:ASP:N	2.35	0.42
2:J:2040:ARG:C	2:J:2042:ASN:H	2.22	0.42
7:G:6018:ASN:ND2	7:G:6019:ASN:HB2	2.31	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:3000:MET:CE	3:C:3002:GLN:NE2	2.80	0.42
6:N:8046:PRO:HB2	6:N:8047:PRO:CD	2.50	0.42
6:F:8188:GLU:OE1	6:F:8190:GLN:HB2	2.19	0.42
6:N:8012:TYR:O	6:N:8016:ARG:HG2	2.20	0.42
1:Y:1001:LEU:HA	1:Y:1001:LEU:HD23	1.86	0.42
7:W:6065:SER:OG	7:W:6066:SER:N	2.52	0.42
6:N:8005:GLU:O	6:N:8009:HIS:ND1	2.53	0.42
2:B:2016:GLU:OE1	6:F:8020:VAL:HG11	2.19	0.42
3:K:3006:LEU:HD11	8:P:5054:MET:HG2	2.02	0.42
4:T:4005:LEU:HD23	4:T:4030:VAL:HG11	2.02	0.42
6:N:8141:LEU:HD12	6:N:8195:TYR:CD1	2.54	0.42
8:X:5008:MET:O	8:X:5026:LEU:O	2.38	0.42
6:V:8046:PRO:HB2	6:V:8047:PRO:CD	2.50	0.42
4:L:4000:ASN:O	4:L:4003:PRO:HD2	2.20	0.42
3:K:3024:GLN:HE22	3:K:3027:MET:CE	2.32	0.42
7:W:6081:GLU:HB2	8:X:5064:MET:HE1	2.02	0.42
3:C:3069:ASN:OD1	4:D:4018:LYS:HG2	2.19	0.42
3:C:3071:THR:HG23	8:H:5061:SER:HB3	2.01	0.42
1:I:1018:LYS:HE2	1:I:1061:ASN:O	2.20	0.42
6:F:8012:TYR:O	6:F:8016:ARG:HG2	2.20	0.41
6:F:8071:GLN:O	6:F:8074:VAL:HB	2.20	0.41
7:W:6072:ILE:HB	7:W:6137:LEU:HB2	2.03	0.41
1:Y:1069:PRO:HD2	1:Y:1072:LEU:HD22	2.02	0.41
6:N:8007:LEU:HG	6:N:8011:PHE:CE1	2.55	0.41
2:Z:2038:ASN:HB2	2:Z:2090:VAL:HG22	2.01	0.41
2:R:2038:ASN:HB2	2:R:2090:VAL:HG22	2.01	0.41
6:N:8196:ASN:HA	6:N:8215:ILE:HD11	2.02	0.41
2:R:2040:ARG:HA	2:R:2089:ILE:HD11	2.02	0.41
6:N:8203:VAL:O	6:N:8207:ALA:HA	2.21	0.41
6:N:8188:GLU:OE2	6:N:8190:GLN:HB2	2.20	0.41
6:F:8005:GLU:O	6:F:8009:HIS:ND1	2.53	0.41
4:D:4000:ASN:O	4:D:4003:PRO:HD2	2.20	0.41
2:J:2049:VAL:HA	2:J:2060:LEU:HD23	2.03	0.41
2:B:2049:VAL:HA	2:B:2060:LEU:HD23	2.03	0.41
6:N:8201:LEU:CD2	6:N:8205:VAL:HG21	2.50	0.41
2:J:2038:ASN:HB2	2:J:2090:VAL:HG22	2.01	0.41
2:J:2092:LEU:CD2	4:L:4056:VAL:HG22	2.38	0.41
3:K:3000:MET:HE2	3:K:3002:GLN:NE2	2.34	0.41
6:V:8054:THR:HG23	6:V:8057:TRP:CB	2.51	0.41
6:F:8054:THR:HG23	6:F:8057:TRP:CB	2.50	0.41
4:L:4000:ASN:ND2	6:N:8010:MET:HB2	2.36	0.41
1:A:1018:LYS:HE2	1:A:1061:ASN:O	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:M:7005:SER:O	5:M:7007:LEU:N	2.53	0.41
6:F:8100:LYS:HD3	6:F:8104:ARG:CZ	2.51	0.41
7:O:6038:GLN:HG2	7:O:6158:LEU:HD23	2.02	0.41
6:F:8162:LEU:HB2	6:F:8167:PHE:CE1	2.56	0.41
5:M:7010:THR:O	5:M:7014:SER:HB2	2.21	0.41
3:S:3071:THR:HG23	8:X:5061:SER:HB3	2.03	0.41
3:C:3016:ARG:CD	3:C:3030:GLU:HG2	2.52	0.40
3:K:3016:ARG:CD	3:K:3030:GLU:HG2	2.51	0.40
1:Q:1069:PRO:HD2	1:Q:1072:LEU:HD22	2.04	0.40
7:O:6072:ILE:HB	7:O:6137:LEU:HB2	2.04	0.40
7:G:6038:GLN:HG2	7:G:6158:LEU:HD23	2.04	0.40
2:R:2089:ILE:HA	4:T:4062:ASN:ND2	2.36	0.40
2:J:2016:GLU:OE1	6:N:8020:VAL:HG11	2.21	0.40
6:N:8215:ILE:HD12	6:N:8215:ILE:HA	1.93	0.40
5:U:7002:TRP:HB2	5:U:7003:ASP:H	1.66	0.40
2:J:2089:ILE:HA	4:L:4062:ASN:ND2	2.37	0.40
7:O:6152:MET:HB2	7:O:6152:MET:HE3	1.91	0.40
4:D:4002:LYS:HG3	6:F:8014:ARG:HB3	2.02	0.40
6:V:8162:LEU:HG	6:V:8166:VAL:HG11	2.04	0.40
2:R:2067:TRP:CE2	2:R:2074:LYS:HB2	2.56	0.40
6:V:8043:PRO:HB2	6:V:8178:ILE:HG21	2.03	0.40
1:Q:1018:LYS:HE2	1:Q:1061:ASN:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	9	42
1	I	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	9	42
1	Q	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	9	42
1	Y	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	9	42
1	g	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	9	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	o	80/119 (67%)	77 (96%)	1 (1%)	2 (2%)	9	42
1	w	80/119 (67%)	77 (96%)	1 (1%)	2 (2%)	9	42
2	B	96/118 (81%)	92 (96%)	4 (4%)	0	100	100
2	J	96/118 (81%)	90 (94%)	6 (6%)	0	100	100
2	R	96/118 (81%)	91 (95%)	5 (5%)	0	100	100
2	Z	96/118 (81%)	92 (96%)	4 (4%)	0	100	100
2	h	96/118 (81%)	90 (94%)	3 (3%)	3 (3%)	7	36
2	p	96/118 (81%)	91 (95%)	5 (5%)	0	100	100
2	x	96/118 (81%)	92 (96%)	3 (3%)	1 (1%)	22	68
3	C	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	K	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	S	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	a	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	i	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	q	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	y	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
4	D	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	L	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	T	69/86 (80%)	67 (97%)	2 (3%)	0	100	100
4	b	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	j	69/86 (80%)	67 (97%)	2 (3%)	0	100	100
4	r	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	z	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
5	l	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	2	14
5	E	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	2	14
5	M	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	2	14
5	U	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	2	14
5	c	15/124 (12%)	9 (60%)	5 (33%)	1 (7%)	2	14
5	k	15/124 (12%)	10 (67%)	4 (27%)	1 (7%)	2	14
5	s	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	2	14
6	2	214/247 (87%)	187 (87%)	17 (8%)	10 (5%)	4	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	214/247 (87%)	182 (85%)	22 (10%)	10 (5%)	4	23
6	N	214/247 (87%)	174 (81%)	31 (14%)	9 (4%)	4	27
6	V	214/247 (87%)	182 (85%)	21 (10%)	11 (5%)	3	22
6	d	214/247 (87%)	183 (86%)	20 (9%)	11 (5%)	3	22
6	l	214/247 (87%)	183 (86%)	21 (10%)	10 (5%)	4	23
6	t	214/247 (87%)	182 (85%)	21 (10%)	11 (5%)	3	22
7	3	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	6	33
7	G	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	6	33
7	O	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	6	33
7	W	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	6	33
7	e	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	6	33
7	m	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	6	33
7	u	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	6	33
8	4	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	H	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	P	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	X	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	f	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	n	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	v	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
All	All	5180/7336 (71%)	4740 (92%)	308 (6%)	132 (2%)	9	42

All (132) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	M	7006	LEU
6	N	8028	ILE
6	N	8185	LYS
6	N	8186	GLU
6	N	8212	LYS
7	O	6162	SER
8	P	5008	MET
5	E	7006	LEU
6	F	8028	ILE
6	F	8185	LYS

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Mol	Chain	Res	Type
6	F	8186	GLU
7	G	6162	SER
8	H	5008	MET
5	U	7006	LEU
6	V	8028	ILE
6	V	8185	LYS
6	V	8186	GLU
7	W	6011	HIS
8	X	5008	MET
5	c	7006	LEU
6	d	8028	ILE
6	d	8185	LYS
6	d	8209	ASN
7	e	6011	HIS
8	f	5008	MET
5	k	7006	LEU
6	l	8028	ILE
6	l	8185	LYS
6	l	8186	GLU
7	m	6011	HIS
8	n	5008	MET
5	s	7006	LEU
6	t	8028	ILE
6	t	8185	LYS
6	t	8186	GLU
6	t	8212	LYS
7	u	6011	HIS
8	v	5008	MET
5	1	7006	LEU
6	2	8028	ILE
6	2	8185	LYS
8	4	5008	MET
2	x	2042	ASN
1	I	1070	ASP
6	N	8133	GLN
7	O	6011	HIS
1	A	1070	ASP
6	F	8133	GLN
6	F	8207	ALA
7	G	6011	HIS
1	Q	1070	ASP
6	V	8026	SER

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Mol	Chain	Res	Type
6	V	8133	GLN
6	V	8207	ALA
7	W	6162	SER
1	Y	1070	ASP
6	d	8026	SER
6	d	8133	GLN
6	d	8186	GLU
7	e	6162	SER
1	g	1070	ASP
6	l	8133	GLN
7	m	6162	SER
7	m	6164	ASN
1	o	1070	ASP
6	t	8026	SER
6	t	8133	GLN
7	u	6162	SER
6	2	8026	SER
6	2	8133	GLN
6	2	8186	GLU
6	2	8209	ASN
7	3	6011	HIS
7	3	6162	SER
1	w	1070	ASP
6	N	8003	GLY
6	N	8026	SER
6	F	8026	SER
6	d	8158	LEU
6	l	8026	SER
6	l	8212	LYS
6	t	8113	LEU
7	3	6164	ASN
6	F	8046	PRO
6	F	8209	ASN
7	G	6164	ASN
6	V	8019	ALA
6	V	8046	PRO
7	W	6164	ASN
6	d	8003	GLY
6	d	8046	PRO
6	d	8110	LEU
7	e	6164	ASN
2	h	2098	ALA

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Mol	Chain	Res	Type
6	l	8003	GLY
6	l	8207	ALA
6	t	8046	PRO
7	u	6067	ASN
7	u	6164	ASN
6	2	8003	GLY
6	2	8034	ASN
6	N	8188	GLU
7	O	6067	ASN
7	O	6164	ASN
6	F	8003	GLY
6	F	8188	GLU
7	G	6067	ASN
6	V	8003	GLY
6	V	8188	GLU
7	W	6067	ASN
6	d	8188	GLU
7	e	6067	ASN
2	h	2041	ASN
2	h	2043	LYS
6	l	8188	GLU
7	m	6067	ASN
6	t	8003	GLY
6	t	8019	ALA
6	2	8188	GLU
7	3	6067	ASN
1	I	1069	PRO
6	N	8046	PRO
1	A	1069	PRO
1	Q	1069	PRO
6	V	8210	ASP
1	o	1069	PRO
6	t	8188	GLU
1	w	1069	PRO
1	Y	1069	PRO
1	g	1069	PRO
6	l	8046	PRO
6	2	8046	PRO

### 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	77/101 (76%)	70 (91%)	7 (9%)	14	45
1	I	77/101 (76%)	72 (94%)	5 (6%)	24	65
1	Q	77/101 (76%)	72 (94%)	5 (6%)	24	65
1	Y	77/101 (76%)	71 (92%)	6 (8%)	18	57
1	g	77/101 (76%)	71 (92%)	6 (8%)	18	57
1	o	77/101 (76%)	73 (95%)	4 (5%)	32	73
1	w	77/101 (76%)	72 (94%)	5 (6%)	24	65
2	B	94/110 (86%)	90 (96%)	4 (4%)	40	80
2	J	94/110 (86%)	92 (98%)	2 (2%)	66	92
2	R	94/110 (86%)	91 (97%)	3 (3%)	51	87
2	Z	94/110 (86%)	90 (96%)	4 (4%)	40	80
2	h	94/110 (86%)	89 (95%)	5 (5%)	32	72
2	p	94/110 (86%)	91 (97%)	3 (3%)	51	87
2	x	94/110 (86%)	90 (96%)	4 (4%)	40	80
3	C	72/84 (86%)	67 (93%)	5 (7%)	22	62
3	K	72/84 (86%)	68 (94%)	4 (6%)	30	70
3	S	72/84 (86%)	68 (94%)	4 (6%)	30	70
3	a	72/84 (86%)	68 (94%)	4 (6%)	30	70
3	i	72/84 (86%)	68 (94%)	4 (6%)	30	70
3	q	72/84 (86%)	68 (94%)	4 (6%)	30	70
3	y	72/84 (86%)	69 (96%)	3 (4%)	40	81
4	D	60/74 (81%)	56 (93%)	4 (7%)	23	63
4	L	60/74 (81%)	57 (95%)	3 (5%)	34	75
4	T	60/74 (81%)	56 (93%)	4 (7%)	23	63
4	b	60/74 (81%)	56 (93%)	4 (7%)	23	63
4	j	60/74 (81%)	56 (93%)	4 (7%)	23	63
4	r	60/74 (81%)	56 (93%)	4 (7%)	23	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	z	60/74 (81%)	57 (95%)	3 (5%)	34	75
5	1	15/97 (16%)	11 (73%)	4 (27%)	1	2
5	E	15/97 (16%)	12 (80%)	3 (20%)	2	8
5	M	15/97 (16%)	12 (80%)	3 (20%)	2	8
5	U	15/97 (16%)	13 (87%)	2 (13%)	6	22
5	c	15/97 (16%)	12 (80%)	3 (20%)	2	8
5	k	15/97 (16%)	13 (87%)	2 (13%)	6	22
5	s	15/97 (16%)	12 (80%)	3 (20%)	2	8
6	2	203/231 (88%)	176 (87%)	27 (13%)	6	22
6	F	203/231 (88%)	170 (84%)	33 (16%)	3	12
6	N	203/231 (88%)	171 (84%)	32 (16%)	4	14
6	V	203/231 (88%)	177 (87%)	26 (13%)	6	24
6	d	203/231 (88%)	178 (88%)	25 (12%)	7	26
6	l	203/231 (88%)	176 (87%)	27 (13%)	6	22
6	t	203/231 (88%)	172 (85%)	31 (15%)	4	15
7	3	108/159 (68%)	98 (91%)	10 (9%)	13	44
7	G	108/159 (68%)	98 (91%)	10 (9%)	13	44
7	O	108/159 (68%)	99 (92%)	9 (8%)	16	53
7	W	108/159 (68%)	99 (92%)	9 (8%)	16	53
7	e	108/159 (68%)	99 (92%)	9 (8%)	16	53
7	m	108/159 (68%)	99 (92%)	9 (8%)	16	53
7	u	108/159 (68%)	99 (92%)	9 (8%)	16	53
8	4	61/66 (92%)	59 (97%)	2 (3%)	50	86
8	H	61/66 (92%)	59 (97%)	2 (3%)	50	86
8	P	61/66 (92%)	59 (97%)	2 (3%)	50	86
8	X	61/66 (92%)	59 (97%)	2 (3%)	50	86
8	f	61/66 (92%)	59 (97%)	2 (3%)	50	86
8	n	61/66 (92%)	59 (97%)	2 (3%)	50	86
8	v	61/66 (92%)	59 (97%)	2 (3%)	50	86
All	All	4830/6454 (75%)	4413 (91%)	417 (9%)	15	51

All (417) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	1002	VAL
1	I	1009	SER
1	I	1047	ASN
1	I	1048	ARG
1	I	1064	ARG
2	J	2054	ARG
2	J	2092	LEU
3	K	3004	ILE
3	K	3016	ARG
3	K	3026	ASN
3	K	3045	ASP
4	L	4021	MET
4	L	4046	ASP
4	L	4053	LEU
5	M	7002	TRP
5	M	7006	LEU
5	M	7014	SER
6	N	8001	GLU
6	N	8009	HIS
6	N	8010	MET
6	N	8024	ARG
6	N	8032	THR
6	N	8037	LEU
6	N	8039	MET
6	N	8054	THR
6	N	8066	GLN
6	N	8073	LEU
6	N	8079	LEU
6	N	8083	ASN
6	N	8093	THR
6	N	8096	GLN
6	N	8106	GLN
6	N	8109	LEU
6	N	8113	LEU
6	N	8117	THR
6	N	8127	MET
6	N	8133	GLN
6	N	8139	VAL
6	N	8147	LEU
6	N	8154	THR
6	N	8160	LEU
6	N	8177	CYS
6	N	8180	LEU

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Mol	Chain	Res	Type
6	N	8184	LEU
6	N	8186	GLU
6	N	8188	GLU
6	N	8198	LEU
6	N	8204	GLN
6	N	8210	ASP
7	O	6010	GLU
7	O	6019	ASN
7	O	6027	LYS
7	O	6031	GLU
7	O	6033	THR
7	O	6131	GLU
7	O	6140	GLU
7	O	6158	LEU
7	O	6162	SER
8	P	5000	HIS
8	P	5058	ARG
1	A	1002	VAL
1	A	1009	SER
1	A	1042	LYS
1	A	1046	LYS
1	A	1047	ASN
1	A	1048	ARG
1	A	1064	ARG
2	B	2040	ARG
2	B	2054	ARG
2	B	2076	ARG
2	B	2092	LEU
3	C	3004	ILE
3	C	3016	ARG
3	C	3024	GLN
3	C	3026	ASN
3	C	3045	ASP
4	D	4002	LYS
4	D	4021	MET
4	D	4046	ASP
4	D	4053	LEU
5	E	7002	TRP
5	E	7006	LEU
5	E	7007	LEU
6	F	8001	GLU
6	F	8010	MET

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Mol	Chain	Res	Type
6	F	8024	ARG
6	F	8037	LEU
6	F	8039	MET
6	F	8054	THR
6	F	8075	LEU
6	F	8077	LYS
6	F	8083	ASN
6	F	8093	THR
6	F	8096	GLN
6	F	8106	GLN
6	F	8109	LEU
6	F	8111	SER
6	F	8119	ASN
6	F	8123	LEU
6	F	8125	LEU
6	F	8127	MET
6	F	8133	GLN
6	F	8139	VAL
6	F	8151	LEU
6	F	8154	THR
6	F	8156	VAL
6	F	8159	HIS
6	F	8162	LEU
6	F	8180	LEU
6	F	8184	LEU
6	F	8186	GLU
6	F	8188	GLU
6	F	8197	LEU
6	F	8202	THR
6	F	8213	ASP
6	F	8215	ILE
7	G	6010	GLU
7	G	6018	ASN
7	G	6019	ASN
7	G	6027	LYS
7	G	6031	GLU
7	G	6033	THR
7	G	6131	GLU
7	G	6140	GLU
7	G	6158	LEU
7	G	6162	SER
8	H	5000	HIS

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Mol	Chain	Res	Type
8	H	5058	ARG
1	Q	1002	VAL
1	Q	1009	SER
1	Q	1046	LYS
1	Q	1047	ASN
1	Q	1048	ARG
2	R	2054	ARG
2	R	2076	ARG
2	R	2092	LEU
3	S	3004	ILE
3	S	3016	ARG
3	S	3026	ASN
3	S	3045	ASP
4	T	4002	LYS
4	T	4021	MET
4	T	4046	ASP
4	T	4053	LEU
5	U	7002	TRP
5	U	7006	LEU
6	V	8001	GLU
6	V	8010	MET
6	V	8024	ARG
6	V	8037	LEU
6	V	8039	MET
6	V	8054	THR
6	V	8073	LEU
6	V	8079	LEU
6	V	8083	ASN
6	V	8093	THR
6	V	8096	GLN
6	V	8106	GLN
6	V	8109	LEU
6	V	8127	MET
6	V	8133	GLN
6	V	8139	VAL
6	V	8147	LEU
6	V	8149	ARG
6	V	8156	VAL
6	V	8162	LEU
6	V	8180	LEU
6	V	8184	LEU
6	V	8186	GLU

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Mol	Chain	Res	Type
6	V	8188	GLU
6	V	8199	LEU
6	V	8213	ASP
7	W	6010	GLU
7	W	6019	ASN
7	W	6027	LYS
7	W	6031	GLU
7	W	6033	THR
7	W	6131	GLU
7	W	6140	GLU
7	W	6158	LEU
7	W	6162	SER
8	X	5000	HIS
8	X	5058	ARG
1	Y	1002	VAL
1	Y	1009	SER
1	Y	1046	LYS
1	Y	1047	ASN
1	Y	1048	ARG
1	Y	1064	ARG
2	Z	2040	ARG
2	Z	2054	ARG
2	Z	2076	ARG
2	Z	2092	LEU
3	a	3004	ILE
3	a	3016	ARG
3	a	3026	ASN
3	a	3045	ASP
4	b	4002	LYS
4	b	4021	MET
4	b	4046	ASP
4	b	4053	LEU
5	c	7002	TRP
5	c	7006	LEU
5	c	7007	LEU
6	d	8001	GLU
6	d	8010	MET
6	d	8024	ARG
6	d	8037	LEU
6	d	8039	MET
6	d	8054	THR
6	d	8066	GLN

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Mol	Chain	Res	Type
6	d	8073	LEU
6	d	8079	LEU
6	d	8083	ASN
6	d	8093	THR
6	d	8094	SER
6	d	8096	GLN
6	d	8106	GLN
6	d	8127	MET
6	d	8133	GLN
6	d	8139	VAL
6	d	8147	LEU
6	d	8159	HIS
6	d	8180	LEU
6	d	8184	LEU
6	d	8186	GLU
6	d	8188	GLU
6	d	8210	ASP
6	d	8213	ASP
7	e	6010	GLU
7	e	6019	ASN
7	e	6027	LYS
7	e	6031	GLU
7	e	6033	THR
7	e	6131	GLU
7	e	6140	GLU
7	e	6158	LEU
7	e	6162	SER
8	f	5000	HIS
8	f	5058	ARG
1	g	1002	VAL
1	g	1009	SER
1	g	1022	GLN
1	g	1047	ASN
1	g	1048	ARG
1	g	1064	ARG
2	h	2002	SER
2	h	2040	ARG
2	h	2054	ARG
2	h	2076	ARG
2	h	2092	LEU
3	i	3004	ILE
3	i	3016	ARG

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Mol	Chain	Res	Type
3	i	3024	GLN
3	i	3045	ASP
4	j	4002	LYS
4	j	4021	MET
4	j	4046	ASP
4	j	4053	LEU
5	k	7002	TRP
5	k	7006	LEU
6	l	8001	GLU
6	l	8010	MET
6	l	8024	ARG
6	l	8032	THR
6	l	8037	LEU
6	l	8039	MET
6	l	8054	THR
6	l	8073	LEU
6	l	8079	LEU
6	l	8083	ASN
6	l	8093	THR
6	l	8096	GLN
6	l	8106	GLN
6	l	8109	LEU
6	l	8127	MET
6	l	8133	GLN
6	l	8139	VAL
6	l	8147	LEU
6	l	8159	HIS
6	l	8160	LEU
6	l	8169	THR
6	l	8170	LEU
6	l	8180	LEU
6	l	8184	LEU
6	l	8186	GLU
6	l	8188	GLU
6	l	8213	ASP
7	m	6010	GLU
7	m	6019	ASN
7	m	6027	LYS
7	m	6031	GLU
7	m	6033	THR
7	m	6131	GLU
7	m	6140	GLU

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Mol	Chain	Res	Type
7	m	6158	LEU
7	m	6162	SER
8	n	5000	HIS
8	n	5058	ARG
1	o	1002	VAL
1	o	1009	SER
1	o	1047	ASN
1	o	1048	ARG
2	p	2042	ASN
2	p	2054	ARG
2	p	2092	LEU
3	q	3004	ILE
3	q	3016	ARG
3	q	3026	ASN
3	q	3045	ASP
4	r	4002	LYS
4	r	4021	MET
4	r	4046	ASP
4	r	4053	LEU
5	s	7002	TRP
5	s	7006	LEU
5	s	7007	LEU
6	t	8001	GLU
6	t	8010	MET
6	t	8024	ARG
6	t	8037	LEU
6	t	8039	MET
6	t	8054	THR
6	t	8066	GLN
6	t	8073	LEU
6	t	8079	LEU
6	t	8083	ASN
6	t	8093	THR
6	t	8096	GLN
6	t	8100	LYS
6	t	8101	GLU
6	t	8106	GLN
6	t	8109	LEU
6	t	8119	ASN
6	t	8126	GLU
6	t	8127	MET
6	t	8139	VAL

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Mol	Chain	Res	Type
6	t	8147	LEU
6	t	8156	VAL
6	t	8160	LEU
6	t	8169	THR
6	t	8177	CYS
6	t	8180	LEU
6	t	8184	LEU
6	t	8186	GLU
6	t	8188	GLU
6	t	8195	TYR
6	t	8213	ASP
7	u	6010	GLU
7	u	6019	ASN
7	u	6027	LYS
7	u	6031	GLU
7	u	6033	THR
7	u	6131	GLU
7	u	6140	GLU
7	u	6158	LEU
7	u	6162	SER
8	v	5000	HIS
8	v	5058	ARG
5	1	7002	TRP
5	1	7006	LEU
5	1	7007	LEU
5	1	7014	SER
6	2	8001	GLU
6	2	8009	HIS
6	2	8010	MET
6	2	8024	ARG
6	2	8032	THR
6	2	8037	LEU
6	2	8039	MET
6	2	8054	THR
6	2	8073	LEU
6	2	8079	LEU
6	2	8083	ASN
6	2	8093	THR
6	2	8096	GLN
6	2	8106	GLN
6	2	8107	GLN
6	2	8119	ASN

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Mol	Chain	Res	Type
6	2	8127	MET
6	2	8133	GLN
6	2	8139	VAL
6	2	8156	VAL
6	2	8177	CYS
6	2	8180	LEU
6	2	8184	LEU
6	2	8186	GLU
6	2	8188	GLU
6	2	8209	ASN
6	2	8210	ASP
7	3	6010	GLU
7	3	6027	LYS
7	3	6031	GLU
7	3	6033	THR
7	3	6079	LYS
7	3	6085	VAL
7	3	6131	GLU
7	3	6140	GLU
7	3	6158	LEU
7	3	6162	SER
8	4	5000	HIS
8	4	5058	ARG
1	w	1002	VAL
1	w	1009	SER
1	w	1047	ASN
1	w	1048	ARG
1	w	1064	ARG
2	x	2002	SER
2	x	2040	ARG
2	x	2054	ARG
2	x	2092	LEU
3	y	3016	ARG
3	y	3026	ASN
3	y	3045	ASP
4	z	4021	MET
4	z	4046	ASP
4	z	4053	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	1047	ASN
2	J	2031	ASN
3	K	3002	GLN
3	K	3024	GLN
6	N	8096	GLN
6	N	8106	GLN
1	A	1047	ASN
2	B	2031	ASN
3	C	3002	GLN
3	C	3024	GLN
6	F	8081	ASN
6	F	8096	GLN
6	F	8106	GLN
7	G	6018	ASN
1	Q	1047	ASN
2	R	2031	ASN
3	S	3002	GLN
3	S	3024	GLN
6	V	8066	GLN
6	V	8096	GLN
1	Y	1022	GLN
1	Y	1047	ASN
2	Z	2031	ASN
3	a	3002	GLN
3	a	3024	GLN
6	d	8096	GLN
6	d	8190	GLN
7	e	6018	ASN
1	g	1047	ASN
2	h	2031	ASN
3	i	3002	GLN
3	i	3024	GLN
6	l	8066	GLN
6	l	8081	ASN
6	l	8096	GLN
6	l	8119	ASN
1	o	1022	GLN
1	o	1047	ASN
2	p	2031	ASN
3	q	3002	GLN
3	q	3024	GLN
6	t	8165	HIS
6	t	8209	ASN

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Mol	Chain	Res	Type
7	u	6018	ASN
1	w	1047	ASN
2	x	2031	ASN
3	y	3002	GLN
3	y	3024	GLN
4	z	4052	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 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	$\# Z  > 2$
9	SO4	2	8301	-	4,4,4	0.25	0	6,6,6	0.38	0
9	SO4	t	8301	-	4,4,4	0.58	0	6,6,6	0.37	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
9	SO4	2	8301	-	-	0/0/0/0	0/0/0/0
9	SO4	t	8301	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.