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PDB ID	:	6HIZ
EMDB ID	:	EMD-0233
Title	:	Cryo-EM structure of the Trypanosoma brucei mitochondrial ribosome - This
		entry contains the head of the small mitoribosomal subunit
Authors	:	Ramrath, D.J.F.; Niemann, M.; Leibundgut, M.; Bieri, P.; Prange, C.; Horn,
		E.K.; Leitner, A.; Boehringer, A.; Schneider, A.; Ban, N.
Deposited on	:	2018-08-31
Resolution	:	3.08 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $ELECTRON\ MICROSCOPY$ 

The reported resolution of this entry is 3.08 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain	-
1	DA	1788	7% • 93%	
2	DL	307	43% •• 53%	
3	DB	1181	85%	9% 6%
4	DC	1165	84%	10% 6%
5	DE	747	71% 7%	21%
6	DF	666	80%	9% 11%
7	DG	631	79%	11% 10%
8	DH	581	87%	10% •



Mol	Chain	Length	Quality of chain					
9	DJ	396	71% 8°	%	20%			
10	DK	324	73% 5	%	21%			
11	DT	247	86%		11% •			
12	DV	183	77%	119	% 13%			
13	DW	179	83%		7% 10%			
14	DX	169	75%	9%	17%			
15	DY	163	83%		12% 6%			
16	CC	74	84%		16%			
17	CI	443	45% 5% 50	)%				
18	CJ	817	88%		10% •			
19	CK	326	14% • 84%					
20	CN	166	83%		12% 5%			
21	CR	320	11% • 86%					
22	CS	244	53% 5%	42%				
23	Cg	498	88%		9% •			
24	Ci	181	79%		12% 9%			
25	Ck	874	73%	7%	20%			
26	CA	611	9% 14% 77%					
27	UO	5	100%					
28	UP	7	100%					

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## 2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 76845 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	DA	131	Total 993	C 629	N 174	O 186	${S \over 4}$	0	0

• Molecule 1 is a protein called mS48.

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DA	894	HIS	ASN	conflict	UNP Q57UJ2
DA	1181	THR	ILE	conflict	UNP Q57UJ2
DA	1333	ALA	VAL	conflict	UNP Q57UJ2
DA	1700	ARG	HIS	conflict	UNP Q57UJ2
DA	1761	LYS	ARG	conflict	UNP Q57UJ2

• Molecule 2 is a protein called mS59.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	DL	143	Total 1153	C 733	N 215	O 202	${ m S} { m 3}$	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DL	274	THR	ALA	conflict	UNP Q38BS2

• Molecule 3 is a protein called mS49.

Mol	Chain	Residues	Atoms				AltConf	Trace	
3	DB	1111	Total 9148	C 5691	N 1717	0 1711	S 29	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DB	23	VAL	ALA	conflict	UNP $Q586P5$
				Continued	on next page
			P	ROTEIN DATA BANK	

Chain	Residue	Modelled	Actual	Comment	Reference
DB	359	ILE	THR	conflict	UNP Q586P5
DB	384	GLN	HIS	conflict	UNP Q586P5
DB	402	THR	ILE	conflict	UNP Q586P5
DB	423	THR	ALA	conflict	UNP Q586P5
DB	586	ARG	HIS	conflict	UNP Q586P5
DB	593	ARG	LYS	conflict	UNP Q586P5
DB	647	SER	GLY	conflict	UNP Q586P5

• Molecule 4 is a protein called mS50.

Mol	Chain	Residues		Α	AltConf	Trace			
4	DC	1095	Total 8748	C 5519	N 1544	0 1654	S 31	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DC	53	ALA	THR	conflict	UNP Q57YB5
DC	365	LYS	GLU	conflict	UNP Q57YB5
DC	385	THR	ALA	conflict	UNP Q57YB5
DC	405	ILE	VAL	conflict	UNP Q57YB5
DC	641	SER	PRO	conflict	UNP Q57YB5
DC	651	LYS	GLU	conflict	UNP Q57YB5
DC	731	GLU	ASP	conflict	UNP Q57YB5
DC	814	GLN	HIS	conflict	UNP Q57YB5
DC	1097	ALA	VAL	conflict	UNP Q57YB5
DC	1113	THR	ILE	conflict	UNP Q57YB5

• Molecule 5 is a protein called mS52.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	DE	590	Total 4831	C 3075	N 874	O 863	S 19	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DE	514	THR	SER	conflict	UNP $Q386Q7$

• Molecule 6 is a protein called mS53.



Mol	Chain	Residues		At	AltConf	Trace			
6	DF	590	Total 4747	C 2979	N 896	0 847	$\begin{array}{c} \mathrm{S} \\ \mathrm{25} \end{array}$	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DF	18	THR	ALA	conflict	UNP Q38ET1
DF	258	ASP	ASN	conflict	UNP Q38ET1
DF	372	ASN	ASP	conflict	UNP Q38ET1
DF	406	ASN	SER	conflict	UNP Q38ET1
DF	510	ASP	GLY	conflict	UNP Q38ET1
DF	577	ALA	VAL	conflict	UNP Q38ET1
DF	636	UNK	GLY	conflict	UNP Q38ET1
DF	638	LYS	ARG	conflict	UNP Q38ET1

• Molecule 7 is a protein called mS54.

Mol	Chain	Residues		At	oms			AltConf	Trace
7	DG	566	Total 4575	C 2875	N 835	0 834	S 31	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DG	428	ASN	SER	conflict	UNP Q57ZP8
DG	429	GLY	SER	conflict	UNP Q57ZP8

• Molecule 8 is a protein called mS55.

Mol	Chain	Residues		At	AltConf	Trace			
8	DH	564	Total 4578	C 2872	N 850	0 834	S 22	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DH	191	HIS	GLN	conflict	UNP $Q580V1$
DH	194	PRO	ARG	conflict	UNP $Q580V1$
DH	488	GLY	SER	conflict	UNP $Q580V1$

• Molecule 9 is a protein called mS57.



Mol	Chain	Residues		At	AltConf	Trace			
9	DJ	315	Total 2572	C 1646	N 452	O 460	S 14	0	0

• Molecule 10 is a protein called mS58.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	DK	255	Total 2007	C 1260	N 365	0 377	${ m S}{ m 5}$	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DK	61	SER	PRO	conflict	UNP Q38BP1
DK	257	GLY	SER	conflict	UNP Q38BP1

• Molecule 11 is a protein called mS67.

Mol	Chain	Residues		At	oms			AltConf	Trace
11	DT	239	Total 2058	C 1321	N 364	O 362	S 11	0	0

• Molecule 12 is a protein called mS69.

Mol	Chain	Residues		At	oms			AltConf	Trace
12	DV	160	Total 1346	C 855	N 252	0 235	$\frac{S}{4}$	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DV	163	ALA	THR	conflict	UNP Q57UZ6

• Molecule 13 is a protein called mS70.

Mol	Chain	Residues		At	oms			AltConf	Trace
13	DW	161	Total 1359	C 866	N 260	0 228	${ m S}{ m 5}$	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DW	74	THR	MET	conflict	UNP Q383N9



• Molecule 14 is a protein called mS71.

Mol	Chain	Residues		At	oms			AltConf	Trace
14	DX	141	Total 1196	C 762	N 226	O 201	${ m S} 7$	0	0

• Molecule 15 is a protein called mS72.

Mol	Chain	Residues		At	oms			AltConf	Trace
15	DY	154	Total 1293	C 827	N 245	0 216	${ m S}{ m 5}$	0	0

• Molecule 16 is a protein called uS3m.

Mol	Chain	Residues		Ato	$\mathbf{ms}$			AltConf	Trace
16	CC	74	Total 646	C 451	N 96	O 98	S 1	0	0

• Molecule 17 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	CI	222	Total 1754	C 1101	N 330	0 313	S 10	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CI	279	UNK	ARG	conflict	UNP $Q57W62$
CI	370	ALA	VAL	conflict	UNP Q57W62

• Molecule 18 is a protein called uS10m.

Mol	Chain	Residues		Α	toms			AltConf	Trace
18	CJ	800	Total 6516	C 4119	N 1151	O 1216	S 30	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CJ	311	LEU	TYR	conflict	UNP $Q57Z45$
CJ	484	HIS	ARG	conflict	UNP $Q57Z45$
CJ	488	SER	ASN	conflict	UNP $Q57Z45$
CJ	594	GLU	VAL	conflict	UNP $Q57Z45$



Chain	Residue	Modelled	Actual	Comment	Reference
CJ	629	ARG	LYS	conflict	UNP $Q57Z45$

• Molecule 19 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	CK	52	Total 438	C 272	N 90	0 74	S 2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CK	3	ARG	GLN	conflict	UNP Q389T7
CK	138	UNK	ILE	conflict	UNP Q389T7

• Molecule 20 is a protein called uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	CN	157	Total 1322	C 843	N 251	O 220	S 8	0	0

• Molecule 21 is a protein called uS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	CR	44	Total 353	C 217	N 64	0 71	S 1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CR	8	ILE	VAL	conflict	UNP Q38AS2

• Molecule 22 is a protein called uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	CS	142	Total 1175	C 761	N 210	0 198	S 6	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CS	-71	MET	-	initiating methionine	UNP $Q584T8$



Chain	Residue	Modelled	Actual	Comment	Reference
CS	-70	ALA	-	expression tag	UNP Q584T8
CS	-69	PHE	-	expression tag	UNP Q584T8
CS	-68	ARG	-	expression tag	UNP Q584T8
CS	-67	ASN	-	expression tag	UNP Q584T8
CS	-66	THR	-	expression tag	UNP Q584T8
CS	-65	PHE	-	expression tag	UNP Q584T8
CS	-64	THR	-	expression tag	UNP Q584T8
CS	-63	THR	-	expression tag	UNP Q584T8
CS	-62	PRO	-	expression tag	UNP Q584T8
CS	-61	GLY	-	expression tag	UNP Q584T8
CS	-60	LYS	-	expression tag	UNP Q584T8
CS	-59	PHE	-	expression tag	UNP Q584T8
CS	-58	SER	-	expression tag	UNP Q584T8
CS	-57	THR	-	expression tag	UNP Q584T8
CS	-56	VAL	-	expression tag	UNP Q584T8
CS	-55	SER	-	expression tag	UNP Q584T8
CS	-54	LYS	-	expression tag	UNP Q584T8
CS	-53	ASN	-	expression tag	UNP Q584T8
CS	-52	ILE	-	expression tag	UNP Q584T8
CS	-51	VAL	-	expression tag	UNP Q584T8
CS	-50	LEU	-	expression tag	UNP Q584T8
CS	-49	LEU	-	expression tag	UNP Q584T8
CS	-48	LEU	-	expression tag	UNP Q584T8
CS	-47	ILE	-	expression tag	UNP Q584T8
CS	-46	TRP	-	expression tag	UNP Q584T8
CS	-45	ARG	-	expression tag	UNP Q584T8
CS	-44	VAL	-	expression tag	UNP Q584T8
CS	-43	LYS	-	expression tag	UNP Q584T8
CS	-42	VAL	-	expression tag	UNP Q584T8
CS	-41	PHE	-	expression tag	UNP Q584T8
CS	-40	LEU	-	expression tag	UNP Q584T8
CS	-39	ARG	-	expression tag	UNP Q584T8
CS	-38	ALA	-	expression tag	UNP Q584T8
CS	-37	GLU	-	expression tag	UNP Q584T8
CS	-36	GLY	-	expression tag	UNP Q584T8
CS	-35	PHE	-	expression tag	UNP Q584T8
CS	-34	ALA	-	expression tag	UNP Q584T8
CS	-33	HIS	-	expression tag	UNP Q584T8
CS	-32	SER	-	expression tag	UNP Q584T8
CS	-31	LEU	-	expression tag	UNP Q584T8
CS	-30	VAL	-	expression tag	UNP Q584T8
CS	-29	MET	-	expression tag	UNP Q584T8



Chain	Residue	Modelled	Actual	Comment	Reference
CS	-28	LEU	-	expression tag	UNP Q584T8
CS	-27	PRO	-	expression tag	UNP Q584T8
CS	-26	VAL	-	expression tag	UNP Q584T8
CS	-25	SER	-	expression tag	UNP Q584T8
CS	-24	LEU	-	expression tag	UNP Q584T8
CS	-23	TYR	-	expression tag	UNP Q584T8
CS	-22	SER	-	expression tag	UNP Q584T8
CS	-21	LYS	-	expression tag	UNP Q584T8
CS	-20	ILE	-	expression tag	UNP Q584T8
CS	-19	LEU	-	expression tag	UNP Q584T8
CS	-18	LEU	-	expression tag	UNP Q584T8
CS	-17	CYS	-	expression tag	UNP Q584T8
CS	-16	ASP	-	expression tag	UNP Q584T8
CS	-15	VAL	-	expression tag	UNP Q584T8
CS	-14	LYS	-	expression tag	UNP Q584T8
CS	-13	LYS	-	expression tag	UNP Q584T8
CS	-12	LYS	-	expression tag	UNP Q584T8
CS	-11	ILE	-	expression tag	UNP Q584T8
CS	-10	VAL	-	expression tag	UNP Q584T8
CS	-9	TYR	-	expression tag	UNP Q584T8
CS	-8	PHE	-	expression tag	UNP Q584T8
CS	-7	HIS	-	expression tag	UNP Q584T8
CS	-6	CYS	-	expression tag	UNP Q584T8
CS	-5	CYS	-	expression tag	UNP Q584T8
CS	-4	THR	-	expression tag	UNP Q584T8
CS	-3	ARG	-	expression tag	UNP $Q584T8$
CS	-2	LYS	-	expression tag	UNP Q584T8
CS	-1	LYS	-	expression tag	UNP Q584T8
CS	0	SER	-	expression tag	UNP Q584T8

• Molecule 23 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Cg	482	Total 3904	C 2499	N 684	0 701	S 20	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cg	181	VAL	ALA	conflict	UNP $Q585C2$
Cg	498	ARG	MET	conflict	UNP $Q585C2$



• Molecule 24 is a protein called mS33.

Mol	Chain	Residues	Atoms				AltConf	Trace	
24	Ci	165	Total 1348	C 848	N 247	0 244	S 9	0	0

• Molecule 25 is a protein called mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ck	703	$\begin{array}{c} \text{Total} \\ 5596 \end{array}$	C 3503	N 1017	O 1050	S 26	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ck	107	SER	LEU	conflict	UNP Q387C7
Ck	144	PHE	LEU	conflict	UNP Q387C7
Ck	253	TYR	PHE	conflict	UNP Q387C7
Ck	339	GLU	VAL	conflict	UNP Q387C7
Ck	871	GLY	GLU	conflict	UNP Q387C7

• Molecule 26 is a RNA chain called RNA (143-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
26	CA	143	Total 3030	C 1364	N 522	O 1001	Р 143	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	473	U	G	conflict	GB 343546

• Molecule 27 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms			AltConf	Trace	
27	UO	5	Total 30	C 20	N 5	O 5	0	0

• Molecule 28 is a protein called Unknown protein.

Mol	Chain	Residues	A	Aton	ıs		AltConf	Trace
28	UP	7	Total 42	C 28	N 7	O 7	0	0





Mol	Chain	Residues	Atoms	AltConf
29	DL	1	Total         C         N           10         7         3	0
29	CA	1	Total         C         N           10         7         3	0

• Molecule 30 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula:  $C_9H_{15}N_2O_{15}P_3$ ).



Mol	Chain	Residues	Atoms				AltConf	
30	DJ	1	Total 29	С 9	N 2	O 15	Р 3	0



• Molecule 31 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



Mol	Chain	Residues	Atoms				AltConf	
31	Cg	1	Total	С	Ν	0	Р	0
01	~0	-	32	10	5	14	3	Ŭ

• Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
32	Cg	1	Total Mg 1 1	0
32	CA	2	Total Mg 2 2	0

• Molecule 33 is water.

Mol	Chain	Residues	Atoms	AltConf
33	Cg	3	Total O 3 3	0



### 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: mS48

Chain DA: 7% ·	93%
MET MET MET ARG ARG VAL ALA SER SER SER SER GLY GLY	HIS TYR TYR SER SER SER SER SER SER ALA SER SER ALA ALA ALA ALA ALA ALA SER TTR MET THR THR THR THR THR THR CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU
LYS ARG TYR GLY ILE PHE SER ASN GLU ARG ALA ALA	LYS ARG ARG ARG ARG ARG CEU PRO FRO FRO FRO FRO FRO ARSN ARSN ARSN ARSN ARSN ARSN ARSN ARSN
ARG PRO HIS SER SER LEU GLU ALA ASN ALA ASN ASP SER SER SER	ASN LEU SER CLU SER THR THR THR ASN CLU CLU CLU CLU CLU THR THR THR THR THR THR THR THR THR THR
PRO ARG SER PRO PRO PRO PRO LYS VAL LYS VAL LEU GLY GLY	LEU NAL ASP ASP ASP ASP ASP LTE LTE CYS ASP ASP ASP ASP ASP ASP ASP ASP ASP AS
PHE PHE VAL ALA ALA ALA ALA ALA ALA SER SER SER SER SER SER	PHE ASP ASP ASP ASP CIEU CIEU CIEU CIEU CIEU CIEU CIEU CIEU
THR ARG CYS CYS CYS GLY GLY GLY GLY GLY ASP ASP ASP THR PHC	ARG LYPS HYPS ARG ARG ARG ALA ALA ALA ALA ALA ALA ALA ALA ALA AL
ALA GLU ALA ALA LEU LEU LEU LYR YAL YAL GLN GLN GLN	ARG ARG ALA ALA ALA ALA ALA ALA ALA ALA ASN ASN ASN ASN ASN ASN ASN ASN ASN AS
GLY PHE THR LEU GLU GLU SER ALA ALA ALA ALA ALA TYR THR CLY	CLU VAL LYS ALLA ALLA ALLA PRO PLEU PLEU PRO CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU
TYR LYS VAL VAL ASP SER LYS SER LYS THR ARG TLE VAL ASN	ARG VILU VAL VAL VAL VAL VAL CLV GLV GLV GLV CLEU CLU CLU CLU CLU ALA ALA ALA ALA ALA ALA ALA ALA ALA A
GLN GLN GLN CLN CLN CLU ASP ASP CLU CVS CLU LVS LVS LVS AIG ARG	GLU ARG ALA SER LLEU LLEU LLEU CLIY SER SER SER SER SER SER SER SER SER SER
THR LEU PHE LYS LYS LYS ALA ALA ALA ALA ALA ARG TYR TYR FRO SER PRO	ALA ALA VAL PRO ASP ASP ASP PRO ASP PRO VAL HIS CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN
GLY GLY ASN ASN ASN ASN ASN ASN ASN ASN ASN CYS ASN CYS ASN ASN ASN ASN ASN ASN ASN ASN ASN AS	THR ASP GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU
ILE ARG GLU ARG ARG CLU CLU CLU SER ARG ALA ALA SER	ALA ALA VAL LYS GLY ARG ARG ARG CLU CLEU CLEU CLU GLU CLN ARG GLU GLU CLN VAL CLV VALV CV VAL CLV VAL CLV VAL CLV VAL CLV VAL CLV VAL CLV VAL CLV VAL CLV VAL CLV VAL CLV VAL CVV VAL CVV VAL CVV VAL CVV VAL CVV VAL CVV VAL CVV VAL CVV VAL CVVV CVV CVVV CV
ARG SER VAL ALA ALA PRO TLE GLY ASP SER THR GLN VAL	ARG ARG GLU LEU VAL CLEU CLEU CLEU CLEU CLEU CLEU CLU CLU CLU CLU CLU CLU CLU CLU CLU CL













M1 T9 R18 R18 K41 R41	L46 R51 D79 R80 R80 K81 K81 K81 K83 K83	884 185 6105 6133 7133 8135 8135 8135 8135 8135 8135 8135 8	S178 C184 CLY ARG ARG CLN THR CLN FRO SER FRO SER H191	Y195 1206 M236 N257	L268 S273 C297	R311
E318 5323 H327 V345	K348 L364 L360 R364 R364 R368 R369 R369	R380 F381 F382 F382 F386 W392 W392 W392 F411 L411 L414 L414	1421 1421 R428 R450 R452 R452 L460	K470 D474 D475 V476 D484	T495 T503 D515	R523
V657 T562 T562 GLY ILLE SFR	SER THR ALA GLY GLY GLY SER ARG					
• Molecule	9: mS57					
Chain DJ:		71%	8%	20%	,	
PHE ARG SER SER ARG ARG ARG ARG	V 10 N 16 N 16 N 33 P 35 C 35 C 35 C 35 C 35 C 35 C 35 C 35 C	R46 T47 F48 N55 S76 S76 L107 L110	L119 M137 A150 E151 S164 R178	A179 L180 F181 D182 S206	D212 V226 E234 A235	R236
T246 L258 Y273 S274 D275 N291	S302 R305 R305 CLY GLY SER SER	HIS ASN PRO ASN ALA ALA ALA ASP ASP ASP ASP ASP ASP ASP ASP ASP AS	LYS LYS GLU GLU LYS ALA GLU GLU LEU LEU	PRO GLU ASP TYR VAL HIS GLU	ASP ARG VAL TYR ASP ARG	SER ALA
ALA PHE LYS LYS ASN VAL ALA ALA GLN GLN	LYS TRP LYS LYS LYS NET PRO LYS LYS SER LSU LYS SER LYS	ARG MET GLY TYR THR GLY ASP PRO				
• Molecule	10: mS58					
Chain DK:		73%	5%	6 21%	, D	
MET S2 L1 18 N34 C35 R36 R36	T54 K65 GLY GLY GLY ARG PRO PRO VAL SER GLY GLY	GLY ASP VAL SER SER GLY GLY GLU THR GLU GLN GLN	SEC SEC THR THR THR GLY GLY ALA LI11	T115 R116 T134 T167	L172 G192 ASP ALA ALA	GLU ALA
THR PRO ARG VAL LYS ASP ASP	VALL LYS GLY GLY ARG ARG CLU LEU SER SER N216 N226	S240 V250 L1270 L1273 S294 S294 B470 B470 B470 B470 S294	A LA LYS ASP ASP ASP GLU GLU CJN CGLU CJN LYS CGLN LEU	ARG PHE THR GLN		
• Molecule	11: mS67					
Chain DT:		86%		1	1% •	
MET LEU VAL SER TYR LEU LEU LEU	A10 D11 R12 F34 F34 F34 F34 F33 F34 F33 F34 F33 F34 F33 F34 F33 F34 F33 F34 F34	H63 188 891 190 091 103 1103 1105 1105	M122 8131 8137 8137 8163 8163 8163 8166	E168 D176 M177 D181	R208 T209 N241 Q247	
• Molecule	12: mS69					
Chain DV:		77%		11%	13%	
MET ARG ARG VAL ARG ASP GLY LEU PHE	LEU SER PRO SER PRO SER LEU LEU CYS SER VAL	ALA VAL 225 726 126 140 141 N43 N43	T57 T68 Q71 K77 V114 V114 Q118	<b>Q131</b> D134 F140	1143 1178 1178 1179 1180 <b>1180</b>	Y182 L183
• Molecule	13: mS70					
Chain DW:		83%		7%	10%	



MET LEU ARG PHE HIS ALA ALA CLEU T10 T22 M37	R58 P59 V60 L70 T74 K125 K125 L128	K133 R145 E163 ARG	LYS SER GLY THR GLY THR PRO SER			
• Molecule 14: mS71	L					
Chain DX:	7	5%		9%	17%	_
MET PHE HIS ARG ARG ALA PHE PHE SER SER SER SER SER SER CTR CYS	THR ILE ILE LEU SER SER VAL CYS CYS CYS CYS CYS	ARG TYR W29 K34 R57 S72	R76 R89 190 L98 L98 I124	M127 G128 T132 R136	V162 V162 Y163 T164	N168 D169
• Molecule 15: mS72	2					
Chain DY:		83%		12	2% 6	6%
MET LEU ARG SER THR THR THR SER T11 11 11 11 11 11 11	823 823 143 143 143 143 143 143 164	L65 T81 R85 86 R87 R87 T93	R111 T124 Q128 V141 V141			
• Molecule 16: uS3m	1					
Chain CC:		84%			16%	_
M4 17 17 114 114 114 114 114 114 114 114	150 150 177 177					
• Molecule 17: uS9m	1					
Chain CI:	45%	5%	50%	,		-
A 12 12 12 12 12 12 12 12 12 12 12 12 12	M65 P66 CLU CLU CLU CLU CLU CLU CLU SER PHE PHE	ALA ASN GLY GLN ALA ALA HIS GLY ASN	LEU PHE TYR PHE ARG GLU TYR PRO MET TYR	PRO GLY GLU TYR VAL PRO	ALA GLU HTS ASN	THR LEU SER SER
ARG ASP GLU LEU LEU LEU ARG ARG ARG ARG ARG ALA ALA CLN CLN GLU GLU	ALA TRP MET ARG VAL SER GLY GLY VAL TYR PHE	GLN SER VAL ASP GLU TYR ALA SER	VAL ASP GLY LEU ASP ALA GLU GLU GLN GLN GLN	GLU VAL LEU ALA ALA LEU LEU	PHE PRO GLU LEU	ASN CYS GLU ALA
GLN ALA ALA LEU VAL GLU GLU CYS SER ARG PRO VAL	SER ALA ALA SER SER GLN LEU LEU SER ARG THR THR	THR ALA GLU GLU VAL CLU CLU ASP ASN	ALA PRO GLY HIS TYR TYR ASN PHE LEU GLU	TRP MET GLY ARG LEU THR	GLU THR ARG ALA	PHE LYS THR GLU HTS
ALA PHE PHE GLU PHE SER ASR ASP ASP ASP ASP VAL VAL	ARG VAL NET PHE GLU GLU ASN TYR ARG LEU MET SER	LYS ALA THR LEU LEU ALA SER ALA	ASP SER TYR SER HIS PHE TYR THR VAL	LYS ASP PHE ALA UNK LYS	VAL ALA GLY GLU	ASP SER ARG HIS D289
230 331 332 333 333 330 330 330 330 330 330 330	335 405 420 420 435 435 435	<b>443</b>				
• Molecule 18: uS10	m					
Chain CJ:		88%			10%	·







• Molecule 19: uS11m

Chain	CK:	14%	•							8	4%										-	
MET MET ARG LYS SER	VAL THR PHE LEU <b>R10</b>	R15 D23	L32 K33	040 R48	<mark>q56</mark>	NG1 ALA	SER GLY GLN	ALA HIS	SER PHE	SER PRO	GLN	GLN MET	ASP TRP	ARG	MET	ALA	SER	SER GLU	GLU SFR	ILE	CTU	GLU MET ARG
GLN LEU ALA GLU ASN	ASP VAL MET GLN HIS	GLN ARG VAL PHE	GLU GLU MET	TRP TYR GLU	CLU GLU	GLU	ARG MET LYS	ALA ARG	CYS	GLU GLU	THR	GLU HIS ALA	UNK SER	ASN	GLY	VAL	PRO	PRO ARG	VAL	dL Y	ASP	TYR PHE LYS
THR ARG PHE GLY TYR	SER LEU VAL LYS ASN	SER GLU MET THR	GLY PRO VAL	ASP TYR SER	GLN LEU ASP	MET TRP	GLY GLU MET	PRO ARG	TYR THR	ASP MET	VAL PHE	LEU TYR LEU	VAL SER	ARG	ARG	THR	1 TK ALA	VAL ALA	TYR THR	TYR	GLY	LYS ARG ILE
LEU ASN THR TYR THR	ALA GLY ASN ARG GLY	CTA CTA CTA CTA	A.S.F A.R.G G.L.Y P.H.E	ARG SER GLU	GLY SER THR	ASP ASN	GLY HIS GLM	VAL THR	NET	LEU ASN	ASP LEU	LEU PRO LYS	LEU ARG	GLU MET	ARG	SER	GLY	ARG PRO	MET GLY	ARG	GLU	LYS VAL GLU
LEU VAL VAL ARG VAL	MET GLY PHE TYR ASN	GLY GLN GLN GLY	ALA VAL ARG ALA	VAL GLN ASP	ARG ALA ASN	GLU	HIS VAL ARG	TYR PHE	GLU ASP	THR PRO	PHE PRO	ASN GLY	PR0 LYS	MET	ARG	VAL	LYS					
• Mole	ecule 20	: uS14	4m																			
Chain	CN:						83'	%										12%	, D	5%	ó	
MET PHE CYS PHE SER	ARG GLY LEU TRP M10	T22 L30	S35 141	H42 S43	S49 K57	V60	K65 M66	K70	V71 T72	N77	L81 F82	V111	M118	1.127	107 F		2 CTN	I166				
• Mole	ecule 21:	: uS18	8m																			
Chain	CR:	11%								86	%											
MET ASN ARG THR GLY	GLY SER ILE TYR ALA	ALA ALA LEU SER	PHE ALA VAL	CYS ARG GLN	PRO TRP ASN	GLU TYR	ILE GLY LEU	LEU THR	GLN	SER THR	PRO TYR	THR	PRO GLN	GLU	PRO	TYR	GLY	ARG LYS	GLN	ARG	GLY	TRP LEU PHE
GLY GLN CLN VAL GLN	LEU HIS TYR HIS ARG	PHE PRO ASP GLU	LEU LEU THR	ASN LEU SER	ARG TRP ARG	THR GLY	GLU THR VAL	GLY ASP	ALA	GLN GLN	PHE ARG	ALA GLN	PRO PHE	ASP TLE	GLU	TAS	PRO	GLY GLY	VAL GLN	ARG	SER	PRO GLU VAL
TYR MET LYS LEU ASN	TYR LYS ASN PRO ALA	IHR ILE SER ARG	LEU THR ARG	THR GLY HIS	MET TYR PRO	ALA ASP	ILE LEU PRO	LEU ASN	PRO GLU	VAL VAL VAL	LYS	ARG VAL ALA	LYS ALA	GLN	ILE	TLE	LEU	TYR PRO	ARG PHE	GLY	PRO	PHE TRP PHE
ARG SER GLN LYS PHE	ARG PRO LYS ALA TYR	GLU GLU ASN TYR	PRO THR THR	TYR SER THR	LYS ARG THR	VAL GLU	HIS PHE ALA	TYR ASN	TRP VAL	THR	ARG ILE	ARG ARG TYR	PHE ARG	GLU	GLU	VAL	THR	SER GLY	SER ALA	SER	ARG	GLY GLY
GLY GLY K248 K248		• 11S10	1283 88	L2 <mark>86</mark> MET SER	THR LYS GLY	MET LYS	LYS LYS PHF	HISN	TYR	SER THR	SER THR	LYS ARG MET	GLY	SER	PRO	TEU	ILE	LYS	VAL			

Chain CS:

42%

5%

MET ALA ALA ALA ALA ASN ASN THR THR THR THR THR THR THR THR THR THR	LYS PHE PHE THR VAL VAL LYS ASN ILEU LEU LEU LEU LEU	TRP ARG VAL LYS VAL LYS PHE PHE LEU ARG ARG ALA GLU GLU	A THE ATAL ATIS SER SER LEU VAL LEU PRO VAL SER	LEU TYR SER LYS LYS LUS CYS CYS CYS CYS LEU VAL LYS LYS
ILE TYR TYR PHE HIE CYS CYS THR ARG LYS	SER MET LLEU ARG ARG CYS PRO CYS VAL TRP PRO ASP PRO CY	THR LYS SER SER VAL SER VAL SER THE GLY MAL	LILL LYS CLU CLV CLN L3 L3 L3 K32 K32 K48 K48	M64 N65 M75 176 176 186 195 195 1107 1107
M140 D152 K172				
• Molecule 23:	mS29			
Chain Cg:		88%		9% •
MET ARG SER LIYS LIYS LIYS LIYS LIYS S9 S9	P50 P50 D73 D73 S76 Q87 R107	R112 E114 E114 L117 L120 H127 T143	C153 N170 T173 W189 L194	V213 S221 S221 S225 C226 C226 C226 C226 C226 C226 C226 C
H296 L308 A309 S310 S310 T316 D317 1318 D319	L325 L325 L344 T355 V373 V373 C391 E391 E391	L422 D436 V464 V468 K480 K480 K480	SER GLY VAL VAL GLY VAL VAL ARG	
• Molecule 24:	mS33			
Chain Ci:		79%		12% 9%
MET VAL LEU LEU ARG ARG PHE PHE LEU LEU LEU	R14 T18 C27 C27 R30 M31 D32 D32 C55 L55	M76 982 M114 M114 M122 M122	H136 K137 D138 D138 R144 N145 D146 D146 S150	L157 M164 A176 A176 CLU GLU GLU GLU ASP
• Molecule 25:	mS35			
Chain Ck:		73%	7%	20%
MET ARG ARG ARG HIS SER SER LEU ASN ASN	LEU LEU GLY GLY GLY GLY GLY GLY GLY HIS SER FHR THR THR	ARG ALA ALA ARG LEU Q30 Q34 Q30 D57 D57	00 00 898 898 898 898 898 804 104 104 111	D136 1137 E161 1176 1176 1185 1185 1185 1188
1214 1230 1231 1242 1254 1254	8291 1292 1316 1316 1317 1320 1330 1350 1350	L359 R373 L401 L401 GLU GLU GLU ASP ASP	ASP ALA ALA VAL OLY GLY PHE VAL SER SER LY GLY	OLU VAL LYAL THR THR LEU SER SER SER SER CLY THR
ASP ALA VAL VAL ARG ASP ASP ALA VAL ALA GLY TLE	PHE GLY GLY GLY GLY TLE TLE THR TLE TRP ASP ASP ASP	MET GLN ASN VAL ASP ASP ASN TRP ASN TRP ASN CLN	ANG LEU ALA ALA LEU LEU SER SER ALA	VAL LEU SER ALA TLE VAL LEU VAL LEU VAL LYS ALA ALA ALA
ALA ALA LYS ALA ALA ALA ALA SER SER HTS FHE FHE THR	ASP GLU TTYR ALA ASP GLN GLN GLU LEU LEU LEU LEU ASP AS3	L568 1573 1573 1575 1575 1575 1597 1697 1607 1611	I618         6619           0619         1620           1628         1627           1629         1623           M633         H634	R652 L653 S654 1661 N682 N687 N687 N690 W690
• Moloculo 26:	RNA (143 MFR)	ARG LYS SER VAL ASP ASP ASP ALA ASP CLU CSP	111R LLEU ASP ALLA CLEU GLN MET MET ASP ASP	GLY ASP OLY CLYS LYS VAL
Chain CA:	149-141111) % 14%		77%	
	D A A U U G U A D I I I I I I I I I I I I I I I I I I	a na	C C C C P P C C C C	A V V V V V V V V V V V V V V V V V V V



<pre>v = 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0</pre>	A U
~~	DA
ADD44D4D4D400044D44000440004000400040004	50
, , , , , , , , , , , , , , , , , , ,	b G
	50
и и и и и и и и и и и и и и и и и и и и	<u></u>
A A A A A A A A A A A A A A	A42
4426 7427 7427 7427 7439 7439 7439 7434 7439 7435 7435 7435 7445 7445 7445 7445 7445	A489 A490
	n
DDD4D440444404400000040D44DD44D4DAD700404444404D4D9	
• Molecule 27: Unknown protein	
Chain UO: 100%	
There are no outlier residues recorded for this chain.	
• Molecule 28: Unknown protein	
Chain IID:	

There are no outlier residues recorded for this chain.



# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101308	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.587	Depositor
Minimum map value	-0.258	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor



## 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: GTP, MG, UTP, SPD

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).

Mal	Chain	Bo	ond lengths	Bond angles			
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5		
1	DA	0.34	0/1010	0.54	1/1369~(0.1%)		
2	DL	0.45	0/1185	0.62	0/1601		
3	DB	0.44	0/9369	0.62	0/12692		
4	DC	0.41	0/8952	0.57	0/12145		
5	DE	0.41	0/4955	0.59	0/6708		
6	DF	0.43	0/4856	0.62	2/6581~(0.0%)		
7	DG	0.40	0/4674	0.58	0/6333		
8	DH	0.46	0/4684	0.62	2/6347~(0.0%)		
9	DJ	0.46	0/2649	0.65	0/3598		
10	DK	0.45	0/2045	0.59	0/2759		
11	DT	0.50	0/2133	0.66	0/2889		
12	DV	0.47	0/1382	0.66	1/1871~(0.1%)		
13	DW	0.41	0/1407	0.55	0/1916		
14	DX	0.45	0/1231	0.66	1/1654~(0.1%)		
15	DY	0.50	0/1334	0.63	0/1810		
16	CC	0.50	0/666	0.72	0/900		
17	CI	0.46	0/1783	0.65	1/2395~(0.0%)		
18	CJ	0.52	1/6705~(0.0%)	0.65	0/9124		
19	CK	0.41	0/448	0.60	0/600		
20	CN	0.50	0/1361	0.67	0/1840		
21	CR	0.43	0/361	0.70	0/490		
22	CS	0.45	0/1209	0.64	0/1626		
23	Cg	0.46	0/4025	0.63	0/5467		
24	Ci	0.49	0/1388	0.73	1/1878~(0.1%)		
25	Ck	0.42	0/5696	0.61	2/7705~(0.0%)		
26	CA	0.59	0/3392	1.07	9/5275~(0.2%)		
All	All	0.45	1/78900~(0.0%)	0.65	$20/\overline{107573}\ (0.0\%)$		

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



Mol	Chain	#Chirality outliers	#Planarity outliers
2	DL	0	2
3	DB	0	2
4	DC	0	2
7	DG	0	2
9	DJ	0	1
11	DT	0	1
14	DX	0	1
18	CJ	0	1
23	Cg	0	1
24	Ci	0	1
25	Ck	0	1
All	All	0	15

sidechain that are expected to be planar.

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
18	CJ	424	HIS	CG-CD2	-8.20	1.21	1.35

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
26	CA	451	U	C2-N1-C1'	7.45	126.64	117.70
26	CA	502	U	C5-C6-N1	-6.87	119.27	122.70
26	CA	422	G	N3-C4-C5	6.34	131.77	128.60
26	CA	451	U	N1-C2-O2	6.29	127.20	122.80
26	CA	451	U	N3-C2-O2	-6.18	117.88	122.20
26	CA	493	U	C2-N1-C1'	6.17	125.11	117.70
8	DH	133	CYS	C-N-CD	6.00	141.01	128.40
17	CI	405	LEU	CA-CB-CG	-5.85	101.84	115.30
24	Ci	55	LEU	CA-CB-CG	5.83	128.71	115.30
14	DX	128	GLY	N-CA-C	5.63	127.17	113.10
26	CA	451	U	C6-N1-C1'	-5.63	113.32	121.20
8	DH	367	LEU	N-CA-C	-5.62	95.84	111.00
25	Ck	687	ARG	N-CA-C	5.57	126.04	111.00
6	DF	55	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	DA	1314	GLY	N-CA-C	5.54	126.95	113.10
26	CA	493	U	N1-C2-O2	5.44	126.61	122.80
25	Ck	359	LEU	CA-CB-CG	5.39	127.71	115.30
26	CA	493	U	N3-C2-O2	-5.22	118.54	122.20
6	DF	510	ASP	CB-CG-OD2	5.20	122.98	118.30
12	DV	183	LEU	CA-CB-CG	5.02	126.86	115.30



There are no chirality outliers.

All (15) planarity outliers are listed below:	
---	--

Mol	Chain	Res	Type	Group
18	CJ	100	ARG	Peptide
23	Cg	50	PRO	Peptide
24	Ci	150	SER	Peptide
25	Ck	230	LEU	Peptide
3	DB	383	ARG	Sidechain
3	DB	586	ARG	Sidechain
4	DC	497	PRO	Peptide
4	DC	775	ALA	Peptide
7	DG	184	ALA	Peptide
7	DG	592	THR	Peptide
9	DJ	35	PRO	Peptide
2	DL	269	MET	Peptide
2	DL	270	THR	Peptide
11	DT	43	ASP	Peptide
14	DX	127	MET	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 PDB entries followed by that with respect to all EM entries.

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	Perce	ntiles
1	DA	129/1788~(7%)	126 (98%)	3~(2%)	0	100	100
2	DL	139/307~(45%)	130 (94%)	9~(6%)	0	100	100
3	DB	1109/1181~(94%)	1078 (97%)	29 (3%)	2 (0%)	47	77
4	DC	1087/1165~(93%)	1052 (97%)	34 (3%)	1 (0%)	51	82
5	DE	576/747~(77%)	564 (98%)	11 (2%)	1 (0%)	47	77



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
6	DF	586/666~(88%)	569~(97%)	16 (3%)	1 (0%)	47	77
7	DG	558/631~(88%)	543~(97%)	14 (2%)	1 (0%)	47	77
8	DH	560/581~(96%)	540 (96%)	20 (4%)	0	100	100
9	DJ	313/396~(79%)	304 (97%)	8 (3%)	1 (0%)	41	71
10	DK	249/324~(77%)	240 (96%)	9 (4%)	0	100	100
11	DT	237/247~(96%)	233~(98%)	4 (2%)	0	100	100
12	DV	158/183~(86%)	151 (96%)	6 (4%)	1 (1%)	25	57
13	DW	159/179~(89%)	153 (96%)	6 (4%)	0	100	100
14	DX	139/169~(82%)	133 (96%)	6 (4%)	0	100	100
15	DY	152/163~(93%)	148 (97%)	4 (3%)	0	100	100
16	CC	72/74~(97%)	68 (94%)	3 (4%)	1 (1%)	11	38
17	CI	218/443~(49%)	210 (96%)	8 (4%)	0	100	100
18	CJ	796/817~(97%)	765 (96%)	30 (4%)	1 (0%)	51	82
19	CK	50/326~(15%)	47 (94%)	3 (6%)	0	100	100
20	CN	155/166~(93%)	150 (97%)	5 (3%)	0	100	100
21	CR	42/320~(13%)	40 (95%)	2(5%)	0	100	100
22	CS	140/244~(57%)	135 (96%)	5 (4%)	0	100	100
23	Cg	480/498~(96%)	461 (96%)	19 (4%)	0	100	100
24	Ci	163/181~(90%)	155~(95%)	8 (5%)	0	100	100
25	Ck	699/874~(80%)	671 (96%)	26 (4%)	2(0%)	41	71
All	All	8966/12670~(71%)	8666 (97%)	288 (3%)	12 (0%)	54	82

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	DJ	36	GLN
12	DV	57	THR
18	CJ	799	ASP
3	DB	1033	TYR
25	Ck	231	GLY
25	Ck	653	LEU
5	DE	71	LEU
4	DC	441	VAL
16	CC	18	LYS
7	DG	48	VAL



Continued from previous page...

Mol	Chain	Res	Type
6	DF	184	VAL
3	DB	946	PRO

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	Pe	erce	entiles
1	DA	111/1514 (7%)	102~(92%)	9~(8%)		11	37
2	DL	123/263~(47%)	112 (91%)	11 (9%)		9	33
3	DB	976/1030~(95%)	874 (90%)	102 (10%)		7	25
4	DC	927/985~(94%)	808~(87%)	119~(13%)		4	17
5	DE	519/644~(81%)	464 (89%)	55 (11%)		6	24
6	DF	500/560~(89%)	443 (89%)	57 (11%)		5	22
7	DG	490/543~(90%)	426 (87%)	64 (13%)		4	16
8	DH	493/504~(98%)	434 (88%)	59 (12%)		5	19
9	DJ	275/347~(79%)	244 (89%)	31 (11%)		6	22
10	DK	209/261~(80%)	192 (92%)	17 (8%)		11	37
11	DT	220/228~(96%)	195~(89%)	25 (11%)		5	22
12	DV	145/165~(88%)	127~(88%)	18 (12%)		4	18
13	DW	148/163~(91%)	136~(92%)	12 (8%)		11	37
14	DX	124/149~(83%)	111 (90%)	13 (10%)		7	25
15	DY	137/146~(94%)	118 (86%)	19 (14%)		3	14
16	CC	73/73~(100%)	62~(85%)	11 (15%)		3	11
17	CI	186/370~(50%)	164 (88%)	22 (12%)		5	20
18	CJ	709/723~(98%)	628~(89%)	81 (11%)		5	22
19	CK	47/283~(17%)	40 (85%)	7 (15%)		3	12
20	CN	142/150~(95%)	122 (86%)	20 (14%)		3	14
21	CR	41/279~(15%)	32 (78%)	9 (22%)		1	3
22	CS	126/220~(57%)	114 (90%)	12 (10%)		8	29



	f = f = f = f = f = f = f = f = f = f =						
Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
23	Cg	424/437~(97%)	380~(90%)	44 (10%)	7 25		
24	Ci	144/160~(90%)	124~(86%)	20 (14%)	3 14		
25	Ck	608/747~(81%)	549~(90%)	59~(10%)	8 28		
All	All	7897/10944~(72%)	7001 (89%)	896 (11%)	9 22		

Continued from previous page...

All (896) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DA	1187	ASP
1	DA	1208	THR
1	DA	1225	HIS
1	DA	1240	LEU
1	DA	1263	VAL
1	DA	1268	LEU
1	DA	1271	LEU
1	DA	1278	THR
1	DA	1292	CYS
2	DL	28	ASN
2	DL	29	PHE
2	DL	39	THR
2	DL	68	LEU
2	DL	102	SER
2	DL	267	HIS
2	DL	268	VAL
2	DL	269	MET
2	DL	270	THR
2	DL	271	PRO
2	DL	286	THR
3	DB	78	ARG
3	DB	99	VAL
3	DB	118	VAL
3	DB	129	TYR
3	DB	173	ARG
3	DB	186	SER
3	DB	189	VAL
3	DB	204	SER
3	DB	213	ASP
3	DB	217	ILE
3	DB	221	HIS
3	DB	233	ASP
3	DB	239	GLN



Mol	Chain	Res	Type
3	DB	249	SER
3	DB	321	SER
3	DB	339	ARG
3	DB	343	VAL
3	DB	368	GLU
3	DB	383	ARG
3	DB	394	ASP
3	DB	416	ASN
3	DB	424	ASP
3	DB	433	ARG
3	DB	435	THR
3	DB	439	VAL
3	DB	445	ASN
3	DB	448	ASP
3	DB	450	MET
3	DB	454	ASP
3	DB	462	ASP
3	DB	490	ARG
3	DB	503	ASN
3	DB	507	LEU
3	DB	511	ARG
3	DB	514	ARG
3	DB	521	LEU
3	DB	522	MET
3	DB	532	GLU
3	DB	539	GLN
3	DB	550	LEU
3	DB	553	LEU
3	DB	554	GLU
3	DB	572	ASP
3	DB	574	ILE
3	DB	587	VAL
3	DB	590	ASP
3	DB	592	MET
3	DB	597	GLU
3	DB	637	THR
3	DB	671	VAL
3	DB	690	ARG
3	DB	693	SER
3	DB	720	LYS
3	DB	744	VAL
3	DB	755	LEU



Mol	Chain	Res	Type
3	DB	756	THR
3	DB	758	SER
3	DB	774	ASN
3	DB	785	ASN
3	DB	790	SER
3	DB	793	ARG
3	DB	810	THR
3	DB	815	ASP
3	DB	820	GLU
3	DB	822	PHE
3	DB	830	LEU
3	DB	831	ASN
3	DB	834	ILE
3	DB	849	ASP
3	DB	850	SER
3	DB	901	VAL
3	DB	908	GLN
3	DB	923	GLN
3	DB	942	ARG
3	DB	958	ASN
3	DB	964	ARG
3	DB	968	VAL
3	DB	984	ASP
3	DB	995	VAL
3	DB	997	ASP
3	DB	1009	ASP
3	DB	1012	THR
3	DB	1013	ARG
3	DB	1020	ASP
3	DB	1026	SER
3	DB	1028	SER
3	DB	1030	ARG
3	DB	1034	ILE
3	DB	1067	ILE
3	DB	1069	THR
3	DB	1080	ARG
3	DB	1104	ASP
3	DB	1110	LYS
3	DB	1117	THR
3	DB	1142	VAL
3	DB	1153	ASP
3	DB	1156	THR



Mol	Chain	Res	Type
3	DB	1165	SER
3	DB	1168	ASP
3	DB	1172	LYS
3	DB	1173	THR
3	DB	1181	LEU
4	DC	30	THR
4	DC	36	ASP
4	DC	46	ARG
4	DC	57	GLU
4	DC	58	VAL
4	DC	82	THR
4	DC	86	THR
4	DC	87	MET
4	DC	92	PHE
4	DC	93	ARG
4	DC	106	SER
4	DC	108	SER
4	DC	114	GLU
4	DC	128	HIS
4	DC	131	GLU
4	DC	148	LEU
4	DC	154	THR
4	DC	162	ILE
4	DC	166	GLU
4	DC	168	PHE
4	DC	227	GLN
4	DC	231	THR
4	DC	268	ASP
4	DC	271	SER
4	DC	279	GLU
4	DC	299	LEU
4	DC	305	ARG
4	DC	313	THR
4	DC	344	MET
4	DC	365	LYS
4	DC	371	ILE
4	DC	379	LEU
4	DC	386	MET
4	DC	406	GLN
4	DC	435	LEU
4	DC	437	LEU
4	DC	442	LEU



Mol	Chain	Res	Type
4	DC	464	THR
4	DC	467	THR
4	DC	471	ARG
4	DC	474	LEU
4	DC	475	LEU
4	DC	491	LEU
4	DC	498	LEU
4	DC	503	ASP
4	DC	506	SER
4	DC	511	ARG
4	DC	513	SER
4	DC	519	SER
4	DC	525	THR
4	DC	533	LEU
4	DC	534	LEU
4	DC	540	LEU
4	DC	544	GLU
4	DC	545	ASP
4	DC	567	ARG
4	DC	569	LEU
4	DC	604	VAL
4	DC	611	MET
4	DC	618	ARG
4	DC	620	VAL
4	DC	632	LEU
4	DC	652	ARG
4	DC	659	LEU
4	DC	669	LEU
4	DC	705	LEU
4	DC	710	THR
4	DC	749	GLU
4	DC	753	LEU
4	DC	755	ASP
4	DC	756	ASP
4	DC	757	ARG
4	DC	766	VAL
4	DC	774	ASP
4	DC	799	ASN
4	DC	809	TYR
4	DC	817	ASP
4	DC	828	ARG
4	DC	865	CYS



Mol	Chain	Res	Type
4	DC	881	MET
4	DC	885	LEU
4	DC	894	HIS
4	DC	928	GLU
4	DC	934	ARG
4	DC	952	GLU
4	DC	953	MET
4	DC	954	LEU
4	DC	955	ASP
4	DC	960	VAL
4	DC	961	THR
4	DC	963	SER
4	DC	970	GLN
4	DC	987	THR
4	DC	1000	LEU
4	DC	1009	THR
4	DC	1019	THR
4	DC	1021	ASN
4	DC	1023	ASN
4	DC	1025	THR
4	DC	1055	ARG
4	DC	1062	GLN
4	DC	1063	SER
4	DC	1071	VAL
4	DC	1076	PHE
4	DC	1104	MET
4	DC	1112	ASP
4	DC	1119	GLN
4	DC	1121	THR
4	DC	1125	SER
4	DC	1128	ARG
4	DC	1132	THR
4	DC	1133	THR
4	DC	1143	VAL
4	DC	1151	THR
4	DC	1153	LEU
4	DC	1159	ASP
4	DC	1161	LYS
4	DC	1162	SER
4	DC	1163	GLU
5	DE	46	SER
5	DE	51	ARG



Mol	Chain	Res	Type
5	DE	54	ARG
5	DE	65	ILE
5	DE	80	LEU
5	DE	149	LEU
5	DE	150	ARG
5	DE	154	SER
5	DE	178	GLN
5	DE	196	ASP
5	DE	203	LEU
5	DE	212	LEU
5	DE	229	ARG
5	DE	246	ILE
5	DE	280	LEU
5	DE	299	LYS
5	DE	319	ASN
5	DE	333	ASP
5	DE	343	LEU
5	DE	398	LEU
5	DE	405	ILE
5	DE	406	ASP
5	DE	408	LEU
5	DE	418	LEU
5	DE	429	ILE
5	DE	445	LEU
5	DE	451	THR
5	DE	484	THR
5	DE	494	ARG
5	DE	503	ASP
5	DE	529	ASP
5	DE	530	TRP
5	DE	538	VAL
5	DE	545	ARG
5	DE	554	LEU
5	DE	566	ARG
5	DE	570	GLU
5	DE	572	VAL
5	DE	573	GLN
5	DE	575	CYS
5	DE	587	MET
5	DE	591	LEU
5	DE	602	LYS
5	DE	604	ASP


Mol	Chain	Res	Type
5	DE	610	LEU
5	DE	615	LEU
5	DE	651	ASN
5	DE	659	ARG
5	DE	698	GLN
5	DE	699	ASN
5	DE	704	LEU
5	DE	717	ARG
5	DE	718	SER
5	DE	721	ASP
5	DE	726	THR
6	DF	8	SER
6	DF	13	ILE
6	DF	15	HIS
6	DF	22	LEU
6	DF	27	ARG
6	DF	33	GLN
6	DF	39	ARG
6	DF	40	GLU
6	DF	50	LEU
6	DF	53	ARG
6	DF	57	ARG
6	DF	69	THR
6	DF	72	THR
6	DF	85	ARG
6	DF	87	GLU
6	DF	110	ASN
6	DF	144	THR
6	DF	154	ASN
6	DF	157	THR
6	DF	170	ARG
6	DF	173	PHE
6	DF	182	ARG
6	DF	188	ARG
6	DF	189	ASP
6	DF	192	LEU
6	DF	194	THR
6	DF	202	LEU
6	DF	238	THR
6	DF	246	LYS
6	DF	255	GLU
6	DF	258	ASP



Mol	Chain	Res	Type
6	DF	259	SER
6	DF	264	VAL
6	DF	274	LEU
6	DF	294	MET
6	DF	297	ARG
6	DF	307	GLU
6	DF	321	LEU
6	DF	326	ASP
6	DF	331	GLU
6	DF	343	GLU
6	DF	362	ILE
6	DF	370	LEU
6	DF	373	ASP
6	DF	394	GLU
6	DF	395	LEU
6	DF	403	LEU
6	DF	437	GLU
6	DF	450	VAL
6	DF	476	LEU
6	DF	491	ARG
6	DF	502	ARG
6	DF	548	ARG
6	DF	550	VAL
6	DF	553	THR
6	DF	568	LEU
6	DF	584	LEU
7	DG	36	THR
7	DG	56	ARG
7	DG	57	GLU
7	DG	62	SER
7	DG	74	LEU
7	DG	78	HIS
7	DG	84	LEU
7	DG	93	ARG
7	DG	95	VAL
7	DG	98	ASP
7	DG	115	ILE
7	DG	125	ASP
7	DG	127	LEU
7	DG	130	LEU
7	DG	141	THR
7	DG	142	LEU



Mol	Chain	Res	Type
7	DG	147	SER
7	DG	149	SER
7	DG	155	GLU
7	DG	179	LEU
7	DG	186	ARG
7	DG	200	GLN
7	DG	206	LEU
7	DG	210	VAL
7	DG	214	TYR
7	DG	220	THR
7	DG	236	VAL
7	DG	296	ASP
7	DG	298	ASP
7	DG	318	ILE
7	DG	326	THR
7	DG	332	GLN
7	DG	334	MET
7	DG	365	GLN
7	DG	367	SER
7	DG	370	ARG
7	DG	377	GLU
7	DG	384	VAL
7	DG	392	ARG
7	DG	399	ARG
7	DG	443	ARG
7	DG	444	THR
7	DG	448	LEU
7	DG	457	ARG
7	DG	466	VAL
7	DG	472	ARG
7	DG	473	CYS
7	DG	494	THR
7	DG	496	ARG
7	DG	497	ARG
7	DG	529	ASP
7	DG	544	ARG
7	DG	547	MET
7	DG	551	MET
7	DG	557	GLN
7	DG	564	GLU
7	DG	577	LEU
7	DG	582	VAL



Mol	Chain	Res	Type
7	DG	608	ARG
7	DG	615	SER
7	DG	616	ARG
7	DG	618	ARG
7	DG	623	MET
7	DG	626	LEU
8	DH	1	MET
8	DH	9	THR
8	DH	18	ARG
8	DH	40	THR
8	DH	42	ARG
8	DH	46	LEU
8	DH	51	ARG
8	DH	76	LEU
8	DH	79	ASP
8	DH	80	ARG
8	DH	81	LYS
8	DH	82	GLN
8	DH	83	GLU
8	DH	84	SER
8	DH	85	LEU
8	DH	105	GLN
8	DH	135	ARG
8	DH	167	GLU
8	DH	174	LEU
8	DH	178	SER
8	DH	195	TYR
8	DH	206	ILE
8	DH	236	MET
8	DH	257	ASN
8	DH	268	LEU
8	DH	273	SER
8	DH	297	CYS
8	DH	311	ARG
8	DH	318	GLU
8	DH	323	SER
8	DH	327	HIS
8	DH	345	VAL
8	DH	348	LYS
8	DH	354	LEU
8	DH	360	LEU
8	DH	364	ARG



Mol	Chain	Res	Type
8	DH	369	ARG
8	DH	380	ARG
8	DH	382	PHE
8	DH	386	ARG
8	DH	392	TRP
8	DH	411	LEU
8	DH	414	LEU
8	DH	418	LYS
8	DH	421	THR
8	DH	428	ARG
8	DH	450	ASN
8	DH	452	ARG
8	DH	460	LEU
8	DH	470	LYS
8	DH	474	ASP
8	DH	476	VAL
8	DH	484	ASP
8	DH	495	THR
8	DH	503	THR
8	DH	515	ASP
8	DH	523	ARG
8	DH	557	VAL
8	DH	562	THR
9	DJ	16	ASN
9	DJ	19	THR
9	DJ	33	ASN
9	DJ	38	MET
9	DJ	46	ARG
9	DJ	48	PHE
9	DJ	55	ASN
9	DJ	76	SER
9	DJ	107	LEU
9	DJ	110	LEU
9	DJ	119	LEU
9	DJ	137	MET
9	DJ	149	THR
9	DJ	151	GLU
9	DJ	164	SER
9	DJ	178	ARG
9	DJ	180	LEU
9	DJ	182	ASP
9	DJ	206	SER



Mol	Chain	Res	Type
9	DJ	212	ASP
9	DJ	226	VAL
9	DJ	234	GLU
9	DJ	236	ARG
9	DJ	246	THR
9	DJ	258	LEU
9	DJ	273	TYR
9	DJ	275	ASP
9	DJ	291	ASN
9	DJ	302	SER
9	DJ	305	ARG
9	DJ	308	ARG
10	DK	2	SER
10	DK	18	LEU
10	DK	34	ASN
10	DK	36	ARG
10	DK	54	THR
10	DK	111	LEU
10	DK	115	THR
10	DK	116	ARG
10	DK	134	THR
10	DK	167	THR
10	DK	172	LEU
10	DK	226	LEU
10	DK	240	SER
10	DK	250	VAL
10	DK	270	LEU
10	DK	273	LEU
10	DK	294	SER
11	DT	11	ASP
11	DT	12	ARG
11	DT	33	HIS
11	DT	35	LYS
11	DT	52	ARG
11	DT	63	HIS
11	DT	88	THR
11	DT	90	THR
11	DT	91	GLN
11	DT	103	LEU
11	DT	105	ARG
11	DT	106	ASP
11	DT	114	LEU



Mol	Chain	Res	Type
11	DT	122	MET
11	DT	131	SER
11	DT	137	LEU
11	DT	163	ARG
11	DT	166	THR
11	DT	168	GLU
11	DT	176	ASP
11	DT	177	MET
11	DT	181	ASP
11	DT	208	ARG
11	DT	209	THR
11	DT	241	ASN
12	DV	26	THR
12	DV	39	ARG
12	DV	41	THR
12	DV	43	ASN
12	DV	56	ARG
12	DV	68	ILE
12	DV	71	GLN
12	DV	77	LYS
12	DV	114	VAL
12	DV	118	GLN
12	DV	131	GLN
12	DV	134	ASP
12	DV	140	PHE
12	DV	143	ILE
12	DV	178	THR
12	DV	179	LEU
12	DV	180	ASP
12	DV	182	TYR
13	DW	10	THR
13	DW	22	THR
13	DW	37	MET
13	DW	58	ARG
13	DW	60	VAL
13	DW	70	LEU
13	DW	74	THR
13	DW	125	LYS
13	DW	128	LEU
13	DW	133	LYS
13	DW	145	ARG
13	DW	163	GLU



Mol	Chain	Res	Type
14	DX	34	LYS
14	DX	57	ARG
14	DX	72	SER
14	DX	76	ARG
14	DX	89	ARG
14	DX	90	ILE
14	DX	98	LEU
14	DX	124	ILE
14	DX	132	THR
14	DX	136	ARG
14	DX	162	VAL
14	DX	164	THR
14	DX	168	ASN
15	DY	11	THR
15	DY	14	THR
15	DY	15	SER
15	DY	23	SER
15	DY	39	VAL
15	DY	43	LEU
15	DY	50	VAL
15	DY	52	GLN
15	DY	64	ASP
15	DY	65	LEU
15	DY	81	THR
15	DY	85	ARG
15	DY	87	ARG
15	DY	93	THR
15	DY	111	ARG
15	DY	124	THR
15	DY	128	GLN
15	DY	141	VAL
15	DY	163	LYS
16	CC	4	MET
16	CC	7	ILE
16	CC	10	VAL
16	CC	13	LYS
16	$\overline{\mathrm{CC}}$	14	THR
16	CC	21	PHE
16	CC	46	TRP
16	CC	47	LEU
16	CC	50	ILE
16	CC	69	GLU



Mol	Chain	Res	Type
16	CC	76	SER
17	CI	18	LEU
17	CI	33	SER
17	CI	34	ASP
17	CI	38	LEU
17	CI	43	SER
17	CI	47	ARG
17	CI	59	ARG
17	CI	65	MET
17	CI	290	ILE
17	CI	303	THR
17	CI	309	ARG
17	CI	311	CYS
17	CI	324	ARG
17	CI	330	ASN
17	CI	338	LYS
17	CI	343	VAL
17	CI	356	MET
17	CI	372	ILE
17	CI	406	THR
17	CI	420	ARG
17	CI	435	LYS
17	CI	439	ARG
18	CJ	17	MET
18	CJ	20	GLN
18	CJ	23	LYS
18	CJ	34	GLN
18	CJ	43	GLU
18	CJ	50	ASP
18	CJ	65	VAL
18	CJ	68	ASP
18	CJ	77	CYS
18	CJ	78	THR
18	CJ	84	MET
18	CJ	93	SER
18	CJ	105	ASN
18	CJ	110	LYS
18	CJ	130	ARG
18	CJ	141	ASP
18	CJ	149	GLU
18	CJ	158	THR
18	CJ	162	ILE



Mol	Chain	Res	Type
18	CJ	178	SER
18	CJ	186	VAL
18	CJ	202	ASP
18	CJ	203	ARG
18	CJ	212	THR
18	CJ	257	VAL
18	CJ	273	ARG
18	CJ	279	LYS
18	CJ	286	LEU
18	CJ	287	LEU
18	CJ	293	ASP
18	CJ	304	ARG
18	CJ	311	LEU
18	CJ	313	GLU
18	CJ	325	SER
18	CJ	330	LEU
18	CJ	345	VAL
18	CJ	346	PRO
18	CJ	380	THR
18	CJ	396	LYS
18	CJ	399	ARG
18	CJ	403	CYS
18	CJ	409	SER
18	CJ	413	GLU
18	CJ	456	THR
18	CJ	457	THR
18	CJ	481	ASP
18	CJ	490	ASP
18	CJ	498	CYS
18	CJ	517	VAL
18	CJ	519	ILE
18	CJ	523	VAL
18	CJ	526	THR
18	CJ	532	PHE
18	CJ	542	LYS
18	CJ	547	LYS
18	CJ	552	ILE
18	CJ	553	ARG
18	CJ	556	GLU
18	CJ	565	THR
18	CJ	569	LEU
18	CJ	585	SER



Mol	Chain	Res	Type
18	CJ	605	THR
18	CJ	618	VAL
18	CJ	629	ARG
18	CJ	648	VAL
18	CJ	654	VAL
18	CJ	671	LEU
18	CJ	684	THR
18	CJ	704	GLU
18	CJ	714	THR
18	CJ	720	THR
18	CJ	727	THR
18	CJ	757	LEU
18	CJ	762	GLN
18	CJ	769	GLN
18	CJ	770	THR
18	CJ	773	GLU
18	CJ	781	HIS
18	CJ	796	ASP
18	CJ	797	LEU
18	CJ	798	GLN
19	CK	15	ARG
19	CK	23	ASP
19	CK	32	LEU
19	CK	33	LYS
19	CK	40	GLN
19	CK	48	ARG
19	CK	56	GLN
20	CN	22	THR
20	CN	30	LEU
20	CN	35	SER
20	CN	41	LEU
20	CN	43	SER
20	CN	49	SER
20	CN	57	LYS
20	CN	60	VAL
20	CN	65	LYS
20	CN	66	MET
20	CN	70	LYS
20	CN	72	THR
20	CN	77	ASN
20	CN	81	LEU
20	CN	83	LYS



Mol	Chain	Res	Type
20	CN	111	VAL
20	CN	118	MET
20	CN	127	LEU
20	CN	135	THR
20	CN	158	ARG
21	CR	243	THR
21	CR	248	LYS
21	CR	250	GLN
21	CR	267	ASN
21	CR	269	SER
21	CR	274	VAL
21	CR	280	ASN
21	CR	282	THR
21	CR	286	LEU
22	CS	32	LYS
22	CS	48	ARG
22	CS	64	MET
22	CS	65	ASN
22	CS	75	MET
22	CS	76	THR
22	CS	86	GLU
22	CS	95	THR
22	CS	107	THR
22	CS	121	SER
22	CS	140	MET
22	CS	152	ASP
23	Cg	20	THR
23	Cg	56	ARG
23	Cg	57	THR
23	Cg	73	ASP
23	Cg	76	SER
23	Cg	87	GLN
23	Cg	107	ARG
23	Cg	112	ARG
23	Cg	114	GLU
23	Cg	117	LEU
23	Cg	120	LEU
23	Cg	127	HIS
23	Cg	143	THR
23	Cg	153	CYS
23	Cg	170	ASN
23	Cg	173	THR



Mol	Chain	Res	Type
23	Cg	189	TRP
23	Cg	194	LEU
23	Cg	213	VAL
23	Cg	221	SER
23	Cg	224	LEU
23	Cg	225	ARG
23	Cg	226	CYS
23	Cg	233	THR
23	Cg	262	GLN
23	Cg	290	LEU
23	Cg	296	HIS
23	Cg	308	LEU
23	Cg	310	SER
23	Cg	316	THR
23	Cg	318	ILE
23	Cg	319	ASP
23	Cg	325	LEU
23	Cg	344	LEU
23	Cg	355	THR
23	Cg	373	VAL
23	Cg	383	ASP
23	Cg	391	GLU
23	Cg	421	GLU
23	Cg	422	LEU
23	Cg	436	ASP
23	Cg	464	VAL
23	Cg	468	ASP
23	Cg	480	LYS
24	Ci	14	ARG
24	Ci	18	THR
24	Ci	27	CYS
24	Ci	30	ARG
24	Ci	32	ASP
24	Ci	54	GLN
24	Ci	76	MET
24	Ci	82	GLN
24	Ci	105	ARG
24	Ci	114	MET
24	Ci	119	LEU
24	Ci	122	MET
24	Ci	136	HIS
24	Ci	138	ASP



Mol	Chain	Res	Type
24	Ci	144	ARG
24	Ci	145	ASN
24	Ci	146	ASP
24	Ci	157	LEU
24	Ci	164	ASN
24	Ci	174	ASP
25	Ck	34	GLN
25	Ck	57	ASP
25	Ck	86	GLU
25	Ck	87	ARG
25	Ck	97	GLN
25	Ck	99	SER
25	Ck	104	SER
25	Ck	108	GLN
25	Ck	111	THR
25	Ck	136	ASP
25	Ck	137	THR
25	Ck	161	GLU
25	Ck	176	THR
25	Ck	185	LEU
25	Ck	188	LEU
25	Ck	207	ARG
25	Ck	214	LEU
25	Ck	242	LEU
25	Ck	254	ILE
25	Ck	290	LEU
25	Ck	292	ASP
25	Ck	316	ASP
25	Ck	317	VAL
25	Ck	320	VAL
25	Ck	341	LEU
25	Ck	350	ASP
25	Ck	353	ARG
25	Ck	373	ARG
25	Ck	401	LEU
25	Ck	568	LEU
25	Ck	573	THR
25	Ck	574	GLU
25	Ck	575	LEU
25	Ck	597	LEU
25	Ck	607	LYS
25	Ck	611	ASN



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Wol	Chain	Res	Type
25	Ck	618	ILE
25	Ck	620	THR
25	Ck	627	ASP
25	Ck	629	LEU
25	Ck	633	MET
25	Ck	634	HIS
25	Ck	652	ARG
25	Ck	654	SER
25	Ck	661	ILE
25	Ck	682	ASN
25	Ck	690	TRP
25	Ck	691	GLN
25	Ck	695	GLN
25	Ck	703	ARG
25	Ck	706	SER
25	Ck	707	LEU
25	Ck	733	LEU
25	Ck	755	ASP
25	Ck	760	VAL
25	Ck	775	ARG
25	Ck	806	ASP
25	Ck	838	LEU
25	Ck	841	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (194) such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	DA	1225	HIS
1	DA	1258	ASN
3	DB	92	HIS
3	DB	114	ASN
3	DB	122	HIS
3	DB	134	HIS
3	DB	153	HIS
3	DB	190	HIS
3	DB	194	GLN
3	DB	209	GLN
3	DB	221	HIS
3	DB	300	GLN
3	DB	414	GLN
3	DB	445	ASN
3	DB	461	GLN



Mol	Chain	Res	Type
3	DB	486	HIS
3	DB	551	HIS
3	DB	562	GLN
3	DB	569	HIS
3	DB	686	GLN
3	DB	703	HIS
3	DB	729	GLN
3	DB	748	HIS
3	DB	774	ASN
3	DB	785	ASN
3	DB	828	HIS
3	DB	908	GLN
3	DB	923	GLN
3	DB	958	ASN
3	DB	981	HIS
3	DB	1004	GLN
3	DB	1051	GLN
3	DB	1055	GLN
3	DB	1124	HIS
4	DC	81	HIS
4	DC	128	HIS
4	DC	242	HIS
4	DC	445	HIS
4	DC	530	GLN
4	DC	574	GLN
4	DC	841	HIS
4	DC	943	HIS
4	DC	970	GLN
4	DC	1110	HIS
4	DC	1134	HIS
4	DC	1141	GLN
4	DC	1160	GLN
5	DE	67	ASN
5	DE	105	ASN
5	DE	194	HIS
5	DE	202	HIS
5	DE	414	ASN
5	DE	442	HIS
5	DE	465	ASN
5	DE	501	HIS
5	DE	567	HIS
5	DE	628	HIS



Mol	Chain	Res	Type
5	DE	658	ASN
5	DE	671	ASN
5	DE	698	GLN
6	DF	41	ASN
6	DF	115	HIS
6	DF	140	HIS
6	DF	154	ASN
6	DF	175	GLN
6	DF	178	ASN
6	DF	187	ASN
6	DF	198	HIS
6	DF	214	HIS
6	DF	283	HIS
6	DF	327	HIS
6	DF	474	GLN
6	DF	543	HIS
7	DG	65	ASN
7	DG	71	ASN
7	DG	92	GLN
7	DG	112	HIS
7	DG	170	ASN
7	DG	191	GLN
7	DG	200	GLN
7	DG	229	HIS
7	DG	230	ASN
7	DG	365	GLN
7	DG	405	GLN
7	DG	476	GLN
7	DG	477	GLN
7	DG	545	HIS
8	DH	4	GLN
8	DH	45	HIS
8	DH	100	HIS
8	DH	123	HIS
8	DH	146	GLN
8	DH	257	ASN
8	DH	302	GLN
8	DH	469	ASN
8	DH	490	HIS
8	DH	498	ASN
8	DH	526	ASN
9	DJ	27	GLN



Mol	Chain	Res	Type
9	DJ	31	HIS
9	DJ	33	ASN
9	DJ	42	HIS
9	DJ	247	ASN
9	DJ	291	ASN
9	DJ	293	ASN
9	DJ	301	HIS
9	DJ	314	GLN
10	DK	171	GLN
10	DK	175	HIS
11	DT	16	HIS
11	DT	45	HIS
11	DT	58	HIS
11	DT	72	HIS
11	DT	82	HIS
11	DT	91	GLN
11	DT	139	HIS
11	DT	140	ASN
11	DT	158	HIS
11	DT	161	ASN
11	DT	219	GLN
12	DV	31	HIS
12	DV	40	HIS
12	DV	48	HIS
12	DV	71	GLN
12	DV	83	GLN
12	DV	131	GLN
13	DW	66	HIS
13	DW	69	GLN
13	DW	87	ASN
13	DW	99	HIS
13	DW	121	HIS
13	DW	154	HIS
14	DX	58	HIS
14	DX	130	GLN
14	DX	167	HIS
14	DX	168	ASN
15	DY	10	ASN
15	DY	99	GLN
15	DY	106	GLN
16	CC	25	HIS
16	CC	48	ASN



Mol	Chain	Res	Type
17	CI	12	HIS
18	CJ	82	HIS
18	CJ	134	GLN
18	CJ	151	ASN
18	CJ	441	HIS
18	CJ	450	HIS
18	CJ	460	HIS
18	CJ	476	ASN
18	CJ	484	HIS
18	CJ	621	ASN
18	CJ	755	ASN
18	CJ	761	GLN
18	CJ	769	GLN
18	CJ	781	HIS
18	CJ	792	HIS
18	CJ	793	HIS
20	CN	133	HIS
20	CN	150	HIS
20	CN	153	ASN
21	CR	249	GLN
21	CR	266	ASN
22	CS	110	HIS
23	Cg	164	HIS
23	Cg	170	ASN
23	Cg	184	HIS
23	Cg	239	GLN
23	Cg	289	ASN
23	Cg	301	HIS
23	Cg	350	ASN
23	Cg	418	ASN
24	Ci	19	HIS
24	Ci	29	GLN
24	Ci	83	ASN
24	Ci	95	ASN
24	Ci	96	ASN
24	Ci	112	ASN
24	Ci	125	HIS
24	Ci	136	HIS
24	Ci	145	ASN
25	Ck	95	HIS
25	Ck	97	GLN
25	Ck	110	HIS



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$\mathbf{Mol}$	Chain	$\mathbf{Res}$	Type
25	Ck	134	HIS
25	Ck	264	ASN
25	Ck	589	GLN
25	Ck	611	ASN
25	Ck	634	HIS
25	Ck	644	HIS
25	Ck	666	HIS
25	Ck	679	GLN
25	Ck	682	ASN
25	Ck	691	GLN
25	Ck	728	GLN

#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	CA	142/611~(23%)	85~(59%)	2(1%)

All (85) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
26	CA	397	U
26	CA	398	U
26	CA	399	А
26	CA	400	U
26	CA	401	А
26	CA	406	U
26	CA	407	U
26	CA	408	С
26	CA	410	U
26	CA	411	А
26	CA	413	А
26	CA	414	А
26	CA	415	U
26	CA	418	А
26	CA	419	U
26	CA	421	G
26	CA	423	А
26	CA	426	А
26	CA	427	U
26	CA	428	А
26	CA	430	U



Mol	Chain	Res	Type
26	CA	431	U
26	CA	433	U
26	CA	434	А
26	CA	435	G
26	CA	438	U
26	CA	441	G
26	CA	442	A
26	CA	444	A
26	CA	445	С
26	CA	446	С
26	CA	448	U
26	CA	449	G
26	CA	450	A
26	CA	451	U
26	CA	452	A
26	CA	453	A
26	CA	455	G
26	CA	457	U
26	CA	458	U
26	CA	459	А
26	CA	460	U
26	CA	461	А
26	CA	462	А
26	CA	463	А
26	CA	464	U
26	CA	467	A
26	CA	468	А
26	CA	469	А
26	CA	470	G
26	CA	471	U
$\overline{26}$	CA	472	G
26	CA	476	А
26	CA	478	A
26	CA	480	C
26	CA	481	A
26	CA	482	U
26	CA	483	A
26	CA	484	A
26	CA	485	U
26	CA	486	C
26	CA	487	A
26	CA	489	А



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Mol	Chain	Res	Type
26	CA	491	U
26	CA	494	А
26	CA	495	U
26	CA	496	U
26	CA	497	А
26	CA	498	U
26	CA	500	U
26	CA	502	U
26	CA	505	U
26	CA	507	А
26	CA	509	U
26	CA	510	А
26	CA	513	U
26	CA	514	А
26	CA	517	U
26	CA	518	G
26	CA	519	U
26	CA	520	А
26	CA	532	А
26	CA	535	U
26	CA	536	U
26	CA	537	А

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	CA	512	G
26	CA	527	А

### 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)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.



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).

Mal	Tune Chain Des Link		Bond lengths			Bond angles				
	Type	Unain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	SPD	CA	703	-	9,9,9	0.40	0	8,8,8	0.58	0
31	GTP	Cg	501	32	26,34,34	1.26	3 (11%)	32,54,54	1.83	9 (28%)
29	SPD	DL	401	-	9,9,9	0.40	0	8,8,8	1.04	0
30	UTP	DJ	401	-	22,30,30	1.86	7 (31%)	27,47,47	1.27	3 (11%)

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
29	SPD	CA	703	-	-	5/7/7/7	-
31	GTP	Cg	501	32	-	6/18/38/38	0/3/3/3
29	SPD	DL	401	-	-	2/7/7/7	-
30	UTP	DJ	401	-	-	11/20/38/38	0/2/2/2

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	DJ	401	UTP	C6-N1	4.09	1.40	1.35
30	DJ	401	UTP	O4'-C1'	3.71	1.46	1.41
31	Cg	501	GTP	C5-C6	-3.70	1.39	1.47
30	DJ	401	UTP	C4-N3	3.65	1.39	1.33
30	DJ	401	UTP	C2'-C1'	2.44	1.57	1.53
31	Cg	501	GTP	C4-N3	-2.32	1.31	1.37
30	DJ	401	UTP	PG-O3G	-2.21	1.46	1.54
30	DJ	401	UTP	PA-O5'	2.13	1.67	1.59
31	Cg	501	GTP	O4'-C4'	-2.06	1.40	1.45
30	DJ	401	UTP	PG-O1G	-2.02	1.47	1.54

All (10) bond length outliers are listed below:

All (12) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
31	Cg	501	GTP	O3G-PG-O3B	4.60	120.05	104.64
31	Cg	501	GTP	C2-N1-C6	-4.23	117.31	125.10
31	Cg	501	GTP	PB-O3B-PG	-2.66	123.69	132.83
31	Cg	501	GTP	N2-C2-N3	-2.66	114.57	119.74
31	Cg	501	GTP	C8-N7-C5	2.63	108.00	102.99
31	Cg	501	GTP	PA-O3A-PB	-2.63	123.82	132.83
31	Cg	501	GTP	O6-C6-C5	-2.56	119.38	124.37
30	DJ	401	UTP	O4'-C4'-C3'	-2.47	100.23	105.11
31	Cg	501	GTP	C5-C6-N1	2.46	118.29	113.95
31	Cg	501	GTP	N2-C2-N1	2.22	121.44	116.71
30	DJ	401	UTP	PB-O3B-PG	-2.09	125.66	132.83
30	DJ	401	UTP	O3B-PG-O2G	-2.07	99.70	111.19

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	DJ	401	UTP	C5'-O5'-PA-O1A
30	DJ	401	UTP	C5'-O5'-PA-O2A
30	DJ	401	UTP	C5'-O5'-PA-O3A
30	DJ	401	UTP	O4'-C4'-C5'-O5'
30	DJ	401	UTP	O4'-C1'-N1-C6
30	DJ	401	UTP	C2'-C1'-N1-C6
31	Cg	501	GTP	PB-O3B-PG-O3G
30	DJ	401	UTP	C3'-C4'-C5'-O5'
29	CA	703	SPD	N6-C7-C8-C9
29	CA	703	SPD	C3-C4-C5-N6
29	CA	703	SPD	C2-C3-C4-C5
29	DL	401	SPD	C4-C5-N6-C7
29	CA	703	SPD	C4-C5-N6-C7
30	DJ	401	UTP	PB-O3B-PG-O2G
31	Cg	501	GTP	PB-O3B-PG-O2G
29	DL	401	SPD	C2-C3-C4-C5
30	DJ	401	UTP	PA-O3A-PB-O2B
31	Cg	501	GTP	PG-O3B-PB-O2B
29	CA	703	SPD	C7-C8-C9-N10
31	Cg	501	GTP	PB-O3B-PG-O1G
30	DJ	401	UTP	C4'-C5'-O5'-PA
30	DJ	401	UTP	PA-O3A-PB-O1B
31	Cg	501	GTP	PG-O3B-PB-O1B
31	Cg	501	GTP	O4'-C4'-C5'-O5'

There are no ring outliers.



No monomer is involved in short contacts.

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







# 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 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0233. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections (i)

#### 6.1.1 Primary map



6.1.2 Raw map



The images above show the map projected in three orthogonal directions.



### 6.2 Central slices (i)

### 6.2.1 Primary map



X Index: 160



Y Index: 160



Z Index: 160

#### 6.2.2 Raw map



X Index: 160

Y Index: 160

Z Index: 160

The images above show central slices of the map in three orthogonal directions.



### 6.3 Largest variance slices (i)

### 6.3.1 Primary map



X Index: 187



Y Index: 167



Z Index: 131

#### 6.3.2 Raw map



X Index: 187

Y Index: 167



The images above show the largest variance slices of the map in three orthogonal directions.



### 6.4 Orthogonal surface views (i)

#### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

#### 6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

### 6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



# 7 Map analysis (i)

This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



### 7.2 Volume estimate (i)



The volume at the recommended contour level is  $1453 \text{ nm}^3$ ; this corresponds to an approximate mass of 1312 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum (i)



\*Reported resolution corresponds to spatial frequency of 0.325  ${\rm \AA^{-1}}$ 



# 8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

#### 8.1 FSC (i)



\*Reported resolution corresponds to spatial frequency of 0.325  $\mathrm{\AA^{-1}}$ 



### 8.2 Resolution estimates (i)

$\mathbf{B}_{\mathrm{assolution ostimato}}(\mathbf{\hat{\lambda}})$	Estimation criterion (FSC cut-off)			
Resolution estimate (A)	0.143	0.5	Half-bit	
Reported by author	3.08	-	-	
Author-provided FSC curve	-	-	-	
Unmasked-calculated*	3.58	4.33	3.67	

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.58 differs from the reported value 3.08 by more than 10 %



# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0233 and PDB model 6HIZ. Per-residue inclusion information can be found in section 3 on page 15.

### 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.


## 9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).



## 9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

$\mathbf{Chain}$	Atom inclusion	Q-score
All	0.9887	0.5340
CA	0.9944	0.5550
CC	0.9719	0.5570
CI	0.9859	0.5660
CJ	0.9880	0.5560
CK	0.9976	0.5570
CN	0.9937	0.5830
CR	0.9798	0.5220
CS	0.9939	0.5730
Cg	0.9937	0.5550
Ci	0.9893	0.5670
Ck	0.9857	0.5040
DA	0.9765	0.4800
DB	0.9832	0.5310
DC	0.9920	0.4960
DE	0.9930	0.5000
DF	0.9930	0.5530
DG	0.9912	0.5060
DH	0.9872	0.5440
DJ	0.9921	0.5570
DK	0.9888	0.5270
DL	0.9540	0.5040
DT	0.9930	0.5690
DV	0.9923	0.5670
DW	0.9901	0.5550
DX	0.9896	0.5560
DY	0.9952	0.5700
UO	1.0000	0.5160
UP	1.0000	0.4590

