

Jan 10, 2024 – 10:21 AM JST

PDB ID	:	7EVO
EMDB ID	:	EMD-31334
Title	:	The cryo-EM structure of the human $17S \text{ U2 snRNP}$
Authors	:	Zhang, X.; Zhan, X.; Shi, Y.
Deposited on	:	2021-05-21
Resolution	:	2.50 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. dev 70
Mogul	:	1.8.5 (274361), 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)	:	2.36

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 2.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM\ structures}\ (\#{ m Entries})$
Clashscore	158937	4297
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 $\geq=3, 2, 1$ and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq=5\%$ The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length		Quality of chain		
			68%			
1	Н	188	45%	25%	8% •	21%
0	1	1904	-			
	1	1304	47%	15% •	38%	
			9%			
3	2	895	17% •	80%		
			16%			
4	3	1217	73	%	23	3% • •
			38%			
5	4	424	38%	6	52%	
6	5	86	60%	16	5%	23%
7	6	110	64%		14%	23%



Mol	Chain	Length	Quality of chain	
8	А	793	16% 16% 84%	
9	В	464	22% 78%	
10	С	501	65%	6% • 16%
11	D	755	13% 22% • 74%	
12	Ε	1052	41%	57%
13	F	255	64% 64%	36%
14	G	225	74%	26%
15	a	118	76% 76%	24%
16	b	86	86%	14%
17	с	92	86%	14%
18	d	76	97% 97%	
19	е	126	66% 66%	34%
20	f	240	30% 30% 70%	6
21	g	119	69% 69%	31%



2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 32104 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.

• Molecule 1 is a RNA chain called U2 snRNA.

Mol	Chain	Residues		Α	AltConf	Trace			
1	Н	148	Total 3142	C 1406	N 551	O 1039	Р 146	0	0

• Molecule 2 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues		Α	AltConf	Trace			
2	1	815	Total 6487	C 4163	N 1121	0 1164	S 39	0	0
			0401	4100	1141	1104	00		

• Molecule 3 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues		At	oms	AltConf	Trace		
3	2	182	Total 1210	C 754	N 229	0 225	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 4 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues		Α	AltConf	Trace			
4	3	1180	Total 9247	C 5872	N 1571	O 1759	S 45	0	0

• Molecule 5 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
5	4	160	Total 664	C 344	N 160	O 160	0	0

• Molecule 6 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
6	5	66	Total 539	C 342	N 93	O 99	${S \atop 5}$	0	0



• Molecule 7 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms	AltConf	Trace		
7	6	85	Total 645	C 396	N 114	0 122	S 13	0	0

• Molecule 8 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
8	А	123	Total 504	C 258	N 123	O 123	0	0

• Molecule 9 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	В	100	Total 421	C 221	N 100	O 100	0	0

• Molecule 10 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
10	С	422	Total 2103	C 1174	N 466	0 459	${S \atop 4}$	0	0

• Molecule 11 is a protein called HIV Tat-specific factor 1.

Mol	Chain	Residues		At	oms			AltConf	Trace
11	D	200	Total 1308	C 788	N 246	O 269	${f S}{5}$	3	0

• Molecule 12 is a protein called RNA helicase.

Mol	Chain	Residues		Ate	AltConf	Trace			
12	Е	455	Total 2153	C 1157	N 487	O 507	${ m S} { m 2}$	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Е	-19	MET	-	initiating methionine	UNP A0A0C4DG89
Е	-18	ALA	-	expression tag	UNP A0A0C4DG89
Е	-17	SER	-	expression tag	UNP A0A0C4DG89
Е	-16	ASP	-	expression tag	UNP A0A0C4DG89



Chain	Residue	Modelled	Actual	Comment	Reference
Е	-15	TYR	-	expression tag	UNP A0A0C4DG89
Е	-14	LYS	-	expression tag	UNP A0A0C4DG89
Е	-13	ASP	-	expression tag	UNP A0A0C4DG89
Е	-12	ASP	-	expression tag	UNP A0A0C4DG89
Е	-11	ASP	-	expression tag	UNP A0A0C4DG89
Е	-10	ASP	-	expression tag	UNP A0A0C4DG89
Е	-9	LYS	-	expression tag	UNP A0A0C4DG89
Е	-8	ALA	-	expression tag	UNP A0A0C4DG89
Е	-7	SER	-	expression tag	UNP A0A0C4DG89
Е	-6	ASP	-	expression tag	UNP A0A0C4DG89
Е	-5	GLU	-	expression tag	UNP A0A0C4DG89
Е	-4	VAL	-	expression tag	UNP A0A0C4DG89
Е	-3	ASP	-	expression tag	UNP A0A0C4DG89
E	-2	ALA	-	expression tag	UNP A0A0C4DG89
Е	-1	GLY	-	expression tag	UNP A0A0C4DG89
E	0	THR	-	expression tag	UNP A0A0C4DG89

• Molecule 13 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
13	F	162	Total 666	C 342	N 162	O 162	0	0

• Molecule 14 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace	
14	G	166	Total 685	C 353	N 166	O 166	0	0

• Molecule 15 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues		Aton	ıs	AltConf	Trace	
15	a	90	Total 372	C 192	N 90	O 90	0	0

• Molecule 16 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	b	74	Total 308	C 160	N 74	0 74	0	0

• Molecule 17 is a protein called Small nuclear ribonucleoprotein E.



Mol	Chain	Residues	Atoms				AltConf	Trace
17	с	79	Total 319	C 161	N 79	O 79	0	0

• Molecule 18 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms			AltConf	Trace	
18	d	74	Total 305	C 157	N 74	О 74	0	0

• Molecule 19 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms			AltConf	Trace	
19	е	83	Total 341	C 175	N 83	O 83	0	0

• Molecule 20 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms			AltConf	Trace	
20	f	71	Total 293	C 151	N 71	O 71	0	0

• Molecule 21 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms			AltConf	Trace	
21	g	82	Total 337	C 173	N 82	O 82	0	0

• Molecule 22 is $[(2 {S},3 {S},4 {E},6 {S},7 {R},10 {R})-3,7-dimethyl-2-[(2 {E},4 {E},6 {R})-6-methyl-6-oxidanyl-7-[(2 {R},3 {R})-3-[(2 {R},3 {S})-3-oxidanylpentan-2-yl]oxiran-2-yl] hepta-2,4-dien-2-yl]-7,10-bis(oxidanyl)-12-oxidanylidene-1-oxacyclododec-4-en-6-yl] 4-cyclo heptylpiperazine-1-carboxylate (three-letter code: 9B0) (formula: C₄₀H₆₆N₂O₉) (labeled as "Ligand of Interest" by depositor).$





Mol	Chain	Residues	Atoms				AltConf
22	1	1	Total 51	C 40	N 2	0 9	0

• Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
23	6	3	Total Zn 3 3	0
23	С	1	Total Zn 1 1	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: U2 snRNA















• Molecule 9: Splicing factor 3A subunit 2













GLU LLEU LLEU ARG GLU LLEU LLEU PRO PRO PRO PRO CGLN THR ASNN THR THR THR TYR LLYS CGLY VAL LLYS LLYS LLYS CGLU

• Molecule 13: U2 small nuclear ribonucleoprotein A'







• Molecule 20: Small nuclear ribonucleoprotein-associated proteins B and B'





65.2
 75.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 74.4
 <li



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	485418	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 $(6k \ge 4k)$	Depositor
Maximum map value	0.257	Depositor
Minimum map value	-0.135	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	347.84, 347.84, 347.84	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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: ZN, $9\mathrm{B}0$

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	nd lengths	B	Bond angles		
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5		
1	Н	0.41	2/3507~(0.1%)	0.95	17/5454~(0.3%)		
2	1	0.27	0/6609	0.45	1/8946~(0.0%)		
3	2	0.25	0/1248	0.45	0/1672		
4	3	0.27	0/9435	0.49	1/12802~(0.0%)		
5	4	0.24	0/670	0.45	0/850		
6	5	0.48	1/555~(0.2%)	0.52	0/750		
7	6	0.25	0/653	0.45	0/877		
8	А	0.24	0/507	0.41	0/640		
9	В	0.24	0/426	0.50	0/543		
10	С	0.25	0/2133	0.45	0/2773		
11	D	0.28	0/1325	0.47	0/1749		
12	Е	0.41	1/2171~(0.0%)	0.52	0/2779		
13	F	0.24	0/671	0.49	0/849		
14	G	0.23	0/689	0.46	0/869		
15	a	0.24	0/374	0.50	0/472		
16	b	0.25	0/311	0.51	0/395		
17	с	0.24	0/319	0.49	0/399		
18	d	0.25	0/307	0.51	0/388		
19	е	0.25	0/343	0.51	0/433		
20	f	0.24	0/294	0.49	0/370		
21	g	0.23	0/339	0.51	0/428		
All	All	0.30	4/32886~(0.0%)	0.56	19/44438~(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
1	Η	0	1
10	С	0	1



Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5	78	PRO	C-N	8.67	1.50	1.34
1	Н	45	С	O3'-P	-7.13	1.52	1.61
1	Н	55	U	P-OP2	5.57	1.58	1.49
12	Е	178	ALA	C-O	5.12	1.33	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Н	28	С	N1-C1'-C2'	-11.54	98.99	114.00
1	Н	120	А	C6-N1-C2	-8.05	113.77	118.60
1	Н	42	G	C4'-C3'-O3'	7.34	127.69	113.00
1	Н	27	U	C3'-C2'-C1'	7.02	107.11	101.50
1	Н	55	U	OP1-P-OP2	6.85	129.88	119.60
1	Н	28	С	C1'-C2'-O2'	-6.80	90.20	110.60
1	Н	55	U	O5'-P-OP2	-6.72	99.65	105.70
4	3	625	LEU	CA-CB-CG	6.71	130.72	115.30
1	Н	120	А	N1-C2-N3	6.31	132.46	129.30
1	Н	19	G	O5'-P-OP1	-6.23	100.09	105.70
1	Н	136	G	C2-N3-C4	6.08	114.94	111.90
1	Н	129	U	N1-C2-O2	5.71	126.80	122.80
1	Н	129	U	N3-C2-O2	-5.48	118.37	122.20
1	Н	136	G	N3-C4-C5	-5.33	125.93	128.60
2	1	563	LEU	CA-CB-CG	5.33	127.57	115.30
1	Н	168	A	C4-N9-C1'	5.25	135.75	126.30
1	Н	28	С	C3'-C2'-C1'	5.21	105.67	101.50
1	Н	121	A	C2-N3-C4	5.06	113.13	110.60
1	Н	137	U	C6-N1-C2	-5.03	117.98	121.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	С	393	PRO	Mainchain
1	Н	43	U	Sidechain



5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Н	3142	0	1594	60	0
2	1	6487	0	6700	136	0
3	2	1210	0	1010	27	0
4	3	9247	0	9179	161	0
5	4	664	0	230	0	0
6	5	539	0	505	10	0
7	6	645	0	626	9	0
8	А	504	0	150	0	0
9	В	421	0	148	0	0
10	С	2103	0	1108	47	0
11	D	1308	0	1061	25	0
12	Е	2153	0	1054	27	0
13	F	666	0	209	0	0
14	G	685	0	226	7	0
15	a	372	0	118	0	0
16	b	308	0	115	0	0
17	с	319	0	92	0	0
18	d	305	0	105	0	0
19	е	341	0	112	0	0
20	f	293	0	99	0	0
21	g	337	0	110	0	0
22	1	51	0	0	9	0
23	6	3	0	0	0	0
23	С	1	0	0	0	0
All	All	32104	0	24551	454	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (454) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:25:G:H1'	10:C:399:LEU:CD2	1.33	1.55
12:E:226:ASP:OD1	12:E:227:PRO:HD2	1.18	1.31
10:C:396:LEU:HD12	10:C:400:HIS:HD2	0.98	1.13



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:25:G:C1'	10:C:399:LEU:CD2	2.25	1.12
10:C:396:LEU:HD12	10:C:400:HIS:CD2	1.88	1.08
1:H:25:G:C1'	10:C:399:LEU:HD22	1.82	1.07
12:E:226:ASP:OD1	12:E:227:PRO:CD	2.04	1.05
10:C:398:LYS:HG2	10:C:403:ASN:ND2	1.72	1.04
1:H:25:G:H1'	10:C:399:LEU:HD21	1.37	1.03
22:1:1500:9B0:C39	7:6:38:ARG:HD2	1.89	1.01
2:1:900:PHE:CD1	2:1:914:PHE:HD2	1.83	0.95
2:1:900:PHE:HD1	2:1:914:PHE:HD2	1.09	0.95
1:H:25:G:C1'	10:C:399:LEU:HD21	1.98	0.90
2:1:900:PHE:CD1	2:1:914:PHE:CD2	2.62	0.87
1:H:25:G:H1'	10:C:399:LEU:HD22	0.88	0.87
4:3:264:GLN:HE22	4:3:322:VAL:H	1.24	0.84
2:1:900:PHE:HD1	2:1:914:PHE:CD2	1.97	0.83
10:C:501:LEU:C	14:G:224:LYS:H	1.84	0.81
1:H:45:C:C2	10:C:395:TRP:CD1	2.70	0.80
4:3:579:GLU:HB3	4:3:625:LEU:HD11	1.65	0.78
10:C:402:LEU:O	10:C:403:ASN:ND2	2.17	0.77
1:H:150:U:H3	1:H:181:G:H1	1.31	0.76
12:E:177:LYS:HB2	12:E:177:LYS:NZ	2.01	0.75
12:E:241:LYS:HA	12:E:241:LYS:HE3	1.69	0.74
1:H:43:U:H4'	1:H:43:U:OP1	1.85	0.74
4:3:463:ARG:HB3	4:3:471:ASP:HA	1.70	0.73
2:1:614:ARG:HH21	12:E:228:LEU:HD13	1.53	0.73
4:3:583:MET:SD	4:3:615:ARG:NH1	2.62	0.72
12:E:166:ARG:NH1	12:E:166:ARG:HB3	2.04	0.72
10:C:501:LEU:HA	14:G:224:LYS:O	1.90	0.72
4:3:1121:THR:HG22	4:3:1125:GLY:H	1.55	0.72
1:H:47:U:H3'	1:H:48:A:H5'	1.71	0.71
4:3:698:PRO:O	4:3:700:LYS:NZ	2.24	0.70
2:1:925:VAL:HG23	2:1:928:TYR:HB2	1.74	0.70
2:1:945:ALA:HA	2:1:948:ARG:HB2	1.74	0.70
4:3:805:ASN:ND2	4:3:858:GLY:O	2.25	0.69
4:3:703:ARG:NH1	4:3:711:ALA:O	2.23	0.69
4:3:1121:THR:HG23	4:3:1123:SER:H	1.54	0.69
1:H:56:A:C2	3:2:478:HIS:CE1	2.81	0.69
2:1:900:PHE:CE1	2:1:954:LEU:HD22	2.27	0.69
4:3:547:CYS:SG	4:3:548:ALA:N	2.65	0.69
7:6:21:ARG:NH2	7:6:68:ASP:OD1	2.26	0.68
12:E:166:ARG:HB3	12:E:166:ARG:HH11	1.58	0.68
10:C:398:LYS:CG	10:C:403:ASN:ND2	2.55	0.68



	the second se	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:3:186:GLU:OE1	4:3:222:ARG:NH2	2.27	0.68
4:3:499:PHE:HD2	4:3:518:GLN:HE21	1.41	0.67
4:3:672:GLY:HA3	4:3:695:GLY:HA3	1.76	0.67
4:3:893:VAL:HG22	4:3:905:VAL:HG22	1.77	0.66
4:3:707:GLN:HG3	4:3:709:GLN:HE22	1.60	0.66
10:C:397:TYR:O	10:C:402:LEU:HB2	1.96	0.66
4:3:673:VAL:HG12	4:3:690:ARG:HA	1.77	0.66
4:3:511:LEU:HB2	4:3:517:VAL:HG23	1.78	0.65
4:3:511:LEU:HD21	4:3:568:MET:HG3	1.78	0.65
4:3:101:LYS:HD3	4:3:104:GLN:HG3	1.77	0.65
2:1:926:LYS:HG2	2:1:927:PRO:HD3	1.79	0.65
1:H:45:C:N3	10:C:395:TRP:CD1	2.65	0.64
2:1:699:GLN:O	2:1:699:GLN:HG3	1.95	0.64
3:2:591:TYR:HA	3:2:595:LYS:HD3	1.77	0.64
1:H:42:G:C5	1:H:43:U:C6	2.85	0.64
10:C:398:LYS:HG2	10:C:403:ASN:HD22	1.60	0.64
2:1:866:LYS:HG3	2:1:909:VAL:HG11	1.79	0.64
4:3:828:GLY:O	4:3:834:LEU:N	2.31	0.64
2:1:731:LEU:HB3	2:1:750:ILE:HD11	1.80	0.63
1:H:56:A:H2	3:2:478:HIS:CE1	2.16	0.63
11:D:201:LEU:HB3	11:D:213:VAL:HG21	1.81	0.63
11:D:248:ASP:OD2	11:D:250:ARG:NH1	2.30	0.63
4:3:707:GLN:O	4:3:709:GLN:NE2	2.32	0.63
4:3:899:THR:HG22	4:3:900:GLY:H	1.64	0.62
2:1:1137:ARG:HH12	3:2:524:LEU:H	1.47	0.62
4:3:864:SER:HB3	4:3:882:LEU:HD12	1.82	0.62
10:C:501:LEU:C	14:G:224:LYS:N	2.52	0.62
2:1:1142:ASN:ND2	11:D:247:LEU:O	2.32	0.62
11:D:138:SER:HB3	11:D:212:HIS:HB3	1.81	0.62
4:3:798:ILE:HD13	4:3:893:VAL:HG21	1.81	0.62
4:3:958:ARG:NH2	4:3:1014:TYR:OH	2.33	0.62
4:3:614:VAL:HG23	4:3:633:LEU:HD21	1.82	0.62
6:5:51:ASN:OD1	6:5:61:LYS:NZ	2.30	0.62
2:1:850:ILE:O	2:1:854:VAL:HB	1.99	0.61
11:D:165:THR:OG1	11:D:166:GLU:N	2.32	0.61
2:1:900:PHE:HE1	2:1:954:LEU:HD22	1.65	0.60
4:3:93:GLN:NE2	4:3:100:GLU:OE1	2.35	0.60
4:3:412:ILE:HG12	4:3:423:LEU:HG	1.83	0.60
12:E:177:LYS:HB2	12:E:177:LYS:HZ3	1.67	0.60
1:H:36:G:N1	11:D:250:ARG:HD2	2.15	0.60
4:3:343:LYS:O	4:3:344:THR:OG1	2.18	0.60



	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:56:A:C5	3:2:504:TRP:CZ3	2.89	0.60
10:C:467:ALA:HA	10:C:470:ARG:HD2	1.84	0.59
22:1:1500:9B0:C39	7:6:38:ARG:CD	2.75	0.59
11:D:206:ILE:HD12	11:D:209:TYR:H	1.68	0.59
1:H:54:U:H2'	1:H:55:U:C6	2.38	0.59
10:C:501:LEU:CA	14:G:224:LYS:O	2.51	0.59
4:3:718:ARG:NH1	4:3:734:LEU:O	2.35	0.59
4:3:294:LYS:HD2	4:3:299:PHE:HB3	1.84	0.58
1:H:20:G:H2'	1:H:21:C:C6	2.38	0.58
2:1:553:VAL:HG22	2:1:596:ILE:HD11	1.85	0.58
4:3:1183:ASN:OD1	4:3:1205:SER:OG	2.22	0.58
1:H:22:U:O2	10:C:395:TRP:CH2	2.56	0.58
1:H:45:C:C2	10:C:395:TRP:HD1	2.20	0.58
1:H:56:A:C5	3:2:504:TRP:HZ3	2.22	0.57
1:H:43:U:H2'	1:H:44:U:C6	2.39	0.57
12:E:207:GLU:OE1	12:E:207:GLU:HA	2.03	0.57
2:1:976:VAL:O	2:1:980:GLU:HG2	2.05	0.57
2:1:1287:ILE:HD13	6:5:32:LEU:HD21	1.85	0.57
4:3:118:GLY:HA2	4:3:132:ILE:HD11	1.87	0.57
4:3:755:VAL:HG13	4:3:764:ILE:HG12	1.87	0.57
4:3:786:ARG:NH1	4:3:802:THR:O	2.38	0.57
4:3:1001:ILE:HG13	4:3:1038:LEU:HD11	1.86	0.57
2:1:823:MET:HG2	2:1:833:LEU:HD22	1.87	0.56
2:1:490:GLU:HB3	2:1:493:LYS:HB2	1.86	0.56
4:3:555:VAL:HG23	4:3:592:LEU:HD11	1.87	0.56
4:3:1008:SER:HB3	4:3:1031:ARG:HB2	1.87	0.56
4:3:675:LEU:HD13	4:3:688:ASP:HB3	1.86	0.56
2:1:1137:ARG:NH1	3:2:522:PHE:O	2.38	0.56
2:1:1000:ILE:O	2:1:1004:ILE:HG22	2.06	0.56
11:D:206:ILE:HD11	11:D:209:TYR:HB2	1.88	0.56
7:6:58:CYS:HB3	7:6:62:GLY:H	1.71	0.56
4:3:507:SER:HB3	4:3:519:VAL:HB	1.88	0.55
4:3:856:LYS:NZ	6:5:58:ASN:O	2.36	0.55
2:1:945:ALA:HB2	2:1:948:ARG:HH11	1.71	0.55
4:3:120:PHE:HB2	4:3:133:SER:HB3	1.87	0.55
7:6:27:ASP:OD1	7:6:67:SER:OG	2.20	0.55
1:H:45:C:H5"	1:H:46:U:H5'	1.89	0.55
12:E:241:LYS:HE3	12:E:241:LYS:CA	2.37	0.55
2:1:494:GLU:HA	2:1:497:ILE:HG22	1.89	0.55
2:1:614:ARG:NH2	12:E:228:LEU:HD13	2.21	0.55
2:1:914:PHE:HZ	2:1:932:ILE:HG12	1.70	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:3:1118:VAL:HG22	4:3:1128:ILE:HG22	1.89	0.55
1:H:42:G:C6	1:H:43:U:C6	2.94	0.54
2:1:954:LEU:O	2:1:958:THR:OG1	2.23	0.54
2:1:1157:TYR:CE1	22:1:1500:9B0:C30	2.91	0.54
10:C:406:TYR:O	10:C:416:TYR:N	2.36	0.54
2:1:1299:GLU:OE2	6:5:71:LYS:NZ	2.39	0.54
4:3:436:ARG:HH11	4:3:776:GLN:HE22	1.55	0.54
4:3:804:HIS:NE2	4:3:859:ASN:O	2.39	0.54
4:3:407:ILE:HG23	4:3:425:VAL:HG13	1.90	0.54
4:3:804:HIS:O	6:5:58:ASN:ND2	2.32	0.54
2:1:658:TRP:CH2	2:1:700:LYS:HE2	2.43	0.54
2:1:963:LYS:HG2	2:1:1003:VAL:HG13	1.89	0.54
2:1:991:GLY:HA3	2:1:1030:LYS:HG2	1.90	0.54
2:1:608:THR:O	2:1:612:THR:HG23	2.09	0.53
2:1:1256:HIS:HD2	2:1:1258:ALA:H	1.55	0.53
1:H:24:A:C6	10:C:396:LEU:HD13	2.44	0.53
4:3:612:ASN:O	4:3:633:LEU:N	2.42	0.53
2:1:1137:ARG:HH12	3:2:524:LEU:N	2.05	0.53
4:3:1159:ASP:HB3	4:3:1162:SER:HB3	1.91	0.53
1:H:151:C:H2'	1:H:152:G:H8	1.74	0.52
2:1:701:VAL:O	2:1:705:SER:OG	2.24	0.52
4:3:476:VAL:HG13	4:3:483:LEU:HG	1.92	0.52
2:1:568:ARG:NH1	12:E:242:PHE:CE1	2.78	0.52
2:1:578:ILE:HD13	2:1:596:ILE:HG21	1.91	0.52
4:3:534:ASN:OD1	4:3:534:ASN:N	2.43	0.52
1:H:46:U:O5'	1:H:47:U:H4'	2.10	0.52
22:1:1500:9B0:C7	22:1:1500:9B0:C29	2.87	0.52
2:1:830:TYR:O	2:1:834:VAL:HG23	2.09	0.52
4:3:463:ARG:HA	4:3:472:ALA:N	2.24	0.52
4:3:506:LEU:HD23	4:3:545:VAL:O	2.10	0.52
2:1:960:VAL:HA	2:1:1003:VAL:HG21	1.92	0.52
4:3:947:GLU:HG2	4:3:964:GLY:HA3	1.91	0.51
1:H:120:A:N1	1:H:137:U:O4	2.43	0.51
2:1:732:TRP:HA	2:1:735:ILE:HG12	1.93	0.51
4:3:797:LEU:HG	4:3:871:PRO:HG3	1.93	0.51
1:H:27:U:H2'	1:H:28:C:C6	2.46	0.51
1:H:42:G:C6	1:H:43:U:C5	2.99	0.51
2:1:763:ASN:HB2	2:1:800:GLY:O	2.11	0.51
4:3:462:VAL:HG23	4:3:510:LEU:HB2	1.92	0.51
10:C:398:LYS:HG2	10:C:403:ASN:HD21	1.66	0.51
2:1:556:ILE:O	2:1:560:LEU:HB2	2.11	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:1:729:LYS:HB3	2:1:730:PRO:HD3	1.93	0.51
4:3:128:ARG:NH2	4:3:178:GLU:O	2.43	0.51
22:1:1500:9B0:C10	22:1:1500:9B0:C5	2.88	0.50
4:3:528:ARG:HH22	4:3:573:GLN:NE2	2.08	0.50
4:3:1133:THR:HG21	4:3:1214:ARG:HH22	1.75	0.50
1:H:36:G:N1	11:D:250:ARG:CD	2.73	0.50
1:H:56:A:N7	3:2:504:TRP:HZ3	2.09	0.50
2:1:851:SER:HA	2:1:854:VAL:HG12	1.92	0.50
2:1:1036:ILE:HD11	2:1:1065:LEU:HD13	1.94	0.50
4:3:747:SER:H	4:3:751:PRO:HA	1.76	0.50
2:1:494:GLU:O	2:1:498:MET:HG3	2.12	0.50
1:H:60:U:H2'	1:H:61:C:C6	2.47	0.50
4:3:236:ILE:HB	4:3:249:LEU:HB2	1.93	0.50
4:3:478:PHE:N	4:3:481:ALA:O	2.42	0.50
1:H:36:G:H1	11:D:250:ARG:HD3	1.77	0.50
2:1:495:ARG:HD2	2:1:534:GLN:NE2	2.27	0.50
2:1:1187:THR:O	2:1:1191:VAL:HG23	2.12	0.50
4:3:739:LEU:HD13	4:3:756:ALA:HB1	1.93	0.50
4:3:663:LEU:HB3	4:3:679:LEU:HB3	1.94	0.50
10:C:438:LEU:HD21	10:C:452:ILE:HG23	1.94	0.50
1:H:22:U:O2	10:C:393:PRO:HB3	2.12	0.49
4:3:34:ARG:NH1	4:3:39:GLU:OE1	2.45	0.49
12:E:177:LYS:NZ	12:E:177:LYS:CB	2.74	0.49
4:3:274:ARG:HD2	4:3:389:PRO:HG3	1.94	0.49
2:1:495:ARG:HD2	2:1:534:GLN:HE21	1.77	0.49
11:D:241:SER:O	11:D:245:LYS:HG3	2.13	0.49
2:1:1125:PRO:HG2	2:1:1165:TYR:CE2	2.48	0.49
4:3:463:ARG:H	4:3:463:ARG:HD2	1.78	0.49
4:3:565:TYR:HD2	4:3:577:TYR:HB2	1.77	0.49
2:1:575:LEU:O	2:1:579:GLU:N	2.46	0.49
2:1:821:HIS:O	2:1:825:LEU:HD23	2.12	0.49
6:5:29:TRP:O	6:5:33:VAL:HG13	2.12	0.49
10:C:501:LEU:CB	14:G:224:LYS:N	2.76	0.49
11:D:136:TYR:HB2	11:D:216:ALA:HA	1.93	0.49
4:3:353:PHE:HB3	4:3:406:PRO:HD3	1.94	0.49
4:3:604:PHE:HB3	4:3:616:ILE:HD11	1.95	0.49
12:E:241:LYS:HA	12:E:241:LYS:CE	2.42	0.49
1:H:42:G:H2'	1:H:43:U:O4'	2.12	0.49
2:1:932:ILE:O	2:1:936:VAL:HG22	2.13	0.49
3:2:473:ASP:N	3:2:473:ASP:OD1	2.46	0.49
4:3:539:PRO:O	4:3:542:LYS:HE2	2.13	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
12:E:166:ARG:NH1	12:E:166:ARG:CB	2.75	0.49
1:H:24:A:C5	10:C:396:LEU:HD13	2.48	0.49
3:2:569:GLN:HA	3:2:572:HIS:HB3	1.95	0.49
12:E:161:ARG:HD2	12:E:165:GLU:OE2	2.13	0.49
4:3:742:ALA:HA	4:3:755:VAL:O	2.13	0.48
10:C:411:CYS:SG	10:C:430:ARG:HD3	2.53	0.48
12:E:177:LYS:HB2	12:E:177:LYS:HZ2	1.78	0.48
1:H:46:U:H3	10:C:398:LYS:HE2	1.79	0.48
10:C:501:LEU:C	14:G:224:LYS:CA	2.81	0.48
1:H:54:U:H2'	1:H:55:U:H6	1.78	0.48
10:C:396:LEU:O	10:C:396:LEU:HG	2.11	0.48
4:3:96:LYS:HB3	4:3:98:MET:HG2	1.94	0.48
4:3:318:ASP:N	4:3:321:MET:O	2.43	0.48
4:3:589:CYS:SG	4:3:637:PRO:HB2	2.54	0.48
2:1:551:LEU:O	2:1:555:VAL:HG23	2.13	0.48
2:1:1005:GLY:HA2	2:1:1045:ARG:NH1	2.28	0.48
12:E:241:LYS:HE3	12:E:241:LYS:O	2.12	0.48
4:3:35:GLY:HA3	6:5:47:PHE:CZ	2.49	0.48
2:1:509:PRO:HA	2:1:512:ARG:HB2	1.96	0.48
2:1:959:ALA:HA	2:1:962:MET:HB2	1.96	0.48
2:1:1106:ARG:HD2	2:1:1106:ARG:HA	1.74	0.48
4:3:546:LYS:HD2	4:3:587:VAL:O	2.14	0.48
11:D:238:LYS:O	11:D:242:MET:HG2	2.14	0.47
4:3:473:TYR:HA	4:3:485:LEU:O	2.13	0.47
4:3:532:ARG:HD3	4:3:533:VAL:H	1.79	0.47
4:3:699:VAL:HA	4:3:715:MET:O	2.14	0.47
3:2:467:GLN:HA	10:C:461:LYS:HE2	1.96	0.47
4:3:671:ASN:HB2	4:3:673:VAL:HG22	1.96	0.47
1:H:120:A:N1	1:H:137:U:C4	2.82	0.47
3:2:495:ARG:HG2	4:3:1083:ASN:O	2.14	0.47
1:H:124:G:H2'	1:H:125:G:C8	2.49	0.47
2:1:925:VAL:CG2	2:1:928:TYR:HB2	2.44	0.47
2:1:1174:GLU:CD	2:1:1210:HIS:HE2	2.17	0.47
2:1:1180:ARG:HH22	3:2:513:GLY:HA2	1.79	0.47
4:3:520:TYR:HE1	4:3:525:ARG:HG2	1.80	0.47
11:D:239:LYS:HA	11:D:242:MET:HG2	1.95	0.47
2:1:914:PHE:CZ	2:1:932:ILE:HG12	2.49	0.47
2:1:1118:ILE:O	2:1:1122:THR:HG23	2.14	0.47
2:1:661:ARG:NH1	2:1:696:ASP:OD2	2.47	0.47
4:3:404:LEU:HD21	4:3:438:LEU:HD11	1.97	0.47
4:3:475:ILE:HG23	4:3:484:VAL:HB	1.97	0.47



Atom-1	Atom-2	Interatomic	Clash
11 D 196 TVD HD9		distance (A)	overlap (A)
11:D:130:1YR:HB3	11:D:214:GLU:HG3	1.97	0.47
10:C:394:TYR:O	10:C:397:TYR:HB3	2.14	0.47
22:1:1500:9B0:C18	22:1:1500:9B0:C23	2.92	0.47
4:3:317:THR:HG22	4:3:318:ASP:O	2.14	0.47
4:3:996:1LE:O	4:3:998:HIS:N	2.47	0.47
7:6:54:TYR:HB3	7:6:57:ARG:HH11	1.80	0.47
1:H:47:U:H3'	1:H:48:A:C5'	2.43	0.47
2:1:746:PHE:O	2:1:750:ILE:HG12	2.15	0.47
3:2:467:GLN:NE2	10:C:457:SER:OG	2.49	0.46
4:3:187:MET:CE	6:5:73:LEU:HD22	2.44	0.46
4:3:451:GLU:HG2	4:3:761:THR:HA	1.97	0.46
4:3:877:LEU:HD23	4:3:935:GLU:HG2	1.96	0.46
4:3:343:LYS:HB3	4:3:343:LYS:HE3	1.66	0.46
4:3:1082:LEU:HD12	4:3:1088:LYS:HE3	1.96	0.46
2:1:492:GLN:OE1	2:1:496:LYS:HD3	2.15	0.46
2:1:505:LYS:NZ	2:1:548:GLU:OE1	2.48	0.46
2:1:945:ALA:HB1	2:1:989:VAL:HG11	1.96	0.46
11:D:147:ASP:HA	11:D:150:ILE:HG13	1.97	0.46
2:1:580:PRO:O	2:1:581:LEU:HB2	2.15	0.46
2:1:850:ILE:HD13	2:1:872:ILE:HG12	1.97	0.46
22:1:1500:9B0:C23	22:1:1500:9B0:C17	2.93	0.46
1:H:30:A:H61	1:H:40:C:H42	1.64	0.46
1:H:36:G:H1	11:D:250:ARG:CD	2.28	0.46
4:3:947:GLU:HG3	4:3:948:VAL:H	1.80	0.46
2:1:830:TYR:OH	2:1:870:GLU:OE1	2.33	0.46
4:3:702:PHE:HE2	4:3:715:MET:HE2	1.80	0.46
4:3:501:GLY:HA2	4:3:525:ARG:HH22	1.80	0.46
7:6:25:LYS:HB3	7:6:25:LYS:HE2	1.84	0.46
1:H:53:U:H2'	1:H:54:U:O4'	2.16	0.46
2:1:1256:HIS:CD2	2:1:1258:ALA:H	2.33	0.46
10:C:393:PRO:HA	10:C:395:TRP:CE2	2.51	0.46
4:3:521:PRO:O	4:3:543:THR:HG23	2.16	0.46
4:3:705:ARG:NH1	4:3:710:GLU:OE1	2.49	0.46
2:1:535:ILE:HG21	2:1:556:ILE:HD11	1.97	0.46
10:C:466:LYS:O	10:C:470:ARG:HG3	2.16	0.46
4:3:230:GLU:OE1	4:3:268:ARG:NH2	2.49	0.45
4:3:330:PHE:O	4:3:390:ARG:NH2	2.49	0.45
4:3:444:VAL:HG11	4:3:736:TYR:HB2	1.98	0.45
4:3:573:GLN:CD	4:3:574:LEU:H	2.20	0.45
12:E:177:LYS:HZ3	12:E:177:LYS:CB	2.28	0.45
1:H:43:U:H2'	1:H:44:U:H6	1.81	0.45



Atom-1	Atom-2	Interatomic	Clash
	1100111 2	distance (Å)	overlap (Å)
10:C:425:HIS:HA	10:C:428:GLU:HG2	1.97	0.45
4:3:463:ARG:NH1	4:3:468:ASP:O	2.49	0.45
1:H:120:A:C6	1:H:137:U:O4	2.69	0.45
2:1:722:GLU:H	2:1:722:GLU:CD	2.19	0.45
4:3:88:VAL:HG12	4:3:104:GLN:HG2	1.98	0.45
7:6:46:CYS:SG	7:6:48:GLU:HG3	2.57	0.45
2:1:822:ARG:H	2:1:822:ARG:HD2	1.82	0.45
2:1:912:ASN:O	2:1:916:THR:HG23	2.16	0.45
2:1:500:LEU:O	2:1:503:LYS:HB3	2.16	0.45
12:E:203:ASP:OD1	12:E:203:ASP:N	2.49	0.45
2:1:668:VAL:HG13	2:1:686:LEU:HD22	1.98	0.45
2:1:696:ASP:OD1	2:1:697:GLU:N	2.50	0.45
2:1:849:ILE:O	2:1:853:ILE:HG12	2.17	0.45
3:2:681:PRO:HB2	3:2:682:LEU:H	1.64	0.45
4:3:294:LYS:HE3	4:3:295:THR:O	2.17	0.45
1:H:166:G:N2	1:H:166:G:OP2	2.50	0.45
2:1:519:ILE:HA	2:1:522:LYS:HB2	1.99	0.45
2:1:522:LYS:HB3	2:1:526:PHE:CE2	2.52	0.45
4:3:1027:ASP:OD2	4:3:1031:ARG:NH1	2.50	0.44
4:3:13:GLY:O	4:3:34:ARG:HG3	2.16	0.44
4:3:200:ALA:O	4:3:204:THR:OG1	2.35	0.44
2:1:766:THR:O	2:1:770:MET:HB2	2.17	0.44
2:1:943:LYS:HB2	2:1:943:LYS:HE2	1.68	0.44
3:2:707:PRO:HA	4:3:1040:ASP:OD2	2.17	0.44
4:3:80:VAL:HB	4:3:88:VAL:HG23	1.98	0.44
10:C:411:CYS:O	10:C:414:TYR:N	2.33	0.44
2:1:812:PRO:HB2	2:1:813:PRO:HD3	2.00	0.44
4:3:449:VAL:HG22	4:3:763:ARG:HG2	1.99	0.44
2:1:503:LYS:HE3	2:1:511:MET:HB2	1.99	0.44
2:1:504:ILE:HD13	2:1:516:LEU:HG	1.98	0.44
11:D:156:PHE:CE2	11:D:201:LEU:HG	2.53	0.44
4:3:1114:SER:HB2	4:3:1215:TYR:CE1	2.53	0.44
6:5:49:LEU:HD12	6:5:49:LEU:HA	1.87	0.44
1:H:25:G:O4'	10:C:399:LEU:HD21	2.16	0.44
3:2:583:LYS:HD2	3:2:583:LYS:HA	1.79	0.44
3:2:592:TYR:CE1	3:2:595:LYS:HD2	2.53	0.44
4:3:552:ARG:HG3	4:3:595:VAL:HG11	2.00	0.44
1:H:26:A:H2'	1:H:27:U:O4'	2.17	0.44
2:1:531:LEU:O	2:1:535:ILE:HG13	2.17	0.44
2:1:614:ARG:N	2:1:615:PRO:HD2	2.33	0.44
2:1:767:ARG:O	2:1:771:LEU:HD23	2.18	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:1:1182:LEU:HD22	2:1:1226:VAL:HG21	2.00	0.44
4:3:899:THR:HG22	4:3:900:GLY:N	2.32	0.44
2:1:553:VAL:HG21	2:1:592:GLU:HG2	2.00	0.43
2:1:714:GLU:O	2:1:717:THR:HG22	2.18	0.43
2:1:945:ALA:HB2	2:1:948:ARG:NH1	2.33	0.43
2:1:982:LEU:HD23	2:1:982:LEU:HA	1.86	0.43
4:3:464:ARG:N	4:3:472:ALA:HB2	2.33	0.43
4:3:534:ASN:HD21	4:3:573:GLN:NE2	2.16	0.43
4:3:716:SER:OG	4:3:717:SER:N	2.51	0.43
4:3:1116:SER:HB3	4:3:1130:VAL:HG12	1.99	0.43
2:1:758:ASP:O	2:1:762:ALA:CB	2.66	0.43
2:1:848:GLU:H	2:1:848:GLU:CD	2.21	0.43
2:1:900:PHE:CE1	2:1:954:LEU:CD2	2.99	0.43
3:2:592:TYR:CZ	3:2:595:LYS:HB3	2.53	0.43
4:3:125:PRO:HG2	4:3:174:ASP:HA	1.99	0.43
1:H:25:G:C2	10:C:395:TRP:HB2	2.53	0.43
1:H:46:U:H3'	1:H:47:U:O3'	2.18	0.43
1:H:151:C:H2'	1:H:152:G:C8	2.53	0.43
2:1:573:LYS:O	2:1:576:VAL:HG12	2.18	0.43
2:1:1193:GLN:HB2	2:1:1233:ALA:HA	1.99	0.43
12:E:166:ARG:CB	12:E:166:ARG:CZ	2.96	0.43
1:H:144:C:H2'	1:H:145:A:H2'	2.00	0.43
2:1:549:ARG:NE	2:1:592:GLU:OE1	2.51	0.43
2:1:684:ARG:O	2:1:688:GLU:HG3	2.18	0.43
4:3:625:LEU:HD12	4:3:625:LEU:O	2.18	0.43
4:3:588:VAL:HG23	4:3:589:CYS:SG	2.59	0.43
4:3:706:MET:HG3	4:3:721:LEU:HD11	2.00	0.43
4:3:875:ASN:OD1	4:3:875:ASN:N	2.51	0.43
1:H:35:A:N6	11:D:250:ARG:HE	2.17	0.43
2:1:1248:GLN:O	3:2:497:SER:HA	2.18	0.43
4:3:704:VAL:HG21	4:3:713:LEU:HB2	2.01	0.43
2:1:1056:MET:HB3	2:1:1056:MET:HE2	1.84	0.43
4:3:83:ASP:O	4:3:111:GLY:N	2.48	0.43
2:1:1021:THR:HG23	2:1:1022:PRO:HD3	2.01	0.43
6:5:53:PHE:O	6:5:57:GLU:HG2	2.19	0.43
10:C:77:GLY:HA3	10:C:78:PRO:HD3	1.84	0.43
10:C:501:LEU:CB	14:G:224:LYS:H	2.31	0.43
1:H:49:U:H2'	1:H:50:C:C6	2.54	0.43
2:1:587:TYR:O	2:1:591:VAL:HG23	2.19	0.43
2:1:864:TYR:O	2:1:868:VAL:HG23	2.19	0.43
2:1:926:LYS:O	2:1:929:LEU:HB2	2.19	0.43



	h h	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
4:3:1141:PHE:HE1	4:3:1208:LEU:HD23	1.84	0.42
2:1:998:LYS:O	2:1:1002:ASN:HB2	2.19	0.42
4:3:635:ALA:HB3	4:3:669:LEU:HD13	2.01	0.42
4:3:773:VAL:HG13	4:3:774:PHE:CD2	2.54	0.42
4:3:866:ILE:HD13	4:3:907:VAL:HG21	2.00	0.42
4:3:1061:ASN:OD1	4:3:1061:ASN:N	2.52	0.42
1:H:13:C:H2'	1:H:14:C:C6	2.54	0.42
2:1:495:ARG:HA	2:1:498:MET:HG3	2.01	0.42
2:1:898:TYR:CZ	12:E:167:VAL:HG11	2.54	0.42
4:3:532:ARG:HE	4:3:532:ARG:HA	1.83	0.42
4:3:565:TYR:OH	4:3:601:ARG:NH1	2.53	0.42
2:1:735:ILE:HG22	2:1:746:PHE:HB3	2.02	0.42
2:1:1103:VAL:HG23	2:1:1103:VAL:O	2.18	0.42
4:3:49:LYS:HD3	4:3:49:LYS:HA	1.70	0.42
4:3:478:PHE:CE2	4:3:483:LEU:HD23	2.52	0.42
4:3:473:TYR:CZ	4:3:497:SER:HA	2.54	0.42
2:1:578:ILE:HG22	2:1:578:ILE:O	2.19	0.42
2:1:1021:THR:N	2:1:1022:PRO:HD2	2.34	0.42
2:1:1067:LYS:HG2	2:1:1111:CYS:SG	2.59	0.42
4:3:279:ASP:HA	4:3:857:ALA:HB2	2.01	0.42
12:E:153:GLN:OE1	12:E:153:GLN:HA	2.20	0.42
2:1:584:ASP:O	2:1:590:ARG:NH2	2.50	0.42
4:3:315:LEU:HD12	4:3:315:LEU:HA	1.92	0.42
4:3:515:ALA:HB1	4:3:526:HIS:NE2	2.34	0.42
4:3:807:TYR:HB2	4:3:812:LYS:HE3	2.00	0.42
10:C:393:PRO:C	10:C:395:TRP:N	2.72	0.42
4:3:700:LYS:HB3	4:3:702:PHE:CZ	2.54	0.42
11:D:172:LEU:HD23	11:D:172:LEU:HA	1.87	0.42
1:H:56:A:C6	3:2:504:TRP:CZ3	3.08	0.42
2:1:498:MET:C	2:1:500:LEU:N	2.74	0.41
2:1:700:LYS:CD	12:E:205:ASP:HB2	2.50	0.41
2:1:893:ILE:HG21	2:1:928:TYR:CG	2.55	0.41
4:3:1165:SER:OG	4:3:1170:VAL:HG23	2.20	0.41
11:D:245:LYS:HB3	11:D:245:LYS:HE2	1.66	0.41
2:1:664:GLY:O	2:1:668:VAL:HG23	2.20	0.41
7:6:29:LYS:HG3	7:6:36:TYR:CZ	2.55	0.41
4:3:511:LEU:HD11	4:3:568:MET:HG3	2.02	0.41
4:3:724:SER:HA	4:3:729:PHE:HA	2.02	0.41
12:E:155:LYS:N	12:E:155:LYS:HD2	2.35	0.41
4:3:473:TYR:HB3	4:3:484:VAL:HG23	2.02	0.41
4:3:594:ASN:H	4:3:594:ASN:ND2	2.18	0.41



Atom-1	Atom-2	Interatomic	Clash
4.2.616.U E.O	4.9.617.II E.IID19	alstance (A)	$\frac{\text{overlap}(\mathbf{A})}{0.41}$
4:3:010:ILE:O	4:3:017:1LE:HD13	2.20	0.41
4:3:702:PHE:CE2	4:3:741:PHE:HA	2.33	0.41
4:3:818:GLN:U	4:3:822:GLU:HG3	2.21	0.41
11:D:201:LEU:HD23	11:D:201:LEU:HA	1.91	0.41
2:1:840:LEU:O	2:1:844:VAL:HG12	2.21	0.41
4:3:703:ARG:NH1	4:3:703:ARG:HA	2.35	0.41
2:1:856:ASP:HB3	2:1:864: TYR:HE2	1.86	0.41
4:3:48:GLY:HA3	4:3:398:VAL:HG11	2.02	0.41
4:3:1128:ILE:HD13	4:3:1216:ALA:HB2	2.01	0.41
12:E:157:GLU:OE2	12:E:157:GLU:N	2.53	0.41
1:H:56:A:C2	3:2:478:HIS:ND1	2.89	0.41
2:1:865:ARG:NH2	2:1:902:GLU:HG2	2.36	0.41
2:1:893:ILE:O	2:1:896:ILE:HG13	2.21	0.41
3:2:459:ARG:NH1	3:2:481:THR:HG22	2.36	0.41
4:3:691:THR:HB	4:3:720:TRP:CH2	2.55	0.41
1:H:35:A:H61	11:D:250:ARG:HD2	1.86	0.41
2:1:926:LYS:HG2	2:1:927:PRO:CD	2.48	0.41
4:3:317:THR:HG22	4:3:318:ASP:N	2.35	0.41
4:3:1020:GLN:HB3	4:3:1022:ILE:HD11	2.03	0.41
2:1:560:LEU:HD12	2:1:560:LEU:HA	1.87	0.40
2:1:892:LEU:HD23	2:1:892:LEU:HA	1.93	0.40
2:1:1074:ARG:HE	22:1:1500:9B0:C1	2.33	0.40
4:3:749:GLN:H	4:3:749:GLN:HG3	1.71	0.40
4:3:515:ALA:HB1	4:3:526:HIS:CE1	2.56	0.40
4:3:569:ASP:O	4:3:571:SER:N	2.55	0.40
2:1:941:ASN:O	2:1:981:TYR:OH	2.36	0.40
2:1:1067:LYS:HD2	2:1:1107:GLN:NE2	2.36	0.40
3:2:496:ASN:O	3:2:497:SER:OG	2.40	0.40
4:3:463:ARG:HA	4:3:472:ALA:H	1.86	0.40
2:1:858:LYS:HD3	12:E:167:VAL:HG22	2.04	0.40
2:1:1074:ARG:NE	22:1:1500:9B0:O2	2.50	0.40
4:3:1095:TYR:HB2	4:3:1173:VAL:HG21	2.03	0.40
11:D:220:LEU:HD23	11:D:220:LEU:HA	1.90	0.40
2:1:1257:PRO:HG3	3:2:482:ALA:HB2	2.02	0.40
3:2:469:VAL:HG11	3:2:489:VAL:HG11	2.02	0.40
4:3:404:LEU:HD23	4:3:407:ILE:HD11	2.04	0.40
4:3:464:ARG:HG3	4:3:514:ASP:OD2	2.22	0.40
4:3:756:ALA:O	4:3:757:ILE:HD13	2.22	0.40
10:C:394:TYR:CE1	10:C:397:TYR:CD2	3.10	0.40
10:C:472:GLN:O	10:C:476:GLU:HB2	2.22	0.40
11:D:160:MET:HB3	11:D:187:CYS:SG	2.62	0.40



There are no symmetry-related clashes.

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	\mathbf{ntiles}
2	1	813/1304~(62%)	782~(96%)	31~(4%)	0	100	100
3	2	172/895~(19%)	156~(91%)	15~(9%)	1 (1%)	25	43
4	3	1168/1217~(96%)	1121 (96%)	46 (4%)	1 (0%)	51	73
5	4	156/424~(37%)	153~(98%)	3~(2%)	0	100	100
6	5	64/86~(74%)	63~(98%)	1 (2%)	0	100	100
7	6	83/110~(76%)	79~(95%)	4(5%)	0	100	100
8	А	121/793~(15%)	121 (100%)	0	0	100	100
9	В	96/464~(21%)	94 (98%)	2(2%)	0	100	100
10	С	416/501 (83%)	398 (96%)	17 (4%)	1 (0%)	47	68
11	D	198/755~(26%)	182 (92%)	16 (8%)	0	100	100
12	Е	447/1052 (42%)	431 (96%)	15 (3%)	1 (0%)	47	68
13	F	160/255~(63%)	160 (100%)	0	0	100	100
14	G	160/225~(71%)	158 (99%)	2(1%)	0	100	100
15	a	86/118 (73%)	84 (98%)	2(2%)	0	100	100
16	b	72/86~(84%)	71 (99%)	1 (1%)	0	100	100
17	с	77/92~(84%)	77 (100%)	0	0	100	100
18	d	72/76~(95%)	72 (100%)	0	0	100	100
19	е	81/126 (64%)	79~(98%)	2(2%)	0	100	100
20	f	67/240~(28%)	67 (100%)	0	0	100	100
21	g	80/119 (67%)	79~(99%)	1 (1%)	0	100	100
All	All	4589/8938~(51%)	4427 (96%)	158 (3%)	4 (0%)	54	73

All (4) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
10	С	412	GLY
3	2	496	ASN
12	Е	585	GLY
4	3	997	GLY

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	Perce	entiles
2	1	701/1104~(64%)	666~(95%)	35~(5%)	24	46
3	2	104/776~(13%)	98~(94%)	6 (6%)	20	38
4	3	1022/1051~(97%)	963 (94%)	59~(6%)	20	38
5	4	8/336~(2%)	8 (100%)	0	100	100
6	5	57/77~(74%)	56~(98%)	1 (2%)	59	81
7	6	73/95~(77%)	72~(99%)	1 (1%)	67	86
8	А	4/709~(1%)	4 (100%)	0	100	100
9	В	7/382~(2%)	7 (100%)	0	100	100
10	С	80/446 (18%)	69~(86%)	11 (14%)	3	6
11	D	108/661~(16%)	100 (93%)	8 (7%)	13	27
12	Е	73/909~(8%)	66 (90%)	7 (10%)	8	16
13	F	6/218~(3%)	6 (100%)	0	100	100
14	G	7/195~(4%)	7 (100%)	0	100	100
15	a	4/110 (4%)	4 (100%)	0	100	100
16	b	4/74~(5%)	4 (100%)	0	100	100
17	с	1/84 (1%)	1 (100%)	0	100	100
18	d	3/66~(4%)	3 (100%)	0	100	100
19	е	3/101~(3%)	3 (100%)	0	100	100
20	f	3/177~(2%)	3 (100%)	0	100	100
21	g	3/101~(3%)	3 (100%)	0	100	100
All	All	2271/7672~(30%)	2143 (94%)	128 (6%)	25	40



Mol	Chain	Res	Type	
2	1	518	GLN	
2	1	546	ASP	
2	1	562	LYS	
2	1	565	ASP	
2	1	576	VAL	
2	1	585	GLU	
2	1	614	ARG	
2	1	637	SER	
2	1	683	LEU	
2	1	700	LYS	
2	1	768	GLU	
2	1	771	LEU	
2	1	778	GLN	
2	1	798	THR	
2	1	823	MET	
2	1	825	LEU	
2	1	892	LEU	
2	1	914	PHE	
2	1	926	LYS	
2	1	941	ASN	
2	1	946	LYS	
2	1	956	SER	
2	1	963	LYS	
2	1	967	GLU	
2	1	1009	MET	
2	1	1014	LYS	
2	1	1017	LEU	
2	1	1027	ARG	
2	1	1053	ARG	
2	1	1070	LYS	
2	1	1105	GLU	
2	1	1126	PHE	
2	1	1209	ASN	
2	1	1271	SER	
2	1	1277	GLN	
3	2	502	ARG	
3	2	508	ARG	
3	2	569	GLN	
3	2	572	HIS	
3	2	577	LYS	
3	2	598	GLU	
4	3	55	THR	

All (128) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
4	3	223	LYS
4	3	230	GLU
4	3	235	LEU
4	3	243	ASP
4	3	246	SER
4	3	298	MET
4	3	316	GLU
4	3	318	ASP
4	3	320	ASP
4	3	369	GLU
4	3	390	ARG
4	3	415	LEU
4	3	429	ARG
4	3	461	THR
4	3	463	ARG
4	3	468	ASP
4	3	480	ASN
4	3	497	SER
4	3	509	SER
4	3	513	ASP
4	3	531	LYS
4	3	546	LYS
4	3	549	VAL
4	3	558	LEU
4	3	573	GLN
4	3	577	TYR
4	3	589	CYS
4	3	590	MET
4	3	591	SER
4	3	629	SER
4	3	633	LEU
4	3	639	SER
4	3	641	CYS
4	3	643	VAL
4	3	645	MET
4	3	670	GLN
4	3	688	ASP
4	3	690	ARG
4	3	697	ARG
4	3	704	VAL
4	3	719	SER
4	3	725	TYR



Mol	Chain	Res	Type
4	3	728	ARG
4	3	738	THR
4	3	809	GLU
4	3	845	GLU
4	3	864	SER
4	3	916	ASN
4	3	919	SER
4	3	959	VAL
4	3	1043	THR
4	3	1048	ASP
4	3	1061	ASN
4	3	1120	THR
4	3	1121	THR
4	3	1166	TYR
4	3	1207	LYS
4	3	1217	PHE
6	5	48	ASP
7	6	73	LYS
10	С	394	TYR
10	С	395	TRP
10	С	396	LEU
10	С	405	ASN
10	С	417	ARG
10	С	437	CYS
10	С	457	SER
10	С	468	SER
10	С	472	GLN
10	С	475	THR
10	С	477	GLU
11	D	162	ASP
11	D	168	PHE
11	D	187	CYS
11	D	201	LEU
11	D	207	ARG
11	D	217	LYS
11	D	237	LYS
11	D	239	LYS
12	E	157	GLU
12	Е	203	ASP
12	Е	207	GLU
12	Е	225	LEU
12	Е	228	LEU



Continued from previous page...

Mol	Chain	\mathbf{Res}	Type
12	Е	229	ASP
12	Е	241	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	506	ASN
2	1	534	GLN
2	1	737	GLN
2	1	903	GLN
2	1	941	ASN
2	1	1007	HIS
2	1	1032	GLN
2	1	1107	GLN
2	1	1144	GLN
2	1	1184	HIS
2	1	1194	HIS
2	1	1252	GLN
2	1	1256	HIS
2	1	1293	ASN
3	2	458	ASN
3	2	467	GLN
3	2	490	HIS
4	3	46	ASN
4	3	93	GLN
4	3	194	ASN
4	3	264	GLN
4	3	363	HIS
4	3	480	ASN
4	3	573	GLN
4	3	594	ASN
4	3	612	ASN
4	3	709	GLN
4	3	776	GLN
4	3	805	ASN
4	3	870	ASN
4	3	916	ASN
4	3	941	HIS
4	3	983	ASN
4	3	1017	ASN
4	3	1052	ASN
10	С	400	HIS



Continued from previous page...

Mol	Chain	Res	Type
10	С	403	ASN
11	D	179	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Н	143/188~(76%)	27 (18%)	0

All (27) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Н	22	U
1	Н	23	А
1	Н	24	А
1	Н	43	U
1	Н	47	U
1	Н	48	А
1	Н	101	U
1	Н	102	U
1	Н	103	U
1	Н	111	G
1	Н	116	А
1	Н	117	U
1	Н	121	А
1	Н	122	U
1	Н	123	А
1	Н	124	G
1	Н	128	С
1	Н	129	U
1	Н	130	U
1	Н	131	G
1	Н	136	G
1	Н	138	С
1	Н	146	С
1	Н	147	G
1	Н	157	G
1	Н	164	С
1	Н	177	А

There are no RNA pucker outliers to report.



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 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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).

Mol	Tuno	Chain	Dog	Link	Bo	ond leng	ths	B	ond ang	les
	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
22	9B0	1	1500	-	52,54,54	0.73	1 (1%)	61,77,77	0.80	2 (3%)

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
22	9B0	1	1500	-	-	25/67/91/91	0/3/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	1500	9B0	C17-C16	-3.63	1.32	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
22	1	1500	9B0	C17-C16-C14	2.91	131.59	127.32
22	1	1500	9B0	O9-C26-C27	-2.47	104.86	109.35



There are no chirality outliers.

Mol	Chain	\mathbf{Res}	Type	Atoms
22	1	1500	9B0	O5-C29-N1-C33
22	1	1500	9B0	O5-C29-N1-C30
22	1	1500	9B0	N1-C29-O5-C8
22	1	1500	9B0	O5-C8-C9-C10
22	1	1500	9B0	C6-C8-C9-C10
22	1	1500	9B0	O3-C3-C4-C5
22	1	1500	9B0	C2-C3-C4-C5
22	1	1500	9B0	C1-C2-C3-C4
22	1	1500	9B0	C1-C2-C3-O3
22	1	1500	9B0	O8-C23-C24-C26
22	1	1500	9B0	C14-C16-C17-C18
22	1	1500	9B0	O6-C29-N1-C30
22	1	1500	9B0	O6-C29-N1-C33
22	1	1500	9B0	O6-C29-O5-C8
22	1	1500	9B0	C4-C5-C6-C7
22	1	1500	9B0	C4-C5-C6-C8
22	1	1500	9B0	C4-C5-C6-O4
22	1	1500	9B0	C9-C10-C11-C12
22	1	1500	9B0	C35-C34-N2-C31
22	1	1500	9B0	O8-C23-C24-C25
22	1	1500	9B0	C9-C8-O5-C29
22	1	1500	9B0	C6-C8-O5-C29
22	1	1500	9B0	C17-C18-C19-C20
22	1	1500	9B0	C17-C18-C19-O7
22	1	1500	9B0	C17-C18-C19-C21

All (25) torsion outliers are listed below:

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1	1500	9B0	9	0

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-31334. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary 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

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: 147

Y Index: 148

Z Index: 191

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

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 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 166 nm^3 ; this corresponds to an approximate mass of 150 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 0.400 ${\rm \AA^{-1}}$



8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-31334 and PDB model 7EVO. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.02 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 (0.02).



9.4 Atom inclusion (i)



At the recommended contour level, 46% of all backbone atoms, 53% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5280	0.3670
1	0.8730	0.5840
2	0.6220	0.4210
3	0.8050	0.5730
4	0.0040	0.0160
5	0.9830	0.6830
6	0.9250	0.6450
А	0.0000	0.0030
В	0.0000	-0.0050
С	0.3010	0.2070
D	0.5410	0.3660
Е	0.0920	0.0680
F	0.0000	0.0180
G	0.0000	-0.0010
Н	0.1450	0.0740
a	0.0000	0.0310
b	0.0000	0.0080
С	0.0000	0.0310
d	0.0000	-0.0240
е	0.0000	0.0410
f	0.0000	0.0290
g	0.0000	0.0440

