



wwPDB EM Validation Summary Report ⓘ

Mar 30, 2026 – 01:46 AM UTC

PDB ID : 6ZSG / pdb_00006zsg
EMDB ID : EMD-11397
Title : Human mitochondrial ribosome in complex with mRNA, A-site tRNA, P-site tRNA and E-site tRNA
Authors : Aibara, S.; Singh, V.; Modelska, A.; Amunts, A.
Deposited on : 2020-07-15
Resolution : 4.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : **FAILED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

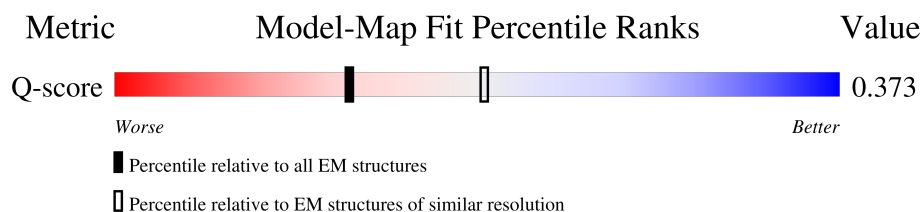
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	7587 (3.50 - 4.50)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 93 unique types of molecules in this entry. The entry contains 315349 atoms, of which 143121 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 protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	0	108	Total	C	H	N	O	S	0	0
			1783	545	903	172	157	6		

- Molecule 2 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1	53	Total	C	H	N	O	S	0	0
			919	281	480	84	72	2		

- Molecule 3 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	2	46	Total	C	H	N	O	S	0	0
			783	233	407	83	59	1		

- Molecule 4 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	3	95	Total	C	H	N	O	S	0	0
			1714	539	883	162	127	3		

- Molecule 5 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	4	38	Total	C	H	N	O	S	0	0
			702	217	361	72	48	4		

- Molecule 6 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	5	393	Total	C	H	N	O	S	0	0
			6405	2070	3201	559	564	11		

- Molecule 7 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	6	354	Total	C	H	N	O	S	0	0
			5788	1881	2841	525	532	9		

- Molecule 8 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	7	291	Total	C	H	N	O	S	0	0
			4740	1514	2375	401	432	18		

- Molecule 9 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	8	139	Total	C	H	N	O	S	0	0
			2377	747	1202	208	218	2		

- Molecule 10 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	9	124	Total	C	H	N	O	S	0	0
			1983	644	987	170	180	2		

- Molecule 11 is a RNA chain called 16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	XA	1499	Total	C	H	N	O	P	0	0
			47993	14284	16160	5756	10294	1499		

- Molecule 12 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	A0	201	Total	C	H	N	O	S	0	0
			3369	1065	1685	322	292	5		

- Molecule 13 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	A1	275	Total	C	H	N	O	S	0	0
			4491	1414	2261	380	425	11		

- Molecule 14 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	A2	116	Total	C	H	N	O	S	0	0
			1889	574	964	181	162	8		

- Molecule 15 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	A3	69	Total	C	H	N	O	S	0	0
			1292	393	682	130	86	1		

- Molecule 16 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	A4	552	Total	C	H	N	O	S	0	0
			8955	2866	4485	756	820	28		

- Molecule 17 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	AA	924	Total	C	H	N	O	P	0	0
			29593	8800	9965	3540	6364	924		

- Molecule 18 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	AB	218	Total	C	H	N	O	S	0	0
			3545	1135	1769	322	309	10		

- Molecule 19 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	AC	132	Total	C	H	N	O	S	0	0
			2170	699	1088	195	184	4		

- Molecule 20 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	AD	343	Total	C	H	N	O	S	0	0
			5500	1706	2784	515	482	13		

- Molecule 21 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	AE	122	Total	C	H	N	O	S	0	0
			1973	614	1001	177	177	4		

- Molecule 22 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	AF	201	Total	C	H	N	O	S	0	0
			3384	1069	1716	305	283	11		

- Molecule 23 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	AG	304	Total	C	H	N	O	S	0	0
			4996	1593	2491	444	454	14		

- Molecule 24 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AH	135	Total	C	H	N	O	S	0	0
			2241	712	1136	187	203	3		

- Molecule 25 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	AI	136	Total	C	H	N	O	S	0	0
			2063	637	1052	192	178	4		

- Molecule 26 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	AJ	108	Total	C	H	N	O	S	0	0
			1725	521	887	169	142	6		

- Molecule 27 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	AK	101	Total	C	H	N	O	S	0	0
			1746	537	885	179	140	5		

- Molecule 28 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	AL	164	Total	C	H	N	O	S	0	0
			2854	883	1472	257	235	7		

- Molecule 29 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	AM	116	Total	C	H	N	O	S	0	0
			1871	582	951	182	150	6		

- Molecule 30 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	AN	107	Total	C	H	N	O	S	0	0
			1754	549	908	153	141	3		

- Molecule 31 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	AO	185	Total	C	H	N	O	S	0	0
			3017	970	1489	285	267	6		

- Molecule 32 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	AP	95	Total	C	H	N	O	S	0	0
			1561	493	796	132	132	8		

- Molecule 33 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	AQ	85	Total	C	H	N	O	S	0	0
			1483	455	749	149	123	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	50	ARG	CYS	conflict	UNP P82921

- Molecule 34 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	AR	250	Total	C	H	N	O	S	0	0
			4134	1314	2074	353	385	8		

- Molecule 35 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	AS	133	Total	C	H	N	O	S	0	0
			2203	709	1103	196	194	1		

- Molecule 36 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	AT	162	Total	C	H	N	O	S	0	0
			2672	850	1342	231	238	11		

- Molecule 37 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	AU	173	Total	C	H	N	O	S	0	0
			2932	900	1471	294	263	4		

- Molecule 38 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	AV	349	Total	C	H	N	O	S	0	0
			5729	1841	2862	478	536	12		

- Molecule 39 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	AW	97	Total	C	H	N	O	S	0	0
			1551	486	785	137	139	4		

- Molecule 40 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	AX	348	Total	C	H	N	O	S	0	0
			5619	1802	2805	491	510	11		

- Molecule 41 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	AY	113	Total	C	H	N	O	S	0	0
			1868	621	912	157	176	2		

- Molecule 42 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	AZ	86	Total	C	H	N	O	S	0	0
			1465	467	734	131	129	4		

- Molecule 43 is a RNA chain called mitochondrial tRNA^{Val}.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	XB	59	Total	C	H	N	O	P	0	0
			1890	563	635	227	406	59		

- Molecule 44 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	XD	236	Total	C	H	N	O	S	0	0
			3739	1145	1897	373	315	9		

- Molecule 45 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	XE	304	Total	C	H	N	O	S	0	0
			4798	1539	2402	416	430	11		

- Molecule 46 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	XF	250	Total	C	H	N	O	S	0	0
			4058	1294	2045	365	348	6		

- Molecule 47 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	XH	95	Total	C	H	N	O		0	0
			1616	498	832	152	134			

- Molecule 48 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	XI	211	Total	C	H	N	O	S	0	0
			3474	1086	1783	303	291	11		

- Molecule 49 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	XJ	170	Total	C	H	N	O	S	0	0
			2657	825	1366	230	234	2		

- Molecule 50 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	XK	177	Total	C	H	N	O	S	0	0
			2899	934	1448	259	251	7		

- Molecule 51 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	XL	115	Total	C	H	N	O	S	0	0
			1830	559	941	171	154	5		

- Molecule 52 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	XM	287	Total	C	H	N	O	S	0	0
			4682	1472	2377	425	402	6		

- Molecule 53 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	XN	221	Total	C	H	N	O	S	0	0
			3586	1138	1808	325	305	10		

- Molecule 54 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	XO	152	Total	C	H	N	O	S	0	0
			2528	784	1283	239	215	7		

- Molecule 55 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	XP	143	Total	C	H	N	O	S	0	0
			2326	729	1162	223	207	5		

- Molecule 56 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	XQ	238	Total	C	H	N	O	S	0	0
			4000	1268	2022	352	349	9		

- Molecule 57 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	XR	140	Total	C	H	N	O	S	0	0
			2367	732	1214	231	186	4		

- Molecule 58 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	XS	160	Total	C	H	N	O	S	0	0
			2638	829	1354	226	225	4		

- Molecule 59 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	XT	166	Total	C	H	N	O	S	0	0
			2778	875	1410	254	232	7		

- Molecule 60 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	XU	141	Total	C	H	N	O	S	0	0
			2335	743	1164	222	203	3		

- Molecule 61 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	XV	202	Total	C	H	N	O	S	0	0
			3304	1051	1656	294	295	8		

- Molecule 62 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	XW	111	Total	C	H	N	O	S	0	0
			1769	558	898	164	146	3		

- Molecule 63 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	XX	243	Total	C	H	N	O	S	0	0
			4089	1317	2054	351	362	5		

- Molecule 64 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	XY	178	Total	C	H	N	O	S	0	0
			3109	981	1575	295	254	4		

- Molecule 65 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	XZ	120	Total	C	H	N	O	S	0	0
			2008	626	1030	183	166	3		

- Molecule 66 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	a	97	Total	C	H	N	O	S	0	0
			1590	512	777	145	151	5		

- Molecule 67 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	b	148	Total	C	H	N	O	S	0	0
			2358	733	1180	229	213	3		

- Molecule 68 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	c	275	Total	C	H	N	O	S	0	0
			4437	1415	2220	383	410	9		

- Molecule 69 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	d	216	Total	C	H	N	O	S	0	0
			3501	1125	1743	305	315	13		

- Molecule 70 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	e	217	Total	C	H	N	O	S	0	0
			3529	1124	1767	310	323	5		

- Molecule 71 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	f	143	Total	C	H	N	O	S	0	0
			2314	737	1165	187	221	4		

- Molecule 72 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	g	132	Total	C	H	N	O	S	0	0
			2183	710	1086	191	194	2		

- Molecule 73 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	h	108	Total	C	H	N	O	S	0	0
			1748	560	866	154	165	3		

- Molecule 74 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	i	97	Total	C	H	N	O	S	0	0
			1684	532	857	165	126	4		

- Molecule 75 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	j	86	Total	C	H	N	O	S	0	0
			1367	426	678	134	127	2		

- Molecule 76 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	k	95	Total	C	H	N	O	S	0	0
			1477	456	745	139	132	5		

- Molecule 77 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	l	80	Total	C	H	N	O	S	0	0
			1327	427	654	118	125	3		

- Molecule 78 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	m	60	Total	C	H	N	O	S	0	0
			1025	309	525	104	85	2		

- Molecule 79 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	o	94	Total	C	H	N	O	S	0	0
			1601	501	804	165	128	3		

- Molecule 80 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	p	127	Total	C	H	N	O	S	0	0
			2141	661	1083	201	192	4		

- Molecule 81 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	q	164	Total	C	H	N	O	S	0	0
			2738	858	1359	267	249	5		

- Molecule 82 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	r	161	Total	C	H	N	O	S	0	0
			2653	834	1341	250	220	8		

- Molecule 83 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	r1	14	Total	C	N	O	P	0	0
			252	126	28	84	14		

- Molecule 84 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	r2	76	Total	C	N	O	P	0	0
			1485	723	230	456	76		

- Molecule 85 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	r3	75	Total	C	N	O	P	0	0
			1459	711	222	451	75		

- Molecule 86 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	r4	75	Total	C	N	O	P	0	0
			1464	713	226	450	75		

- Molecule 87 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	s	370	Total	C	H	N	O	S	
			6059	1946	3023	542	534	14	0

- Molecule 88 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	t1	46	Total	C	H	N	O	2	0
			733	228	379	56	70		
88	t2	30	Total	C	H	N	O	0	0
			506	154	268	38	46		
88	t3	30	Total	C	H	N	O	0	0
			506	154	268	38	46		
88	t4	29	Total	C	H	N	O	0	0
			484	148	255	36	45		
88	t5	29	Total	C	H	N	O	0	0
			484	148	255	36	45		
88	t6	27	Total	C	H	N	O	0	0
			450	137	236	34	43		

- Molecule 89 is a protein called Quinupristin.

Mol	Chain	Residues	Atoms						AltConf	Trace
89	A	8	Total	C	H	N	O	S	0	0
			140	53	67	9	10	1		

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
90	0	1	Total	Zn	0
			1	1	
90	4	1	Total	Zn	0
			1	1	
90	AB	1	Total	Zn	0
			1	1	
90	AO	1	Total	Zn	0
			1	1	
90	AP	1	Total	Zn	0
			1	1	
90	AT	1	Total	Zn	0
			1	1	
90	r	1	Total	Zn	0
			1	1	

- Molecule 91 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

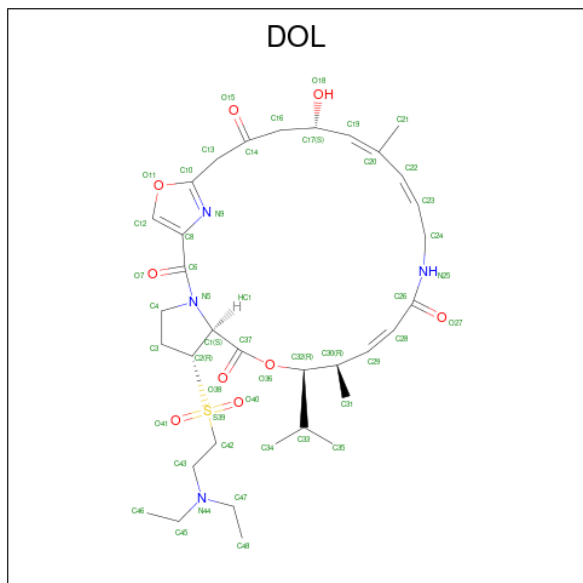
Mol	Chain	Residues	Atoms		AltConf
91	2	1	Total	Mg	0
			1	1	
91	9	1	Total	Mg	0
			1	1	
91	XA	141	Total	Mg	0
			141	141	
91	AA	46	Total	Mg	0
			46	46	
91	XD	1	Total	Mg	0
			1	1	
91	XE	1	Total	Mg	0
			1	1	
91	XI	1	Total	Mg	0
			1	1	
91	XM	1	Total	Mg	0
			1	1	
91	XW	1	Total	Mg	0
			1	1	

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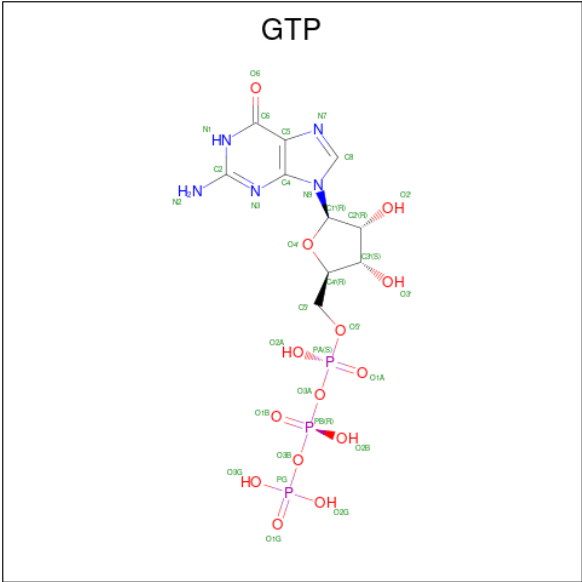
Mol	Chain	Residues	Atoms		AltConf
91	g	1	Total	Mg	0
			1	1	

- Molecule 92 is 5-(2-DIETHYLAMINO-ETHANESULFONYL)-21-HYDROXY-10-ISOPROPYL-11,19-DIMETHYL-9,26-DIOXA-3,15,28-TRIAZA-TRICYCLO[23.2.1.00,255]OCTACOSA-1(27),12,17,19,25(28)-PENTAENE-2,8,14,23-TETRAONE (CCD ID: DOL) (formula: $C_{34}H_{50}N_4O_9S$).



Mol	Chain	Residues	Atoms						AltConf
92	XA	1	Total	C	H	N	O	S	0
			98	34	50	4	9	1	

- Molecule 93 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13350	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.310	Depositor
Minimum map value	-0.193	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	546.0, 546.0, 546.0	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

245 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
84	P5P	r2	30	84	20,23,24	1.29	3 (15%)	27,33,36	2.47	11 (40%)
84	P5P	r2	64	84	20,23,24	1.28	3 (15%)	27,33,36	2.49	11 (40%)
86	P5P	r4	14	86	20,23,24	1.27	3 (15%)	27,33,36	2.49	11 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	Y5P	r2	20	84	14,19,20	7.39	3 (21%)	18,26,29	0.58	0
86	P5P	r4	1	86	20,23,24	1.29	3 (15%)	27,33,36	2.49	11 (40%)
84	Y5P	r2	39	84	14,19,20	7.31	3 (21%)	18,26,29	0.56	0
86	Y5P	r4	42	86	14,19,20	7.33	3 (21%)	18,26,29	0.56	0
86	P5P	r4	52	86	20,23,24	1.29	3 (15%)	27,33,36	2.49	11 (40%)
84	Y5P	r2	25	84	14,19,20	7.39	3 (21%)	18,26,29	0.57	0
84	P5P	r2	35	84	20,23,24	1.31	3 (15%)	27,33,36	2.49	11 (40%)
85	P5P	r3	52	85	20,23,24	1.28	3 (15%)	27,33,36	2.49	11 (40%)
84	Y5P	r2	33	84	14,19,20	7.38	3 (21%)	18,26,29	0.57	0
85	Y5P	r3	62	85	14,19,20	7.39	3 (21%)	18,26,29	0.53	0
85	Y5P	r3	40	85	14,19,20	7.37	3 (21%)	18,26,29	0.51	0
84	Y5P	r2	55	84	14,19,20	7.37	3 (21%)	18,26,29	0.56	0
86	P5P	r4	44	86	20,23,24	1.29	3 (15%)	27,33,36	2.49	11 (40%)
85	P5P	r3	11	85	20,23,24	1.29	3 (15%)	27,33,36	2.48	11 (40%)
85	Y5P	r3	37	85	14,19,20	7.35	3 (21%)	18,26,29	0.62	0
83	Y5P	r1	50	83	14,19,20	7.28	3 (21%)	18,26,29	0.59	0
84	P5P	r2	53	84	20,23,24	1.28	3 (15%)	27,33,36	2.46	10 (37%)
85	Y5P	r3	70	85	14,19,20	7.34	3 (21%)	18,26,29	0.54	0
86	P5P	r4	15	86	20,23,24	1.28	3 (15%)	27,33,36	2.48	10 (37%)
86	P5P	r4	71	86	20,23,24	1.28	3 (15%)	27,33,36	2.48	11 (40%)
85	Y5P	r3	61	85	14,19,20	7.35	3 (21%)	18,26,29	0.54	0
84	P5P	r2	22	84	20,23,24	1.28	3 (15%)	27,33,36	2.50	11 (40%)
85	Y5P	r3	65	85	14,19,20	7.33	3 (21%)	18,26,29	0.56	0
84	P5P	r2	63	84	20,23,24	1.30	3 (15%)	27,33,36	2.49	10 (37%)
84	Y5P	r2	48	84	14,19,20	7.36	3 (21%)	18,26,29	0.56	0
85	Y5P	r3	59	85	14,19,20	7.40	3 (21%)	18,26,29	0.58	0
86	P5P	r4	10	86	20,23,24	1.28	3 (15%)	27,33,36	2.49	11 (40%)
84	Y5P	r2	45	84	14,19,20	7.35	3 (21%)	18,26,29	0.54	0
84	Y5P	r2	51	84	14,19,20	7.32	3 (21%)	18,26,29	0.56	0
85	P5P	r3	6	85	20,23,24	1.30	3 (15%)	27,33,36	2.49	10 (37%)
84	P5P	r2	37	84	20,23,24	1.32	3 (15%)	27,33,36	2.51	11 (40%)
86	Y5P	r4	67	86	14,19,20	7.36	3 (21%)	18,26,29	0.55	0
85	Y5P	r3	7	85	14,19,20	7.40	3 (21%)	18,26,29	0.58	0
86	Y5P	r4	62	86	14,19,20	7.38	3 (21%)	18,26,29	0.55	0
86	Y5P	r4	51	86	14,19,20	7.38	3 (21%)	18,26,29	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	P5P	r3	32	85	20,23,24	1.28	3 (15%)	27,33,36	2.48	11 (40%)
86	P5P	r4	37	86	20,23,24	1.27	3 (15%)	27,33,36	2.47	10 (37%)
86	P5P	r4	24	86	20,23,24	1.28	3 (15%)	27,33,36	2.47	11 (40%)
83	Y5P	r1	54	83	14,19,20	7.42	3 (21%)	18,26,29	0.54	0
85	Y5P	r3	63	85	14,19,20	7.42	3 (21%)	18,26,29	0.61	0
85	Y5P	r3	66	85	14,19,20	7.38	3 (21%)	18,26,29	0.62	0
86	P5P	r4	35	86	20,23,24	1.27	3 (15%)	27,33,36	2.49	11 (40%)
85	P5P	r3	46	85	20,23,24	1.29	3 (15%)	27,33,36	2.49	11 (40%)
86	P5P	r4	23	86	20,23,24	1.28	3 (15%)	27,33,36	2.48	11 (40%)
84	P5P	r2	9	84	20,23,24	1.28	3 (15%)	27,33,36	2.50	11 (40%)
85	Y5P	r3	64	85	14,19,20	7.40	3 (21%)	18,26,29	0.55	0
84	Y5P	r2	62	84	14,19,20	7.39	3 (21%)	18,26,29	0.57	0
84	P5P	r2	7	84	20,23,24	1.27	3 (15%)	27,33,36	2.47	11 (40%)
84	Y5P	r2	43	84	14,19,20	7.35	3 (21%)	18,26,29	0.57	0
85	Y5P	r3	2	85	14,19,20	7.37	3 (21%)	18,26,29	0.53	0
85	Y5P	r3	21	85	14,19,20	7.40	3 (21%)	18,26,29	0.55	0
85	P5P	r3	23	85	20,23,24	1.29	3 (15%)	27,33,36	2.47	11 (40%)
84	Y5P	r2	16	84	14,19,20	7.41	3 (21%)	18,26,29	0.54	0
85	Y5P	r3	34	85	14,19,20	7.35	3 (21%)	18,26,29	0.54	0
85	P5P	r3	44	85	20,23,24	1.29	3 (15%)	27,33,36	2.48	11 (40%)
85	P5P	r3	36	85	20,23,24	1.30	3 (15%)	27,33,36	2.49	11 (40%)
86	P5P	r4	18	86	20,23,24	1.26	3 (15%)	27,33,36	2.47	11 (40%)
89	MHU	A	5	89	14,15,16	0.44	0	18,19,21	1.25	3 (16%)
85	P5P	r3	9	85	20,23,24	1.27	3 (15%)	27,33,36	2.52	11 (40%)
83	Y5P	r1	44	83	14,19,20	7.36	3 (21%)	18,26,29	0.58	0
83	Y5P	r1	56	83	14,19,20	7.36	3 (21%)	18,26,29	0.59	0
86	Y5P	r4	20	86	14,19,20	7.41	3 (21%)	18,26,29	0.56	0
84	Y5P	r2	12	84	14,19,20	7.38	3 (21%)	18,26,29	0.55	0
86	Y5P	r4	11	86	14,19,20	7.39	3 (21%)	18,26,29	0.55	0
86	Y5P	r4	48	86	14,19,20	7.39	3 (21%)	18,26,29	0.56	0
83	Y5P	r1	46	83	14,19,20	7.32	3 (21%)	18,26,29	0.56	0
83	Y5P	r1	55	83	14,19,20	7.39	3 (21%)	18,26,29	0.54	0
84	P5P	r2	21	84	20,23,24	1.28	3 (15%)	27,33,36	2.47	11 (40%)
85	P5P	r3	45	85	20,23,24	1.29	3 (15%)	27,33,36	2.49	11 (40%)
84	P5P	r2	6	84	20,23,24	1.29	3 (15%)	27,33,36	2.48	11 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	P5P	r2	34	84	20,23,24	1.30	3 (15%)	27,33,36	2.48	11 (40%)
85	P5P	r3	43	85	20,23,24	1.30	3 (15%)	27,33,36	2.48	11 (40%)
85	Y5P	r3	48	85	14,19,20	7.38	3 (21%)	18,26,29	0.58	0
86	Y5P	r4	25	86	14,19,20	7.37	3 (21%)	18,26,29	0.56	0
86	P5P	r4	46	86	20,23,24	1.28	3 (15%)	27,33,36	2.46	10 (37%)
86	Y5P	r4	54	86	14,19,20	7.36	3 (21%)	18,26,29	0.54	0
84	Y5P	r2	68	84	14,19,20	7.36	3 (21%)	18,26,29	0.53	0
85	Y5P	r3	54	85	14,19,20	7.38	3 (21%)	18,26,29	0.53	0
85	Y5P	r3	13	85	14,19,20	7.41	3 (21%)	18,26,29	0.59	0
85	Y5P	r3	57	85	14,19,20	7.41	3 (21%)	18,26,29	0.60	0
84	P5P	r2	27	84	20,23,24	1.27	3 (15%)	27,33,36	2.50	11 (40%)
85	Y5P	r3	12	85	14,19,20	7.35	3 (21%)	18,26,29	0.56	0
85	P5P	r3	20	85	20,23,24	1.28	3 (15%)	27,33,36	2.48	11 (40%)
84	P5P	r2	19	84	20,23,24	1.28	3 (15%)	27,33,36	2.48	11 (40%)
86	Y5P	r4	4	86	14,19,20	7.38	3 (21%)	18,26,29	0.56	0
86	Y5P	r4	47	86	14,19,20	7.39	3 (21%)	18,26,29	0.56	0
86	P5P	r4	36	86	20,23,24	1.27	3 (15%)	27,33,36	2.50	11 (40%)
84	Y5P	r2	60	84	14,19,20	7.38	3 (21%)	18,26,29	0.58	0
86	Y5P	r4	2	86	14,19,20	7.35	3 (21%)	18,26,29	0.54	0
85	P5P	r3	27	85	20,23,24	1.29	3 (15%)	27,33,36	2.48	11 (40%)
84	Y5P	r2	49	84	14,19,20	7.37	3 (21%)	18,26,29	0.56	0
85	P5P	r3	53	85	20,23,24	1.26	3 (15%)	27,33,36	2.47	10 (37%)
86	Y5P	r4	59	86	14,19,20	7.41	3 (21%)	18,26,29	0.58	0
83	Y5P	r1	48	83	14,19,20	7.34	3 (21%)	18,26,29	0.55	0
83	Y5P	r1	52	83	14,19,20	7.35	3 (21%)	18,26,29	0.55	0
84	P5P	r2	57	84	20,23,24	1.29	3 (15%)	27,33,36	2.50	11 (40%)
85	P5P	r3	19	85	20,23,24	1.27	3 (15%)	27,33,36	2.50	11 (40%)
84	Y5P	r2	75	84	14,19,20	7.32	3 (21%)	18,26,29	0.59	0
84	P5P	r2	38	84	20,23,24	1.30	3 (15%)	27,33,36	2.48	11 (40%)
84	P5P	r2	44	84	20,23,24	1.28	3 (15%)	27,33,36	2.48	11 (40%)
86	Y5P	r4	13	86	14,19,20	7.40	3 (21%)	18,26,29	0.55	0
86	Y5P	r4	49	86	14,19,20	7.38	3 (21%)	18,26,29	0.56	0
84	P5P	r2	18	84	20,23,24	1.26	3 (15%)	27,33,36	2.49	11 (40%)
85	Y5P	r3	18	85	14,19,20	7.32	3 (21%)	18,26,29	0.55	0
86	P5P	r4	63	86	20,23,24	1.28	3 (15%)	27,33,36	2.47	10 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	MHV	A	6	89	7,9,10	0.34	0	8,11,13	1.75	3 (37%)
86	Y5P	r4	75	86	14,19,20	7.38	3 (21%)	18,26,29	0.58	0
84	P5P	r2	52	84	20,23,24	1.30	3 (15%)	27,33,36	2.49	11 (40%)
84	Y5P	r2	66	84	14,19,20	7.41	3 (21%)	18,26,29	0.57	0
86	Y5P	r4	45	86	14,19,20	7.41	3 (21%)	18,26,29	0.54	0
85	P5P	r3	38	85	20,23,24	1.30	3 (15%)	27,33,36	2.49	11 (40%)
86	P5P	r4	64	86	20,23,24	1.30	3 (15%)	27,33,36	2.48	10 (37%)
86	Y5P	r4	61	86	14,19,20	7.37	3 (21%)	18,26,29	0.55	0
86	P5P	r4	34	86	20,23,24	1.27	3 (15%)	27,33,36	2.50	11 (40%)
83	Y5P	r1	47	83	14,19,20	7.37	3 (21%)	18,26,29	0.63	0
86	Y5P	r4	66	86	14,19,20	7.38	3 (21%)	18,26,29	0.55	0
85	P5P	r3	47	85	20,23,24	1.28	3 (15%)	27,33,36	2.47	11 (40%)
85	Y5P	r3	51	85	14,19,20	7.35	3 (21%)	18,26,29	0.55	0
86	P5P	r4	6	86	20,23,24	1.27	3 (15%)	27,33,36	2.48	11 (40%)
86	P5P	r4	19	86	20,23,24	1.28	3 (15%)	27,33,36	2.47	11 (40%)
84	Y5P	r2	42	84	14,19,20	7.37	3 (21%)	18,26,29	0.58	0
84	Y5P	r2	56	84	14,19,20	7.43	3 (21%)	18,26,29	0.56	0
85	P5P	r3	30	85	20,23,24	1.29	3 (15%)	27,33,36	2.49	11 (40%)
84	P5P	r2	65	84	20,23,24	1.29	3 (15%)	27,33,36	2.47	11 (40%)
85	Y5P	r3	39	85	14,19,20	7.36	3 (21%)	18,26,29	0.56	0
83	Y5P	r1	45	83	14,19,20	7.39	3 (21%)	18,26,29	0.58	0
84	P5P	r2	69	84	20,23,24	1.28	3 (15%)	27,33,36	2.50	11 (40%)
84	Y5P	r2	11	84	14,19,20	7.36	3 (21%)	18,26,29	0.56	0
84	P5P	r2	24	84	20,23,24	1.28	3 (15%)	27,33,36	2.51	11 (40%)
86	Y5P	r4	43	86	14,19,20	7.39	3 (21%)	18,26,29	0.55	0
85	Y5P	r3	26	85	14,19,20	7.38	3 (21%)	18,26,29	0.58	0
85	Y5P	r3	55	85	14,19,20	7.38	3 (21%)	18,26,29	0.53	0
86	P5P	r4	57	86	20,23,24	1.29	3 (15%)	27,33,36	2.50	10 (37%)
86	Y5P	r4	16	86	14,19,20	7.46	3 (21%)	18,26,29	0.61	0
85	P5P	r3	67	85	20,23,24	1.28	3 (15%)	27,33,36	2.49	11 (40%)
85	P5P	r3	69	85	20,23,24	1.28	3 (15%)	27,33,36	2.50	11 (40%)
86	Y5P	r4	68	86	14,19,20	7.35	3 (21%)	18,26,29	0.56	0
86	Y5P	r4	3	86	14,19,20	7.33	3 (21%)	18,26,29	0.55	0
85	Y5P	r3	68	85	14,19,20	7.37	3 (21%)	18,26,29	0.58	0
85	P5P	r3	22	85	20,23,24	1.29	3 (15%)	27,33,36	2.49	11 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	P5P	r3	56	85	20,23,24	1.28	3 (15%)	27,33,36	2.48	11 (40%)
84	Y5P	r2	59	84	14,19,20	7.36	3 (21%)	18,26,29	0.56	0
85	P5P	r3	3	85	20,23,24	1.31	3 (15%)	27,33,36	2.49	11 (40%)
83	Y5P	r1	49	83	14,19,20	7.35	3 (21%)	18,26,29	0.54	0
84	P5P	r2	29	84	20,23,24	1.29	3 (15%)	27,33,36	2.49	11 (40%)
86	P5P	r4	21	86	20,23,24	1.28	3 (15%)	27,33,36	2.47	11 (40%)
86	P5P	r4	70	86	20,23,24	1.27	3 (15%)	27,33,36	2.47	11 (40%)
84	P5P	r2	14	84	20,23,24	1.29	3 (15%)	27,33,36	2.48	10 (37%)
83	Y5P	r1	51	83	14,19,20	7.35	3 (21%)	18,26,29	0.59	0
85	P5P	r3	72	85	20,23,24	1.28	3 (15%)	27,33,36	2.46	10 (37%)
86	P5P	r4	9	86	20,23,24	1.27	3 (15%)	27,33,36	2.48	11 (40%)
86	P5P	r4	65	86	20,23,24	1.28	3 (15%)	27,33,36	2.46	10 (37%)
84	Y5P	r2	47	84	14,19,20	7.44	3 (21%)	18,26,29	0.55	0
86	P5P	r4	29	86	20,23,24	1.27	3 (15%)	27,33,36	2.52	11 (40%)
86	P5P	r4	58	86	20,23,24	1.27	3 (15%)	27,33,36	2.47	11 (40%)
86	P5P	r4	26	86	20,23,24	1.27	3 (15%)	27,33,36	2.49	11 (40%)
84	P5P	r2	76	84	20,23,24	1.25	3 (15%)	27,33,36	2.49	11 (40%)
85	P5P	r3	14	85	20,23,24	1.28	3 (15%)	27,33,36	2.50	11 (40%)
89	MHW	A	1	89	9,9,10	0.79	0	10,11,13	2.49	3 (30%)
86	P5P	r4	7	86	20,23,24	1.28	3 (15%)	27,33,36	2.49	11 (40%)
84	Y5P	r2	61	84	14,19,20	7.34	3 (21%)	18,26,29	0.57	0
89	DBB	A	3	89	4,5,6	0.58	0	1,5,7	0.28	0
84	Y5P	r2	72	84	14,19,20	7.38	3 (21%)	18,26,29	0.54	0
83	Y5P	r1	53	83	14,19,20	7.41	3 (21%)	18,26,29	0.63	0
86	Y5P	r4	60	86	14,19,20	7.41	3 (21%)	18,26,29	0.56	0
85	P5P	r3	49	85	20,23,24	1.28	3 (15%)	27,33,36	2.46	11 (40%)
89	004	A	7	89	9,10,11	1.14	1 (11%)	9,12,14	1.60	2 (22%)
85	Y5P	r3	50	85	14,19,20	7.39	3 (21%)	18,26,29	0.56	0
85	P5P	r3	75	85	20,23,24	1.33	3 (15%)	27,33,36	2.48	11 (40%)
86	P5P	r4	38	86	20,23,24	1.28	3 (15%)	27,33,36	2.48	11 (40%)
84	Y5P	r2	3	84	14,19,20	7.41	3 (21%)	18,26,29	0.57	0
86	Y5P	r4	72	86	14,19,20	7.36	3 (21%)	18,26,29	0.56	0
86	Y5P	r4	12	86	14,19,20	7.39	3 (21%)	18,26,29	0.58	0
85	Y5P	r3	60	85	14,19,20	7.37	3 (21%)	18,26,29	0.55	0
84	Y5P	r2	17	84	14,19,20	7.37	3 (21%)	18,26,29	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	P5P	r3	4	85	20,23,24	1.31	3 (15%)	27,33,36	2.50	10 (37%)
86	Y5P	r4	56	86	14,19,20	7.39	3 (21%)	18,26,29	0.54	0
86	Y5P	r4	17	86	14,19,20	7.41	3 (21%)	18,26,29	0.54	0
84	P5P	r2	71	84	20,23,24	1.29	3 (15%)	27,33,36	2.47	10 (37%)
85	P5P	r3	5	85	20,23,24	1.30	3 (15%)	27,33,36	2.52	11 (40%)
84	P5P	r2	10	84	20,23,24	1.28	3 (15%)	27,33,36	2.49	11 (40%)
85	P5P	r3	17	85	20,23,24	1.28	3 (15%)	27,33,36	2.49	11 (40%)
86	P5P	r4	27	86	20,23,24	1.28	3 (15%)	27,33,36	2.48	11 (40%)
84	Y5P	r2	8	84	14,19,20	7.38	3 (21%)	18,26,29	0.58	0
84	Y5P	r2	32	84	14,19,20	7.36	3 (21%)	18,26,29	0.57	0
84	P5P	r2	46	84	20,23,24	1.28	3 (15%)	27,33,36	2.49	11 (40%)
84	Y5P	r2	40	84	14,19,20	7.38	3 (21%)	18,26,29	0.57	0
84	Y5P	r2	50	84	14,19,20	7.38	3 (21%)	18,26,29	0.55	0
84	Y5P	r2	2	84	14,19,20	7.37	3 (21%)	18,26,29	0.54	0
85	P5P	r3	10	85	20,23,24	1.29	3 (15%)	27,33,36	2.47	11 (40%)
85	P5P	r3	58	85	20,23,24	1.27	3 (15%)	27,33,36	2.49	11 (40%)
84	P5P	r2	23	84	20,23,24	1.29	3 (15%)	27,33,36	2.46	10 (37%)
86	Y5P	r4	8	86	14,19,20	7.36	3 (21%)	18,26,29	0.57	0
84	P5P	r2	70	84	20,23,24	1.28	3 (15%)	27,33,36	2.48	11 (40%)
86	Y5P	r4	40	86	14,19,20	7.37	3 (21%)	18,26,29	0.55	0
86	Y5P	r4	55	86	14,19,20	7.39	3 (21%)	18,26,29	0.54	0
84	P5P	r2	26	84	20,23,24	1.29	3 (15%)	27,33,36	2.48	11 (40%)
84	Y5P	r2	41	84	14,19,20	7.36	3 (21%)	18,26,29	0.54	0
84	P5P	r2	15	84	20,23,24	1.29	3 (15%)	27,33,36	2.48	10 (37%)
84	P5P	r2	28	84	20,23,24	1.28	3 (15%)	27,33,36	2.48	11 (40%)
84	P5P	r2	58	84	20,23,24	1.29	3 (15%)	27,33,36	2.48	11 (40%)
86	Y5P	r4	41	86	14,19,20	7.42	3 (21%)	18,26,29	0.55	0
85	Y5P	r3	41	85	14,19,20	7.36	3 (21%)	18,26,29	0.61	0
85	Y5P	r3	33	85	14,19,20	7.33	3 (21%)	18,26,29	0.54	0
85	P5P	r3	15	85	20,23,24	1.28	3 (15%)	27,33,36	2.49	11 (40%)
86	P5P	r4	28	86	20,23,24	1.28	3 (15%)	27,33,36	2.46	11 (40%)
85	Y5P	r3	74	85	14,19,20	7.31	3 (21%)	18,26,29	0.54	0
86	P5P	r4	30	86	20,23,24	1.28	3 (15%)	27,33,36	2.47	11 (40%)
84	Y5P	r2	13	84	14,19,20	7.39	3 (21%)	18,26,29	0.57	0
85	Y5P	r3	16	85	14,19,20	7.39	3 (21%)	18,26,29	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	Y5P	r3	28	85	14,19,20	7.38	3 (21%)	18,26,29	0.56	0
86	P5P	r4	73	86	20,23,24	1.27	3 (15%)	27,33,36	2.53	11 (40%)
84	Y5P	r2	4	84	14,19,20	7.36	3 (21%)	18,26,29	0.56	0
85	Y5P	r3	71	85	14,19,20	7.32	3 (21%)	18,26,29	0.58	0
85	Y5P	r3	35	85	14,19,20	7.32	3 (21%)	18,26,29	0.58	0
85	Y5P	r3	25	85	14,19,20	7.37	3 (21%)	18,26,29	0.62	0
85	Y5P	r3	29	85	14,19,20	7.38	3 (21%)	18,26,29	0.57	0
86	Y5P	r4	32	86	14,19,20	7.37	3 (21%)	18,26,29	0.55	0
84	P5P	r2	5	84	20,23,24	1.28	3 (15%)	27,33,36	2.48	11 (40%)
85	P5P	r3	8	85	20,23,24	1.28	3 (15%)	27,33,36	2.48	11 (40%)
86	Y5P	r4	50	86	14,19,20	7.37	3 (21%)	18,26,29	0.55	0
84	P5P	r2	31	84	20,23,24	1.29	3 (15%)	27,33,36	2.49	11 (40%)
84	P5P	r2	36	84	20,23,24	1.30	3 (15%)	27,33,36	2.50	11 (40%)
86	P5P	r4	69	86	20,23,24	1.29	3 (15%)	27,33,36	2.48	11 (40%)
85	Y5P	r3	42	85	14,19,20	7.35	3 (21%)	18,26,29	0.59	0
84	P5P	r2	73	84	20,23,24	1.27	3 (15%)	27,33,36	2.52	11 (40%)
84	Y5P	r2	74	84	14,19,20	7.37	3 (21%)	18,26,29	0.58	0
85	Y5P	r3	1	85	18,20,20	6.53	3 (16%)	25,29,29	0.66	0
86	P5P	r4	5	86	20,23,24	1.28	3 (15%)	27,33,36	2.48	11 (40%)
86	Y5P	r4	33	86	14,19,20	7.42	3 (21%)	18,26,29	0.54	0
86	Y5P	r4	74	86	14,19,20	7.37	3 (21%)	18,26,29	0.57	0
86	P5P	r4	31	86	20,23,24	1.30	3 (15%)	27,33,36	2.48	11 (40%)
85	P5P	r3	31	85	20,23,24	1.31	3 (15%)	27,33,36	2.45	10 (37%)
86	P5P	r4	22	86	20,23,24	1.28	3 (15%)	27,33,36	2.48	11 (40%)
86	Y5P	r4	39	86	14,19,20	7.35	3 (21%)	18,26,29	0.55	0
84	Y5P	r2	67	84	14,19,20	7.34	3 (21%)	18,26,29	0.54	0
84	Y5P	r2	54	84	14,19,20	7.38	3 (21%)	18,26,29	0.55	0
85	P5P	r3	24	85	20,23,24	1.31	3 (15%)	27,33,36	2.48	10 (37%)
83	Y5P	r1	57	83	14,19,20	7.40	3 (21%)	18,26,29	0.57	0
84	P5P	r2	1	84	20,23,24	1.28	3 (15%)	27,33,36	2.49	11 (40%)
86	P5P	r4	53	86	20,23,24	1.29	3 (15%)	27,33,36	2.48	10 (37%)
85	Y5P	r3	73	85	14,19,20	7.31	3 (21%)	18,26,29	0.59	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	P5P	r2	30	84	-	0/7/25/26	0/3/3/3
84	P5P	r2	64	84	-	0/7/25/26	0/3/3/3
86	P5P	r4	14	86	-	0/7/25/26	0/3/3/3
84	Y5P	r2	20	84	-	1/7/33/34	0/2/2/2
86	P5P	r4	1	86	-	3/7/25/26	0/3/3/3
84	Y5P	r2	39	84	-	1/7/33/34	0/2/2/2
86	Y5P	r4	42	86	-	1/7/33/34	0/2/2/2
86	P5P	r4	52	86	-	2/7/25/26	0/3/3/3
84	Y5P	r2	25	84	-	1/7/33/34	0/2/2/2
84	P5P	r2	35	84	-	2/7/25/26	0/3/3/3
85	P5P	r3	52	85	-	2/7/25/26	0/3/3/3
84	Y5P	r2	33	84	-	6/7/33/34	0/2/2/2
85	Y5P	r3	62	85	-	1/7/33/34	0/2/2/2
85	Y5P	r3	40	85	-	1/7/33/34	0/2/2/2
84	Y5P	r2	55	84	-	1/7/33/34	0/2/2/2
86	P5P	r4	44	86	-	0/7/25/26	0/3/3/3
85	P5P	r3	11	85	-	0/7/25/26	0/3/3/3
85	Y5P	r3	37	85	-	1/7/33/34	0/2/2/2
83	Y5P	r1	50	83	-	2/7/33/34	0/2/2/2
84	P5P	r2	53	84	-	0/7/25/26	0/3/3/3
85	Y5P	r3	70	85	-	1/7/33/34	0/2/2/2
86	P5P	r4	15	86	-	0/7/25/26	0/3/3/3
86	P5P	r4	71	86	-	0/7/25/26	0/3/3/3
85	Y5P	r3	61	85	-	2/7/33/34	0/2/2/2
84	P5P	r2	22	84	-	1/7/25/26	0/3/3/3
85	Y5P	r3	65	85	-	1/7/33/34	0/2/2/2
84	P5P	r2	63	84	-	0/7/25/26	0/3/3/3
84	Y5P	r2	48	84	-	1/7/33/34	0/2/2/2
85	Y5P	r3	59	85	-	1/7/33/34	0/2/2/2
86	P5P	r4	10	86	-	2/7/25/26	0/3/3/3
84	Y5P	r2	45	84	-	3/7/33/34	0/2/2/2
84	Y5P	r2	51	84	-	1/7/33/34	0/2/2/2
85	P5P	r3	6	85	-	0/7/25/26	0/3/3/3
84	P5P	r2	37	84	-	0/7/25/26	0/3/3/3
86	Y5P	r4	67	86	-	5/7/33/34	0/2/2/2
85	Y5P	r3	7	85	-	3/7/33/34	0/2/2/2
86	Y5P	r4	62	86	-	1/7/33/34	0/2/2/2
86	Y5P	r4	51	86	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	P5P	r3	32	85	-	0/7/25/26	0/3/3/3
86	P5P	r4	37	86	-	0/7/25/26	0/3/3/3
86	P5P	r4	24	86	-	2/7/25/26	0/3/3/3
83	Y5P	r1	54	83	-	1/7/33/34	0/2/2/2
85	Y5P	r3	63	85	-	1/7/33/34	0/2/2/2
85	Y5P	r3	66	85	-	3/7/33/34	0/2/2/2
86	P5P	r4	35	86	-	0/7/25/26	0/3/3/3
85	P5P	r3	46	85	-	0/7/25/26	0/3/3/3
86	P5P	r4	23	86	-	3/7/25/26	0/3/3/3
84	P5P	r2	9	84	-	4/7/25/26	0/3/3/3
85	Y5P	r3	64	85	-	3/7/33/34	0/2/2/2
84	Y5P	r2	62	84	-	1/7/33/34	0/2/2/2
84	P5P	r2	7	84	-	1/7/25/26	0/3/3/3
84	Y5P	r2	43	84	-	1/7/33/34	0/2/2/2
85	Y5P	r3	2	85	-	1/7/33/34	0/2/2/2
85	Y5P	r3	21	85	-	1/7/33/34	0/2/2/2
85	P5P	r3	23	85	-	0/7/25/26	0/3/3/3
84	Y5P	r2	16	84	-	1/7/33/34	0/2/2/2
85	Y5P	r3	34	85	-	1/7/33/34	0/2/2/2
85	P5P	r3	44	85	-	1/7/25/26	0/3/3/3
85	P5P	r3	36	85	-	0/7/25/26	0/3/3/3
86	P5P	r4	18	86	-	1/7/25/26	0/3/3/3
89	MHU	A	5	89	-	5/9/12/14	0/1/1/1
85	P5P	r3	9	85	-	3/7/25/26	0/3/3/3
83	Y5P	r1	44	83	-	1/7/33/34	0/2/2/2
83	Y5P	r1	56	83	-	4/7/33/34	0/2/2/2
86	Y5P	r4	20	86	-	2/7/33/34	0/2/2/2
84	Y5P	r2	12	84	-	1/7/33/34	0/2/2/2
86	Y5P	r4	11	86	-	1/7/33/34	0/2/2/2
86	Y5P	r4	48	86	-	3/7/33/34	0/2/2/2
83	Y5P	r1	46	83	-	2/7/33/34	0/2/2/2
83	Y5P	r1	55	83	-	3/7/33/34	0/2/2/2
84	P5P	r2	21	84	-	2/7/25/26	0/3/3/3
85	P5P	r3	45	85	-	0/7/25/26	0/3/3/3
84	P5P	r2	6	84	-	1/7/25/26	0/3/3/3
84	P5P	r2	34	84	-	0/7/25/26	0/3/3/3
85	P5P	r3	43	85	-	0/7/25/26	0/3/3/3
85	Y5P	r3	48	85	-	4/7/33/34	0/2/2/2
86	Y5P	r4	25	86	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	P5P	r4	46	86	-	3/7/25/26	0/3/3/3
86	Y5P	r4	54	86	-	1/7/33/34	0/2/2/2
84	Y5P	r2	68	84	-	3/7/33/34	0/2/2/2
85	Y5P	r3	54	85	-	3/7/33/34	0/2/2/2
85	Y5P	r3	13	85	-	5/7/33/34	0/2/2/2
85	Y5P	r3	57	85	-	3/7/33/34	0/2/2/2
84	P5P	r2	27	84	-	0/7/25/26	0/3/3/3
85	Y5P	r3	12	85	-	1/7/33/34	0/2/2/2
85	P5P	r3	20	85	-	2/7/25/26	0/3/3/3
84	P5P	r2	19	84	-	6/7/25/26	0/3/3/3
86	Y5P	r4	4	86	-	1/7/33/34	0/2/2/2
86	Y5P	r4	47	86	-	4/7/33/34	0/2/2/2
86	P5P	r4	36	86	-	0/7/25/26	0/3/3/3
84	Y5P	r2	60	84	-	1/7/33/34	0/2/2/2
86	Y5P	r4	2	86	-	1/7/33/34	0/2/2/2
85	P5P	r3	27	85	-	0/7/25/26	0/3/3/3
84	Y5P	r2	49	84	-	3/7/33/34	0/2/2/2
85	P5P	r3	53	85	-	0/7/25/26	0/3/3/3
86	Y5P	r4	59	86	-	2/7/33/34	0/2/2/2
83	Y5P	r1	48	83	-	1/7/33/34	0/2/2/2
83	Y5P	r1	52	83	-	1/7/33/34	0/2/2/2
84	P5P	r2	57	84	-	0/7/25/26	0/3/3/3
85	P5P	r3	19	85	-	3/7/25/26	0/3/3/3
84	Y5P	r2	75	84	-	4/7/33/34	0/2/2/2
84	P5P	r2	38	84	-	0/7/25/26	0/3/3/3
84	P5P	r2	44	84	-	0/7/25/26	0/3/3/3
86	Y5P	r4	13	86	-	3/7/33/34	0/2/2/2
86	Y5P	r4	49	86	-	3/7/33/34	0/2/2/2
84	P5P	r2	18	84	-	1/7/25/26	0/3/3/3
85	Y5P	r3	18	85	-	4/7/33/34	0/2/2/2
86	P5P	r4	63	86	-	0/7/25/26	0/3/3/3
89	MHV	A	6	89	-	0/1/12/14	0/1/1/1
86	Y5P	r4	75	86	-	4/7/33/34	0/2/2/2
84	P5P	r2	52	84	-	1/7/25/26	0/3/3/3
84	Y5P	r2	66	84	-	3/7/33/34	0/2/2/2
86	Y5P	r4	45	86	-	4/7/33/34	0/2/2/2
85	P5P	r3	38	85	-	2/7/25/26	0/3/3/3
86	P5P	r4	64	86	-	2/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	Y5P	r4	61	86	-	2/7/33/34	0/2/2/2
86	P5P	r4	34	86	-	1/7/25/26	0/3/3/3
83	Y5P	r1	47	83	-	3/7/33/34	0/2/2/2
86	Y5P	r4	66	86	-	3/7/33/34	0/2/2/2
85	P5P	r3	47	85	-	1/7/25/26	0/3/3/3
85	Y5P	r3	51	85	-	4/7/33/34	0/2/2/2
86	P5P	r4	6	86	-	2/7/25/26	0/3/3/3
86	P5P	r4	19	86	-	0/7/25/26	0/3/3/3
84	Y5P	r2	42	84	-	1/7/33/34	0/2/2/2
84	Y5P	r2	56	84	-	1/7/33/34	0/2/2/2
85	P5P	r3	30	85	-	2/7/25/26	0/3/3/3
84	P5P	r2	65	84	-	0/7/25/26	0/3/3/3
85	Y5P	r3	39	85	-	1/7/33/34	0/2/2/2
83	Y5P	r1	45	83	-	3/7/33/34	0/2/2/2
84	P5P	r2	69	84	-	3/7/25/26	0/3/3/3
84	Y5P	r2	11	84	-	1/7/33/34	0/2/2/2
84	P5P	r2	24	84	-	2/7/25/26	0/3/3/3
86	Y5P	r4	43	86	-	1/7/33/34	0/2/2/2
85	Y5P	r3	26	85	-	1/7/33/34	0/2/2/2
85	Y5P	r3	55	85	-	1/7/33/34	0/2/2/2
86	P5P	r4	57	86	-	0/7/25/26	0/3/3/3
86	Y5P	r4	16	86	-	1/7/33/34	0/2/2/2
85	P5P	r3	67	85	-	1/7/25/26	0/3/3/3
85	P5P	r3	69	85	-	0/7/25/26	0/3/3/3
86	Y5P	r4	68	86	-	1/7/33/34	0/2/2/2
86	Y5P	r4	3	86	-	1/7/33/34	0/2/2/2
85	Y5P	r3	68	85	-	1/7/33/34	0/2/2/2
85	P5P	r3	22	85	-	3/7/25/26	0/3/3/3
85	P5P	r3	56	85	-	2/7/25/26	0/3/3/3
84	Y5P	r2	59	84	-	1/7/33/34	0/2/2/2
85	P5P	r3	3	85	-	3/7/25/26	0/3/3/3
83	Y5P	r1	49	83	-	3/7/33/34	0/2/2/2
84	P5P	r2	29	84	-	0/7/25/26	0/3/3/3
86	P5P	r4	21	86	-	1/7/25/26	0/3/3/3
86	P5P	r4	70	86	-	0/7/25/26	0/3/3/3
84	P5P	r2	14	84	-	3/7/25/26	0/3/3/3
83	Y5P	r1	51	83	-	2/7/33/34	0/2/2/2
85	P5P	r3	72	85	-	0/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	P5P	r4	9	86	-	2/7/25/26	0/3/3/3
86	P5P	r4	65	86	-	0/7/25/26	0/3/3/3
84	Y5P	r2	47	84	-	2/7/33/34	0/2/2/2
86	P5P	r4	29	86	-	4/7/25/26	0/3/3/3
86	P5P	r4	58	86	-	0/7/25/26	0/3/3/3
86	P5P	r4	26	86	-	2/7/25/26	0/3/3/3
84	P5P	r2	76	84	-	3/7/25/26	0/3/3/3
85	P5P	r3	14	85	-	3/7/25/26	0/3/3/3
89	MHW	A	1	89	-	0/2/2/4	0/1/1/1
86	P5P	r4	7	86	-	2/7/25/26	0/3/3/3
84	Y5P	r2	61	84	-	2/7/33/34	0/2/2/2
89	DBB	A	3	89	-	0/3/4/6	-
84	Y5P	r2	72	84	-	3/7/33/34	0/2/2/2
83	Y5P	r1	53	83	-	6/7/33/34	0/2/2/2
86	Y5P	r4	60	86	-	1/7/33/34	0/2/2/2
85	P5P	r3	49	85	-	1/7/25/26	0/3/3/3
89	004	A	7	89	-	0/4/6/8	0/1/1/1
85	Y5P	r3	50	85	-	3/7/33/34	0/2/2/2
85	P5P	r3	75	85	-	2/7/25/26	0/3/3/3
86	P5P	r4	38	86	-	2/7/25/26	0/3/3/3
84	Y5P	r2	3	84	-	3/7/33/34	0/2/2/2
86	Y5P	r4	72	86	-	3/7/33/34	0/2/2/2
86	Y5P	r4	12	86	-	2/7/33/34	0/2/2/2
85	Y5P	r3	60	85	-	2/7/33/34	0/2/2/2
84	Y5P	r2	17	84	-	4/7/33/34	0/2/2/2
85	P5P	r3	4	85	-	3/7/25/26	0/3/3/3
86	Y5P	r4	56	86	-	3/7/33/34	0/2/2/2
86	Y5P	r4	17	86	-	3/7/33/34	0/2/2/2
84	P5P	r2	71	84	-	0/7/25/26	0/3/3/3
85	P5P	r3	5	85	-	2/7/25/26	0/3/3/3
84	P5P	r2	10	84	-	2/7/25/26	0/3/3/3
85	P5P	r3	17	85	-	5/7/25/26	0/3/3/3
86	P5P	r4	27	86	-	3/7/25/26	0/3/3/3
84	Y5P	r2	8	84	-	1/7/33/34	0/2/2/2
84	Y5P	r2	32	84	-	1/7/33/34	0/2/2/2
84	P5P	r2	46	84	-	6/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	Y5P	r2	40	84	-	1/7/33/34	0/2/2/2
84	Y5P	r2	50	84	-	3/7/33/34	0/2/2/2
84	Y5P	r2	2	84	-	2/7/33/34	0/2/2/2
85	P5P	r3	10	85	-	0/7/25/26	0/3/3/3
85	P5P	r3	58	85	-	2/7/25/26	0/3/3/3
84	P5P	r2	23	84	-	2/7/25/26	0/3/3/3
86	Y5P	r4	8	86	-	1/7/33/34	0/2/2/2
84	P5P	r2	70	84	-	0/7/25/26	0/3/3/3
86	Y5P	r4	40	86	-	1/7/33/34	0/2/2/2
86	Y5P	r4	55	86	-	1/7/33/34	0/2/2/2
84	P5P	r2	26	84	-	0/7/25/26	0/3/3/3
84	Y5P	r2	41	84	-	1/7/33/34	0/2/2/2
84	P5P	r2	15	84	-	4/7/25/26	0/3/3/3
84	P5P	r2	28	84	-	0/7/25/26	0/3/3/3
84	P5P	r2	58	84	-	0/7/25/26	0/3/3/3
86	Y5P	r4	41	86	-	3/7/33/34	0/2/2/2
85	Y5P	r3	41	85	-	3/7/33/34	0/2/2/2
85	Y5P	r3	33	85	-	1/7/33/34	0/2/2/2
85	P5P	r3	15	85	-	0/7/25/26	0/3/3/3
86	P5P	r4	28	86	-	2/7/25/26	0/3/3/3
85	Y5P	r3	74	85	-	1/7/33/34	0/2/2/2
86	P5P	r4	30	86	-	1/7/25/26	0/3/3/3
84	Y5P	r2	13	84	-	3/7/33/34	0/2/2/2
85	Y5P	r3	16	85	-	2/7/33/34	0/2/2/2
85	Y5P	r3	28	85	-	1/7/33/34	0/2/2/2
86	P5P	r4	73	86	-	5/7/25/26	0/3/3/3
84	Y5P	r2	4	84	-	1/7/33/34	0/2/2/2
85	Y5P	r3	71	85	-	3/7/33/34	0/2/2/2
85	Y5P	r3	35	85	-	3/7/33/34	0/2/2/2
85	Y5P	r3	25	85	-	1/7/33/34	0/2/2/2
85	Y5P	r3	29	85	-	1/7/33/34	0/2/2/2
86	Y5P	r4	32	86	-	3/7/33/34	0/2/2/2
84	P5P	r2	5	84	-	0/7/25/26	0/3/3/3
85	P5P	r3	8	85	-	0/7/25/26	0/3/3/3
86	Y5P	r4	50	86	-	2/7/33/34	0/2/2/2
84	P5P	r2	31	84	-	0/7/25/26	0/3/3/3
84	P5P	r2	36	84	-	3/7/25/26	0/3/3/3
86	P5P	r4	69	86	-	0/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	Y5P	r3	42	85	-	1/7/33/34	0/2/2/2
84	P5P	r2	73	84	-	3/7/25/26	0/3/3/3
84	Y5P	r2	74	84	-	3/7/33/34	0/2/2/2
85	Y5P	r3	1	85	-	1/10/34/34	0/2/2/2
86	P5P	r4	5	86	-	0/7/25/26	0/3/3/3
86	Y5P	r4	33	86	-	2/7/33/34	0/2/2/2
86	Y5P	r4	74	86	-	4/7/33/34	0/2/2/2
86	P5P	r4	31	86	-	2/7/25/26	0/3/3/3
85	P5P	r3	31	85	-	1/7/25/26	0/3/3/3
86	P5P	r4	22	86	-	3/7/25/26	0/3/3/3
86	Y5P	r4	39	86	-	1/7/33/34	0/2/2/2
84	Y5P	r2	67	84	-	3/7/33/34	0/2/2/2
84	Y5P	r2	54	84	-	1/7/33/34	0/2/2/2
85	P5P	r3	24	85	-	2/7/25/26	0/3/3/3
83	Y5P	r1	57	83	-	1/7/33/34	0/2/2/2
84	P5P	r2	1	84	-	3/7/25/26	0/3/3/3
86	P5P	r4	53	86	-	3/7/25/26	0/3/3/3
85	Y5P	r3	73	85	-	3/7/33/34	0/2/2/2

The worst 5 of 721 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	r4	16	Y5P	C2-N3	27.01	1.48	1.27
84	r2	47	Y5P	C2-N3	26.91	1.48	1.27
84	r2	56	Y5P	C2-N3	26.86	1.48	1.27
86	r4	33	Y5P	C2-N3	26.86	1.48	1.27
83	r1	53	Y5P	C2-N3	26.85	1.48	1.27

The worst 5 of 1234 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	A	1	MHW	O-C-CA	-6.19	116.60	124.37
85	r3	6	P5P	N9-C8-N7	-5.38	106.30	113.94
86	r4	64	P5P	N9-C8-N7	-5.36	106.33	113.94
86	r4	57	P5P	N9-C8-N7	-5.34	106.35	113.94
85	r3	4	P5P	N9-C8-N7	-5.33	106.37	113.94

There are no chirality outliers.

5 of 413 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	r1	51	Y5P	O4'-C1'-N1-C2
83	r1	53	Y5P	O4'-C4'-C5'-O5'
84	r2	12	Y5P	O4'-C1'-N1-C2
84	r2	13	Y5P	O4'-C4'-C5'-O5'
84	r2	17	Y5P	O4'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 204 ligands modelled in this entry, 202 are monoatomic - leaving 2 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
93	GTP	AX	500	-	33,34,34	0.93	1 (3%)	50,54,54	1.57	8 (16%)
92	DOL	XA	5143	-	47,50,50	3.92	18 (38%)	57,70,70	3.08	15 (26%)

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
93	GTP	AX	500	-	-	7/22/38/38	0/3/3/3
92	DOL	XA	5143	-	-	19/64/77/77	0/2/3/3

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
92	XA	5143	DOL	C28-C29	10.46	1.55	1.32
92	XA	5143	DOL	C6-N5	10.29	1.49	1.34
92	XA	5143	DOL	C22-C23	9.03	1.57	1.32
92	XA	5143	DOL	C10-N9	8.83	1.38	1.29
92	XA	5143	DOL	C19-C20	8.75	1.57	1.34

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
92	XA	5143	DOL	O40-S39-O41	-15.75	100.27	118.13
92	XA	5143	DOL	O11-C10-C13	9.21	126.22	117.70
92	XA	5143	DOL	C24-N25-C26	-5.55	113.18	122.17
92	XA	5143	DOL	O11-C10-N9	-5.37	108.28	114.09
93	AX	500	GTP	C5-C4-N3	-5.16	120.17	128.39

There are no chirality outliers.

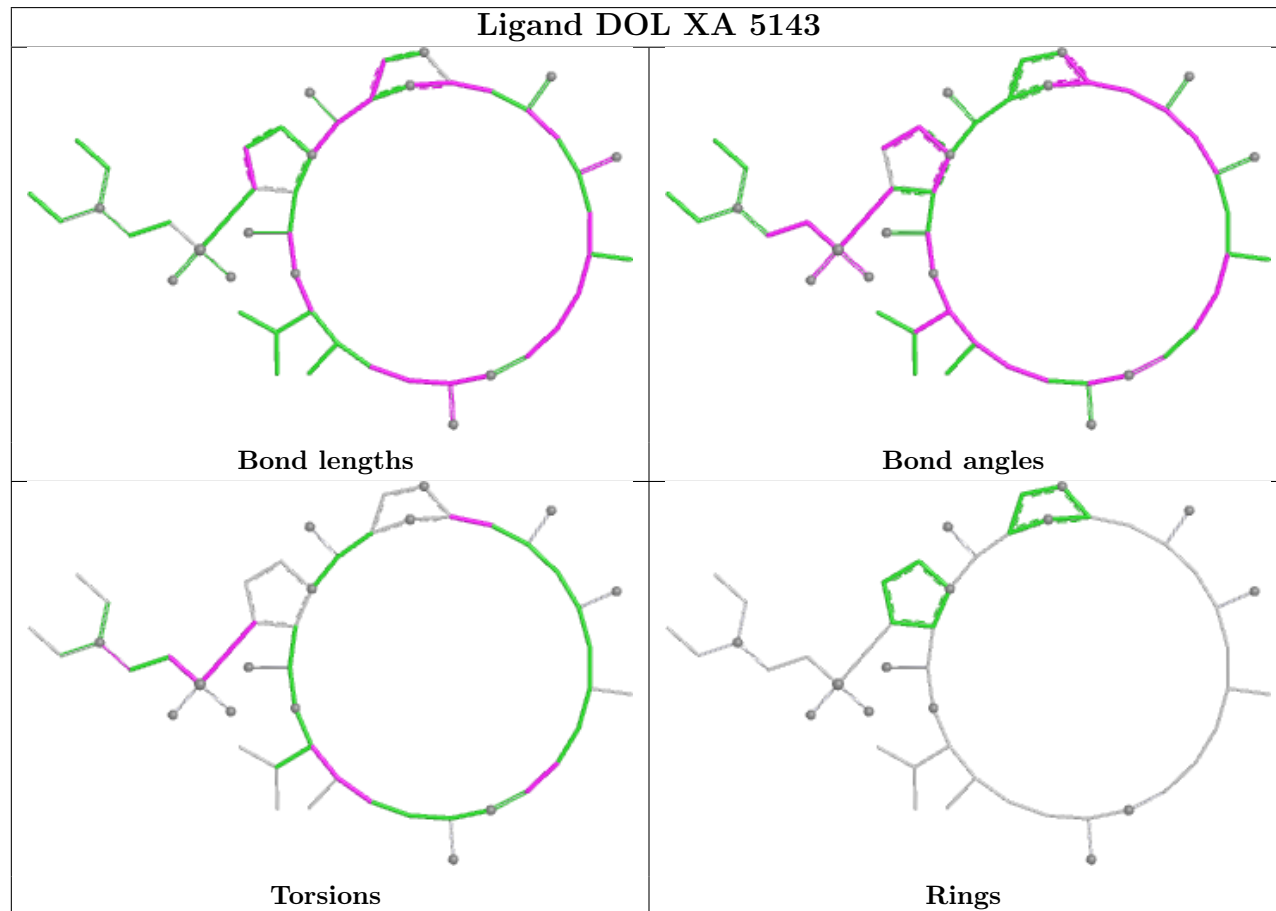
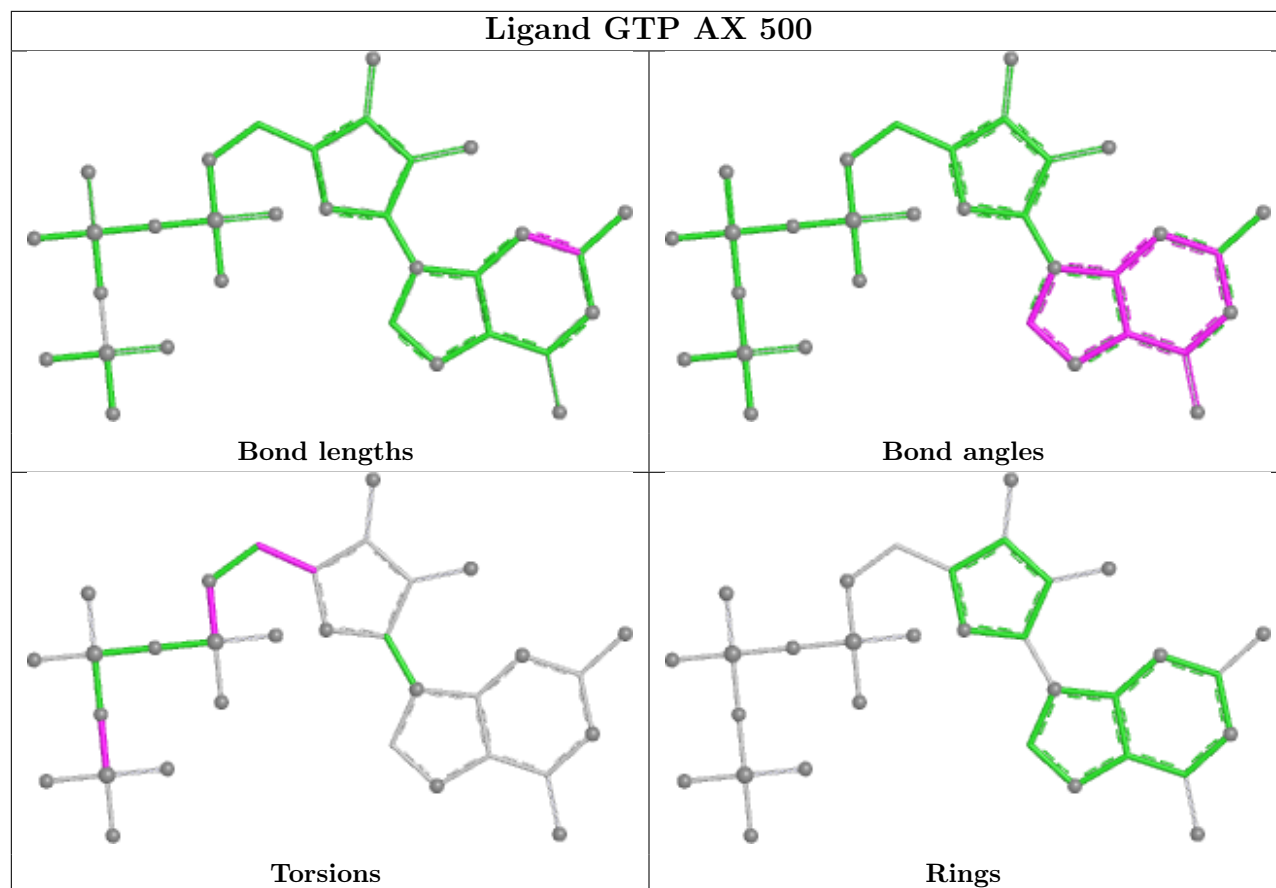
5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
92	XA	5143	DOL	C3-C2-S39-O41
92	XA	5143	DOL	C3-C2-S39-C42
92	XA	5143	DOL	C1-C2-S39-O41
92	XA	5143	DOL	C1-C2-S39-O40
92	XA	5143	DOL	C43-C42-S39-C2

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 than 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.



4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
85	r3	3
16	A4	2
38	AV	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r3	18:Y5P	O3'	19:P5P	P	6.45
1	A4	537:ARG	C	538:ASP	N	6.17
1	r3	17:P5P	O3'	18:Y5P	P	5.79
1	r3	16:Y5P	O3'	17:P5P	P	5.56
1	AV	269:SER	C	270:PRO	N	4.72

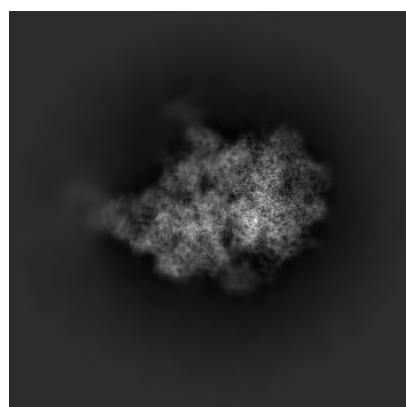
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11397. These allow visual inspection of the internal detail of the map and identification of artifacts.

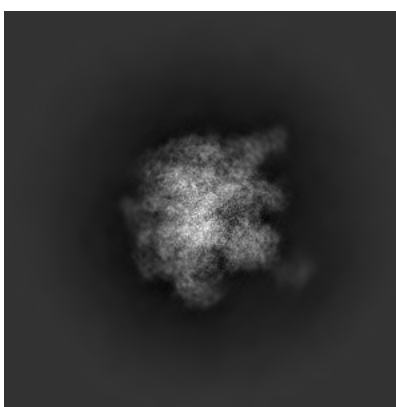
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections [i](#)

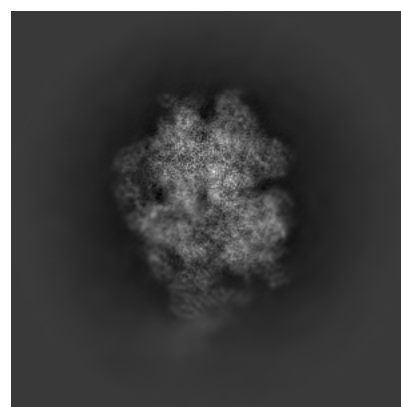
5.1.1 Primary map



X



Y

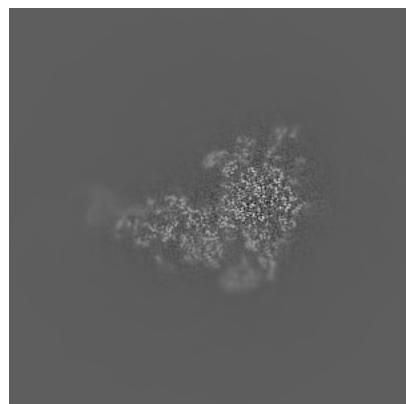


Z

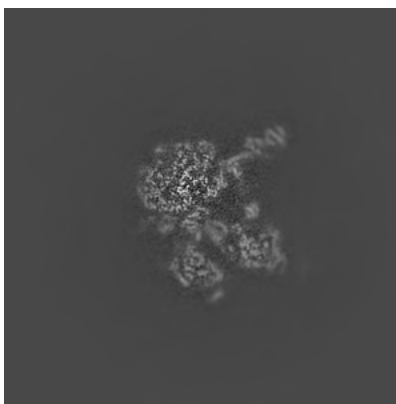
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

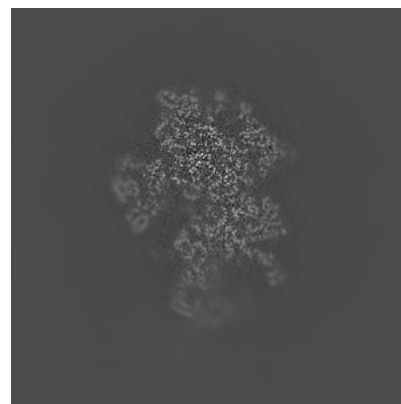
5.2.1 Primary map



X Index: 260



Y Index: 260

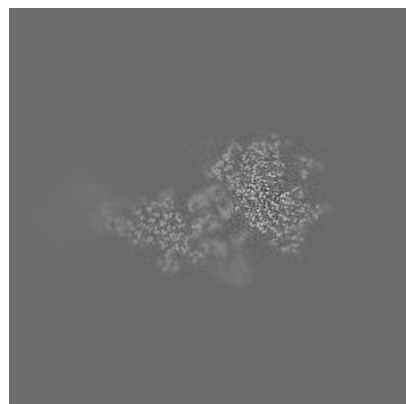


Z Index: 260

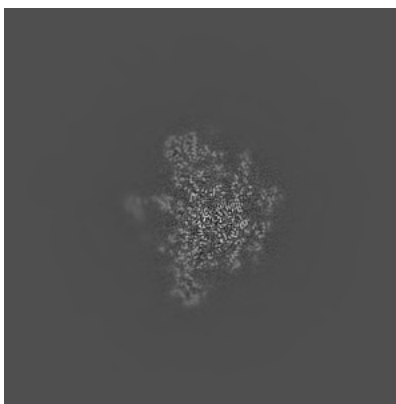
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

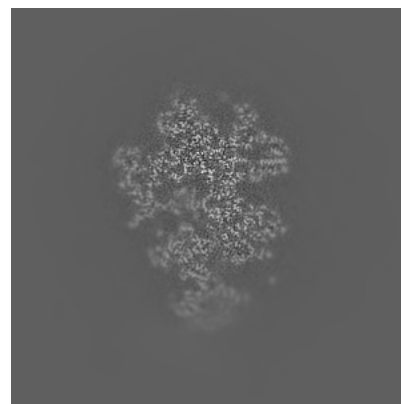
5.3.1 Primary map



X Index: 238



Y Index: 319

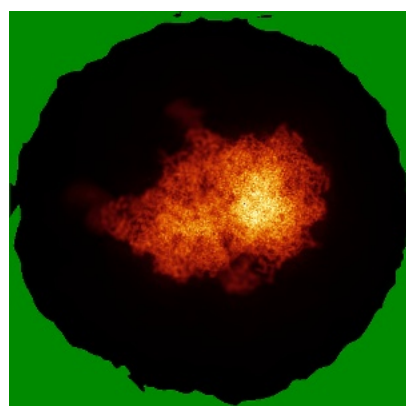


Z Index: 247

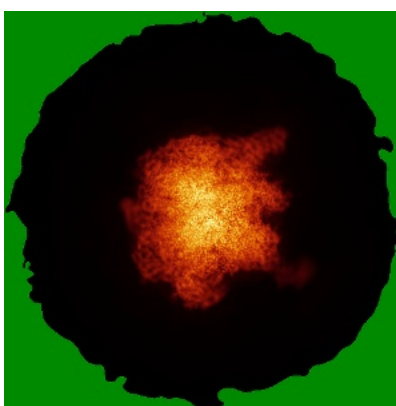
The images above show the largest variance slices of the map in three orthogonal directions.

5.4 Orthogonal standard-deviation projections (False-color) [i](#)

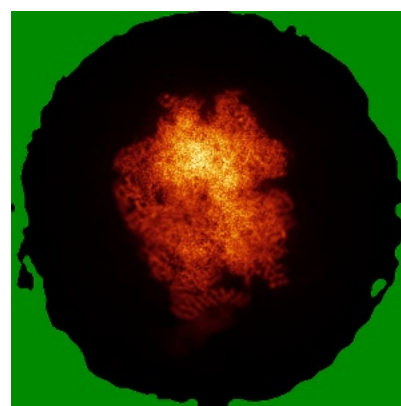
5.4.1 Primary map



X



Y

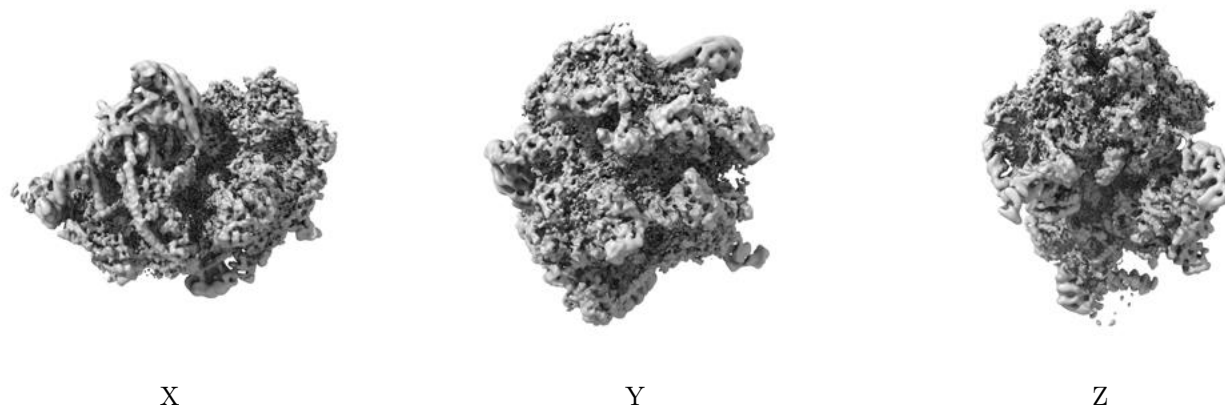


Z

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.

5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

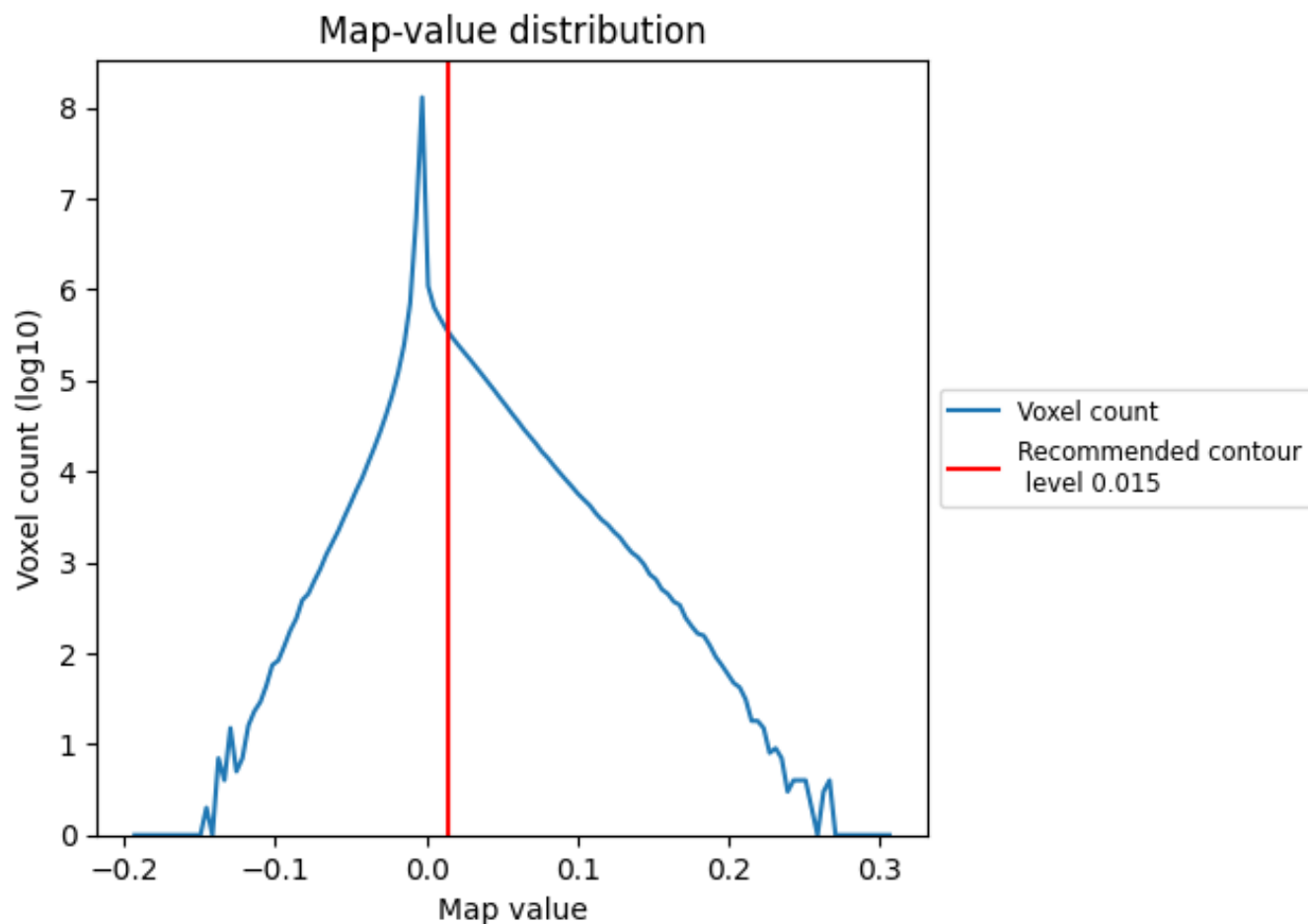
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

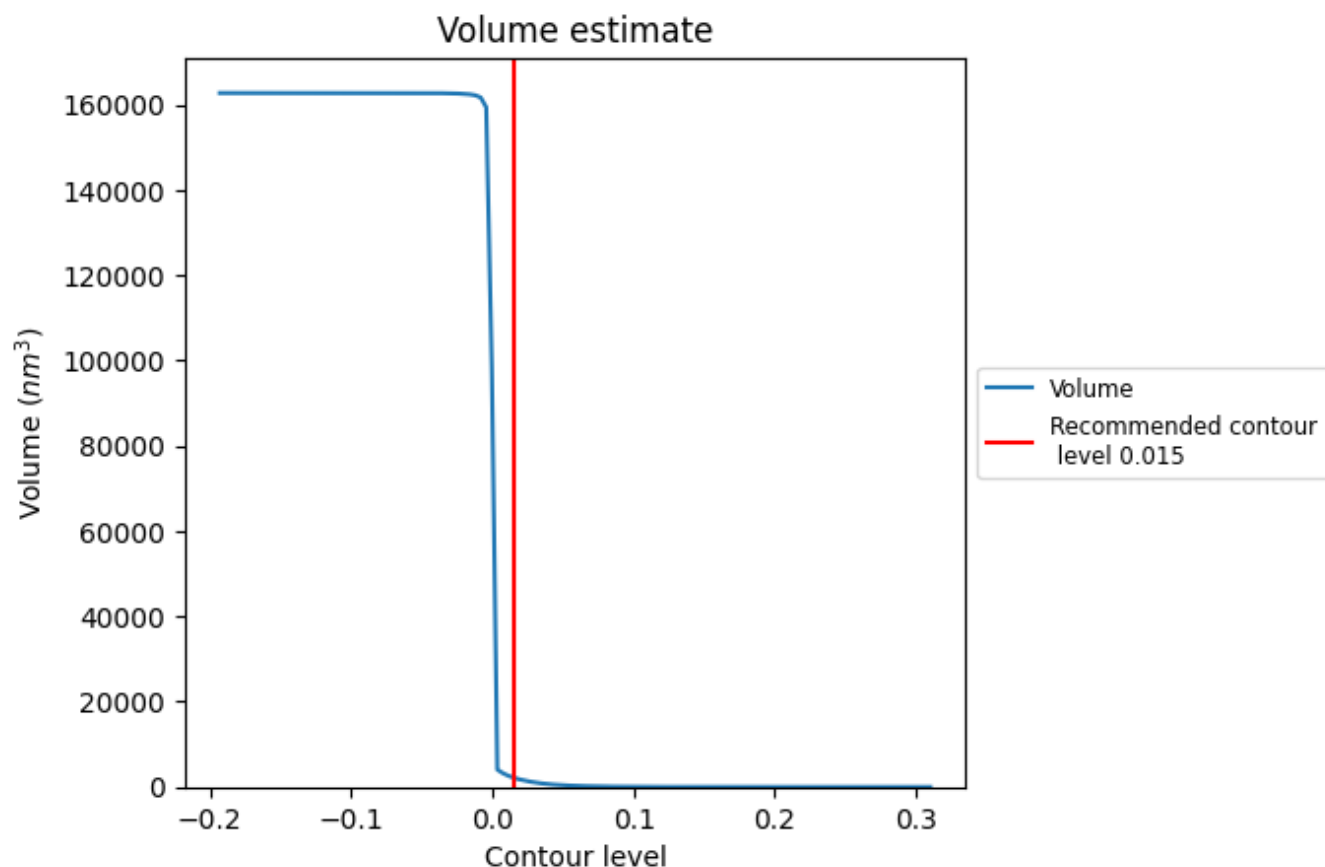
This section contains the results of statistical analysis of the map.

6.1 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.

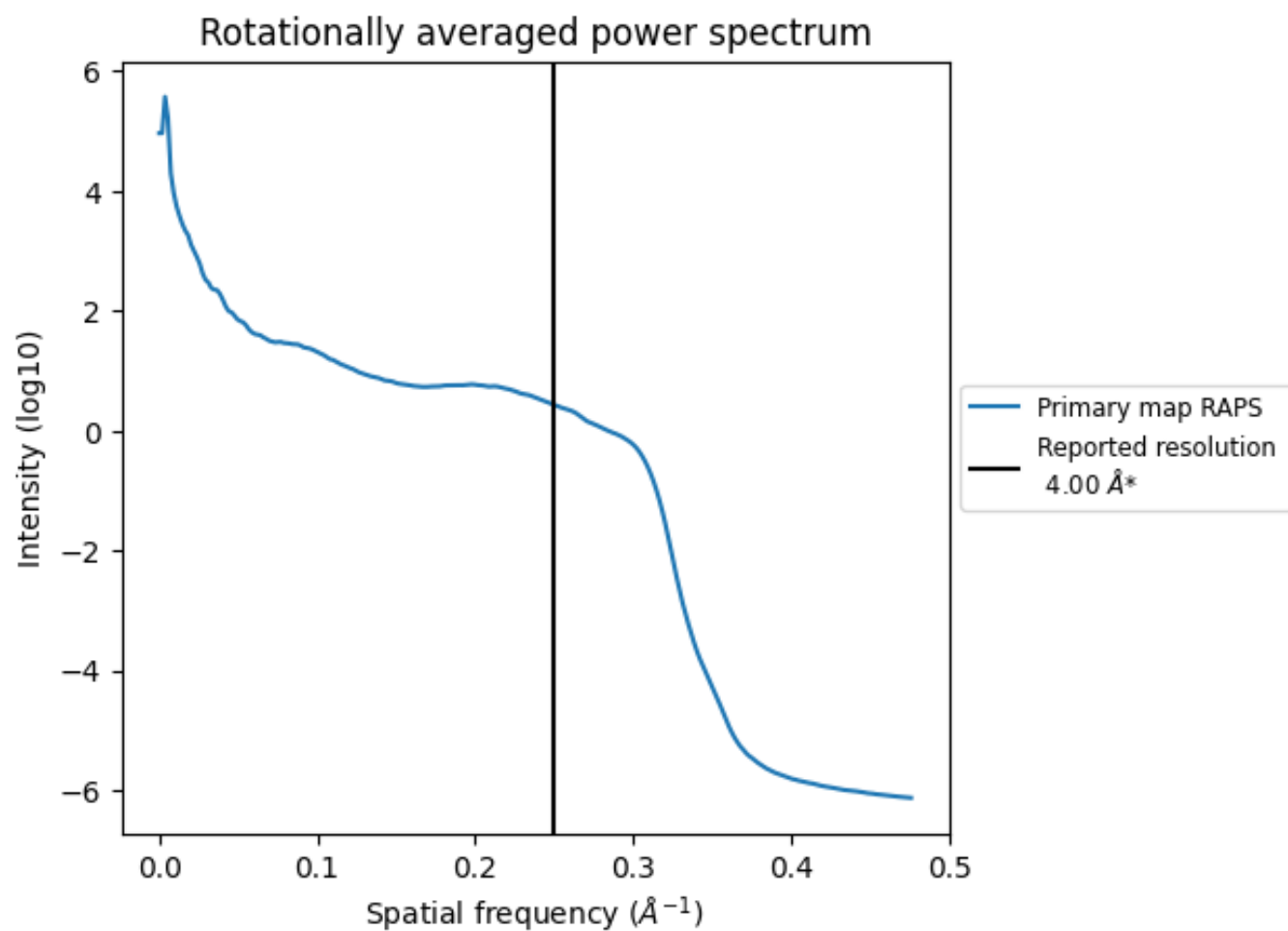
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 2190 nm³; this corresponds to an approximate mass of 1978 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.

6.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

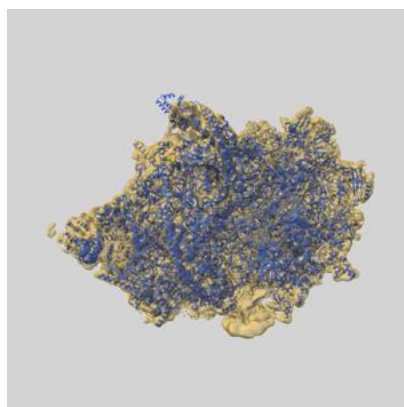
7 Fourier-Shell correlation ⓘ

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

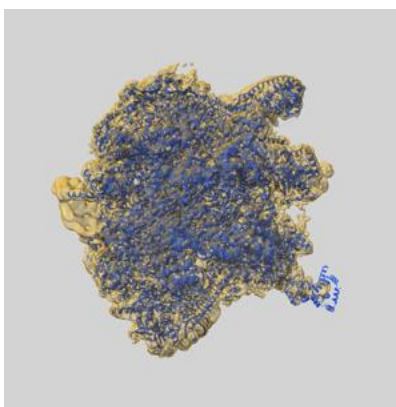
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11397 and PDB model 6ZSG. Per-residue inclusion information can be found in section ?? on page ??.

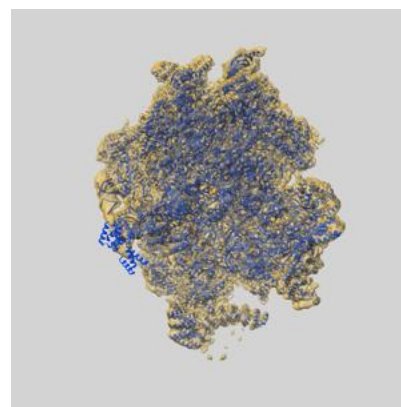
8.1 Map-model overlay [i](#)



X



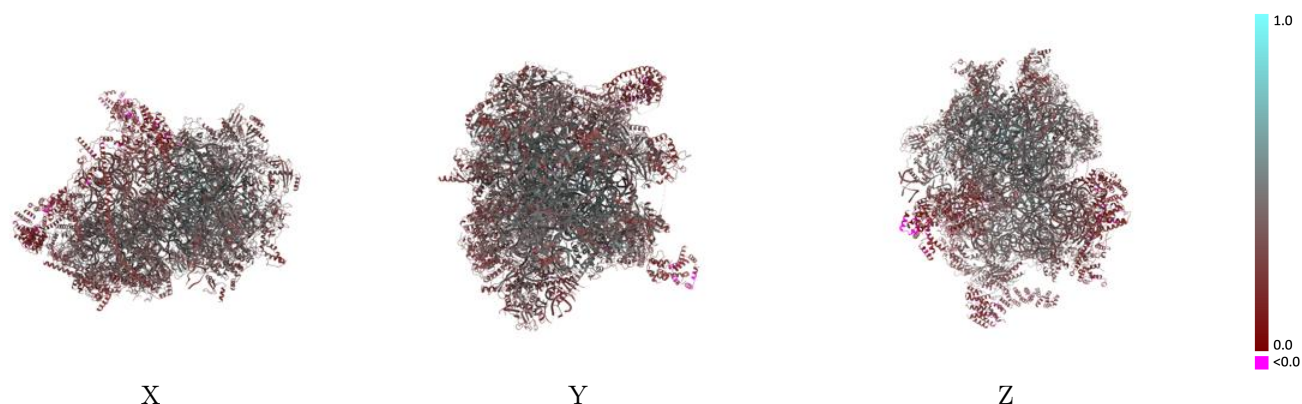
Y



Z

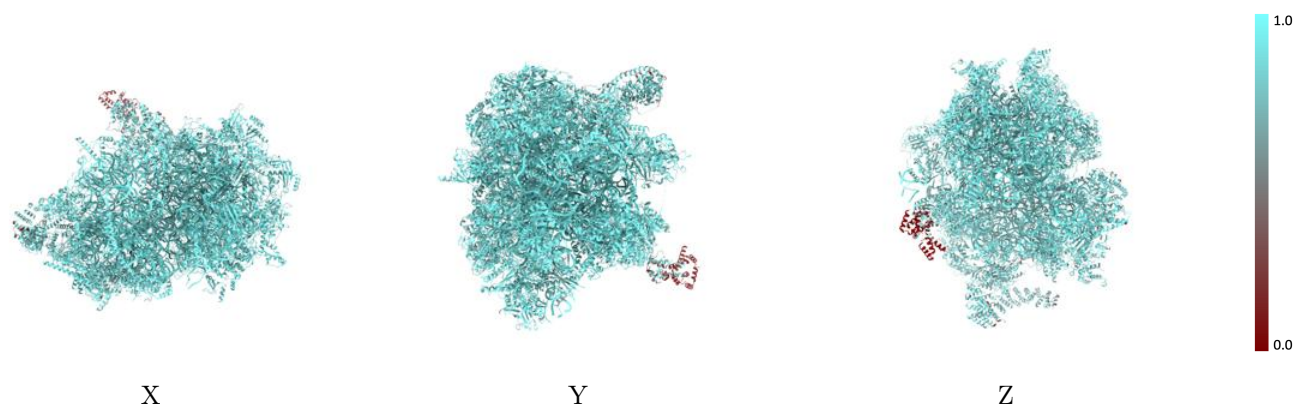
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

8.2 Q-score mapped to coordinate model [i](#)



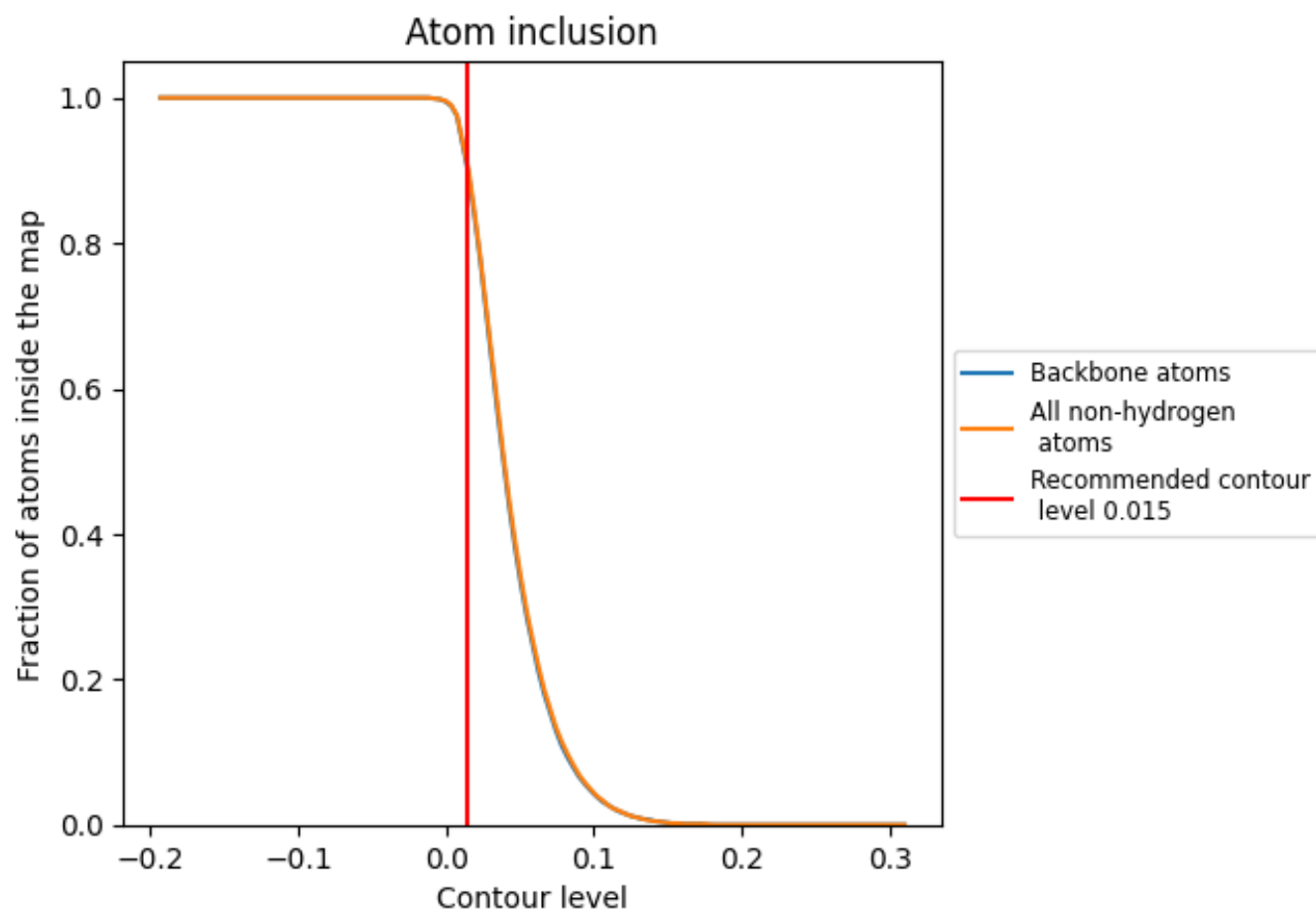
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

8.3 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 (0.015).

8.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9040	 0.3730
0	 0.9100	 0.4150
1	 0.8970	 0.3910
2	 0.9390	 0.5100
3	 0.9310	 0.4870
4	 0.9320	 0.4330
5	 0.9170	 0.3870
6	 0.8920	 0.3470
7	 0.8890	 0.3420
8	 0.8220	 0.2690
9	 0.9030	 0.3820
A	 0.8900	 0.4360
A0	 0.8450	 0.2290
A1	 0.8340	 0.2720
A2	 0.8490	 0.3250
A3	 0.8870	 0.4190
A4	 0.7720	 0.1860
AA	 0.9770	 0.4050
AB	 0.9120	 0.3660
AC	 0.8740	 0.3850
AD	 0.8730	 0.3690
AE	 0.9050	 0.3860
AF	 0.8520	 0.3070
AG	 0.8640	 0.3230
AH	 0.8620	 0.3500
AI	 0.9050	 0.3780
AJ	 0.8750	 0.3800
AK	 0.8860	 0.3540
AL	 0.8810	 0.3460
AM	 0.8530	 0.2850
AN	 0.9100	 0.3650
AO	 0.8790	 0.3050
AP	 0.8980	 0.3980
AQ	 0.8980	 0.3860
AR	 0.8410	 0.2320



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Chain	Atom inclusion	Q-score
AS	 0.8620	 0.3120
AT	 0.8860	 0.3380
AU	 0.8610	 0.2570
AV	 0.7900	 0.1720
AW	 0.8760	 0.3370
AX	 0.8490	 0.2390
AY	 0.8370	 0.2630
AZ	 0.8700	 0.3130
XA	 0.9750	 0.4690
XB	 0.9870	 0.3280
XD	 0.9340	 0.4600
XE	 0.9160	 0.4320
XF	 0.9290	 0.4520
XH	 0.8860	 0.3570
XI	 0.7310	 0.2570
XJ	 0.8320	 0.2130
XK	 0.9180	 0.4380
XL	 0.9090	 0.4280
XM	 0.9140	 0.4240
XN	 0.9040	 0.4270
XO	 0.9120	 0.4090
XP	 0.9090	 0.3870
XQ	 0.8840	 0.3820
XR	 0.9100	 0.4470
XS	 0.9040	 0.4430
XT	 0.9220	 0.4490
XU	 0.9180	 0.4120
XV	 0.8930	 0.3580
XW	 0.9440	 0.4710
XX	 0.9070	 0.3850
XY	 0.9170	 0.4030
XZ	 0.9290	 0.4520
a	 0.8900	 0.4040
b	 0.9310	 0.4510
c	 0.9010	 0.3780
d	 0.8750	 0.3440
e	 0.8330	 0.2220
f	 0.8390	 0.3080
g	 0.9190	 0.4320
h	 0.9010	 0.3340
i	 0.9080	 0.4650
j	 0.9080	 0.4040

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Chain	Atom inclusion	Q-score
k	 0.8450	 0.2520
l	 0.8380	 0.2420
m	 0.8540	 0.2680
o	 0.9360	 0.4610
p	 0.9040	 0.3280
q	 0.8440	 0.2860
r	 0.9090	 0.3880
r1	 0.9210	 0.3550
r2	 0.9240	 0.2820
r3	 0.9380	 0.3480
r4	 0.9050	 0.2140
s	 0.9090	 0.3950
t1	 0.5670	 0.1930
t2	 0.6220	 0.1920
t3	 0.2940	 0.1650
t4	 0.2440	 0.1000
t5	 0.0040	 0.1170
t6	 0.0000	 -0.0110