



wwPDB EM Validation Summary Report ⓘ

Aug 26, 2026 – 10:02 am BST

PDB ID : 9SH6 / pdb_00009sh6
EMDB ID : EMD-54889
Title : Structure of a GPCR dimer bound to two G proteins
Authors : Velazhahan, V.; Tate, C.
Deposited on : 2025-08-25
Resolution : 2.77 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:

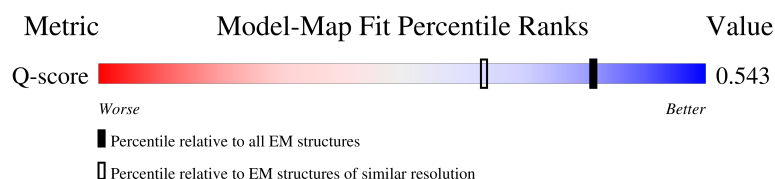
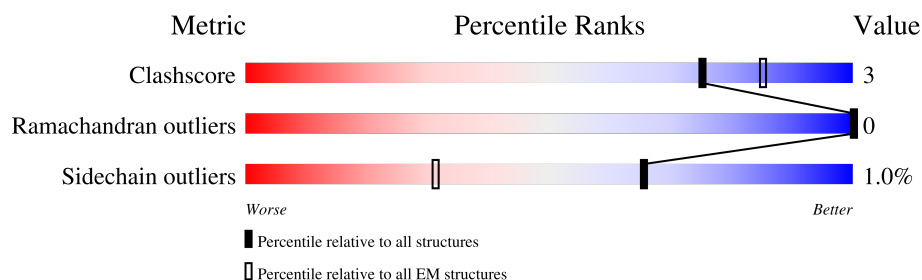
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 2.77 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



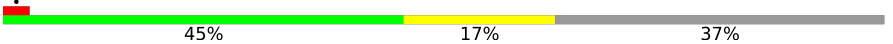
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10695 (2.27 - 3.27)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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
1	A	430	
1	B	430	
2	I	13	
2	K	13	

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Mol	Chain	Length	Quality of chain
3	G	110	
3	H	110	
4	C	423	
4	F	423	
5	D	472	
5	E	472	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 27678 atoms, of which 12792 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 Pheromone alpha factor receptor.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	309	Total	C	H	N	O	S	0	0
			4701	1549	2334	374	433	11		
1	A	309	Total	C	H	N	O	S	0	0
			4669	1543	2312	370	433	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP D6VTK4
A	?	-	THR	deletion	UNP D6VTK4

- Molecule 2 is a protein called Mating factor alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	K	13	Total	C	H	N	O	S	0	0
			235	82	115	20	17	1		
2	I	13	Total	C	H	N	O	S	0	0
			235	82	115	20	17	1		

- Molecule 3 is a protein called Guanine nucleotide-binding protein subunit gamma.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	69	Total	C	H	N	O	S	0	0
			572	280	126	78	87	1		
3	H	69	Total	C	H	N	O	S	0	0
			572	280	126	78	87	1		

- Molecule 4 is a protein called Guanine nucleotide-binding protein subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	C	358	Total	C	H	N	O	S	0	0
			4758	1625	2152	450	515	16		

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Mol	Chain	Residues	Atoms						AltConf	Trace
4	F	358	Total	C	H	N	O	S	0	0
			4758	1625	2152	450	515	16		

- Molecule 5 is a protein called Guanine nucleotide-binding protein alpha-1 subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	224	Total	C	H	N	O	S	0	0
			3155	1110	1435	284	318	8		
5	D	224	Total	C	H	N	O	S	0	0
			3155	1110	1435	284	318	8		

There are 600 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MET	-	initiating methionine	UNP P08539
E	2	GLY	-	expression tag	UNP P08539
E	3	CYS	-	expression tag	UNP P08539
E	4	THR	-	expression tag	UNP P08539
E	5	VAL	-	expression tag	UNP P08539
E	6	SER	-	expression tag	UNP P08539
E	7	THR	-	expression tag	UNP P08539
E	8	GLN	-	expression tag	UNP P08539
E	9	THR	-	expression tag	UNP P08539
E	10	ILE	-	expression tag	UNP P08539
E	11	GLY	-	expression tag	UNP P08539
E	12	ASP	-	expression tag	UNP P08539
E	13	GLU	-	expression tag	UNP P08539
E	14	SER	-	expression tag	UNP P08539
E	15	ASP	-	expression tag	UNP P08539
E	16	PRO	-	expression tag	UNP P08539
E	17	PHE	-	expression tag	UNP P08539
E	18	LEU	-	expression tag	UNP P08539
E	19	GLN	-	expression tag	UNP P08539
E	20	ASN	-	expression tag	UNP P08539
E	21	LYS	-	expression tag	UNP P08539
E	22	ARG	-	expression tag	UNP P08539
E	23	ALA	-	expression tag	UNP P08539
E	24	ASN	-	expression tag	UNP P08539
E	25	ASP	-	expression tag	UNP P08539
E	26	VAL	-	expression tag	UNP P08539
E	27	ILE	-	expression tag	UNP P08539
E	28	GLU	-	expression tag	UNP P08539

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Chain	Residue	Modelled	Actual	Comment	Reference
E	29	GLN	-	expression tag	UNP P08539
E	30	SER	-	expression tag	UNP P08539
E	31	LEU	-	expression tag	UNP P08539
E	32	GLN	-	expression tag	UNP P08539
E	33	LEU	-	expression tag	UNP P08539
E	34	GLU	-	expression tag	UNP P08539
E	35	LYS	-	expression tag	UNP P08539
E	36	GLN	-	expression tag	UNP P08539
E	37	ARG	-	expression tag	UNP P08539
E	38	ASP	-	expression tag	UNP P08539
E	39	LYS	-	expression tag	UNP P08539
E	40	ASN	-	expression tag	UNP P08539
E	41	GLU	-	expression tag	UNP P08539
E	42	ILE	-	expression tag	UNP P08539
E	43	LYS	-	expression tag	UNP P08539
E	44	LEU	-	expression tag	UNP P08539
E	45	LEU	-	expression tag	UNP P08539
E	46	LEU	-	expression tag	UNP P08539
E	47	LEU	-	expression tag	UNP P08539
E	48	GLY	-	expression tag	UNP P08539
E	49	ALA	-	expression tag	UNP P08539
E	50	GLY	-	expression tag	UNP P08539
E	51	GLU	-	expression tag	UNP P08539
E	52	SER	-	expression tag	UNP P08539
E	53	GLY	-	expression tag	UNP P08539
E	54	LYS	-	expression tag	UNP P08539
E	55	SER	-	expression tag	UNP P08539
E	56	THR	-	expression tag	UNP P08539
E	57	VAL	-	expression tag	UNP P08539
E	58	LEU	-	expression tag	UNP P08539
E	59	LYS	-	expression tag	UNP P08539
E	60	GLN	-	expression tag	UNP P08539
E	61	LEU	-	expression tag	UNP P08539
E	62	LYS	-	expression tag	UNP P08539
E	63	LEU	-	expression tag	UNP P08539
E	64	LEU	-	expression tag	UNP P08539
E	65	HIS	-	expression tag	UNP P08539
E	66	GLN	-	expression tag	UNP P08539
E	67	GLY	-	expression tag	UNP P08539
E	68	GLY	-	expression tag	UNP P08539
E	69	PHE	-	expression tag	UNP P08539
E	70	SER	-	expression tag	UNP P08539

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Chain	Residue	Modelled	Actual	Comment	Reference
E	71	HIS	-	expression tag	UNP P08539
E	72	GLN	-	expression tag	UNP P08539
E	73	GLU	-	expression tag	UNP P08539
E	74	ARG	-	expression tag	UNP P08539
E	75	LEU	-	expression tag	UNP P08539
E	76	GLN	-	expression tag	UNP P08539
E	77	TYR	-	expression tag	UNP P08539
E	78	ALA	-	expression tag	UNP P08539
E	79	GLN	-	expression tag	UNP P08539
E	80	VAL	-	expression tag	UNP P08539
E	81	ILE	-	expression tag	UNP P08539
E	82	TRP	-	expression tag	UNP P08539
E	83	ALA	-	expression tag	UNP P08539
E	84	ASP	-	expression tag	UNP P08539
E	85	ALA	-	expression tag	UNP P08539
E	86	ILE	-	expression tag	UNP P08539
E	87	GLN	-	expression tag	UNP P08539
E	88	SER	-	expression tag	UNP P08539
E	89	MET	-	expression tag	UNP P08539
E	90	LYS	-	expression tag	UNP P08539
E	91	ILE	-	expression tag	UNP P08539
E	92	LEU	-	expression tag	UNP P08539
E	93	ILE	-	expression tag	UNP P08539
E	94	ILE	-	expression tag	UNP P08539
E	95	GLN	-	expression tag	UNP P08539
E	96	ALA	-	expression tag	UNP P08539
E	97	ARG	-	expression tag	UNP P08539
E	98	LYS	-	expression tag	UNP P08539
E	99	LEU	-	expression tag	UNP P08539
E	100	GLY	-	expression tag	UNP P08539
E	101	ILE	-	expression tag	UNP P08539
E	102	GLN	-	expression tag	UNP P08539
E	103	LEU	-	expression tag	UNP P08539
E	104	ASP	-	expression tag	UNP P08539
E	105	CYS	-	expression tag	UNP P08539
E	106	ASP	-	expression tag	UNP P08539
E	107	ASP	-	expression tag	UNP P08539
E	108	PRO	-	expression tag	UNP P08539
E	109	ILE	-	expression tag	UNP P08539
E	110	ASN	-	expression tag	UNP P08539
E	111	ASN	-	expression tag	UNP P08539
E	112	LYS	-	expression tag	UNP P08539

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Chain	Residue	Modelled	Actual	Comment	Reference
E	113	ASP	-	expression tag	UNP P08539
E	114	LEU	-	expression tag	UNP P08539
E	115	PHE	-	expression tag	UNP P08539
E	116	ALA	-	expression tag	UNP P08539
E	117	CYS	-	expression tag	UNP P08539
E	118	LYS	-	expression tag	UNP P08539
E	119	ARG	-	expression tag	UNP P08539
E	120	ILE	-	expression tag	UNP P08539
E	121	LEU	-	expression tag	UNP P08539
E	122	LEU	-	expression tag	UNP P08539
E	123	LYS	-	expression tag	UNP P08539
E	124	ALA	-	expression tag	UNP P08539
E	125	LYS	-	expression tag	UNP P08539
E	126	ALA	-	expression tag	UNP P08539
E	127	LEU	-	expression tag	UNP P08539
E	128	ASP	-	expression tag	UNP P08539
E	129	TYR	-	expression tag	UNP P08539
E	130	ILE	-	expression tag	UNP P08539
E	131	ASN	-	expression tag	UNP P08539
E	132	ALA	-	expression tag	UNP P08539
E	133	SER	-	expression tag	UNP P08539
E	134	VAL	-	expression tag	UNP P08539
E	135	ALA	-	expression tag	UNP P08539
E	136	GLY	-	expression tag	UNP P08539
E	137	GLY	-	expression tag	UNP P08539
E	138	SER	-	expression tag	UNP P08539
E	139	ASP	-	expression tag	UNP P08539
E	140	PHE	-	expression tag	UNP P08539
E	141	LEU	-	expression tag	UNP P08539
E	142	ASN	-	expression tag	UNP P08539
E	143	ASP	-	expression tag	UNP P08539
E	144	TYR	-	expression tag	UNP P08539
E	145	VAL	-	expression tag	UNP P08539
E	146	LEU	-	expression tag	UNP P08539
E	147	LYS	-	expression tag	UNP P08539
E	148	TYR	-	expression tag	UNP P08539
E	149	SER	-	expression tag	UNP P08539
E	150	GLU	-	expression tag	UNP P08539
E	151	ARG	-	expression tag	UNP P08539
E	152	TYR	-	expression tag	UNP P08539
E	153	GLU	-	expression tag	UNP P08539
E	154	THR	-	expression tag	UNP P08539

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Chain	Residue	Modelled	Actual	Comment	Reference
E	155	ARG	-	expression tag	UNP P08539
E	156	ARG	-	expression tag	UNP P08539
E	157	ARG	-	expression tag	UNP P08539
E	158	VAL	-	expression tag	UNP P08539
E	159	GLN	-	expression tag	UNP P08539
E	160	SER	-	expression tag	UNP P08539
E	161	THR	-	expression tag	UNP P08539
E	162	GLY	-	expression tag	UNP P08539
E	163	ARG	-	expression tag	UNP P08539
E	164	ALA	-	expression tag	UNP P08539
E	165	LYS	-	expression tag	UNP P08539
E	166	ALA	-	expression tag	UNP P08539
E	167	ALA	-	expression tag	UNP P08539
E	168	PHE	-	expression tag	UNP P08539
E	169	ASP	-	expression tag	UNP P08539
E	170	GLU	-	expression tag	UNP P08539
E	171	ASP	-	expression tag	UNP P08539
E	172	GLY	-	expression tag	UNP P08539
E	173	ASN	-	expression tag	UNP P08539
E	174	ILE	-	expression tag	UNP P08539
E	175	SER	-	expression tag	UNP P08539
E	176	ASN	-	expression tag	UNP P08539
E	177	VAL	-	expression tag	UNP P08539
E	178	LYS	-	expression tag	UNP P08539
E	179	SER	-	expression tag	UNP P08539
E	180	ASP	-	expression tag	UNP P08539
E	181	THR	-	expression tag	UNP P08539
E	182	ASP	-	expression tag	UNP P08539
E	183	ARG	-	expression tag	UNP P08539
E	184	ASP	-	expression tag	UNP P08539
E	185	ALA	-	expression tag	UNP P08539
E	186	GLU	-	expression tag	UNP P08539
E	187	THR	-	expression tag	UNP P08539
E	188	VAL	-	expression tag	UNP P08539
E	189	THR	-	expression tag	UNP P08539
E	190	GLN	-	expression tag	UNP P08539
E	191	ASN	-	expression tag	UNP P08539
E	192	GLU	-	expression tag	UNP P08539
E	193	ASP	-	expression tag	UNP P08539
E	194	ALA	-	expression tag	UNP P08539
E	195	ASP	-	expression tag	UNP P08539
E	196	ARG	-	expression tag	UNP P08539

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Chain	Residue	Modelled	Actual	Comment	Reference
E	197	ASN	-	expression tag	UNP P08539
E	198	ASN	-	expression tag	UNP P08539
E	199	SER	-	expression tag	UNP P08539
E	200	SER	-	expression tag	UNP P08539
E	201	ARG	-	expression tag	UNP P08539
E	202	ILE	-	expression tag	UNP P08539
E	203	ASN	-	expression tag	UNP P08539
E	204	LEU	-	expression tag	UNP P08539
E	205	GLN	-	expression tag	UNP P08539
E	206	ASP	-	expression tag	UNP P08539
E	207	ILE	-	expression tag	UNP P08539
E	208	CYS	-	expression tag	UNP P08539
E	209	LYS	-	expression tag	UNP P08539
E	210	ASP	-	expression tag	UNP P08539
E	211	LEU	-	expression tag	UNP P08539
E	212	ASN	-	expression tag	UNP P08539
E	213	GLN	-	expression tag	UNP P08539
E	214	GLU	-	expression tag	UNP P08539
E	215	GLY	-	expression tag	UNP P08539
E	216	ASP	-	expression tag	UNP P08539
E	217	ASP	-	expression tag	UNP P08539
E	218	GLN	-	expression tag	UNP P08539
E	219	MET	-	expression tag	UNP P08539
E	220	PHE	-	expression tag	UNP P08539
E	221	VAL	-	expression tag	UNP P08539
E	222	ARG	-	expression tag	UNP P08539
E	223	LYS	-	expression tag	UNP P08539
E	224	THR	-	expression tag	UNP P08539
E	225	SER	-	expression tag	UNP P08539
E	226	ARG	-	expression tag	UNP P08539
E	227	GLU	-	expression tag	UNP P08539
E	228	ILE	-	expression tag	UNP P08539
E	229	GLN	-	expression tag	UNP P08539
E	230	GLY	-	expression tag	UNP P08539
E	231	GLN	-	expression tag	UNP P08539
E	232	ASN	-	expression tag	UNP P08539
E	233	ARG	-	expression tag	UNP P08539
E	234	ARG	-	expression tag	UNP P08539
E	235	ASN	-	expression tag	UNP P08539
E	236	LEU	-	expression tag	UNP P08539
E	237	ILE	-	expression tag	UNP P08539
E	238	HIS	-	expression tag	UNP P08539

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Chain	Residue	Modelled	Actual	Comment	Reference
E	239	GLU	-	expression tag	UNP P08539
E	240	ASP	-	expression tag	UNP P08539
E	241	ILE	-	expression tag	UNP P08539
E	242	ALA	-	expression tag	UNP P08539
E	243	LYS	-	expression tag	UNP P08539
E	244	ALA	-	expression tag	UNP P08539
E	245	ILE	-	expression tag	UNP P08539
E	246	LYS	-	expression tag	UNP P08539
E	247	GLN	-	expression tag	UNP P08539
E	248	LEU	-	expression tag	UNP P08539
E	249	TRP	-	expression tag	UNP P08539
E	250	ASN	-	expression tag	UNP P08539
E	251	ASN	-	expression tag	UNP P08539
E	252	ASP	-	expression tag	UNP P08539
E	253	LYS	-	expression tag	UNP P08539
E	254	GLY	-	expression tag	UNP P08539
E	255	ILE	-	expression tag	UNP P08539
E	256	LYS	-	expression tag	UNP P08539
E	257	GLN	-	expression tag	UNP P08539
E	258	CYS	-	expression tag	UNP P08539
E	259	PHE	-	expression tag	UNP P08539
E	260	ALA	-	expression tag	UNP P08539
E	261	ARG	-	expression tag	UNP P08539
E	262	SER	-	expression tag	UNP P08539
E	263	ASN	-	expression tag	UNP P08539
E	264	GLU	-	expression tag	UNP P08539
E	265	PHE	-	expression tag	UNP P08539
E	266	GLN	-	expression tag	UNP P08539
E	267	LEU	-	expression tag	UNP P08539
E	268	GLU	-	expression tag	UNP P08539
E	269	GLY	-	expression tag	UNP P08539
E	270	SER	-	expression tag	UNP P08539
E	271	ALA	-	expression tag	UNP P08539
E	272	ALA	-	expression tag	UNP P08539
E	273	TYR	-	expression tag	UNP P08539
E	274	TYR	-	expression tag	UNP P08539
E	275	PHE	-	expression tag	UNP P08539
E	276	ASP	-	expression tag	UNP P08539
E	277	ASN	-	expression tag	UNP P08539
E	278	ILE	-	expression tag	UNP P08539
E	279	GLU	-	expression tag	UNP P08539
E	280	LYS	-	expression tag	UNP P08539

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Chain	Residue	Modelled	Actual	Comment	Reference
E	281	PHE	-	expression tag	UNP P08539
E	282	ALA	-	expression tag	UNP P08539
E	283	SER	-	expression tag	UNP P08539
E	284	PRO	-	expression tag	UNP P08539
E	285	ASN	-	expression tag	UNP P08539
E	286	TYR	-	expression tag	UNP P08539
E	287	VAL	-	expression tag	UNP P08539
E	288	CYS	-	expression tag	UNP P08539
E	289	THR	-	expression tag	UNP P08539
E	290	ASP	-	expression tag	UNP P08539
E	291	GLU	-	expression tag	UNP P08539
E	292	ASP	-	expression tag	UNP P08539
E	293	ILE	-	expression tag	UNP P08539
E	294	LEU	-	expression tag	UNP P08539
E	295	LYS	-	expression tag	UNP P08539
E	296	GLY	-	expression tag	UNP P08539
E	297	ARG	-	expression tag	UNP P08539
E	298	ILE	-	expression tag	UNP P08539
E	299	LYS	-	expression tag	UNP P08539
E	300	THR	-	expression tag	UNP P08539
D	1	MET	-	initiating methionine	UNP P08539
D	2	GLY	-	expression tag	UNP P08539
D	3	CYS	-	expression tag	UNP P08539
D	4	THR	-	expression tag	UNP P08539
D	5	VAL	-	expression tag	UNP P08539
D	6	SER	-	expression tag	UNP P08539
D	7	THR	-	expression tag	UNP P08539
D	8	GLN	-	expression tag	UNP P08539
D	9	THR	-	expression tag	UNP P08539
D	10	ILE	-	expression tag	UNP P08539
D	11	GLY	-	expression tag	UNP P08539
D	12	ASP	-	expression tag	UNP P08539
D	13	GLU	-	expression tag	UNP P08539
D	14	SER	-	expression tag	UNP P08539
D	15	ASP	-	expression tag	UNP P08539
D	16	PRO	-	expression tag	UNP P08539
D	17	PHE	-	expression tag	UNP P08539
D	18	LEU	-	expression tag	UNP P08539
D	19	GLN	-	expression tag	UNP P08539
D	20	ASN	-	expression tag	UNP P08539
D	21	LYS	-	expression tag	UNP P08539
D	22	ARG	-	expression tag	UNP P08539

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Chain	Residue	Modelled	Actual	Comment	Reference
D	23	ALA	-	expression tag	UNP P08539
D	24	ASN	-	expression tag	UNP P08539
D	25	ASP	-	expression tag	UNP P08539
D	26	VAL	-	expression tag	UNP P08539
D	27	ILE	-	expression tag	UNP P08539
D	28	GLU	-	expression tag	UNP P08539
D	29	GLN	-	expression tag	UNP P08539
D	30	SER	-	expression tag	UNP P08539
D	31	LEU	-	expression tag	UNP P08539
D	32	GLN	-	expression tag	UNP P08539
D	33	LEU	-	expression tag	UNP P08539
D	34	GLU	-	expression tag	UNP P08539
D	35	LYS	-	expression tag	UNP P08539
D	36	GLN	-	expression tag	UNP P08539
D	37	ARG	-	expression tag	UNP P08539
D	38	ASP	-	expression tag	UNP P08539
D	39	LYS	-	expression tag	UNP P08539
D	40	ASN	-	expression tag	UNP P08539
D	41	GLU	-	expression tag	UNP P08539
D	42	ILE	-	expression tag	UNP P08539
D	43	LYS	-	expression tag	UNP P08539
D	44	LEU	-	expression tag	UNP P08539
D	45	LEU	-	expression tag	UNP P08539
D	46	LEU	-	expression tag	UNP P08539
D	47	LEU	-	expression tag	UNP P08539
D	48	GLY	-	expression tag	UNP P08539
D	49	ALA	-	expression tag	UNP P08539
D	50	GLY	-	expression tag	UNP P08539
D	51	GLU	-	expression tag	UNP P08539
D	52	SER	-	expression tag	UNP P08539
D	53	GLY	-	expression tag	UNP P08539
D	54	LYS	-	expression tag	UNP P08539
D	55	SER	-	expression tag	UNP P08539
D	56	THR	-	expression tag	UNP P08539
D	57	VAL	-	expression tag	UNP P08539
D	58	LEU	-	expression tag	UNP P08539
D	59	LYS	-	expression tag	UNP P08539
D	60	GLN	-	expression tag	UNP P08539
D	61	LEU	-	expression tag	UNP P08539
D	62	LYS	-	expression tag	UNP P08539
D	63	LEU	-	expression tag	UNP P08539
D	64	LEU	-	expression tag	UNP P08539

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Chain	Residue	Modelled	Actual	Comment	Reference
D	65	HIS	-	expression tag	UNP P08539
D	66	GLN	-	expression tag	UNP P08539
D	67	GLY	-	expression tag	UNP P08539
D	68	GLY	-	expression tag	UNP P08539
D	69	PHE	-	expression tag	UNP P08539
D	70	SER	-	expression tag	UNP P08539
D	71	HIS	-	expression tag	UNP P08539
D	72	GLN	-	expression tag	UNP P08539
D	73	GLU	-	expression tag	UNP P08539
D	74	ARG	-	expression tag	UNP P08539
D	75	LEU	-	expression tag	UNP P08539
D	76	GLN	-	expression tag	UNP P08539
D	77	TYR	-	expression tag	UNP P08539
D	78	ALA	-	expression tag	UNP P08539
D	79	GLN	-	expression tag	UNP P08539
D	80	VAL	-	expression tag	UNP P08539
D	81	ILE	-	expression tag	UNP P08539
D	82	TRP	-	expression tag	UNP P08539
D	83	ALA	-	expression tag	UNP P08539
D	84	ASP	-	expression tag	UNP P08539
D	85	ALA	-	expression tag	UNP P08539
D	86	ILE	-	expression tag	UNP P08539
D	87	GLN	-	expression tag	UNP P08539
D	88	SER	-	expression tag	UNP P08539
D	89	MET	-	expression tag	UNP P08539
D	90	LYS	-	expression tag	UNP P08539
D	91	ILE	-	expression tag	UNP P08539
D	92	LEU	-	expression tag	UNP P08539
D	93	ILE	-	expression tag	UNP P08539
D	94	ILE	-	expression tag	UNP P08539
D	95	GLN	-	expression tag	UNP P08539
D	96	ALA	-	expression tag	UNP P08539
D	97	ARG	-	expression tag	UNP P08539
D	98	LYS	-	expression tag	UNP P08539
D	99	LEU	-	expression tag	UNP P08539
D	100	GLY	-	expression tag	UNP P08539
D	101	ILE	-	expression tag	UNP P08539
D	102	GLN	-	expression tag	UNP P08539
D	103	LEU	-	expression tag	UNP P08539
D	104	ASP	-	expression tag	UNP P08539
D	105	CYS	-	expression tag	UNP P08539
D	106	ASP	-	expression tag	UNP P08539

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Chain	Residue	Modelled	Actual	Comment	Reference
D	107	ASP	-	expression tag	UNP P08539
D	108	PRO	-	expression tag	UNP P08539
D	109	ILE	-	expression tag	UNP P08539
D	110	ASN	-	expression tag	UNP P08539
D	111	ASN	-	expression tag	UNP P08539
D	112	LYS	-	expression tag	UNP P08539
D	113	ASP	-	expression tag	UNP P08539
D	114	LEU	-	expression tag	UNP P08539
D	115	PHE	-	expression tag	UNP P08539
D	116	ALA	-	expression tag	UNP P08539
D	117	CYS	-	expression tag	UNP P08539
D	118	LYS	-	expression tag	UNP P08539
D	119	ARG	-	expression tag	UNP P08539
D	120	ILE	-	expression tag	UNP P08539
D	121	LEU	-	expression tag	UNP P08539
D	122	LEU	-	expression tag	UNP P08539
D	123	LYS	-	expression tag	UNP P08539
D	124	ALA	-	expression tag	UNP P08539
D	125	LYS	-	expression tag	UNP P08539
D	126	ALA	-	expression tag	UNP P08539
D	127	LEU	-	expression tag	UNP P08539
D	128	ASP	-	expression tag	UNP P08539
D	129	TYR	-	expression tag	UNP P08539
D	130	ILE	-	expression tag	UNP P08539
D	131	ASN	-	expression tag	UNP P08539
D	132	ALA	-	expression tag	UNP P08539
D	133	SER	-	expression tag	UNP P08539
D	134	VAL	-	expression tag	UNP P08539
D	135	ALA	-	expression tag	UNP P08539
D	136	GLY	-	expression tag	UNP P08539
D	137	GLY	-	expression tag	UNP P08539
D	138	SER	-	expression tag	UNP P08539
D	139	ASP	-	expression tag	UNP P08539
D	140	PHE	-	expression tag	UNP P08539
D	141	LEU	-	expression tag	UNP P08539
D	142	ASN	-	expression tag	UNP P08539
D	143	ASP	-	expression tag	UNP P08539
D	144	TYR	-	expression tag	UNP P08539
D	145	VAL	-	expression tag	UNP P08539
D	146	LEU	-	expression tag	UNP P08539
D	147	LYS	-	expression tag	UNP P08539
D	148	TYR	-	expression tag	UNP P08539

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Chain	Residue	Modelled	Actual	Comment	Reference
D	149	SER	-	expression tag	UNP P08539
D	150	GLU	-	expression tag	UNP P08539
D	151	ARG	-	expression tag	UNP P08539
D	152	TYR	-	expression tag	UNP P08539
D	153	GLU	-	expression tag	UNP P08539
D	154	THR	-	expression tag	UNP P08539
D	155	ARG	-	expression tag	UNP P08539
D	156	ARG	-	expression tag	UNP P08539
D	157	ARG	-	expression tag	UNP P08539
D	158	VAL	-	expression tag	UNP P08539
D	159	GLN	-	expression tag	UNP P08539
D	160	SER	-	expression tag	UNP P08539
D	161	THR	-	expression tag	UNP P08539
D	162	GLY	-	expression tag	UNP P08539
D	163	ARG	-	expression tag	UNP P08539
D	164	ALA	-	expression tag	UNP P08539
D	165	LYS	-	expression tag	UNP P08539
D	166	ALA	-	expression tag	UNP P08539
D	167	ALA	-	expression tag	UNP P08539
D	168	PHE	-	expression tag	UNP P08539
D	169	ASP	-	expression tag	UNP P08539
D	170	GLU	-	expression tag	UNP P08539
D	171	ASP	-	expression tag	UNP P08539
D	172	GLY	-	expression tag	UNP P08539
D	173	ASN	-	expression tag	UNP P08539
D	174	ILE	-	expression tag	UNP P08539
D	175	SER	-	expression tag	UNP P08539
D	176	ASN	-	expression tag	UNP P08539
D	177	VAL	-	expression tag	UNP P08539
D	178	LYS	-	expression tag	UNP P08539
D	179	SER	-	expression tag	UNP P08539
D	180	ASP	-	expression tag	UNP P08539
D	181	THR	-	expression tag	UNP P08539
D	182	ASP	-	expression tag	UNP P08539
D	183	ARG	-	expression tag	UNP P08539
D	184	ASP	-	expression tag	UNP P08539
D	185	ALA	-	expression tag	UNP P08539
D	186	GLU	-	expression tag	UNP P08539
D	187	THR	-	expression tag	UNP P08539
D	188	VAL	-	expression tag	UNP P08539
D	189	THR	-	expression tag	UNP P08539
D	190	GLN	-	expression tag	UNP P08539

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Chain	Residue	Modelled	Actual	Comment	Reference
D	191	ASN	-	expression tag	UNP P08539
D	192	GLU	-	expression tag	UNP P08539
D	193	ASP	-	expression tag	UNP P08539
D	194	ALA	-	expression tag	UNP P08539
D	195	ASP	-	expression tag	UNP P08539
D	196	ARG	-	expression tag	UNP P08539
D	197	ASN	-	expression tag	UNP P08539
D	198	ASN	-	expression tag	UNP P08539
D	199	SER	-	expression tag	UNP P08539
D	200	SER	-	expression tag	UNP P08539
D	201	ARG	-	expression tag	UNP P08539
D	202	ILE	-	expression tag	UNP P08539
D	203	ASN	-	expression tag	UNP P08539
D	204	LEU	-	expression tag	UNP P08539
D	205	GLN	-	expression tag	UNP P08539
D	206	ASP	-	expression tag	UNP P08539
D	207	ILE	-	expression tag	UNP P08539
D	208	CYS	-	expression tag	UNP P08539
D	209	LYS	-	expression tag	UNP P08539
D	210	ASP	-	expression tag	UNP P08539
D	211	LEU	-	expression tag	UNP P08539
D	212	ASN	-	expression tag	UNP P08539
D	213	GLN	-	expression tag	UNP P08539
D	214	GLU	-	expression tag	UNP P08539
D	215	GLY	-	expression tag	UNP P08539
D	216	ASP	-	expression tag	UNP P08539
D	217	ASP	-	expression tag	UNP P08539
D	218	GLN	-	expression tag	UNP P08539
D	219	MET	-	expression tag	UNP P08539
D	220	PHE	-	expression tag	UNP P08539
D	221	VAL	-	expression tag	UNP P08539
D	222	ARG	-	expression tag	UNP P08539
D	223	LYS	-	expression tag	UNP P08539
D	224	THR	-	expression tag	UNP P08539
D	225	SER	-	expression tag	UNP P08539
D	226	ARG	-	expression tag	UNP P08539
D	227	GLU	-	expression tag	UNP P08539
D	228	ILE	-	expression tag	UNP P08539
D	229	GLN	-	expression tag	UNP P08539
D	230	GLY	-	expression tag	UNP P08539
D	231	GLN	-	expression tag	UNP P08539
D	232	ASN	-	expression tag	UNP P08539

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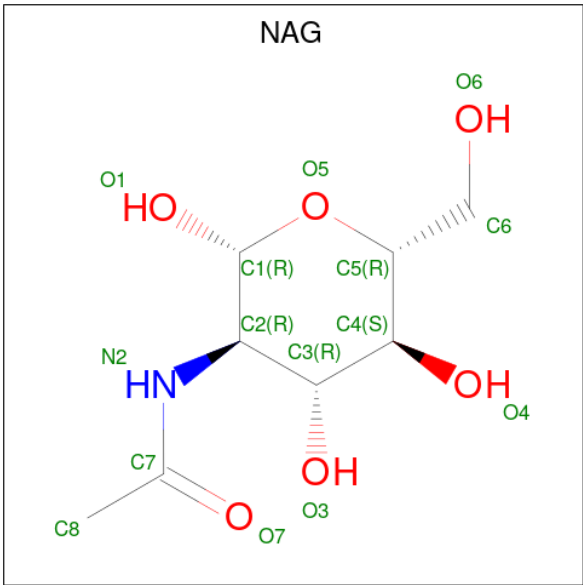
Chain	Residue	Modelled	Actual	Comment	Reference
D	233	ARG	-	expression tag	UNP P08539
D	234	ARG	-	expression tag	UNP P08539
D	235	ASN	-	expression tag	UNP P08539
D	236	LEU	-	expression tag	UNP P08539
D	237	ILE	-	expression tag	UNP P08539
D	238	HIS	-	expression tag	UNP P08539
D	239	GLU	-	expression tag	UNP P08539
D	240	ASP	-	expression tag	UNP P08539
D	241	ILE	-	expression tag	UNP P08539
D	242	ALA	-	expression tag	UNP P08539
D	243	LYS	-	expression tag	UNP P08539
D	244	ALA	-	expression tag	UNP P08539
D	245	ILE	-	expression tag	UNP P08539
D	246	LYS	-	expression tag	UNP P08539
D	247	GLN	-	expression tag	UNP P08539
D	248	LEU	-	expression tag	UNP P08539
D	249	TRP	-	expression tag	UNP P08539
D	250	ASN	-	expression tag	UNP P08539
D	251	ASN	-	expression tag	UNP P08539
D	252	ASP	-	expression tag	UNP P08539
D	253	LYS	-	expression tag	UNP P08539
D	254	GLY	-	expression tag	UNP P08539
D	255	ILE	-	expression tag	UNP P08539
D	256	LYS	-	expression tag	UNP P08539
D	257	GLN	-	expression tag	UNP P08539
D	258	CYS	-	expression tag	UNP P08539
D	259	PHE	-	expression tag	UNP P08539
D	260	ALA	-	expression tag	UNP P08539
D	261	ARG	-	expression tag	UNP P08539
D	262	SER	-	expression tag	UNP P08539
D	263	ASN	-	expression tag	UNP P08539
D	264	GLU	-	expression tag	UNP P08539
D	265	PHE	-	expression tag	UNP P08539
D	266	GLN	-	expression tag	UNP P08539
D	267	LEU	-	expression tag	UNP P08539
D	268	GLU	-	expression tag	UNP P08539
D	269	GLY	-	expression tag	UNP P08539
D	270	SER	-	expression tag	UNP P08539
D	271	ALA	-	expression tag	UNP P08539
D	272	ALA	-	expression tag	UNP P08539
D	273	TYR	-	expression tag	UNP P08539
D	274	TYR	-	expression tag	UNP P08539

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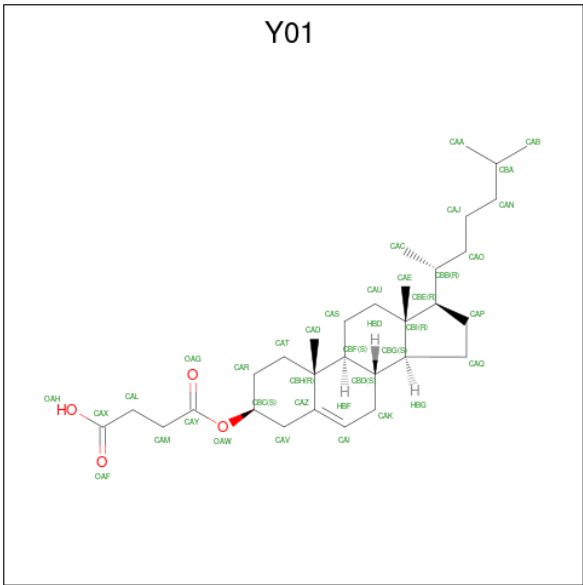
Chain	Residue	Modelled	Actual	Comment	Reference
D	275	PHE	-	expression tag	UNP P08539
D	276	ASP	-	expression tag	UNP P08539
D	277	ASN	-	expression tag	UNP P08539
D	278	ILE	-	expression tag	UNP P08539
D	279	GLU	-	expression tag	UNP P08539
D	280	LYS	-	expression tag	UNP P08539
D	281	PHE	-	expression tag	UNP P08539
D	282	ALA	-	expression tag	UNP P08539
D	283	SER	-	expression tag	UNP P08539
D	284	PRO	-	expression tag	UNP P08539
D	285	ASN	-	expression tag	UNP P08539
D	286	TYR	-	expression tag	UNP P08539
D	287	VAL	-	expression tag	UNP P08539
D	288	CYS	-	expression tag	UNP P08539
D	289	THR	-	expression tag	UNP P08539
D	290	ASP	-	expression tag	UNP P08539
D	291	GLU	-	expression tag	UNP P08539
D	292	ASP	-	expression tag	UNP P08539
D	293	ILE	-	expression tag	UNP P08539
D	294	LEU	-	expression tag	UNP P08539
D	295	LYS	-	expression tag	UNP P08539
D	296	GLY	-	expression tag	UNP P08539
D	297	ARG	-	expression tag	UNP P08539
D	298	ILE	-	expression tag	UNP P08539
D	299	LYS	-	expression tag	UNP P08539
D	300	THR	-	expression tag	UNP P08539

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 7 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).



Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	H	O	0
			84	31	49	4	
7	B	1	Total	C	H	O	0
			84	31	49	4	

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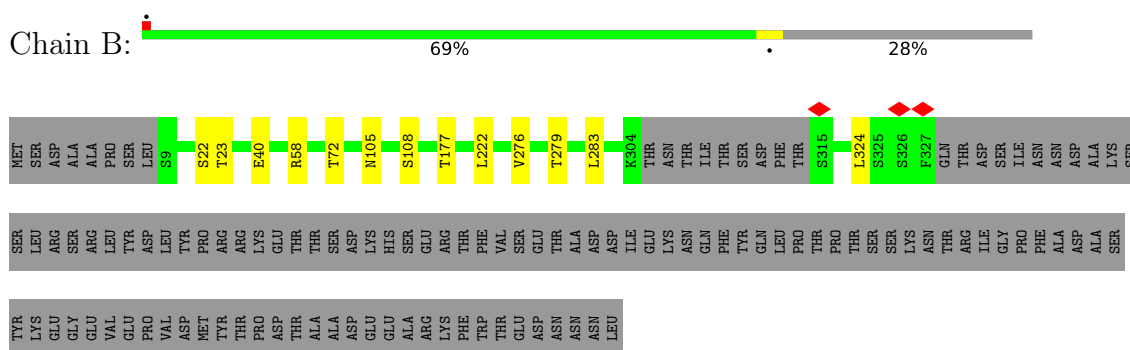
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Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	H	O	0
			84	31	49	4	
7	B	1	Total	C	H	O	0
			84	31	49	4	
7	B	1	Total	C	H	O	0
			84	31	49	4	
7	A	1	Total	C	H	O	0
			84	31	49	4	
7	A	1	Total	C	H	O	0
			84	31	49	4	
7	A	1	Total	C	H	O	0
			84	31	49	4	
7	A	1	Total	C	H	O	0
			84	31	49	4	

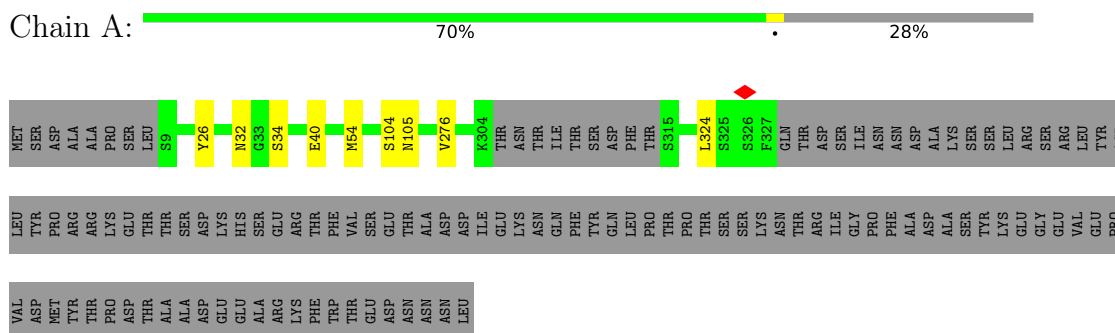
3 Residue-property plots [i](#)

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: Pheromone alpha factor receptor



- Molecule 1: Pheromone alpha factor receptor



- Molecule 2: Mating factor alpha



There are no outlier residues recorded for this chain.

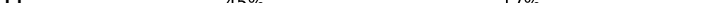
- Molecule 2: Mating factor alpha



There are no outlier residues recorded for this chain.

- Molecule 3: Guanine nucleotide-binding protein subunit gamma

SER	ASN	SER	SER	VAL	CYS	CYS	THR	LEU	MET																																						
MET	THR	THR	VAL	GLN	ASN	ASN	SER	PRO	ARG	LEU	GLN	GLN	PRO	GLN	GLN	GLN	GLN	GLN	LEU	SER	LEU	LYS	ILE	LYS	GLN	R50	151	752	A56	T64	T67	X68	D69	P73	E74	L75	V76	G77	Y78	P79	V80	A81	G82	L90	Q98	MET	ASN

- Chain H:  45% 17% 37%

[illegible]

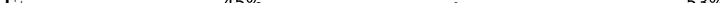
- Chain C:  74% 11% 15%

GLU	TYR	ASN	THR	A333	Q337	T338	L339	L347	S358	A359	S360	G361	R362	D370	V375	G385	K386	R398	S410	W411	M415	K416	G421	TYR	GLN																										
II30	ALA	ALA	ALA	ALA	II30	DI33	II42	LI54	YI61	R168	II87	II95	II96	II97	II98	S199	G200	D220	P234	ASN	SER	GLU	ASN	SER	S240	P241	T242	S271	S284	D290	R300	L310	F311	GLY	TYR	GLU	GLU	ARG	THR	PRO	THR	PRO	THR	TYR	MET	ALA	ALA	ALA	ASN	ASN	MET

- Chain F: 74% 10% 15%

Relative frequencies of amino acids in the protein. The chart shows the relative frequency of each amino acid on the x-axis (0 to 1.0) and the amino acid name on the y-axis. The bars are color-coded: grey for common, yellow for less common, orange for rare, and red for very rare. A red diamond marker is placed above the K38 bar.

Amino Acid	Relative Frequency (approx.)	Category
T338	0.05	Common
L339	0.05	Common
D348	0.05	Common
N349	0.05	Common
S358	0.05	Common
A359	0.05	Common
S360	0.05	Common
G361	0.05	Common
R362	0.05	Common
D370	0.05	Common
L379	0.05	Common
K386	0.05	Rare
R398	0.05	Common
D402	0.05	Common
G403	0.05	Common
S410	0.05	Common
W411	0.05	Common
G421	0.05	Common
T421	0.05	Common
GLN	0.05	Common
I142	0.05	Common
Y161	0.05	Common
D186	0.05	Common
I187	0.05	Common
I195	0.05	Common
L196	0.05	Common
T197	0.05	Common
H221	0.05	Common
P234	0.05	Common
ASN	0.05	Common
GLU	0.05	Common
ASN	0.05	Common
S240	0.05	Common
N241	0.05	Common
T242	0.05	Common
D249	0.05	Common
G250	0.05	Common
D256	0.05	Common
L273	0.05	Common
G288	0.05	Common
R300	0.05	Common
L310	0.05	Common
F311	0.05	Common
ARG	0.05	Common
GLY	0.05	Common
TYR	0.05	Common
GLU	0.05	Common
GLU	0.05	Common
ARG	0.05	Common
THR	0.05	Common
PRO	0.05	Common
THR	0.05	Common
PRO	0.05	Common
THR	0.05	Common
THR	0.05	Common
TYR	0.05	Common
MET	0.05	Common
ALA	0.05	Common
ALA	0.05	Common
ASN	0.05	Common
MET	0.05	Common
GLU	0.05	Common
TYR	0.05	Common
ASN	0.05	Common
THR	0.05	Common
A333	0.05	Common
G334	0.05	Common
S335	0.05	Common
MET	0.05	Common
ALA	0.05	Common
HIS	0.05	Common
GLN	0.05	Common
MET	0.05	Common
ASP	0.05	Common
SER	0.05	Common
SER	0.05	Common
ILE	0.05	Common
THR	0.05	Common
TYR	0.05	Common
SER	0.05	Common
ASN	0.05	Common
ASN	0.05	Common
VAL	0.05	Common
THR	0.05	Common
THR	0.05	Common
GLN	0.05	Common
GLN	0.05	Common
TYR	0.05	Common
ILE	0.05	Common
GLN	0.05	Common
PRO	0.05	Common
GLN	0.05	Common
SER	0.05	Common
LEU	0.05	Common
GLN	0.05	Common
ASP	0.05	Common
ILE	0.05	Common
SER	0.05	Common
ALA	0.05	Common
VAL	0.05	Common
GLU	0.05	Common
GLU	0.05	Common
ASP	0.05	Common
GLU	0.05	Common
ILE	0.05	Common
GLN	0.05	Common
ASN	0.05	Common
K38	0.05	Very Rare
R43	0.05	Less Common
Q44	0.05	Less Common
E45	0.05	Less Common
S46	0.05	Less Common
K47	0.05	Less Common
Q48	0.05	Less Common
L49	0.05	Less Common
M68	0.05	Less Common
I107	0.05	Less Common
D120	0.05	Less Common
S121	0.05	Less Common
K126	0.05	Less Common
I130	0.05	Rare
D133	0.05	Less Common

- Chain E:  45% . 53%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	393315	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.750	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.0136	Depositor
Map size (Å)	240.8, 240.8, 240.8	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	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: Y01, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.23	0/2404	0.35	0/3278
1	B	0.23	0/2414	0.40	2/3289 (0.1%)
2	I	0.23	0/127	0.38	0/172
2	K	0.27	0/127	0.64	0/172
3	G	0.24	0/454	0.76	3/628 (0.5%)
3	H	0.25	0/454	0.78	5/628 (0.8%)
4	C	0.25	0/2656	0.68	12/3617 (0.3%)
4	F	0.26	0/2656	0.74	13/3617 (0.4%)
5	D	0.22	0/1748	0.46	2/2359 (0.1%)
5	E	0.22	0/1748	0.40	0/2359
All	All	0.24	0/14788	0.56	37/20119 (0.2%)

There are no bond length outliers.

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	126	LYS	CA-C-N	11.66	140.50	122.42
4	F	126	LYS	C-N-CA	11.66	140.50	122.42
4	F	256	ASP	CA-C-N	10.29	135.10	120.28
4	F	256	ASP	C-N-CA	10.29	135.10	120.28
4	C	126	LYS	CA-C-N	10.10	140.30	121.81

There are no chirality outliers.

There are no planarity outliers.

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	A	2357	2312	2395	5	0
1	B	2367	2334	2417	7	0
2	I	120	115	115	0	0
2	K	120	115	115	0	0
3	G	446	126	339	8	0
3	H	446	126	339	16	0
4	C	2606	2152	2405	22	0
4	F	2606	2152	2405	26	0
5	D	1720	1435	1695	10	0
5	E	1720	1435	1695	7	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
7	A	175	245	245	0	0
7	B	175	245	245	0	0
All	All	14886	12792	14436	90	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 3.

The worst 5 of 90 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)
5:E:63:LEU:HD12	5:E:64:LEU:HG	1.58	0.85
3:H:74:GLU:HG2	3:H:75:LEU:HD12	1.61	0.80
4:C:271:SER:OG	4:C:290:ASP:OD2	2.07	0.73
3:H:65:SER:OG	3:H:66:ASN:OD1	2.09	0.69
1:A:26:TYR:O	1:A:34:SER:OG	2.11	0.69

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	Percentiles	
1	A	305/430 (71%)	295 (97%)	10 (3%)	0	100	100
1	B	305/430 (71%)	291 (95%)	14 (5%)	0	100	100
2	I	11/13 (85%)	11 (100%)	0	0	100	100
2	K	11/13 (85%)	11 (100%)	0	0	100	100
3	G	67/110 (61%)	61 (91%)	6 (9%)	0	100	100
3	H	67/110 (61%)	63 (94%)	4 (6%)	0	100	100
4	C	352/423 (83%)	331 (94%)	21 (6%)	0	100	100
4	F	352/423 (83%)	328 (93%)	24 (7%)	0	100	100
5	D	220/472 (47%)	206 (94%)	14 (6%)	0	100	100
5	E	220/472 (47%)	207 (94%)	13 (6%)	0	100	100
All	All	1910/2896 (66%)	1804 (94%)	106 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	Percentiles	
1	A	263/382 (69%)	262 (100%)	1 (0%)	84	93
1	B	265/382 (69%)	264 (100%)	1 (0%)	84	93
2	I	12/12 (100%)	12 (100%)	0	100	100
2	K	12/12 (100%)	12 (100%)	0	100	100
3	G	31/103 (30%)	30 (97%)	1 (3%)	34	67
3	H	31/103 (30%)	30 (97%)	1 (3%)	34	67
4	C	268/364 (74%)	264 (98%)	4 (2%)	57	81
4	F	268/364 (74%)	266 (99%)	2 (1%)	76	90
5	D	179/417 (43%)	177 (99%)	2 (1%)	65	85
5	E	179/417 (43%)	176 (98%)	3 (2%)	53	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1508/2556 (59%)	1493 (99%)	15 (1%)	65 86

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	63	LEU
5	D	450	MET
5	E	305	GLU
3	H	51	ILE
4	F	221	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
4	C	112	GLN
4	F	127	GLN
5	D	434	ASN
1	B	301	ASN
1	A	21	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	Y01	B	502	-	38,38,38	0.48	0	57,57,57	0.54	0
7	Y01	B	505	-	38,38,38	0.48	0	57,57,57	0.55	0
6	NAG	A	501	1	14,14,15	1.89	3 (21%)	17,19,21	1.03	1 (5%)
7	Y01	A	503	-	38,38,38	0.48	0	57,57,57	0.53	0
7	Y01	A	502	-	38,38,38	0.47	0	57,57,57	0.44	0
7	Y01	B	504	-	38,38,38	0.47	0	57,57,57	0.46	0
7	Y01	B	506	-	38,38,38	0.47	0	57,57,57	0.44	0
7	Y01	A	506	-	38,38,38	0.46	0	57,57,57	0.44	0
6	NAG	B	501	1	14,14,15	1.87	3 (21%)	17,19,21	1.03	1 (5%)
7	Y01	A	504	-	38,38,38	0.47	0	57,57,57	0.47	0
7	Y01	B	503	-	38,38,38	0.48	0	57,57,57	0.48	0
7	Y01	A	505	-	38,38,38	0.48	0	57,57,57	0.44	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
7	Y01	B	502	-	-	7/19/77/77	0/4/4/4
7	Y01	B	505	-	-	5/19/77/77	0/4/4/4
6	NAG	A	501	1	-	2/6/23/26	0/1/1/1
7	Y01	A	503	-	-	4/19/77/77	0/4/4/4
7	Y01	A	502	-	-	4/19/77/77	0/4/4/4
7	Y01	B	504	-	-	8/19/77/77	0/4/4/4
7	Y01	B	506	-	-	3/19/77/77	0/4/4/4
7	Y01	A	506	-	-	6/19/77/77	0/4/4/4
6	NAG	B	501	1	-	2/6/23/26	0/1/1/1
7	Y01	A	504	-	-	8/19/77/77	0/4/4/4
7	Y01	B	503	-	-	5/19/77/77	0/4/4/4
7	Y01	A	505	-	-	2/19/77/77	0/4/4/4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	501	NAG	O5-C1	4.40	1.50	1.43
6	B	501	NAG	O5-C1	4.31	1.50	1.43
6	B	501	NAG	C7-N2	3.22	1.45	1.34
6	A	501	NAG	C7-N2	3.21	1.45	1.34
6	A	501	NAG	C2-N2	2.14	1.50	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	501	NAG	C8-C7-N2	2.26	119.92	116.10
6	A	501	NAG	C8-C7-N2	2.20	119.82	116.10

There are no chirality outliers.

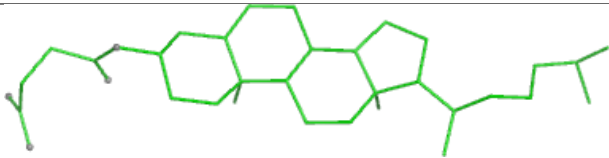
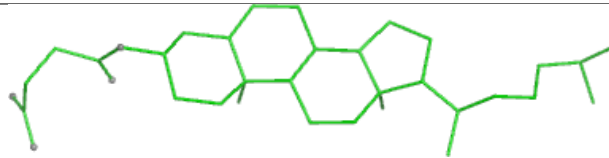
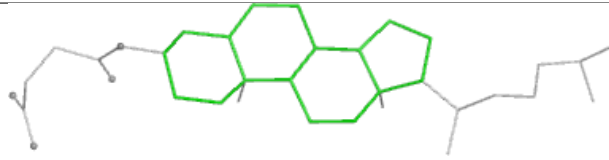
5 of 56 torsion outliers are listed below:

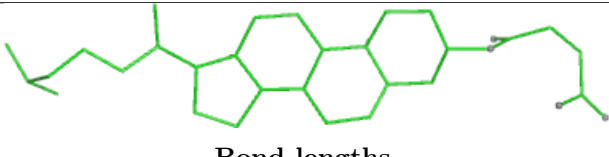
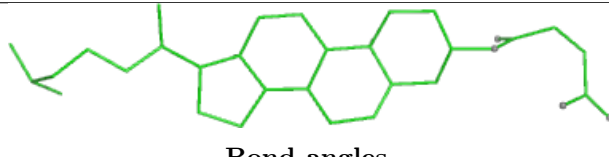
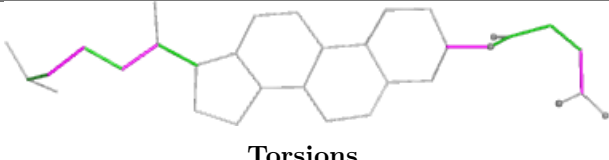
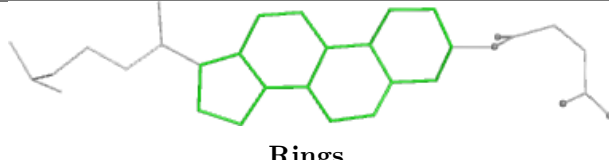
Mol	Chain	Res	Type	Atoms
7	B	504	Y01	OAG-CAY-OAW-CBC
7	B	504	Y01	CAM-CAY-OAW-CBC
7	B	505	Y01	CAR-CBC-OAW-CAY
7	A	503	Y01	CAV-CBC-OAW-CAY
7	A	504	Y01	OAG-CAY-OAW-CBC

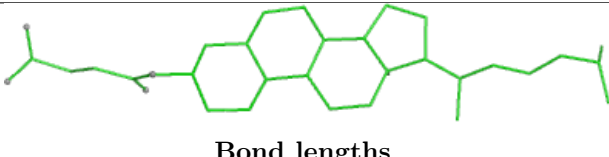
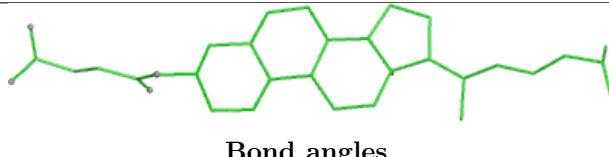
There are no ring outliers.

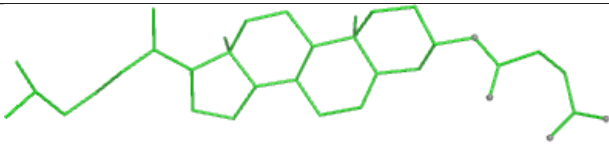
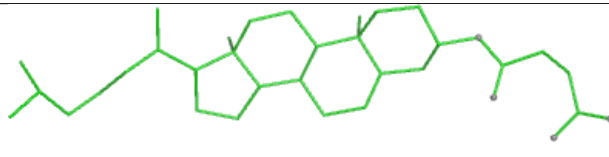
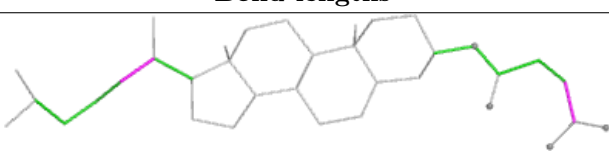
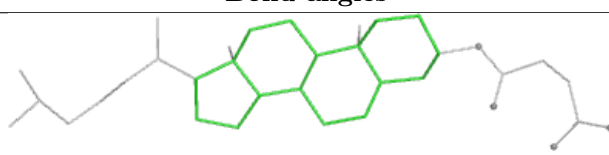
No monomer is involved in short contacts.

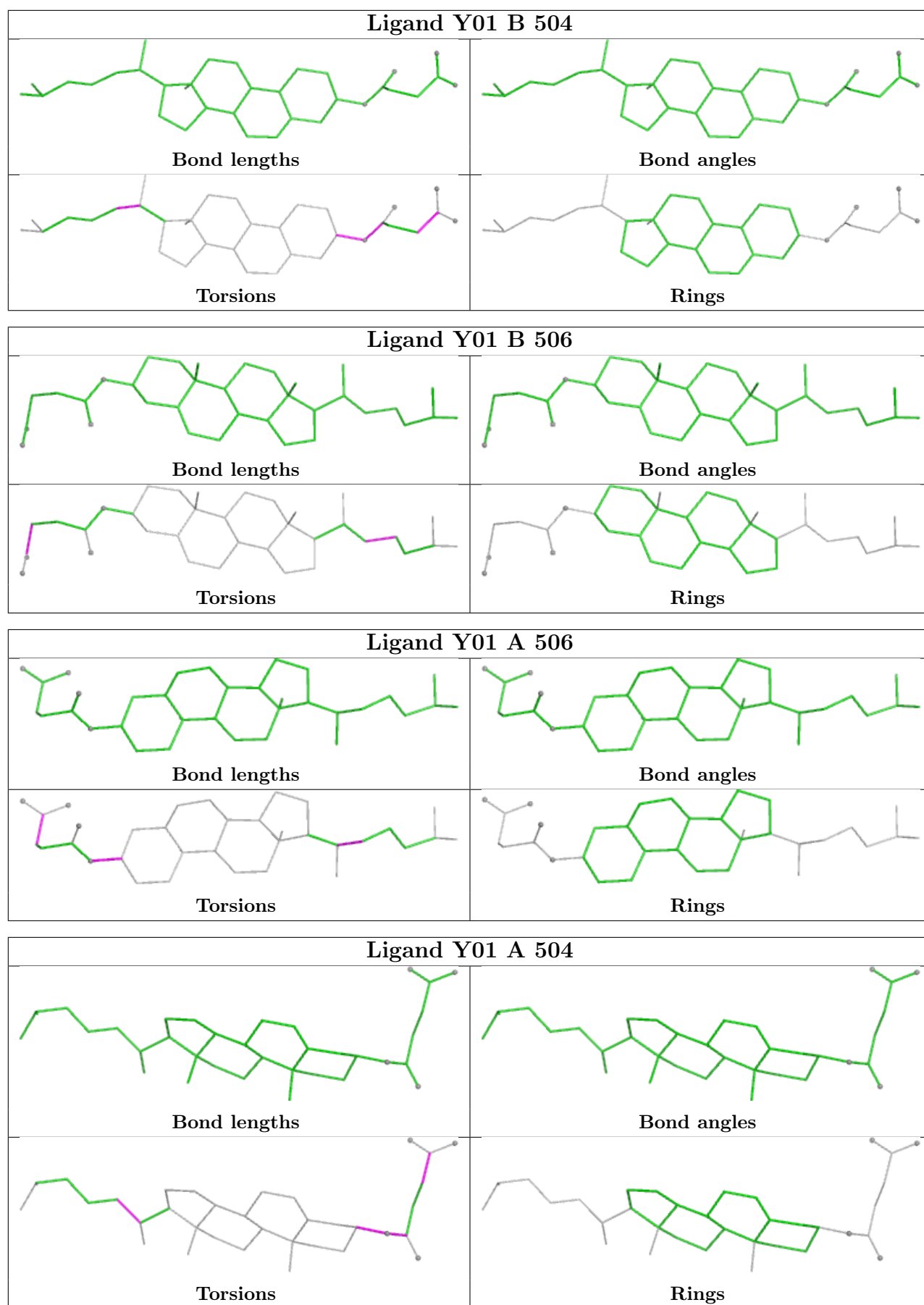
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

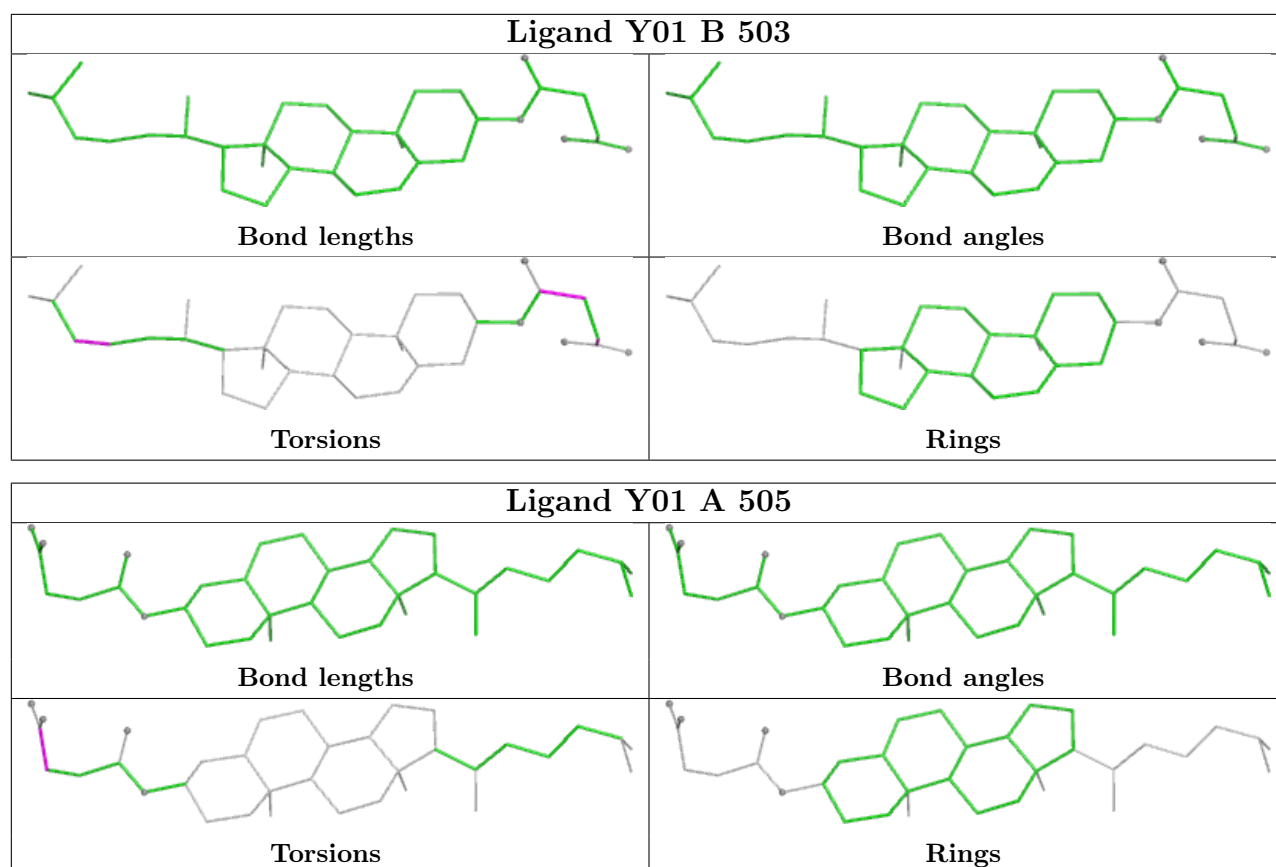
Ligand Y01 B 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand Y01 B 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand Y01 A 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand Y01 A 502	
	
Bond lengths	Bond angles
	
Torsions	Rings





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-54889. These allow visual inspection of the internal detail of the map and identification of artifacts.

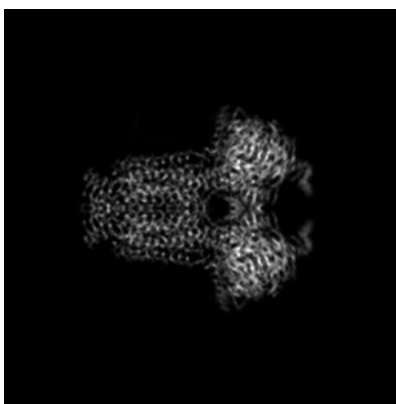
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

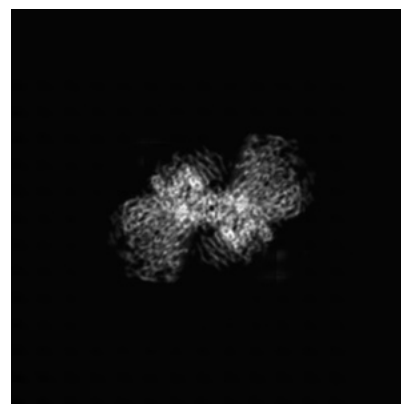
6.1.1 Primary map



X

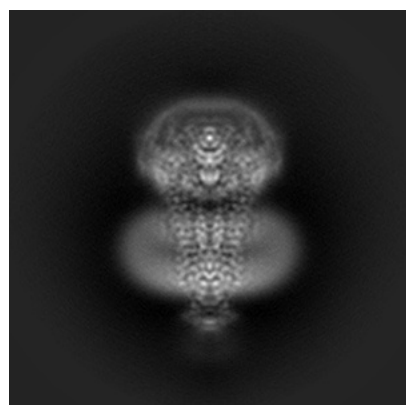


Y

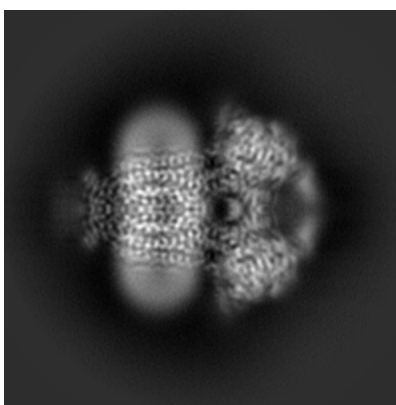


Z

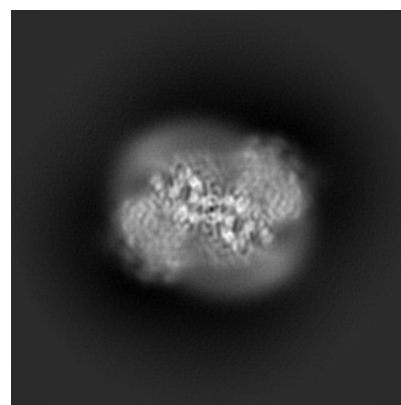
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

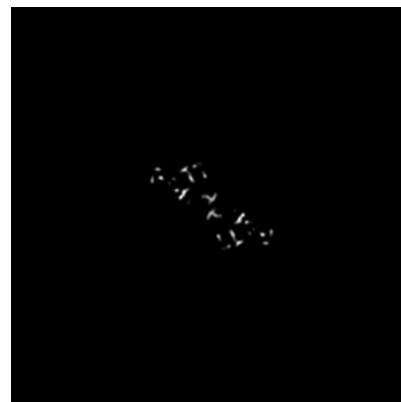
6.2.1 Primary map



X Index: 140

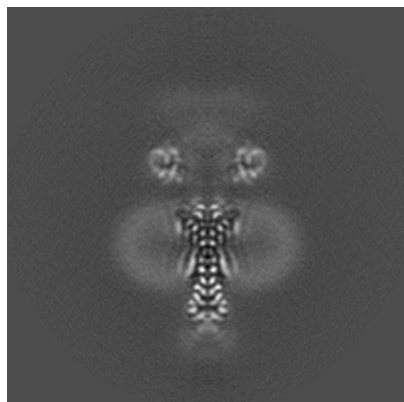


Y Index: 140

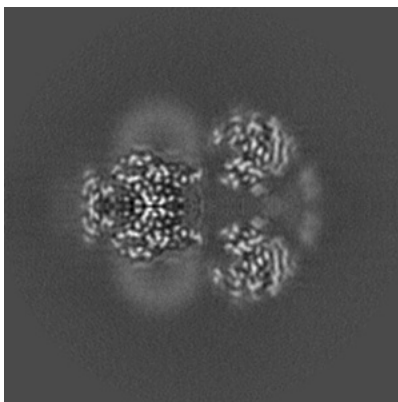


Z Index: 140

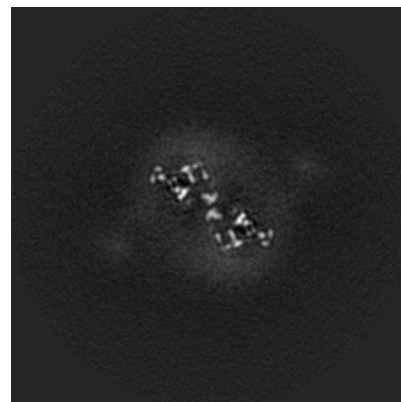
6.2.2 Raw map



X Index: 140



Y Index: 140



Z Index: 140

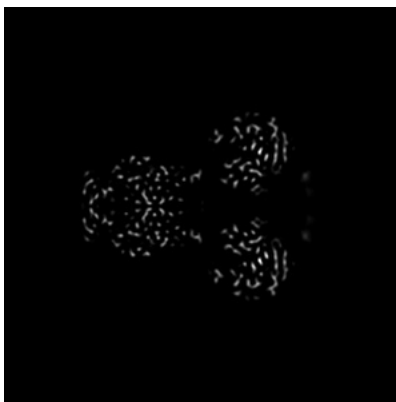
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 164

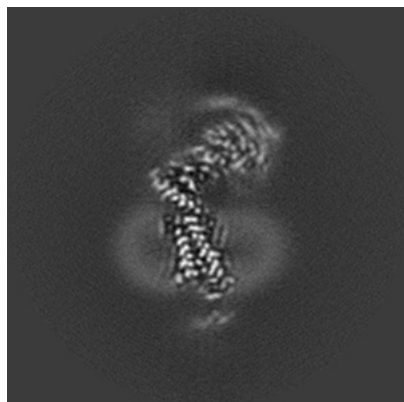


Y Index: 140

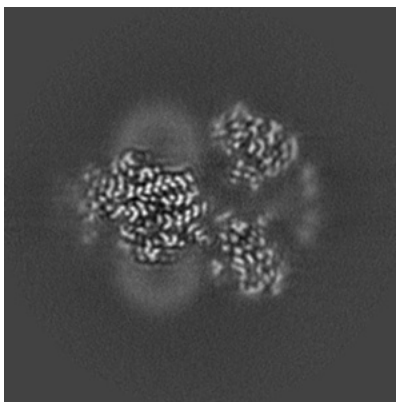


Z Index: 174

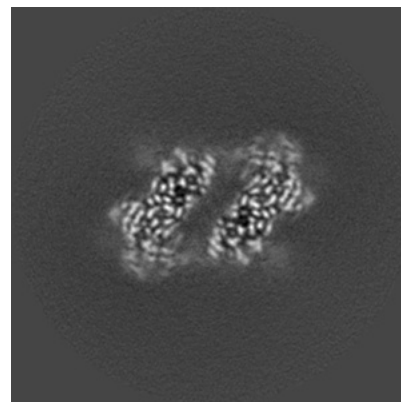
6.3.2 Raw map



X Index: 165



Y Index: 145



Z Index: 163

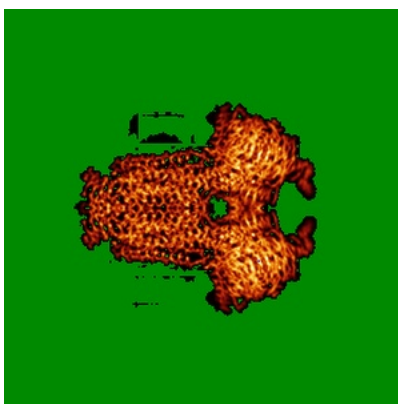
The images above show the largest variance slices of the map in three orthogonal directions.

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

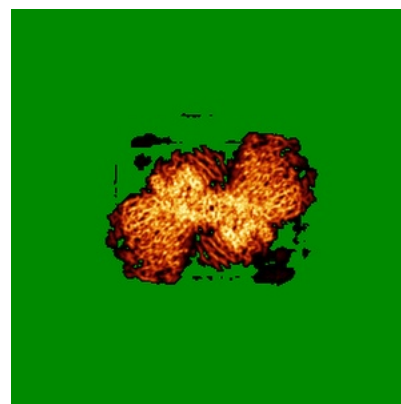
6.4.1 Primary map



X

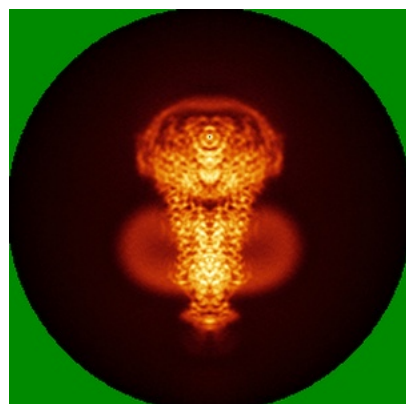


Y

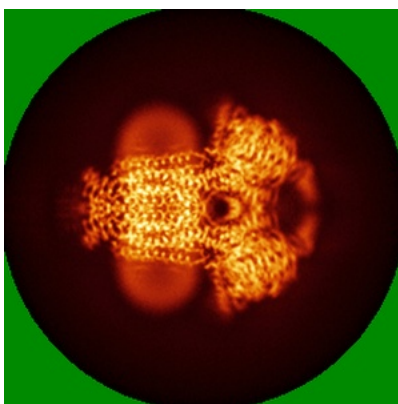


Z

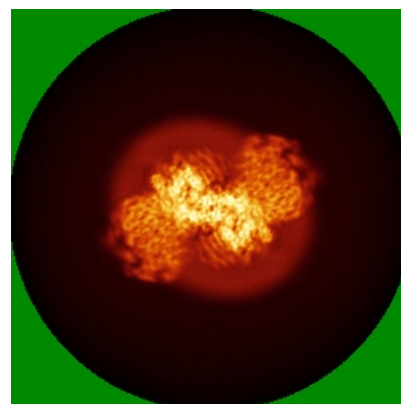
6.4.2 Raw map



X



Y

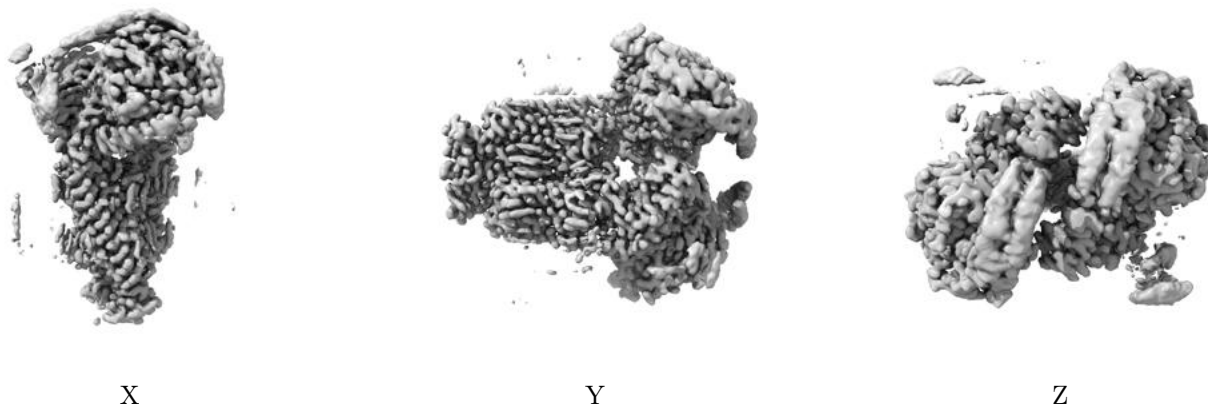


Z

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.

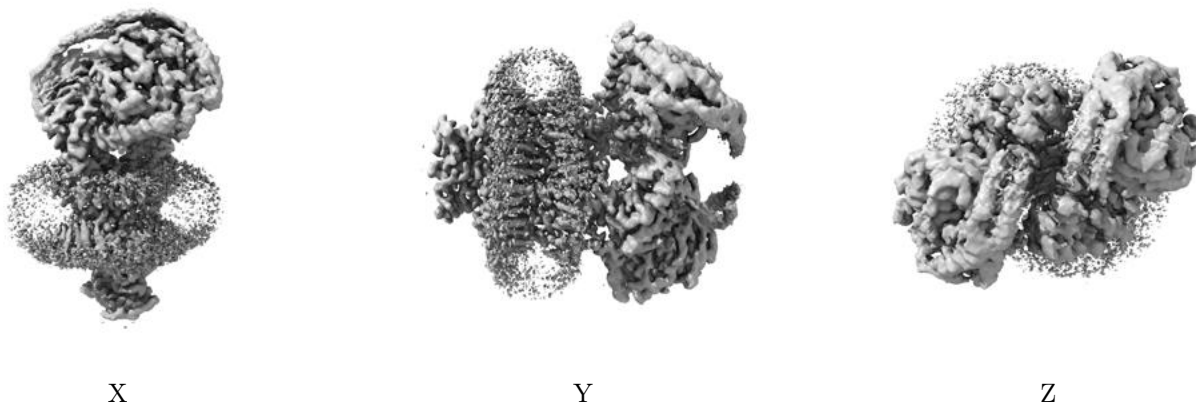
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0136. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

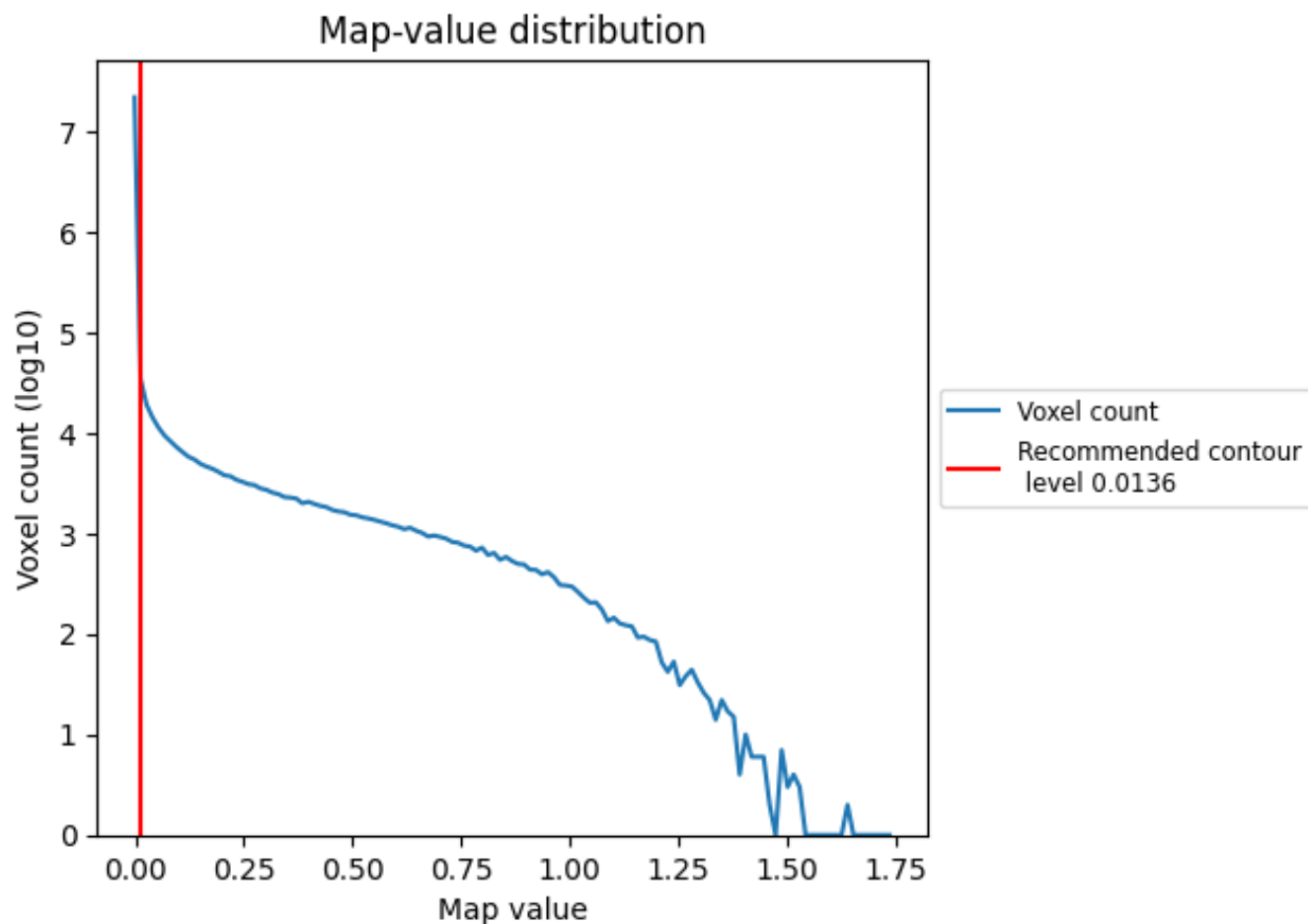
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

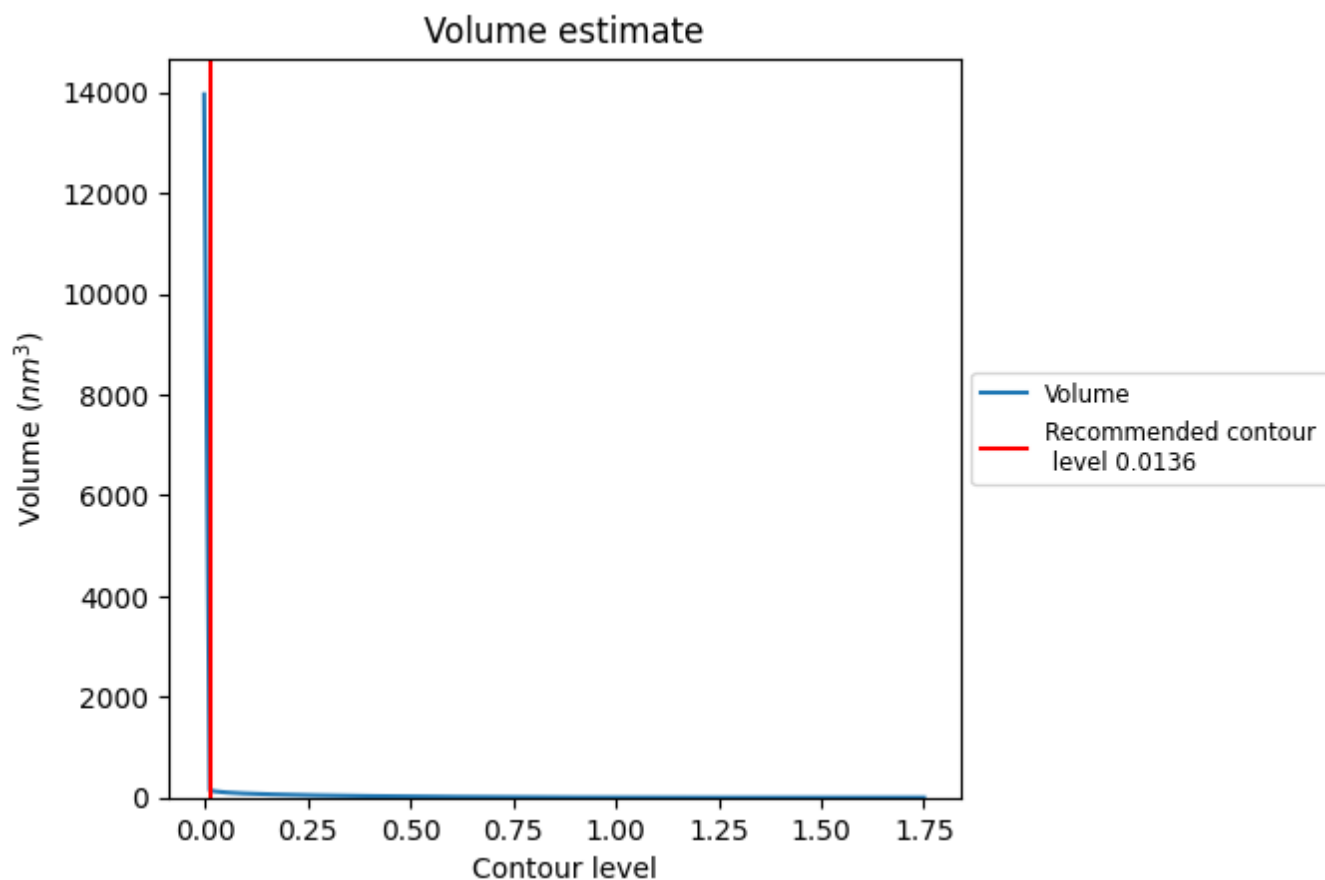
This section contains the results of statistical analysis of the map.

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.

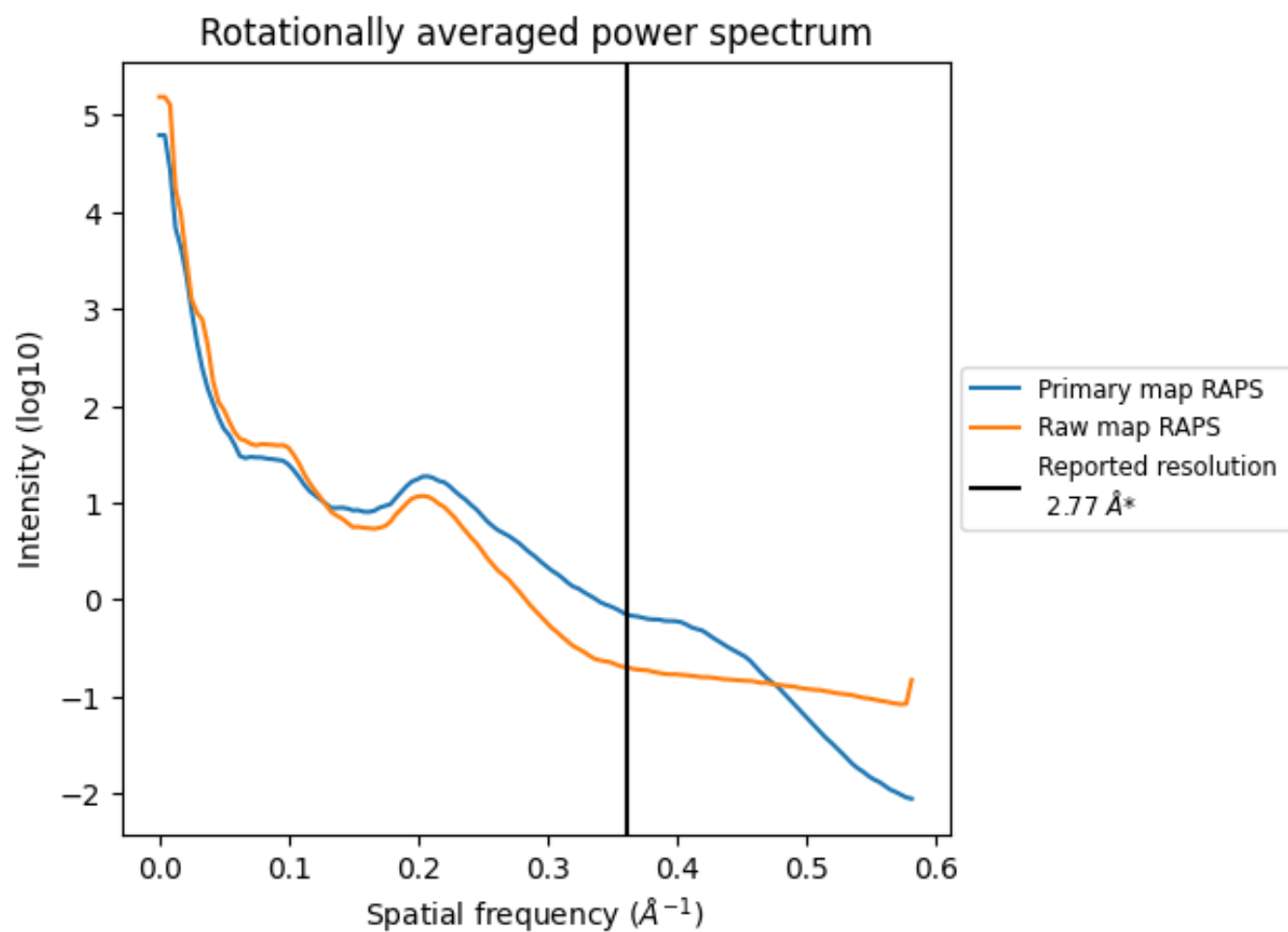
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 141 nm³; this corresponds to an approximate mass of 127 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 ⓘ

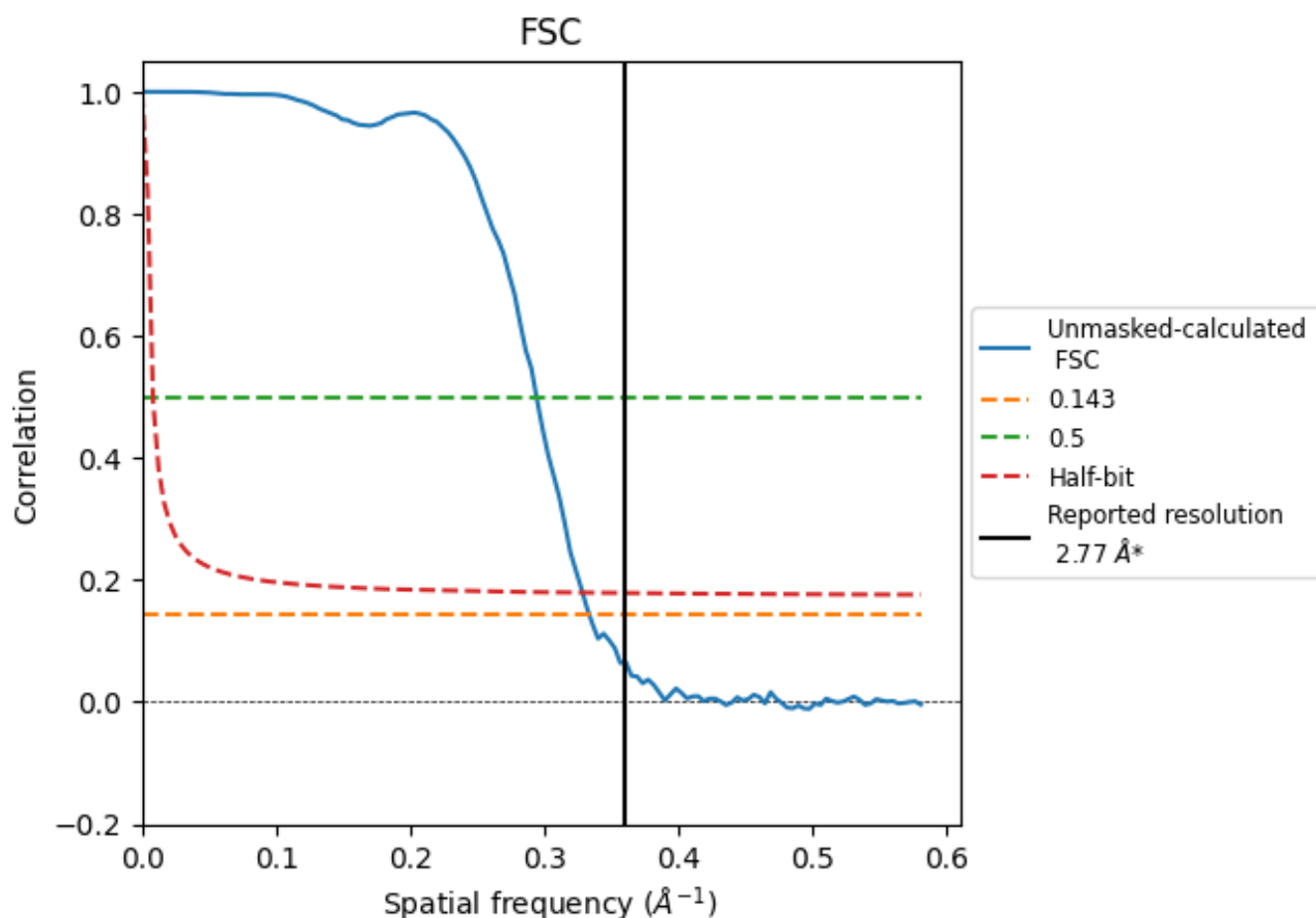


*Reported resolution corresponds to spatial frequency of 0.361 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.361 Å⁻¹

8.2 Resolution estimates [i](#)

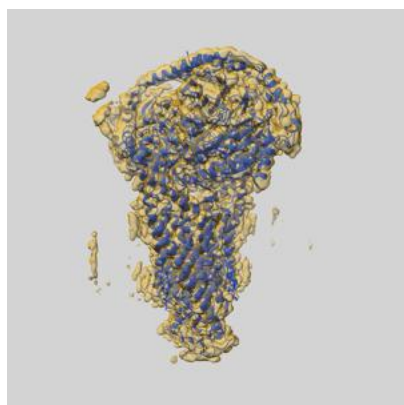
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.77	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.99	3.40	3.04

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

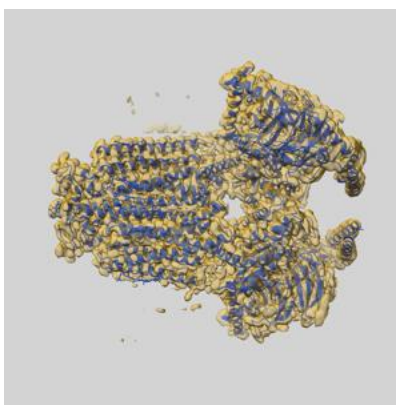
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54889 and PDB model 9SH6. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

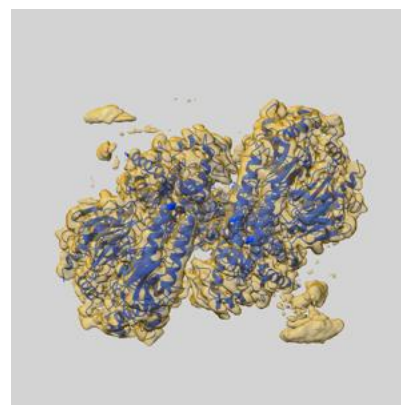
9.1 Map-model overlay [i](#)



X



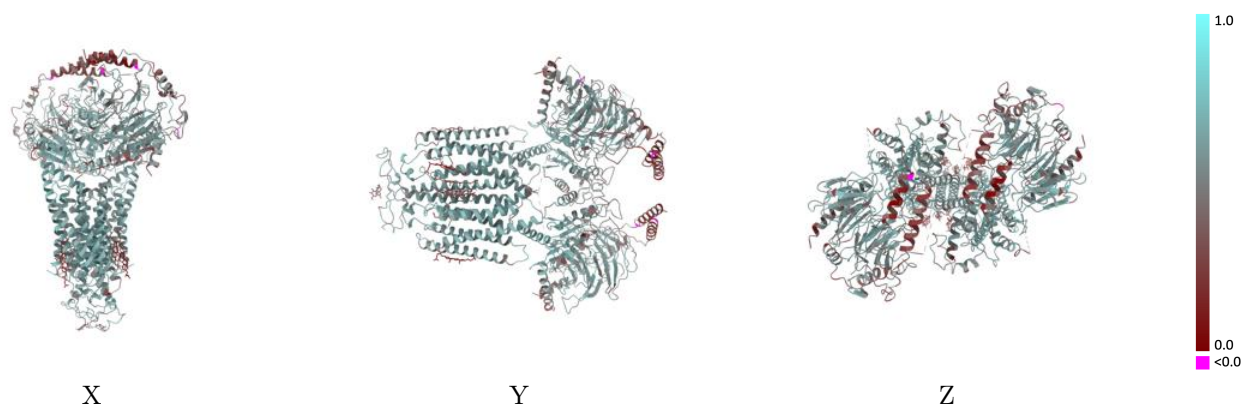
Y



Z

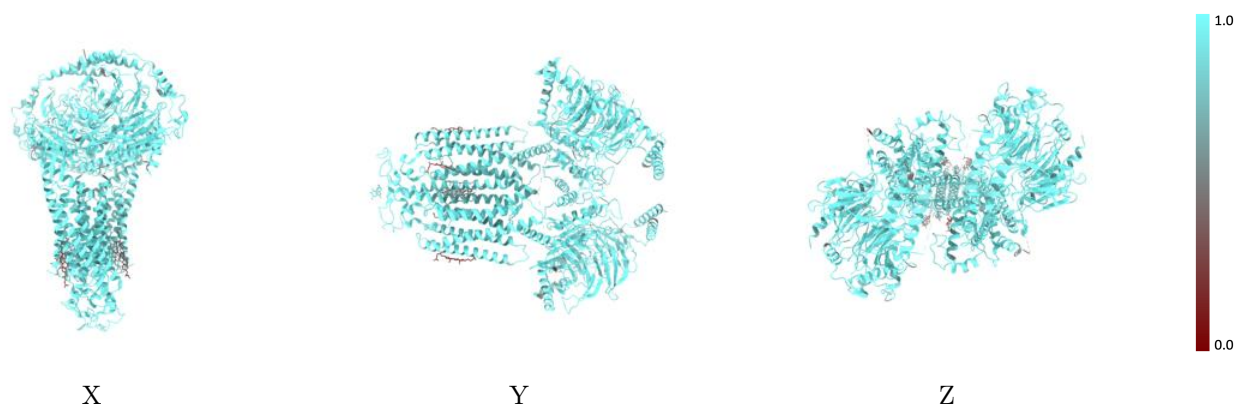
The images above show the 3D surface view of the map at the recommended contour level 0.0136 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



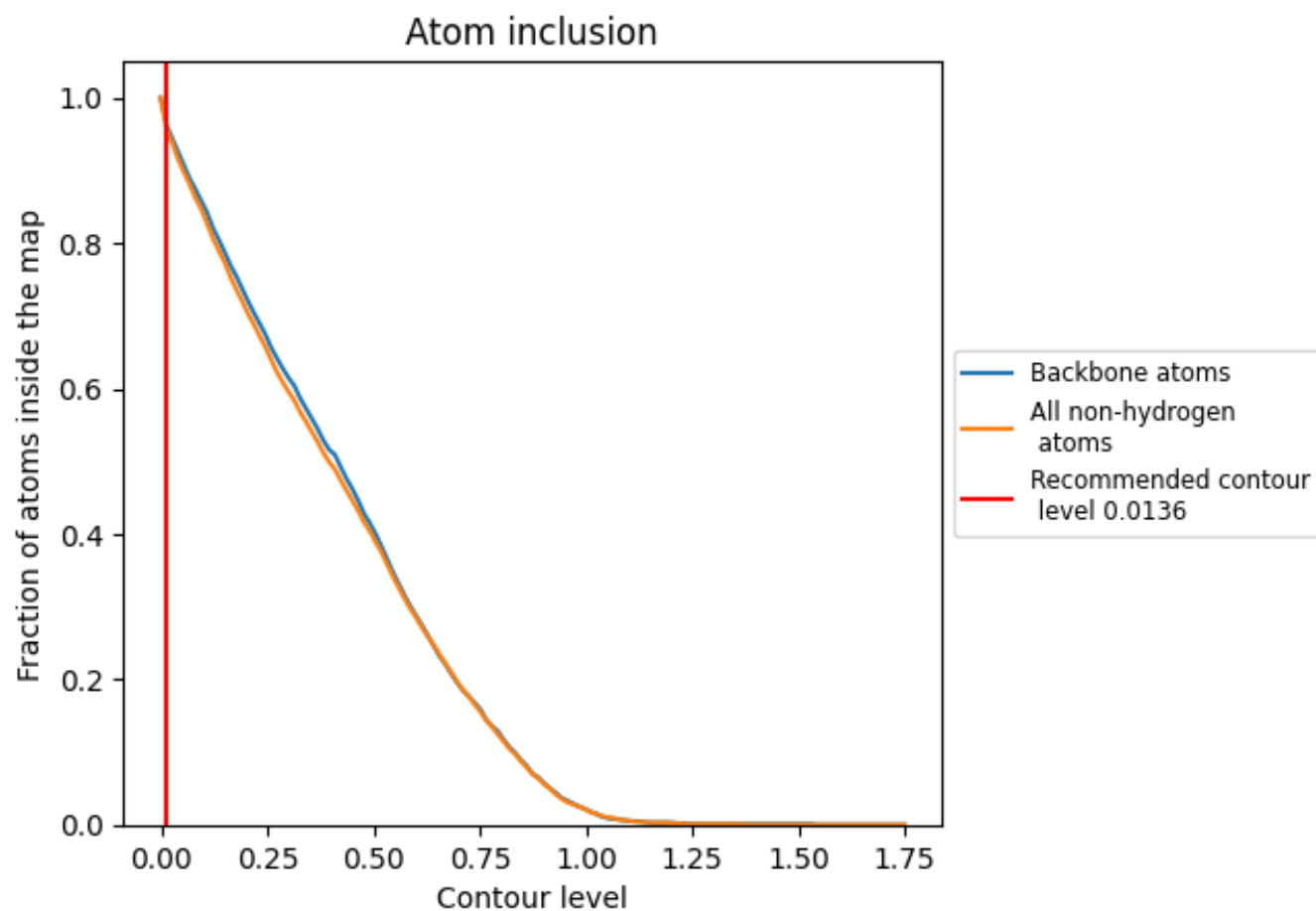
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0136).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0136) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9540	0.5430
A	0.9420	0.5680
B	0.9420	0.5690
C	0.9680	0.5340
D	0.9570	0.5490
E	0.9530	0.5470
F	0.9640	0.5340
G	0.9500	0.4220
H	0.9340	0.4190
I	0.9920	0.6110
K	0.9740	0.5930

1.0

0.0

<0.0