wwPDB EM Validation Summary Report

Oct 14, 2024 – 03:16 PM JST

PDB ID	:	7DW9
EMDB ID	:	EMD-30877
Title	:	Cryo-EM structure of human V2 vasopressin receptor in complex with an Gs protein
Authors	:	Zhou, F.; Jiang, Y.
Deposited on	:	2021-01-15
Resolution	:	2.60 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:

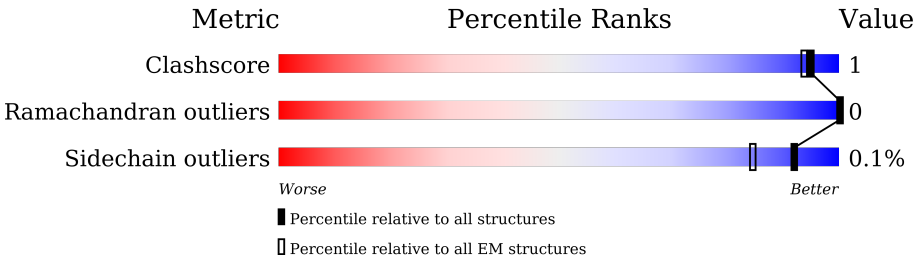
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	R	645	42% 57%
2	A	361	65% 34%
3	B	371	5% 89% 8%
4	Y	71	24% 82% 18%
5	N	140	5% 89% 10%
6	S	247	5% 91% 6%
7	C	10	30% 90% 10%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 10105 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Vasopressin V2 receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	R	278	2177	1432	378	351	16	0	0

There are 274 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-115	HIS	-	expression tag	UNP P30518
R	-114	HIS	-	expression tag	UNP P30518
R	-113	HIS	-	expression tag	UNP P30518
R	-112	HIS	-	expression tag	UNP P30518
R	-111	HIS	-	expression tag	UNP P30518
R	-110	HIS	-	expression tag	UNP P30518
R	-109	HIS	-	expression tag	UNP P30518
R	-108	HIS	-	expression tag	UNP P30518
R	-107	HIS	-	expression tag	UNP P30518
R	-106	HIS	-	expression tag	UNP P30518
R	-105	ALA	-	expression tag	UNP P30518
R	-104	ASP	-	expression tag	UNP P30518
R	-103	LEU	-	expression tag	UNP P30518
R	-102	GLU	-	expression tag	UNP P30518
R	-101	ASP	-	expression tag	UNP P30518
R	-100	ASN	-	expression tag	UNP P30518
R	-99	TRP	-	expression tag	UNP P30518
R	-98	GLU	-	expression tag	UNP P30518
R	-97	THR	-	expression tag	UNP P30518
R	-96	LEU	-	expression tag	UNP P30518
R	-95	ASN	-	expression tag	UNP P30518
R	-94	ASP	-	expression tag	UNP P30518
R	-93	ASN	-	expression tag	UNP P30518
R	-92	LEU	-	expression tag	UNP P30518
R	-91	LYS	-	expression tag	UNP P30518
R	-90	VAL	-	expression tag	UNP P30518
R	-89	ILE	-	expression tag	UNP P30518
R	-88	GLU	-	expression tag	UNP P30518

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-87	LYS	-	expression tag	UNP P30518
R	-86	ALA	-	expression tag	UNP P30518
R	-85	ASP	-	expression tag	UNP P30518
R	-84	ASN	-	expression tag	UNP P30518
R	-83	ALA	-	expression tag	UNP P30518
R	-82	ALA	-	expression tag	UNP P30518
R	-81	GLN	-	expression tag	UNP P30518
R	-80	VAL	-	expression tag	UNP P30518
R	-79	LYS	-	expression tag	UNP P30518
R	-78	ASP	-	expression tag	UNP P30518
R	-77	ALA	-	expression tag	UNP P30518
R	-76	LEU	-	expression tag	UNP P30518
R	-75	THR	-	expression tag	UNP P30518
R	-74	LYS	-	expression tag	UNP P30518
R	-73	MET	-	expression tag	UNP P30518
R	-72	ARG	-	expression tag	UNP P30518
R	-71	ALA	-	expression tag	UNP P30518
R	-70	ALA	-	expression tag	UNP P30518
R	-69	ALA	-	expression tag	UNP P30518
R	-68	LEU	-	expression tag	UNP P30518
R	-67	ASP	-	expression tag	UNP P30518
R	-66	ALA	-	expression tag	UNP P30518
R	-65	GLN	-	expression tag	UNP P30518
R	-64	LYS	-	expression tag	UNP P30518
R	-63	ALA	-	expression tag	UNP P30518
R	-62	THR	-	expression tag	UNP P30518
R	-61	PRO	-	expression tag	UNP P30518
R	-60	PRO	-	expression tag	UNP P30518
R	-59	LYS	-	expression tag	UNP P30518
R	-58	LEU	-	expression tag	UNP P30518
R	-57	GLU	-	expression tag	UNP P30518
R	-56	ASP	-	expression tag	UNP P30518
R	-55	LYS	-	expression tag	UNP P30518
R	-54	SER	-	expression tag	UNP P30518
R	-53	PRO	-	expression tag	UNP P30518
R	-52	ASP	-	expression tag	UNP P30518
R	-51	SER	-	expression tag	UNP P30518
R	-50	PRO	-	expression tag	UNP P30518
R	-49	GLU	-	expression tag	UNP P30518
R	-48	MET	-	expression tag	UNP P30518
R	-47	LYS	-	expression tag	UNP P30518
R	-46	ASP	-	expression tag	UNP P30518

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-45	PHE	-	expression tag	UNP P30518
R	-44	ARG	-	expression tag	UNP P30518
R	-43	HIS	-	expression tag	UNP P30518
R	-42	GLY	-	expression tag	UNP P30518
R	-41	PHE	-	expression tag	UNP P30518
R	-40	ASP	-	expression tag	UNP P30518
R	-39	ILE	-	expression tag	UNP P30518
R	-38	LEU	-	expression tag	UNP P30518
R	-37	VAL	-	expression tag	UNP P30518
R	-36	GLY	-	expression tag	UNP P30518
R	-35	GLN	-	expression tag	UNP P30518
R	-34	ILE	-	expression tag	UNP P30518
R	-33	ASP	-	expression tag	UNP P30518
R	-32	ASP	-	expression tag	UNP P30518
R	-31	ALA	-	expression tag	UNP P30518
R	-30	LEU	-	expression tag	UNP P30518
R	-29	LYS	-	expression tag	UNP P30518
R	-28	LEU	-	expression tag	UNP P30518
R	-27	ALA	-	expression tag	UNP P30518
R	-26	ASN	-	expression tag	UNP P30518
R	-25	GLU	-	expression tag	UNP P30518
R	-24	GLY	-	expression tag	UNP P30518
R	-23	LYS	-	expression tag	UNP P30518
R	-22	VAL	-	expression tag	UNP P30518
R	-21	LYS	-	expression tag	UNP P30518
R	-20	GLU	-	expression tag	UNP P30518
R	-19	ALA	-	expression tag	UNP P30518
R	-18	GLN	-	expression tag	UNP P30518
R	-17	ALA	-	expression tag	UNP P30518
R	-16	ALA	-	expression tag	UNP P30518
R	-15	ALA	-	expression tag	UNP P30518
R	-14	GLU	-	expression tag	UNP P30518
R	-13	GLN	-	expression tag	UNP P30518
R	-12	LEU	-	expression tag	UNP P30518
R	-11	LYS	-	expression tag	UNP P30518
R	-10	THR	-	expression tag	UNP P30518
R	-9	THR	-	expression tag	UNP P30518
R	-8	ARG	-	expression tag	UNP P30518
R	-7	ASN	-	expression tag	UNP P30518
R	-6	ALA	-	expression tag	UNP P30518
R	-5	TYR	-	expression tag	UNP P30518
R	-4	ILE	-	expression tag	UNP P30518

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-3	GLN	-	expression tag	UNP P30518
R	-2	LYS	-	expression tag	UNP P30518
R	-1	TYR	-	expression tag	UNP P30518
R	0	LEU	-	expression tag	UNP P30518
R	372	VAL	-	expression tag	UNP P30518
R	373	PHE	-	expression tag	UNP P30518
R	374	THR	-	expression tag	UNP P30518
R	375	LEU	-	expression tag	UNP P30518
R	376	GLU	-	expression tag	UNP P30518
R	377	ASP	-	expression tag	UNP P30518
R	378	PHE	-	expression tag	UNP P30518
R	379	VAL	-	expression tag	UNP P30518
R	380	GLY	-	expression tag	UNP P30518
R	381	ASP	-	expression tag	UNP P30518
R	382	TRP	-	expression tag	UNP P30518
R	383	GLU	-	expression tag	UNP P30518
R	384	GLN	-	expression tag	UNP P30518
R	385	THR	-	expression tag	UNP P30518
R	386	ALA	-	expression tag	UNP P30518
R	387	ALA	-	expression tag	UNP P30518
R	388	TYR	-	expression tag	UNP P30518
R	389	ASN	-	expression tag	UNP P30518
R	390	LEU	-	expression tag	UNP P30518
R	391	ASP	-	expression tag	UNP P30518
R	392	GLN	-	expression tag	UNP P30518
R	393	VAL	-	expression tag	UNP P30518
R	394	LEU	-	expression tag	UNP P30518
R	395	GLU	-	expression tag	UNP P30518
R	396	GLN	-	expression tag	UNP P30518
R	397	GLY	-	expression tag	UNP P30518
R	398	GLY	-	expression tag	UNP P30518
R	399	VAL	-	expression tag	UNP P30518
R	400	SER	-	expression tag	UNP P30518
R	401	SER	-	expression tag	UNP P30518
R	402	LEU	-	expression tag	UNP P30518
R	403	LEU	-	expression tag	UNP P30518
R	404	GLN	-	expression tag	UNP P30518
R	405	ASN	-	expression tag	UNP P30518
R	406	LEU	-	expression tag	UNP P30518
R	407	ALA	-	expression tag	UNP P30518
R	408	VAL	-	expression tag	UNP P30518
R	409	SER	-	expression tag	UNP P30518

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Chain	Residue	Modelled	Actual	Comment	Reference
R	410	VAL	-	expression tag	UNP P30518
R	411	THR	-	expression tag	UNP P30518
R	412	PRO	-	expression tag	UNP P30518
R	413	ILE	-	expression tag	UNP P30518
R	414	GLN	-	expression tag	UNP P30518
R	415	ARG	-	expression tag	UNP P30518
R	416	ILE	-	expression tag	UNP P30518
R	417	VAL	-	expression tag	UNP P30518
R	418	ARG	-	expression tag	UNP P30518
R	419	SER	-	expression tag	UNP P30518
R	420	GLY	-	expression tag	UNP P30518
R	421	GLU	-	expression tag	UNP P30518
R	422	ASN	-	expression tag	UNP P30518
R	423	ALA	-	expression tag	UNP P30518
R	424	LEU	-	expression tag	UNP P30518
R	425	LYS	-	expression tag	UNP P30518
R	426	ILE	-	expression tag	UNP P30518
R	427	ASP	-	expression tag	UNP P30518
R	428	ILE	-	expression tag	UNP P30518
R	429	HIS	-	expression tag	UNP P30518
R	430	VAL	-	expression tag	UNP P30518
R	431	ILE	-	expression tag	UNP P30518
R	432	ILE	-	expression tag	UNP P30518
R	433	PRO	-	expression tag	UNP P30518
R	434	TYR	-	expression tag	UNP P30518
R	435	GLU	-	expression tag	UNP P30518
R	436	GLY	-	expression tag	UNP P30518
R	437	LEU	-	expression tag	UNP P30518
R	438	SER	-	expression tag	UNP P30518
R	439	ALA	-	expression tag	UNP P30518
R	440	ASP	-	expression tag	UNP P30518
R	441	GLN	-	expression tag	UNP P30518
R	442	MET	-	expression tag	UNP P30518
R	443	ALA	-	expression tag	UNP P30518
R	444	GLN	-	expression tag	UNP P30518
R	445	ILE	-	expression tag	UNP P30518
R	446	GLU	-	expression tag	UNP P30518
R	447	GLU	-	expression tag	UNP P30518
R	448	VAL	-	expression tag	UNP P30518
R	449	PHE	-	expression tag	UNP P30518
R	450	LYS	-	expression tag	UNP P30518
R	451	VAL	-	expression tag	UNP P30518

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Chain	Residue	Modelled	Actual	Comment	Reference
R	452	VAL	-	expression tag	UNP P30518
R	453	TYR	-	expression tag	UNP P30518
R	454	PRO	-	expression tag	UNP P30518
R	455	VAL	-	expression tag	UNP P30518
R	456	ASP	-	expression tag	UNP P30518
R	457	ASP	-	expression tag	UNP P30518
R	458	HIS	-	expression tag	UNP P30518
R	459	HIS	-	expression tag	UNP P30518
R	460	PHE	-	expression tag	UNP P30518
R	461	LYS	-	expression tag	UNP P30518
R	462	VAL	-	expression tag	UNP P30518
R	463	ILE	-	expression tag	UNP P30518
R	464	LEU	-	expression tag	UNP P30518
R	465	PRO	-	expression tag	UNP P30518
R	466	TYR	-	expression tag	UNP P30518
R	467	GLY	-	expression tag	UNP P30518
R	468	THR	-	expression tag	UNP P30518
R	469	LEU	-	expression tag	UNP P30518
R	470	VAL	-	expression tag	UNP P30518
R	471	ILE	-	expression tag	UNP P30518
R	472	ASP	-	expression tag	UNP P30518
R	473	GLY	-	expression tag	UNP P30518
R	474	VAL	-	expression tag	UNP P30518
R	475	THR	-	expression tag	UNP P30518
R	476	PRO	-	expression tag	UNP P30518
R	477	ASN	-	expression tag	UNP P30518
R	478	MET	-	expression tag	UNP P30518
R	479	LEU	-	expression tag	UNP P30518
R	480	ASN	-	expression tag	UNP P30518
R	481	TYR	-	expression tag	UNP P30518
R	482	PHE	-	expression tag	UNP P30518
R	483	GLY	-	expression tag	UNP P30518
R	484	ARG	-	expression tag	UNP P30518
R	485	PRO	-	expression tag	UNP P30518
R	486	TYR	-	expression tag	UNP P30518
R	487	GLU	-	expression tag	UNP P30518
R	488	GLY	-	expression tag	UNP P30518
R	489	ILE	-	expression tag	UNP P30518
R	490	ALA	-	expression tag	UNP P30518
R	491	VAL	-	expression tag	UNP P30518
R	492	PHE	-	expression tag	UNP P30518
R	493	ASP	-	expression tag	UNP P30518

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Chain	Residue	Modelled	Actual	Comment	Reference
R	494	GLY	-	expression tag	UNP P30518
R	495	LYS	-	expression tag	UNP P30518
R	496	LYS	-	expression tag	UNP P30518
R	497	ILE	-	expression tag	UNP P30518
R	498	THR	-	expression tag	UNP P30518
R	499	VAL	-	expression tag	UNP P30518
R	500	THR	-	expression tag	UNP P30518
R	501	GLY	-	expression tag	UNP P30518
R	502	THR	-	expression tag	UNP P30518
R	503	LEU	-	expression tag	UNP P30518
R	504	TRP	-	expression tag	UNP P30518
R	505	ASN	-	expression tag	UNP P30518
R	506	GLY	-	expression tag	UNP P30518
R	507	ASN	-	expression tag	UNP P30518
R	508	LYS	-	expression tag	UNP P30518
R	509	ILE	-	expression tag	UNP P30518
R	510	ILE	-	expression tag	UNP P30518
R	511	ASP	-	expression tag	UNP P30518
R	512	GLU	-	expression tag	UNP P30518
R	513	ARG	-	expression tag	UNP P30518
R	514	LEU	-	expression tag	UNP P30518
R	515	ILE	-	expression tag	UNP P30518
R	516	THR	-	expression tag	UNP P30518
R	517	PRO	-	expression tag	UNP P30518
R	518	ASP	-	expression tag	UNP P30518
R	519	GLY	-	expression tag	UNP P30518
R	520	SER	-	expression tag	UNP P30518
R	521	MET	-	expression tag	UNP P30518
R	522	LEU	-	expression tag	UNP P30518
R	523	PHE	-	expression tag	UNP P30518
R	524	ARG	-	expression tag	UNP P30518
R	525	VAL	-	expression tag	UNP P30518
R	526	THR	-	expression tag	UNP P30518
R	527	ILE	-	expression tag	UNP P30518
R	528	ASN	-	expression tag	UNP P30518
R	529	SER	-	expression tag	UNP P30518

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	238	Total	C	N	O	S	0	0
			1971	1246	353	363	9		

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	341	Total	C	N	O	S	0	0
			2605	1607	469	508	21		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	initiating methionine	UNP P54311
B	-3	GLY	-	expression tag	UNP P54311
B	-2	SER	-	expression tag	UNP P54311
B	-1	LEU	-	expression tag	UNP P54311
B	0	LEU	-	expression tag	UNP P54311
B	1	GLN	-	expression tag	UNP P54311
B	341	GLY	-	expression tag	UNP P54311
B	342	SER	-	expression tag	UNP P54311
B	343	SER	-	expression tag	UNP P54311
B	344	GLY	-	expression tag	UNP P54311
B	345	GLY	-	expression tag	UNP P54311
B	346	GLY	-	expression tag	UNP P54311
B	347	GLY	-	expression tag	UNP P54311
B	348	SER	-	expression tag	UNP P54311
B	349	GLY	-	expression tag	UNP P54311
B	350	GLY	-	expression tag	UNP P54311
B	351	GLY	-	expression tag	UNP P54311
B	352	GLY	-	expression tag	UNP P54311
B	353	SER	-	expression tag	UNP P54311
B	354	SER	-	expression tag	UNP P54311
B	355	GLY	-	expression tag	UNP P54311
B	356	VAL	-	expression tag	UNP P54311
B	357	SER	-	expression tag	UNP P54311
B	358	GLY	-	expression tag	UNP P54311
B	359	TRP	-	expression tag	UNP P54311
B	360	ARG	-	expression tag	UNP P54311
B	361	LEU	-	expression tag	UNP P54311
B	362	PHE	-	expression tag	UNP P54311
B	363	LYS	-	expression tag	UNP P54311
B	364	LYS	-	expression tag	UNP P54311
B	365	ILE	-	expression tag	UNP P54311
B	366	SER	-	expression tag	UNP P54311

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Y	58	Total	C	N	O	S	0	0
			445	278	78	86	3		

- Molecule 5 is a protein called Nanobody35.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	126	Total	C	N	O	S	0	0
			961	599	168	188	6		

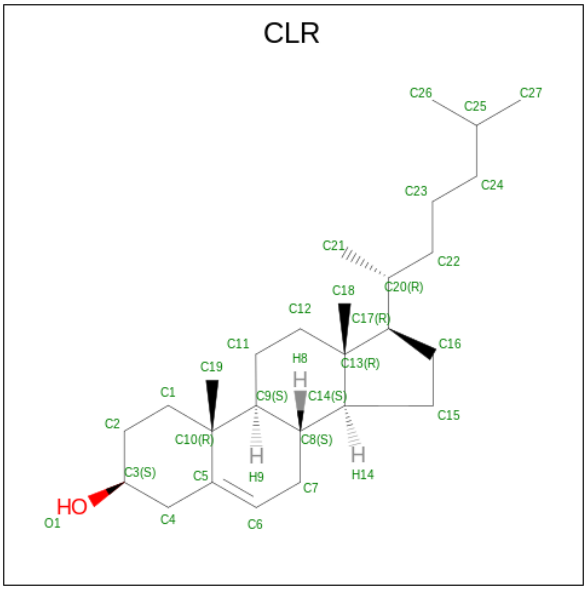
- Molecule 6 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	233	Total	C	N	O	S	0	0
			1787	1134	296	347	10		

- Molecule 7 is a protein called CYS-TYR-PHE-GLN-ASN-CYS-PRO-ARG-GLY-NH2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	10	Total	C	N	O	S	0	1
			75	46	15	12	2		

- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			AltConf
8	R	1	Total	C	O	0
			28	27	1	

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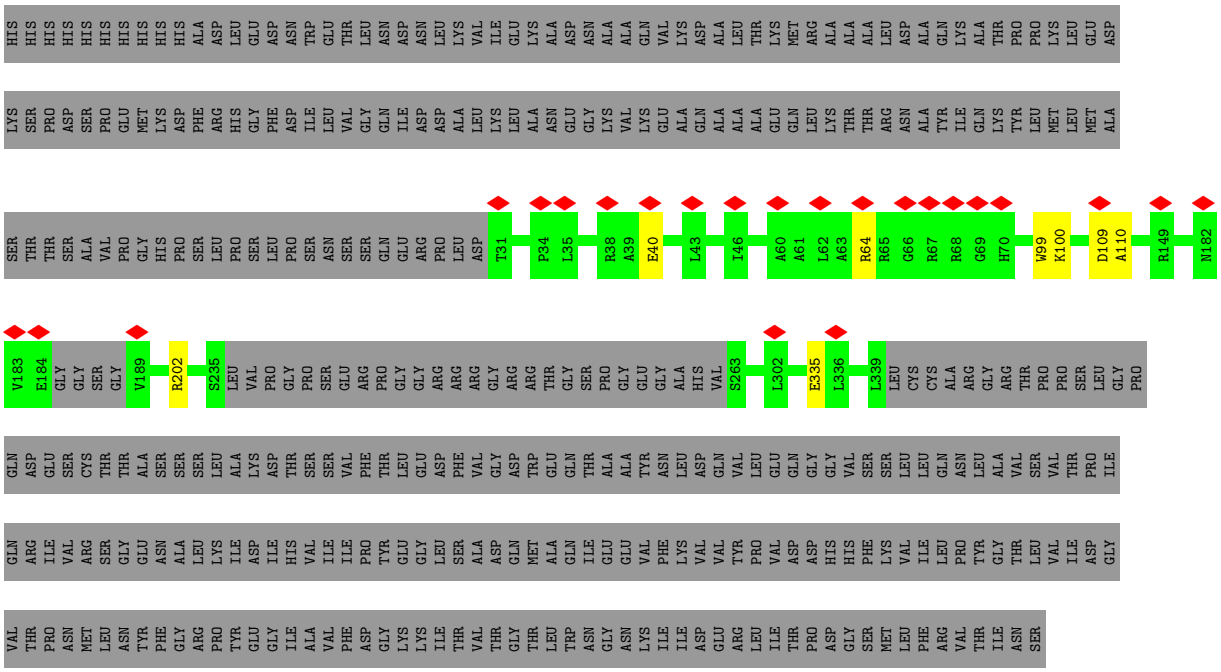
Mol	Chain	Residues	Atoms			AltConf
8	R	1	Total	C	O	0
			28	27	1	
8	R	1	Total	C	O	0
			28	27	1	

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.

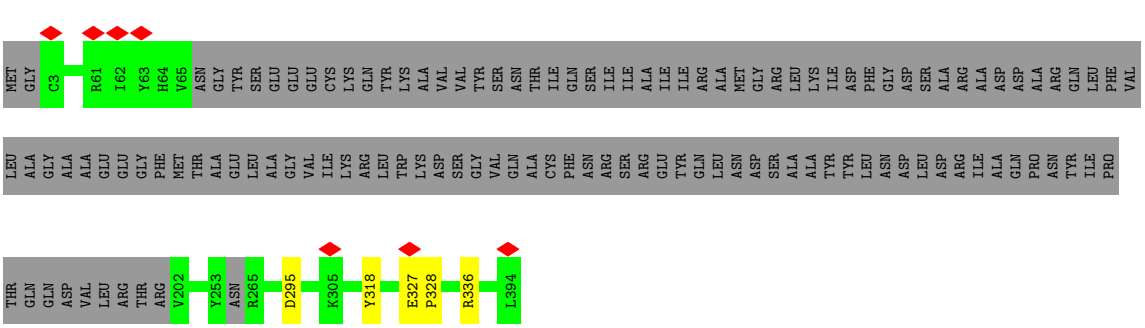
• Molecule 1: Vasopressin V2 receptor

Chain R:



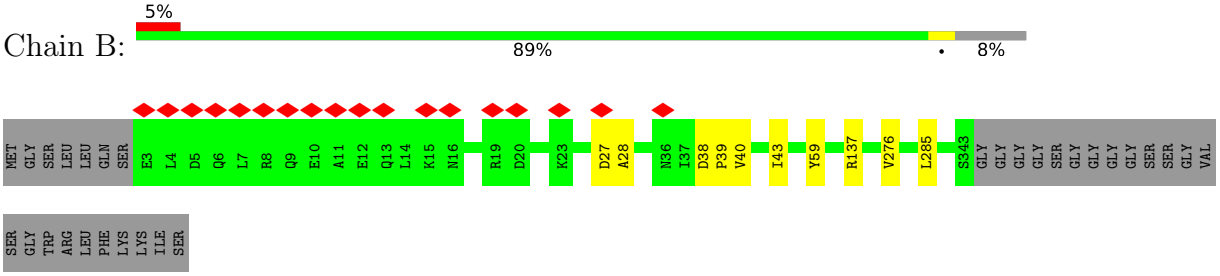
• Molecule 2: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short

Chain A:



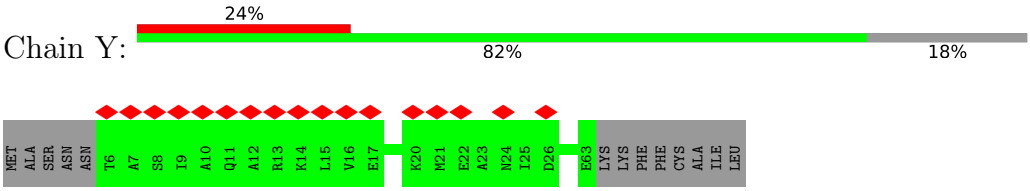
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:



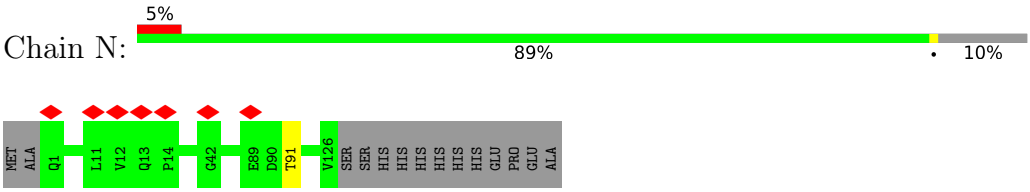
• Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain Y:



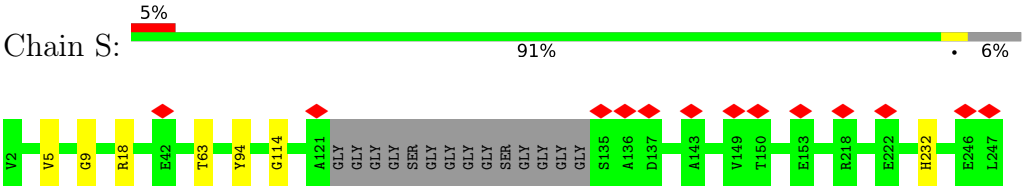
• Molecule 5: Nanobody35

Chain N:



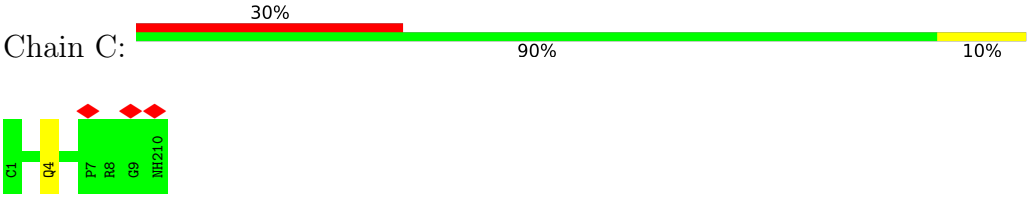
• Molecule 6: scFv16

Chain S:



• Molecule 7: CYS-TYR-PHE-GLN-ASN-CYS-PRO-ARG-GLY-NH2

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	577084	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	OTHER	Depositor
Maximum map value	0.053	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	151.2, 151.2, 151.2	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NH2, CLR

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	R	0.30	0/2238	0.52	0/3058
2	A	0.36	0/2009	0.56	0/2702
3	B	0.39	0/2652	0.58	0/3596
4	Y	0.29	0/451	0.49	0/609
5	N	0.38	0/981	0.58	0/1329
6	S	0.38	0/1831	0.55	0/2483
7	C	0.41	0/76	0.67	0/101
All	All	0.36	0/10238	0.55	0/13878

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	137	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	2177	0	2228	6	0
2	A	1971	0	1952	3	0
3	B	2605	0	2506	5	0
4	Y	445	0	454	0	0
5	N	961	0	930	1	0
6	S	1787	0	1722	5	0
7	C	75	0	65	2	0
8	R	84	0	135	1	0
All	All	10105	0	9992	21	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 1.

The worst 5 of 21 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)
6:S:9:GLY:O	6:S:18:ARG:NH1	2.31	0.64
1:R:202:ARG:NE	7:C:4:GLN:OE1	2.39	0.53
1:R:40:GLU:OE1	1:R:100:LYS:NZ	2.32	0.51
1:R:202:ARG:NH2	7:C:4:GLN:OE1	2.43	0.49
1:R:109:ASP:OD1	1:R:110:ALA:N	2.46	0.49

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	R	272/645 (42%)	269 (99%)	3 (1%)	0	100	100
2	A	232/361 (64%)	228 (98%)	4 (2%)	0	100	100
3	B	339/371 (91%)	323 (95%)	16 (5%)	0	100	100
4	Y	56/71 (79%)	56 (100%)	0	0	100	100
5	N	124/140 (89%)	121 (98%)	3 (2%)	0	100	100
6	S	229/247 (93%)	225 (98%)	4 (2%)	0	100	100
7	C	8/10 (80%)	8 (100%)	0	0	100	100
All	All	1260/1845 (68%)	1230 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	R	225/534 (42%)	225 (100%)	0	100	100
2	A	215/315 (68%)	215 (100%)	0	100	100
3	B	280/302 (93%)	279 (100%)	1 (0%)	89	96
4	Y	47/58 (81%)	47 (100%)	0	100	100
5	N	104/116 (90%)	104 (100%)	0	100	100
6	S	196/198 (99%)	196 (100%)	0	100	100
7	C	8/8 (100%)	8 (100%)	0	100	100
All	All	1075/1531 (70%)	1074 (100%)	1 (0%)	92	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	59	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	138	HIS
3	B	293	ASN

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)

3 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	$\#\|Z\| > 2$
8	CLR	R	602	-	31,31,31	0.56	0	48,48,48	2.15	8 (16%)
8	CLR	R	603	-	31,31,31	0.56	0	48,48,48	2.14	7 (14%)
8	CLR	R	601	-	31,31,31	0.59	0	48,48,48	2.13	7 (14%)

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
8	CLR	R	602	-	-	1/10/68/68	0/4/4/4
8	CLR	R	603	-	-	0/10/68/68	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CLR	R	601	-	-	5/10/68/68	0/4/4/4

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	R	603	CLR	C7-C8-C9	8.01	119.42	109.71
8	R	601	CLR	C7-C8-C14	7.84	122.27	110.91
8	R	602	CLR	C7-C8-C14	7.79	122.20	110.91
8	R	601	CLR	C7-C8-C9	7.65	118.98	109.71
8	R	603	CLR	C7-C8-C14	7.34	121.54	110.91

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	R	602	CLR	C20-C22-C23-C24
8	R	601	CLR	C13-C17-C20-C21
8	R	601	CLR	C16-C17-C20-C21
8	R	601	CLR	C13-C17-C20-C22
8	R	601	CLR	C16-C17-C20-C22

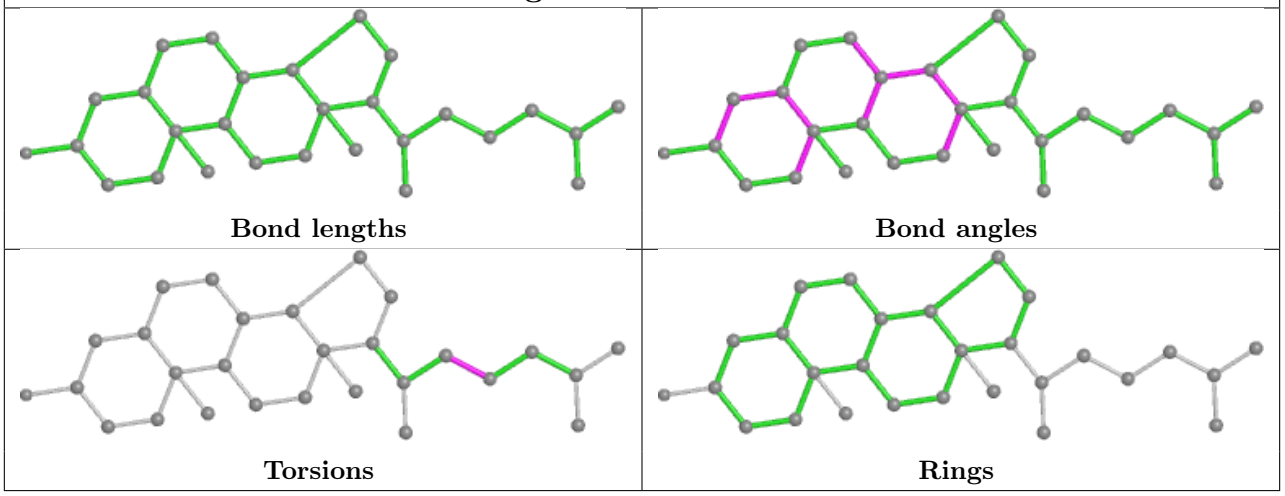
There are no ring outliers.

1 monomer is involved in 1 short contact:

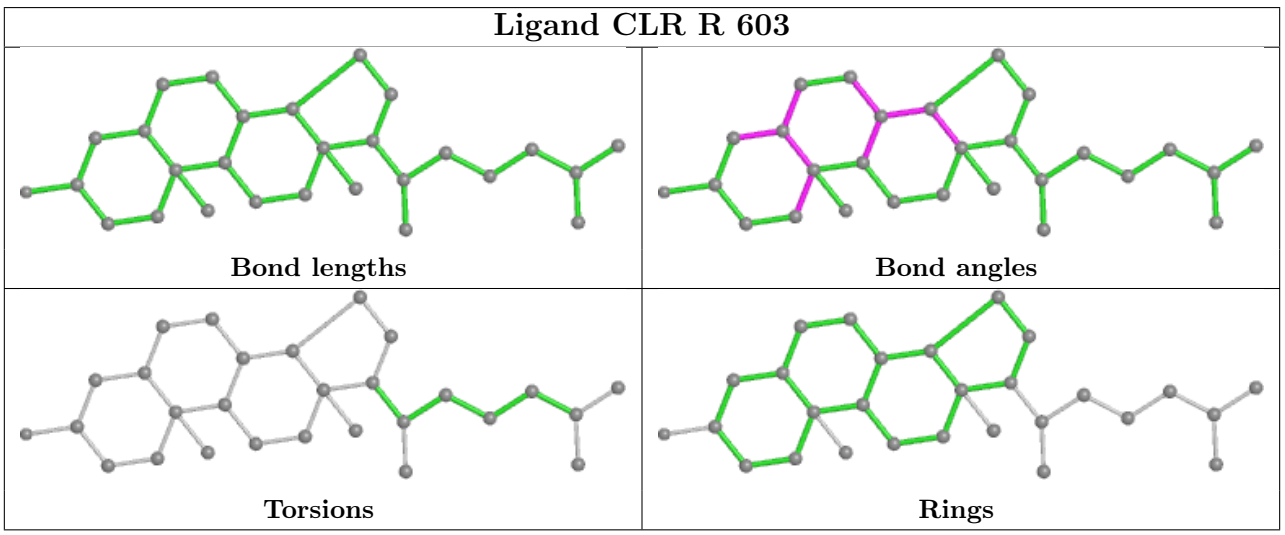
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	R	603	CLR	1	0

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

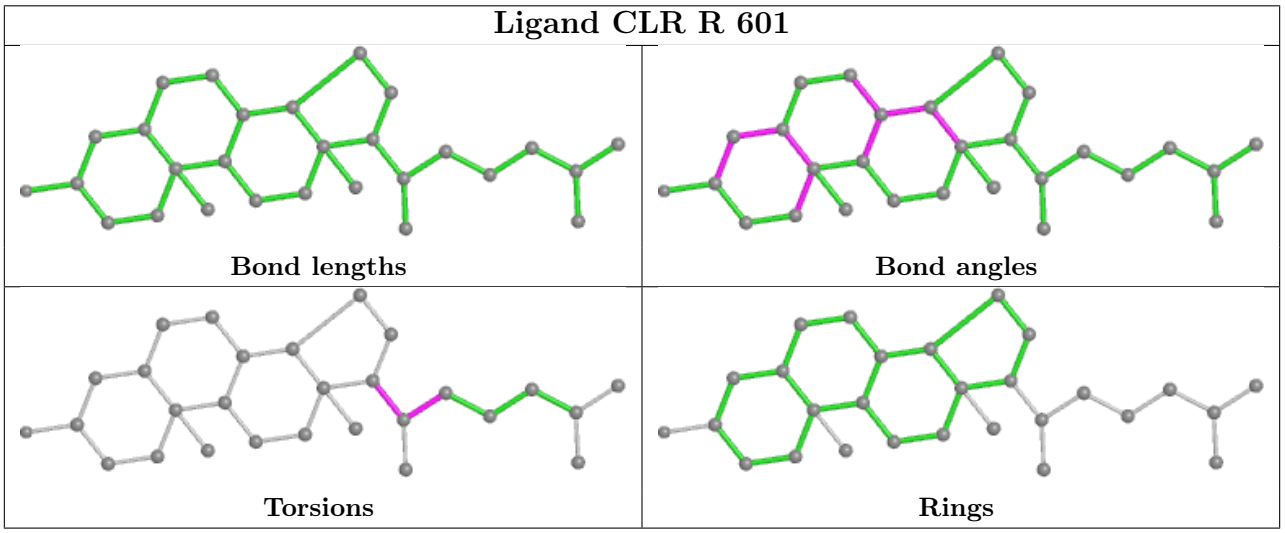
Ligand CLR R 602



Ligand CLR R 603



Ligand CLR R 601



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

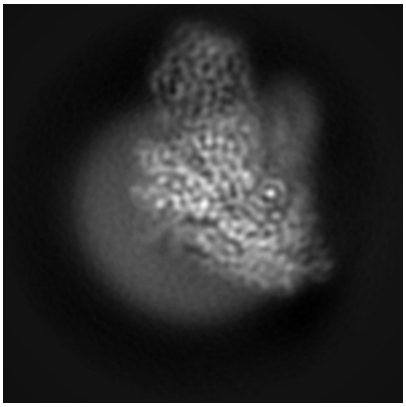
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30877. These allow visual inspection of the internal detail of the map and identification of artifacts.

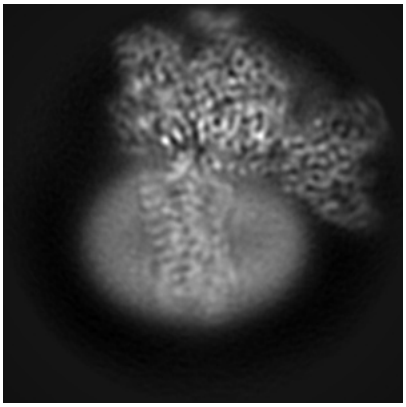
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

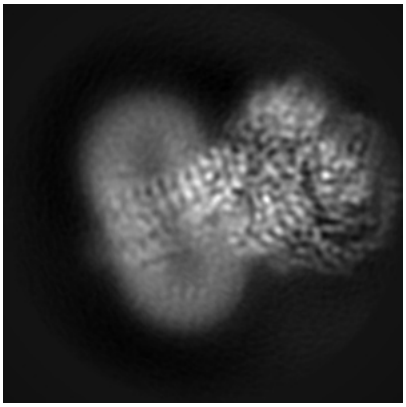
6.1.1 Primary map



X



Y

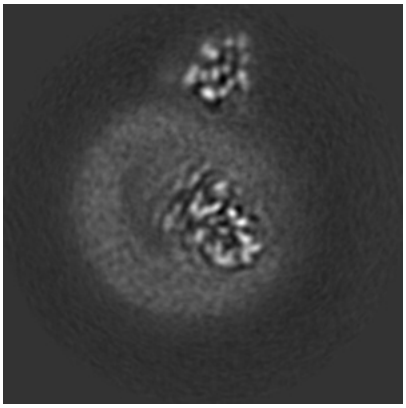


Z

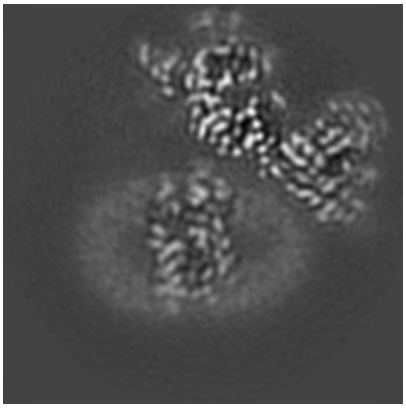
The images above show the map projected in three orthogonal directions.

6.2 Central slices

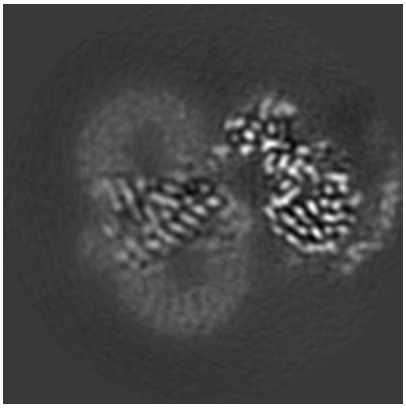
6.2.1 Primary map



X Index: 90



Y Index: 90

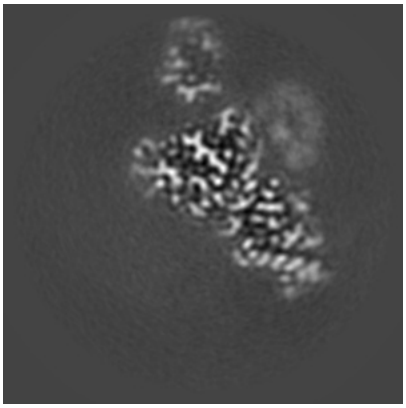


Z Index: 90

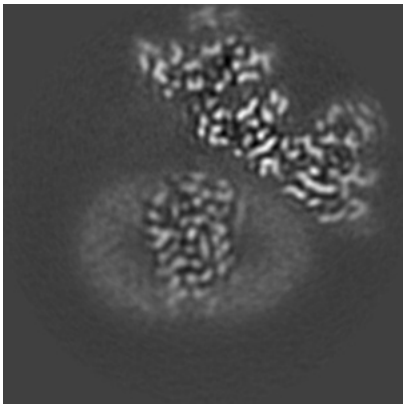
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

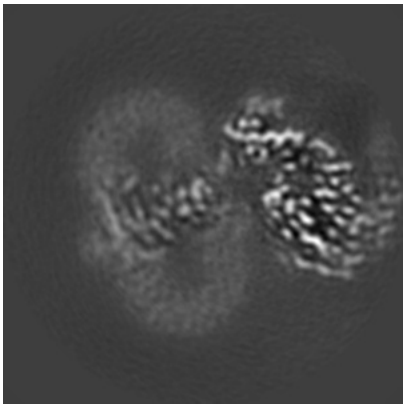
6.3.1 Primary map



X Index: 125



Y Index: 92

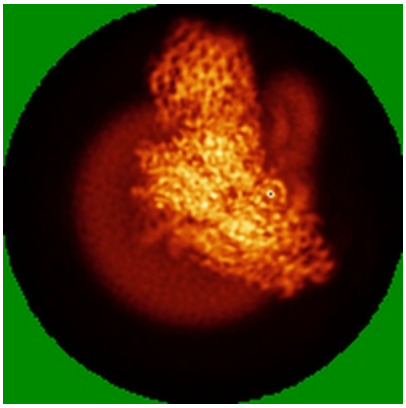


Z Index: 94

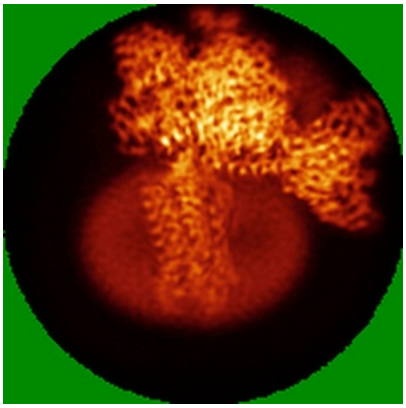
The images above show the largest variance slices of the map in three orthogonal directions.

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

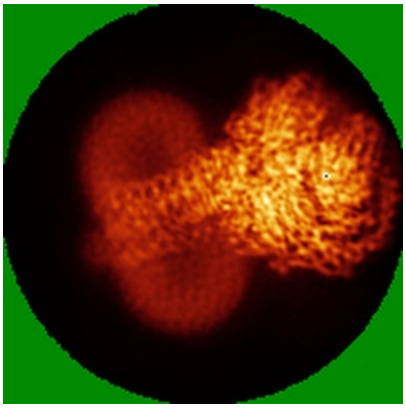
6.4.1 Primary map



X



Y



Z

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

X Y Z

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

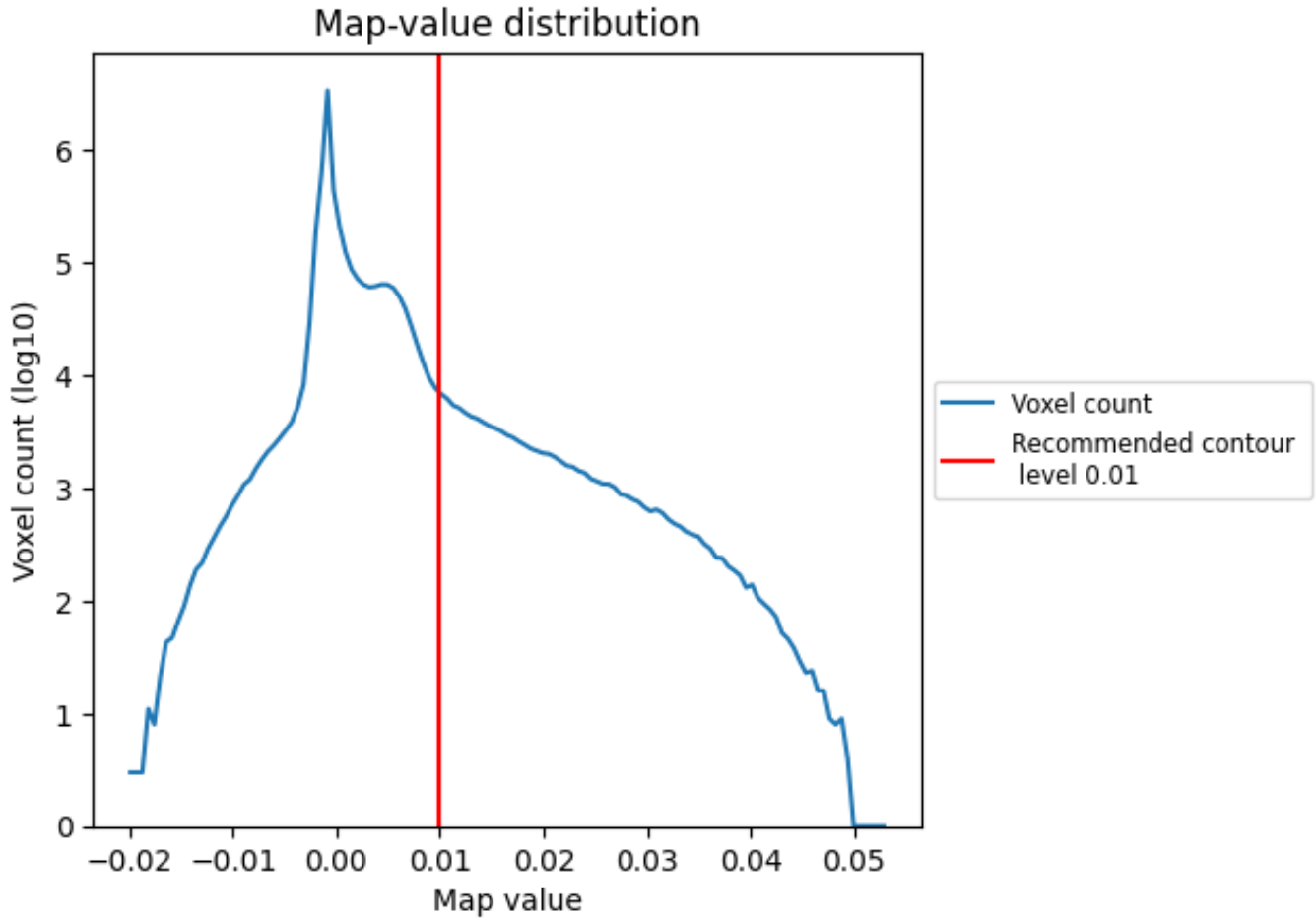
6.6 Mask visualisation (i)

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

7 Map analysis

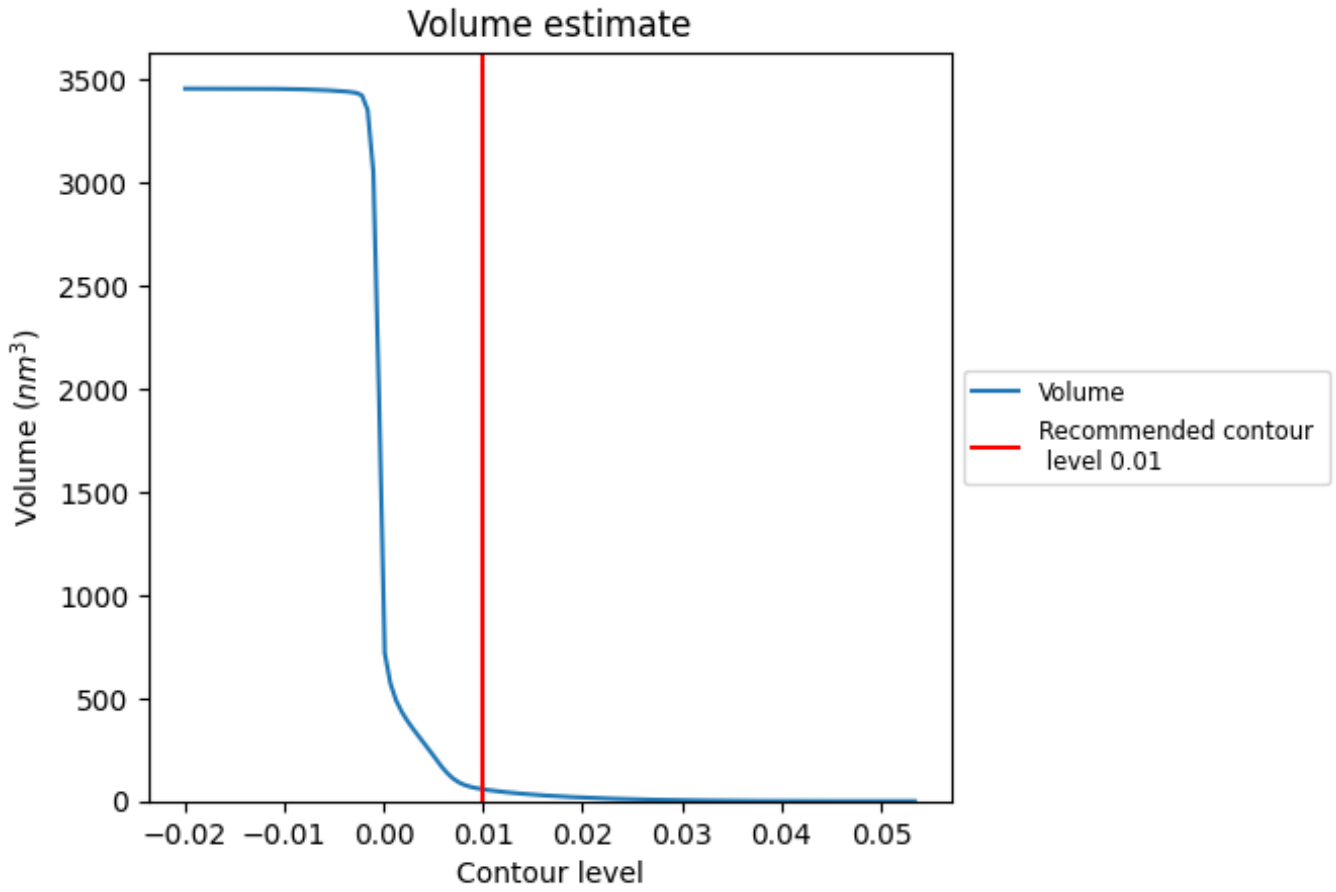
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

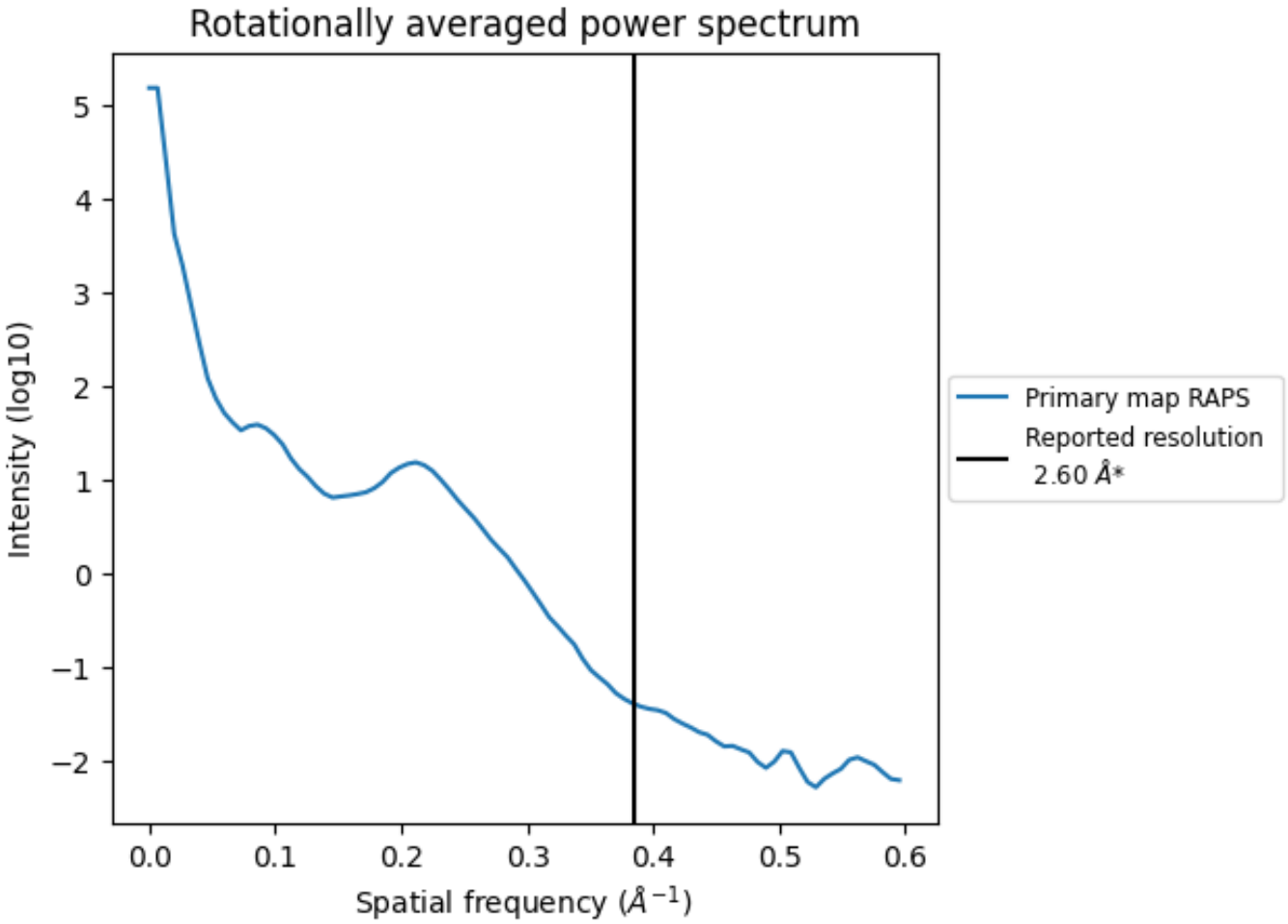
7.2 Volume estimate (i)



The volume at the recommended contour level is 58 nm^3; this corresponds to an approximate mass of 52 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

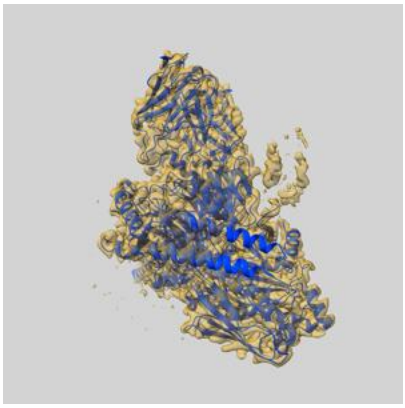
8 Fourier-Shell correlation (i)

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

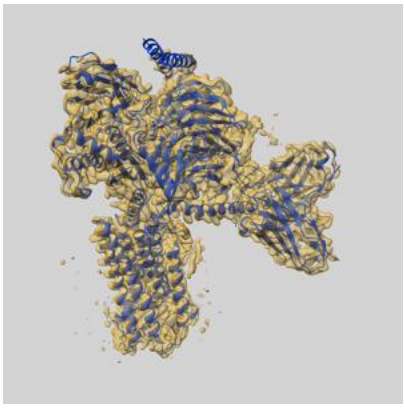
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30877 and PDB model 7DW9. Per-residue inclusion information can be found in section 3 on page 13.

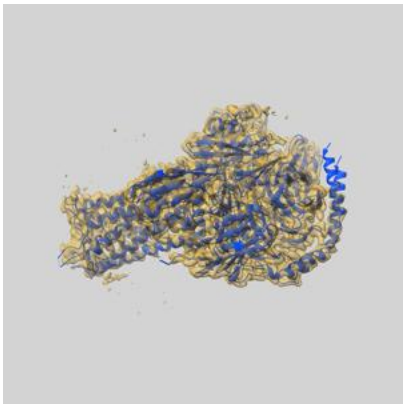
9.1 Map-model overlay



X



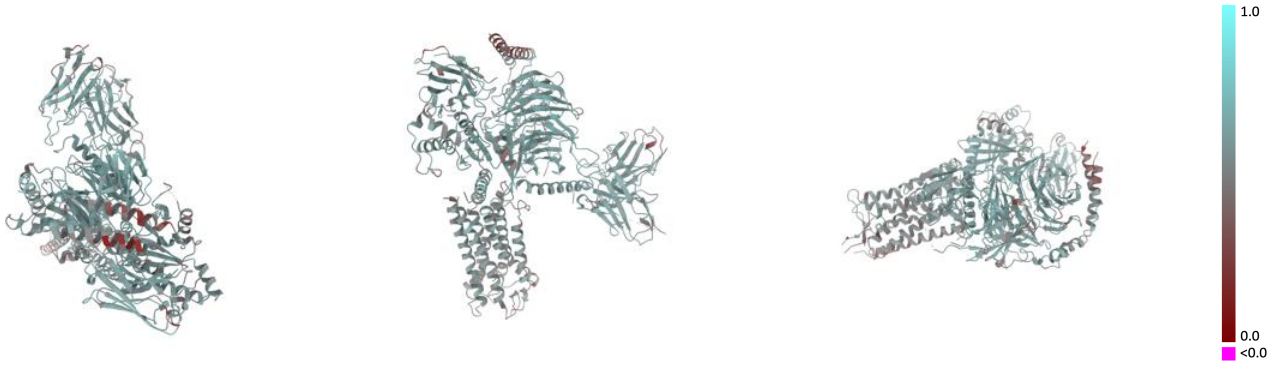
Y



Z

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

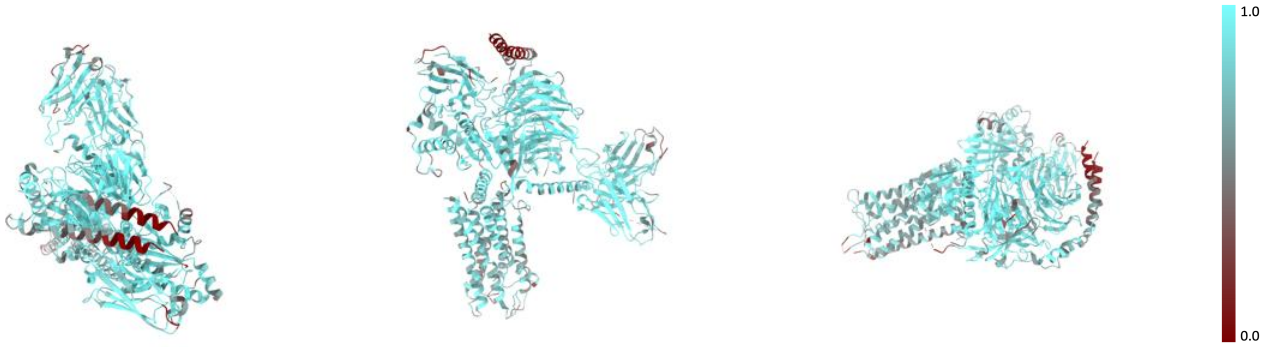
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

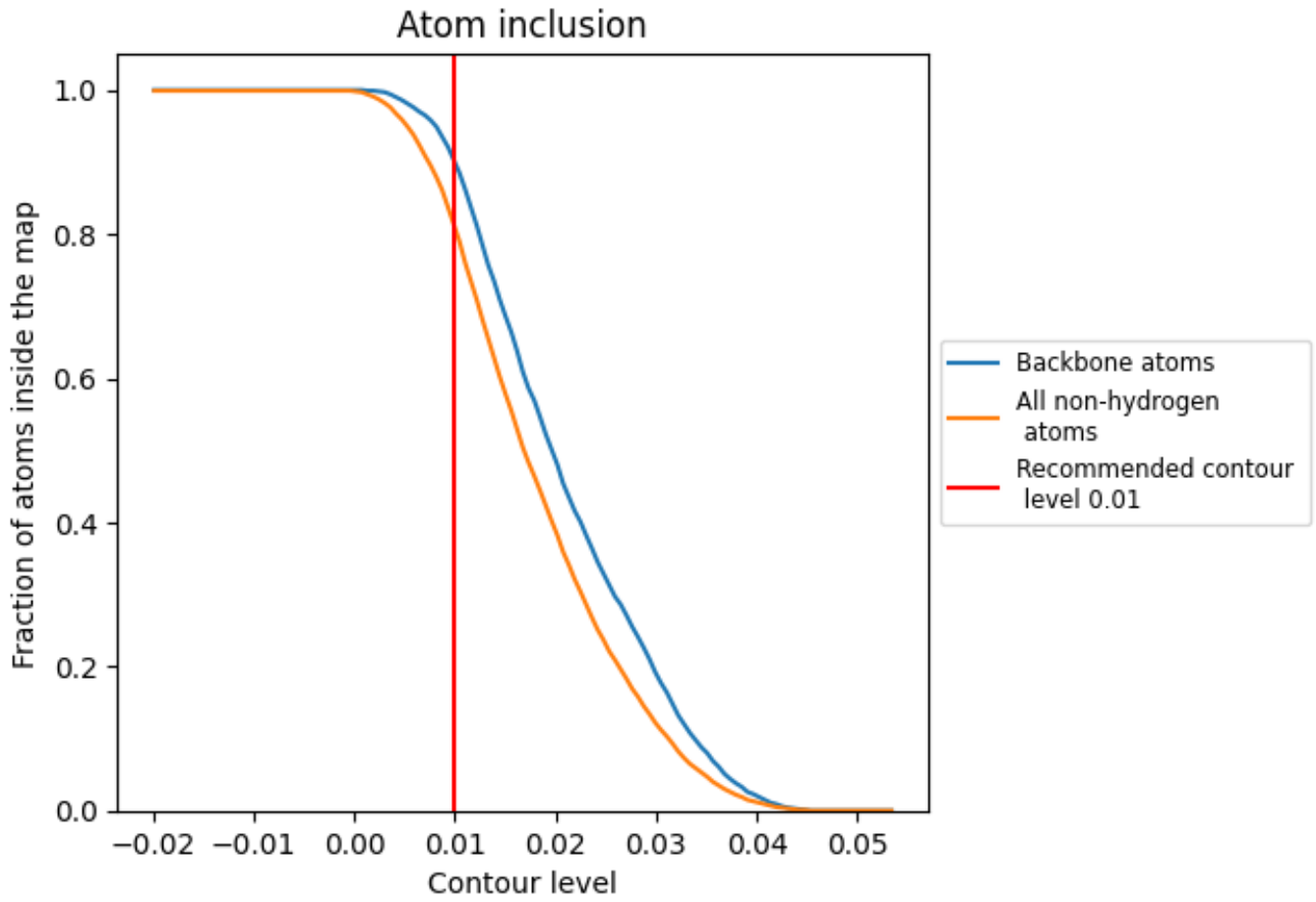
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 81% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8090	0.5510
A	0.8460	0.5690
B	0.8750	0.5870
C	0.7080	0.4690
N	0.8270	0.5680
R	0.7150	0.4900
S	0.8360	0.5670
Y	0.5980	0.4940