Full wwPDB EM Validation Report ⓘ

Dec 12, 2023 – 12:08 PM EST

PDB ID	:	8U1U
EMDB ID	:	EMD-41829
Title	:	Structure of a class A GPCR/agonist complex
Authors	:	Sun, D.; Johnson, M.; Masureel, M.
Deposited on	:	2023-09-02
Resolution	:	3.10 Å(reported)

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

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

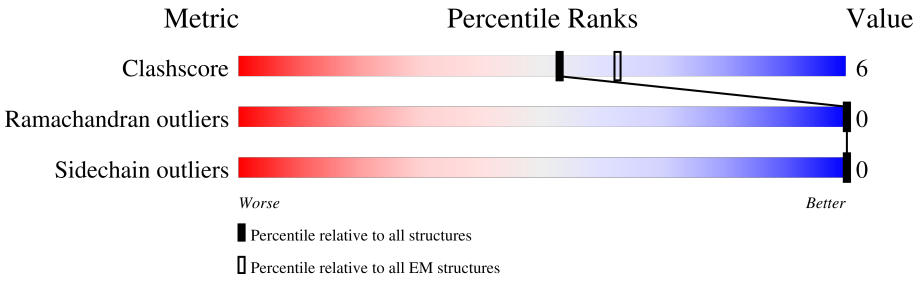
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	743	41% 8% 51%
2	B	376	51% 6% 43%
3	C	357	5% 83% 12% 5%
4	D	71	23% 72% 7% 21%
5	E	259	78% 11% 10%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9507 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 C-C motif chemokine 1,C-C chemokine receptor type 8,EGFP fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	366	2952	1955	476	492	29	0	0

There are 89 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	CYS	ALA	conflict	UNP P22362
A	93D	GLY	-	linker	UNP P22362
A	93E	SER	-	linker	UNP P22362
A	93F	GLY	-	linker	UNP P22362
A	93G	SER	-	linker	UNP P22362
A	93H	GLY	-	linker	UNP P22362
A	93I	SER	-	linker	UNP P22362
A	93J	GLY	-	linker	UNP P22362
A	93K	SER	-	linker	UNP P22362
A	93L	GLY	-	linker	UNP P22362
A	93M	SER	-	linker	UNP P22362
A	93N	GLY	-	linker	UNP P22362
A	93O	SER	-	linker	UNP P22362
A	93P	GLY	-	linker	UNP P22362
A	93Q	SER	-	linker	UNP P22362
A	93R	GLY	-	linker	UNP P22362
A	93S	SER	-	linker	UNP P22362
A	93T	GLY	-	linker	UNP P22362
A	93U	SER	-	linker	UNP P22362
A	93V	GLY	-	linker	UNP P22362
A	93W	SER	-	linker	UNP P22362
A	93X	GLY	-	linker	UNP P22362
A	93Y	SER	-	linker	UNP P22362
A	93Z	GLY	-	linker	UNP P22362
A	94A	SER	-	linker	UNP P22362
A	117	CYS	PHE	conflict	UNP P51685
A	452	GLY	-	linker	UNP P51685

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Chain	Residue	Modelled	Actual	Comment	Reference
A	453	GLY	-	linker	UNP P51685
A	454	SER	-	linker	UNP P51685
A	455	ASP	-	linker	UNP P51685
A	456	TYR	-	linker	UNP P51685
A	457	LYS	-	linker	UNP P51685
A	458	ASP	-	linker	UNP P51685
A	459	ASP	-	linker	UNP P51685
A	460	ASP	-	linker	UNP P51685
A	461	ASP	-	linker	UNP P51685
A	462	LYS	-	linker	UNP P51685
A	463	GLY	-	linker	UNP P51685
A	464	GLY	-	linker	UNP P51685
A	465	SER	-	linker	UNP P51685
A	466	LEU	-	linker	UNP P51685
A	467	GLU	-	linker	UNP P51685
A	468	VAL	-	linker	UNP P51685
A	469	LEU	-	linker	UNP P51685
A	470	PHE	-	linker	UNP P51685
A	471	GLN	-	linker	UNP P51685
A	472	GLY	-	linker	UNP P51685
A	473	PRO	-	linker	UNP P51685
A	520	LEU	PHE	conflict	UNP A0A6M5E0N3
A	539	GLY	THR	conflict	UNP A0A6M5E0N3
A	542	LEU	VAL	conflict	UNP A0A6M5E0N3
A	546	ALA	SER	conflict	UNP A0A6M5E0N3
A	627	THR	MET	conflict	UNP A0A6M5E0N3
A	637	ALA	VAL	conflict	UNP A0A6M5E0N3
A	649	GLY	SER	conflict	UNP A0A6M5E0N3
A	658	GLN	HIS	conflict	UNP A0A6M5E0N3
A	677	TYR	THR	conflict	UNP A0A6M5E0N3
A	680	LYS	ALA	conflict	UNP A0A6M5E0N3
A	713	GLY	-	expression tag	UNP A0A6M5E0N3
A	714	SER	-	expression tag	UNP A0A6M5E0N3
A	715	ALA	-	expression tag	UNP A0A6M5E0N3
A	716	TRP	-	expression tag	UNP A0A6M5E0N3
A	717	SER	-	expression tag	UNP A0A6M5E0N3
A	718	HIS	-	expression tag	UNP A0A6M5E0N3
A	719	PRO	-	expression tag	UNP A0A6M5E0N3
A	720	GLN	-	expression tag	UNP A0A6M5E0N3
A	721	PHE	-	expression tag	UNP A0A6M5E0N3
A	722	GLU	-	expression tag	UNP A0A6M5E0N3
A	723	LYS	-	expression tag	UNP A0A6M5E0N3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	724	GLY	-	expression tag	UNP A0A6M5E0N3
A	725	GLY	-	expression tag	UNP A0A6M5E0N3
A	726	GLY	-	expression tag	UNP A0A6M5E0N3
A	727	SER	-	expression tag	UNP A0A6M5E0N3
A	728	GLY	-	expression tag	UNP A0A6M5E0N3
A	729	GLY	-	expression tag	UNP A0A6M5E0N3
A	730	GLY	-	expression tag	UNP A0A6M5E0N3
A	731	SER	-	expression tag	UNP A0A6M5E0N3
A	732	GLY	-	expression tag	UNP A0A6M5E0N3
A	733	GLY	-	expression tag	UNP A0A6M5E0N3
A	734	SER	-	expression tag	UNP A0A6M5E0N3
A	735	ALA	-	expression tag	UNP A0A6M5E0N3
A	736	TRP	-	expression tag	UNP A0A6M5E0N3
A	737	SER	-	expression tag	UNP A0A6M5E0N3
A	738	HIS	-	expression tag	UNP A0A6M5E0N3
A	739	PRO	-	expression tag	UNP A0A6M5E0N3
A	740	GLN	-	expression tag	UNP A0A6M5E0N3
A	741	PHE	-	expression tag	UNP A0A6M5E0N3
A	742	GLU	-	expression tag	UNP A0A6M5E0N3
A	743	LYS	-	expression tag	UNP A0A6M5E0N3

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	214	Total	C	N	O	S	0	0
			1726	1097	288	329	12		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	MET	-	initiating methionine	UNP P63096
B	-20	LYS	-	expression tag	UNP P63096
B	-19	LYS	-	expression tag	UNP P63096
B	-18	HIS	-	expression tag	UNP P63096
B	-17	HIS	-	expression tag	UNP P63096
B	-16	HIS	-	expression tag	UNP P63096
B	-15	HIS	-	expression tag	UNP P63096
B	-14	HIS	-	expression tag	UNP P63096
B	-13	HIS	-	expression tag	UNP P63096
B	-12	HIS	-	expression tag	UNP P63096
B	-11	HIS	-	expression tag	UNP P63096
B	-10	HIS	-	expression tag	UNP P63096

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	HIS	-	expression tag	UNP P63096
B	-8	GLU	-	expression tag	UNP P63096
B	-7	ASN	-	expression tag	UNP P63096
B	-6	LEU	-	expression tag	UNP P63096
B	-5	TYR	-	expression tag	UNP P63096
B	-4	PHE	-	expression tag	UNP P63096
B	-3	GLN	-	expression tag	UNP P63096
B	-2	GLY	-	expression tag	UNP P63096
B	-1	GLY	-	expression tag	UNP P63096
B	0	SER	-	expression tag	UNP P63096

- 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	C	338	Total	C	N	O	S	0	0
			2601	1604	467	509	21		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	MET	-	initiating methionine	UNP P62873
C	-15	HIS	-	expression tag	UNP P62873
C	-14	HIS	-	expression tag	UNP P62873
C	-13	HIS	-	expression tag	UNP P62873
C	-12	HIS	-	expression tag	UNP P62873
C	-11	HIS	-	expression tag	UNP P62873
C	-10	HIS	-	expression tag	UNP P62873
C	-9	HIS	-	expression tag	UNP P62873
C	-8	HIS	-	expression tag	UNP P62873
C	-7	GLY	-	expression tag	UNP P62873
C	-6	GLU	-	expression tag	UNP P62873
C	-5	ASN	-	expression tag	UNP P62873
C	-4	LEU	-	expression tag	UNP P62873
C	-3	TYR	-	expression tag	UNP P62873
C	-2	PHE	-	expression tag	UNP P62873
C	-1	GLN	-	expression tag	UNP P62873
C	0	GLY	-	expression tag	UNP P62873
C	1	SER	-	expression tag	UNP P62873

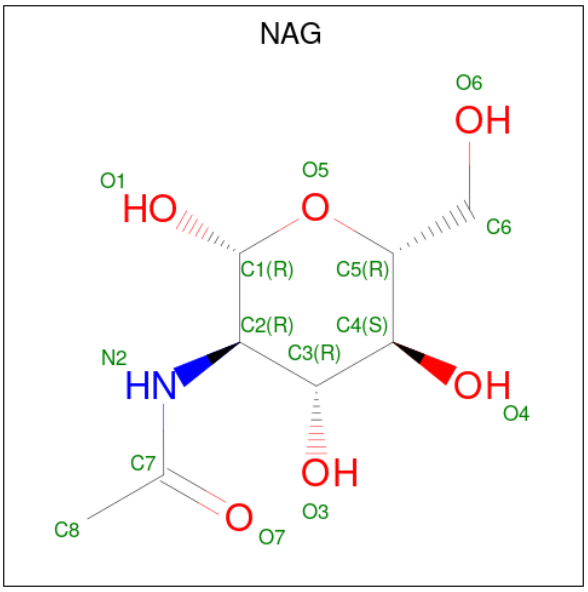
- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	56	Total	C	N	O	S	0	0
			429	269	76	81	3		

- Molecule 5 is a protein called scFv fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	232	Total	C	N	O	S	0	0
			1785	1132	295	348	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



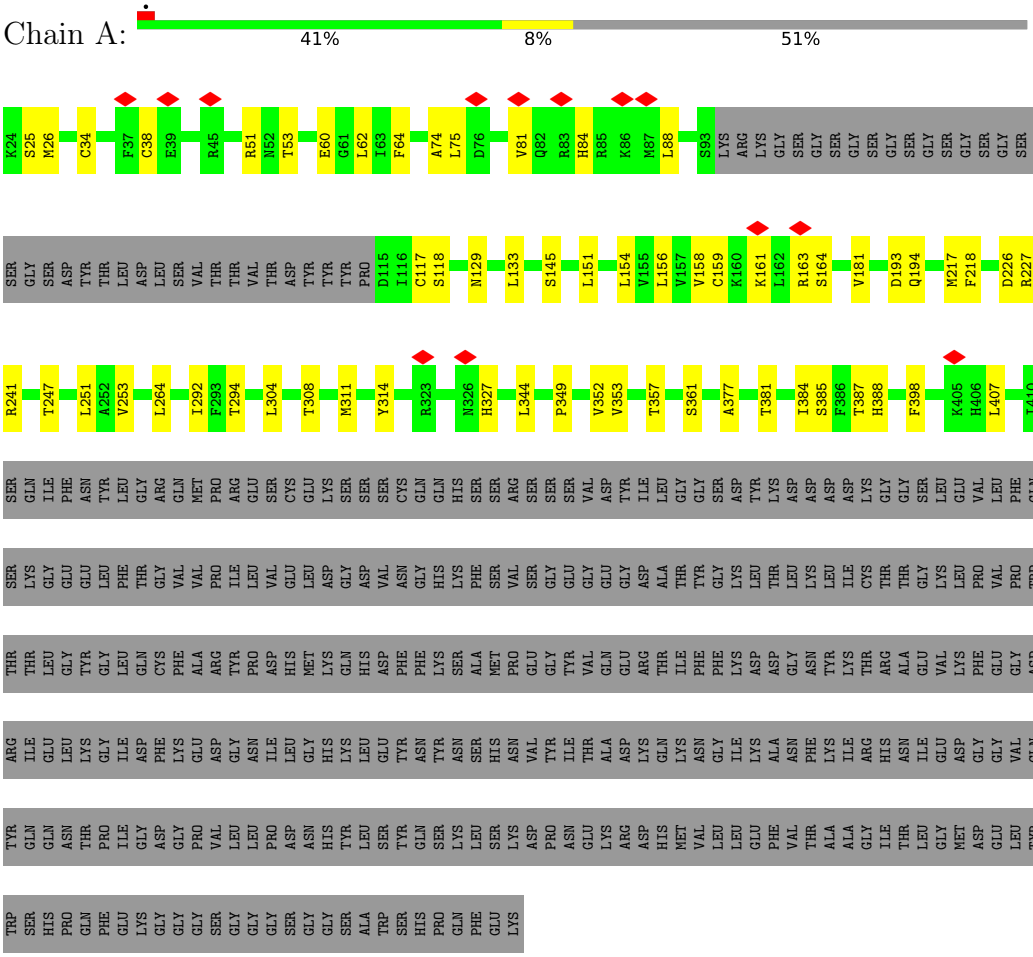
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	

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.

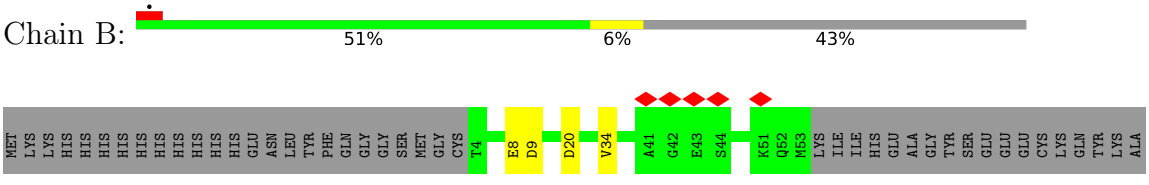
• Molecule 1: C-C motif chemokine 1,C-C chemokine receptor type 8,EGFP fusion protein

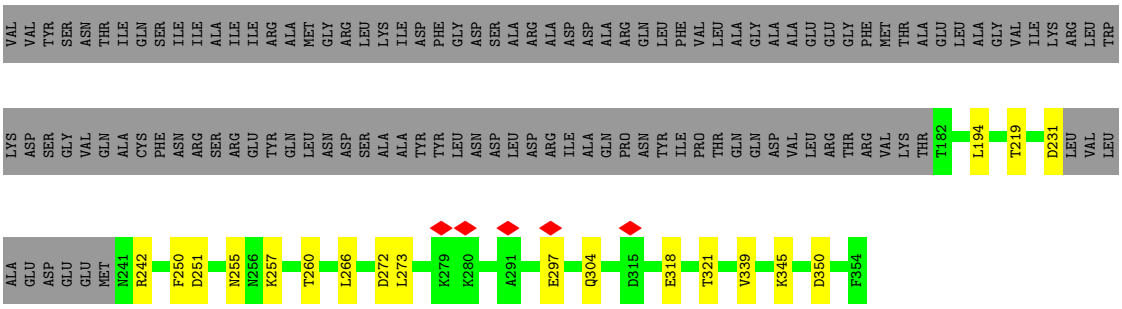
Chain A:



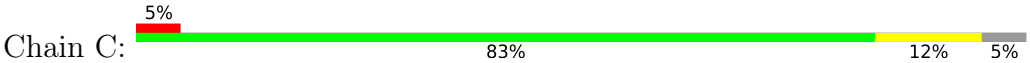
• Molecule 2: Guanine nucleotide-binding protein G(i) subunit alpha-1

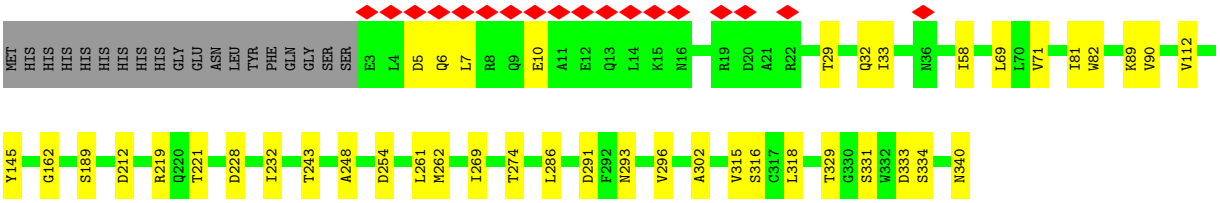
Chain B:



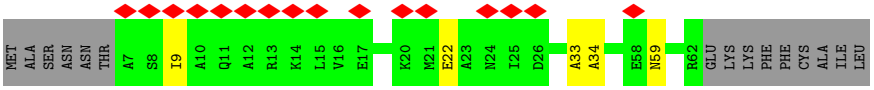


• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

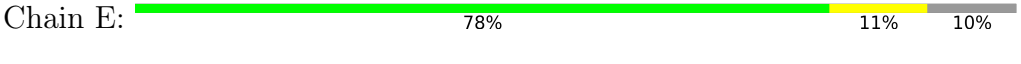


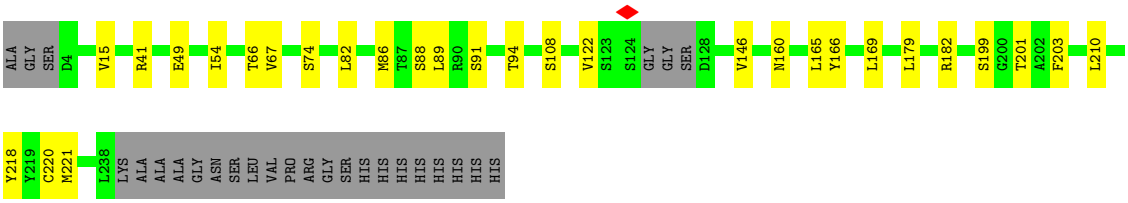


• Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



• Molecule 5: scFv fragment





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	201761	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.814	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	70.168	Depositor
Minimum map value	-28.687	Depositor
Average map value	0.007	Depositor
Map value standard deviation	1.145	Depositor
Recommended contour level	8.33	Depositor
Map size (Å)	292.4064, 292.4064, 292.4064	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0153, 1.0153, 1.0153	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.33	0/3024	0.56	0/4099
2	B	0.28	0/1755	0.51	0/2352
3	C	0.29	0/2648	0.60	0/3589
4	D	0.29	0/435	0.54	0/587
5	E	0.32	0/1829	0.59	0/2480
All	All	0.31	0/9691	0.57	0/13107

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2952	0	3044	39	0
2	B	1726	0	1711	19	0
3	C	2601	0	2505	31	0
4	D	429	0	441	5	0
5	E	1785	0	1716	23	0
6	A	14	0	13	0	0
All	All	9507	0	9430	106	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 6.

All (106) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:VAL:O	1:A:161:LYS:NZ	2.07	0.86
1:A:304:LEU:O	1:A:308:THR:OG1	2.00	0.80
3:C:29:THR:OG1	3:C:32:GLN:OE1	2.04	0.76
2:B:8:GLU:OE2	5:E:166:TYR:OH	2.04	0.75
3:C:69:LEU:HD11	3:C:90:VAL:HG21	1.70	0.74
5:E:94:THR:HG22	5:E:122:VAL:H	1.55	0.70
5:E:41:ARG:NH2	5:E:49:GLU:OE2	2.26	0.69
3:C:318:LEU:CD2	3:C:329:THR:HG22	2.27	0.65
5:E:165:LEU:HD11	5:E:220:CYS:HB2	1.79	0.65
2:B:251:ASP:OD1	2:B:255:ASN:ND2	2.29	0.65
1:A:84:HIS:O	1:A:88:LEU:N	2.30	0.64
1:A:154:LEU:O	1:A:158:VAL:HG22	1.98	0.64
5:E:165:LEU:HD22	5:E:203:PHE:HD2	1.64	0.62
5:E:91:SER:O	5:E:94:THR:HG23	2.01	0.61
3:C:212:ASP:OD2	3:C:219:ARG:NH2	2.34	0.60
2:B:34:VAL:CG2	2:B:194:LEU:HD11	2.31	0.60
1:A:164:SER:OG	2:B:350:ASP:OD2	2.20	0.60
3:C:145:TYR:O	3:C:162:GLY:N	2.34	0.59
1:A:226:ASP:OD1	1:A:241:ARG:NE	2.33	0.59
1:A:353:VAL:O	1:A:357:THR:HG23	2.02	0.59
2:B:297:GLU:N	2:B:297:GLU:OE1	2.35	0.59
3:C:58:ILE:O	3:C:316:SER:OG	2.18	0.59
3:C:333:ASP:O	3:C:334:SER:OG	2.21	0.57
5:E:146:VAL:HG22	5:E:210:LEU:HD21	1.85	0.57
1:A:64:PHE:HZ	1:A:81:VAL:HG23	1.70	0.57
2:B:34:VAL:HG11	2:B:339:VAL:HG11	1.87	0.57
3:C:286:LEU:HD13	3:C:296:VAL:HG22	1.89	0.55
3:C:286:LEU:CD1	3:C:296:VAL:HG22	2.37	0.54
5:E:169:LEU:HD13	5:E:218:TYR:CZ	2.42	0.53
1:A:145:SER:OG	1:A:181:VAL:HG11	2.09	0.53
5:E:94:THR:HG22	5:E:122:VAL:N	2.23	0.53
3:C:10:GLU:N	3:C:10:GLU:OE1	2.42	0.52
2:B:304:GLN:CD	2:B:321:THR:HG21	2.30	0.52
3:C:331:SER:OG	3:C:333:ASP:OD1	2.28	0.52
1:A:117:CYS:SG	1:A:118:SER:N	2.83	0.51
1:A:384:ILE:O	1:A:387:THR:OG1	2.21	0.51
5:E:165:LEU:HD12	5:E:221:MET:O	2.11	0.51
5:E:165:LEU:HD22	5:E:203:PHE:CD2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:VAL:HG23	2:B:194:LEU:HD11	1.91	0.51
1:A:64:PHE:CZ	1:A:81:VAL:HG23	2.45	0.50
1:A:227:ARG:NH1	1:A:314:TYR:OH	2.45	0.49
2:B:34:VAL:HG11	2:B:339:VAL:CG1	2.42	0.49
1:A:51:ARG:O	1:A:62:LEU:HD12	2.12	0.49
1:A:264:LEU:HG	1:A:294:THR:HG22	1.95	0.49
1:A:156:LEU:O	1:A:156:LEU:HD23	2.12	0.49
1:A:377:ALA:O	1:A:381:THR:HG23	2.13	0.48
3:C:274:THR:OG1	3:C:315:VAL:O	2.27	0.48
1:A:151:LEU:HD21	1:A:407:LEU:CD2	2.43	0.48
1:A:398:PHE:HD1	1:A:407:LEU:HD11	1.78	0.48
2:B:34:VAL:HG21	2:B:194:LEU:HD11	1.96	0.48
1:A:217:MET:HA	1:A:217:MET:HE2	1.96	0.48
3:C:228:ASP:N	3:C:228:ASP:OD1	2.44	0.48
1:A:158:VAL:HG23	1:A:159:CYS:SG	2.54	0.48
1:A:327:HIS:HE2	2:B:318:GLU:CD	2.18	0.47
5:E:66:THR:HG23	5:E:67:VAL:HG13	1.96	0.47
1:A:311:MET:SD	1:A:344:LEU:HD11	2.54	0.47
2:B:231:ASP:OD2	2:B:242:ARG:NH2	2.47	0.47
2:B:20:ASP:OD1	3:C:89:LYS:NZ	2.43	0.47
3:C:7:LEU:HD11	4:D:9:ILE:HD12	1.97	0.47
3:C:189:SER:OG	3:C:232:ILE:HG22	2.15	0.47
5:E:108:SER:O	5:E:182:ARG:NH2	2.46	0.47
5:E:54:ILE:HG23	5:E:54:ILE:O	2.16	0.46
1:A:193:ASP:OD1	1:A:194:GLN:N	2.46	0.46
2:B:34:VAL:HG13	2:B:219:THR:HG21	1.98	0.46
3:C:254:ASP:OD2	4:D:33:ALA:HB1	2.16	0.46
3:C:248:ALA:HB1	3:C:269:ILE:HG22	1.97	0.46
1:A:129:ASN:O	1:A:133:LEU:HD23	2.16	0.46
3:C:340:ASN:ND2	4:D:59:ASN:OD1	2.50	0.45
1:A:327:HIS:CE1	2:B:345:LYS:HZ1	2.35	0.45
3:C:69:LEU:HD12	3:C:81:ILE:HG22	1.99	0.45
3:C:69:LEU:HD13	3:C:82:TRP:O	2.18	0.44
1:A:53:THR:HG21	1:A:60:GLU:O	2.18	0.44
3:C:232:ILE:HG13	3:C:243:THR:HG22	1.98	0.44
1:A:53:THR:HG21	1:A:60:GLU:C	2.37	0.44
1:A:247:THR:O	1:A:251:LEU:HD13	2.17	0.44
2:B:257:LYS:O	2:B:260:THR:OG1	2.35	0.44
1:A:218:PHE:HB2	1:A:253:VAL:HG13	2.00	0.44
1:A:385:SER:O	1:A:388:HIS:ND1	2.47	0.43
2:B:9:ASP:OD2	5:E:160:ASN:ND2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:199:SER:O	5:E:201:THR:N	2.52	0.43
2:B:272:ASP:OD1	2:B:273:LEU:N	2.49	0.43
1:A:34:CYS:CB	1:A:75:LEU:HD21	2.49	0.43
2:B:250:PHE:CE2	2:B:266:LEU:HD13	2.53	0.43
1:A:233:HIS:O	1:A:237:ALA:N	2.48	0.42
5:E:169:LEU:HD13	5:E:218:TYR:CE2	2.54	0.42
5:E:74:SER:O	5:E:82:LEU:HD12	2.20	0.42
3:C:5:ASP:OD1	3:C:6:GLN:N	2.53	0.42
5:E:169:LEU:HB2	5:E:179:LEU:HD11	2.02	0.42
3:C:33:ILE:HD11	4:D:34:ALA:CB	2.49	0.42
1:A:25:SER:OG	1:A:26:MET:N	2.53	0.41
5:E:15:VAL:HG11	5:E:89:LEU:HD13	2.03	0.41
1:A:349:PRO:HA	1:A:352:VAL:HG12	2.03	0.41
5:E:86:MET:CE	5:E:89:LEU:HD21	2.50	0.41
5:E:88:SER:O	5:E:88:SER:OG	2.34	0.41
1:A:38:CYS:SG	1:A:117:CYS:N	2.93	0.41
1:A:62:LEU:HB3	1:A:74:ALA:HB3	2.03	0.41
1:A:292:ILE:HD11	1:A:361:SER:HB2	2.03	0.41
3:C:254:ASP:HB2	3:C:261:LEU:HD11	2.02	0.41
3:C:221:THR:HG22	4:D:22:GLU:OE1	2.21	0.41
3:C:81:ILE:HD11	3:C:112:VAL:HG11	2.03	0.40
5:E:86:MET:HE3	5:E:89:LEU:HD21	2.02	0.40
3:C:71:VAL:HG23	3:C:81:ILE:HD13	2.03	0.40
3:C:262:MET:HE3	3:C:302:ALA:HB2	2.02	0.40
3:C:291:ASP:O	3:C:293:ASN:N	2.53	0.40
3:C:262:MET:CE	3:C:302:ALA:HB2	2.51	0.40
1:A:163:ARG:HE	1:A:163:ARG:HA	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	362/743 (49%)	347 (96%)	15 (4%)	0	100	100
2	B	208/376 (55%)	205 (99%)	3 (1%)	0	100	100
3	C	336/357 (94%)	326 (97%)	10 (3%)	0	100	100
4	D	54/71 (76%)	50 (93%)	4 (7%)	0	100	100
5	E	228/259 (88%)	219 (96%)	9 (4%)	0	100	100
All	All	1188/1806 (66%)	1147 (96%)	41 (4%)	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	A	336/651 (52%)	336 (100%)	0	100	100
2	B	190/325 (58%)	190 (100%)	0	100	100
3	C	281/298 (94%)	281 (100%)	0	100	100
4	D	45/58 (78%)	45 (100%)	0	100	100
5	E	197/215 (92%)	197 (100%)	0	100	100
All	All	1049/1547 (68%)	1049 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
6	NAG	A	900	1	14,14,15	0.20	0	17,19,21	0.37	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
6	NAG	A	900	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

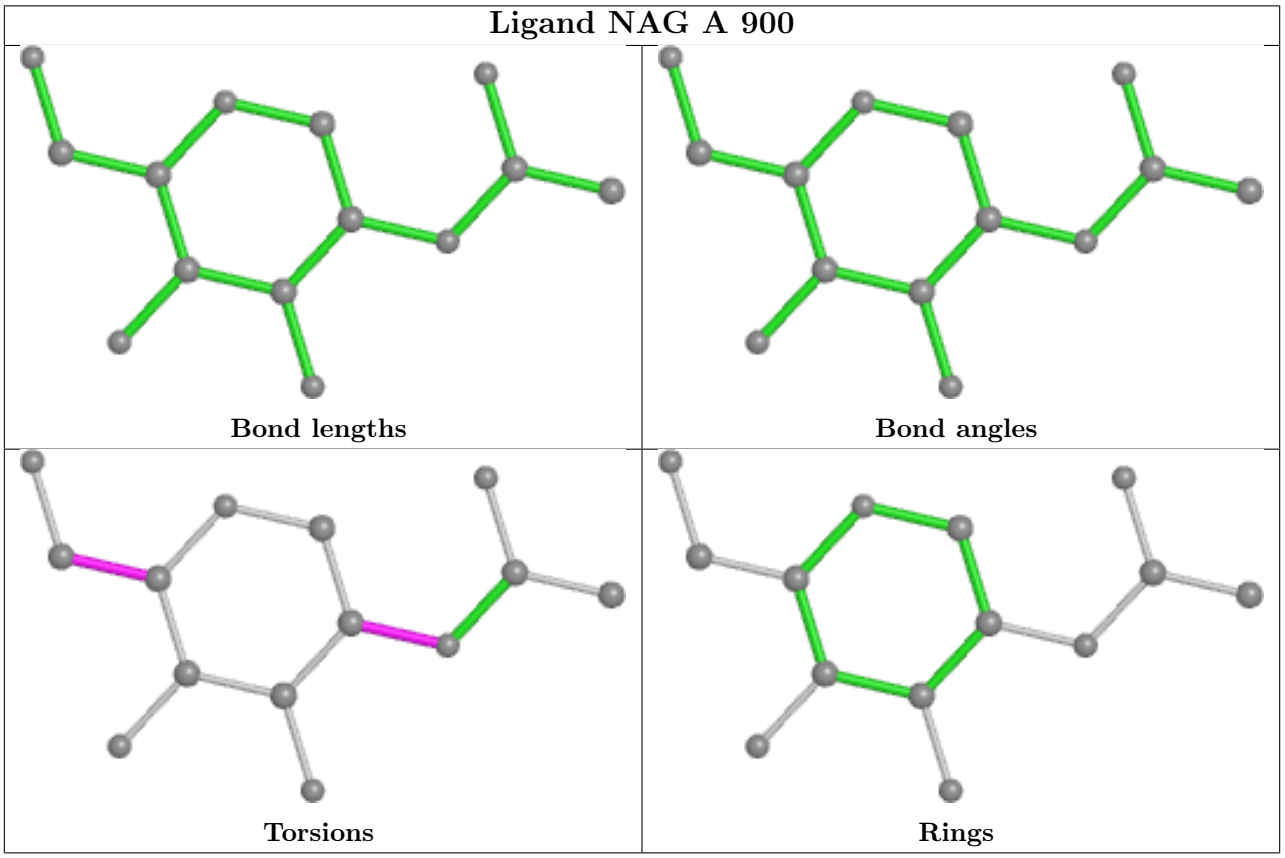
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	900	NAG	O5-C5-C6-O6
6	A	900	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

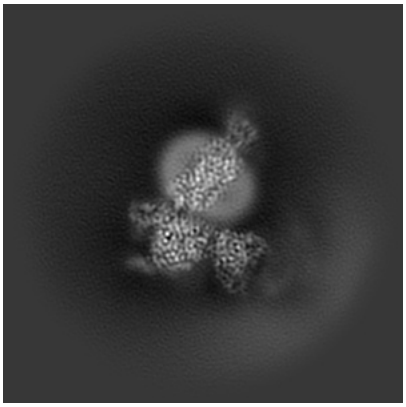
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41829. These allow visual inspection of the internal detail of the map and identification of artifacts.

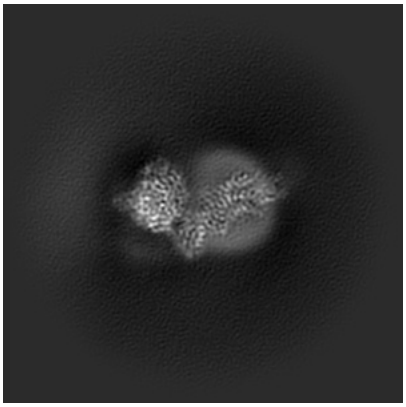
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

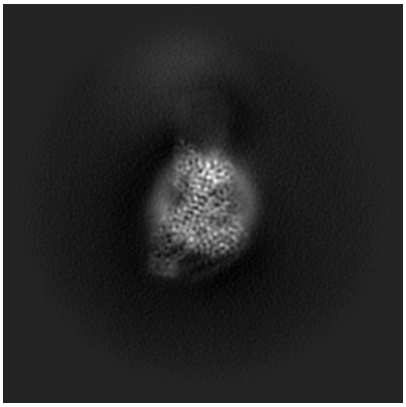
6.1.1 Primary map



X



Y

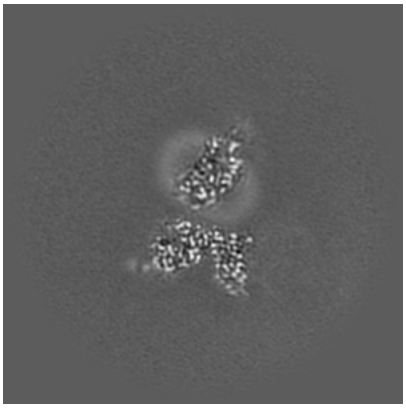


Z

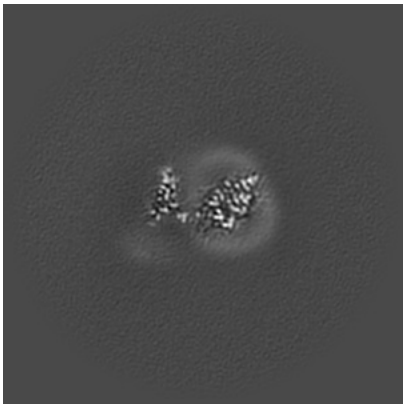
The images above show the map projected in three orthogonal directions.

6.2 Central slices

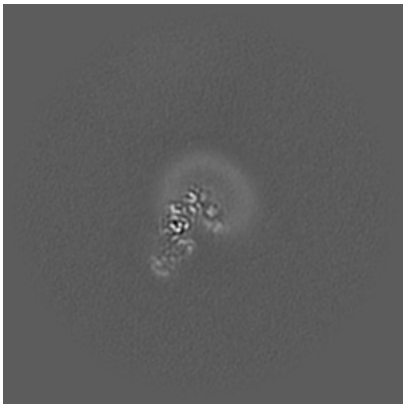
6.2.1 Primary map



X Index: 144



Y Index: 144

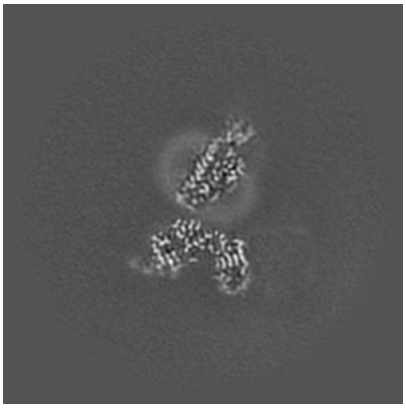


Z Index: 144

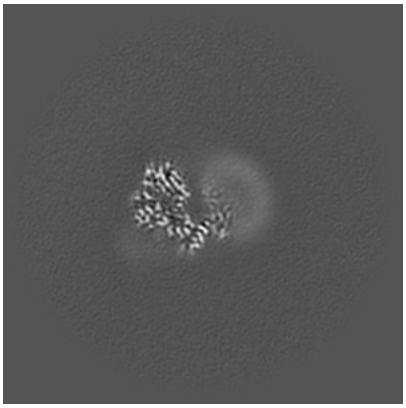
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

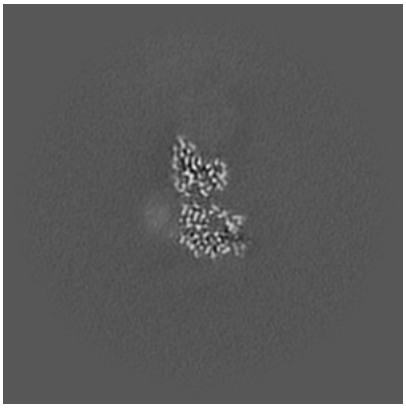
6.3.1 Primary map



X Index: 147



Y Index: 124

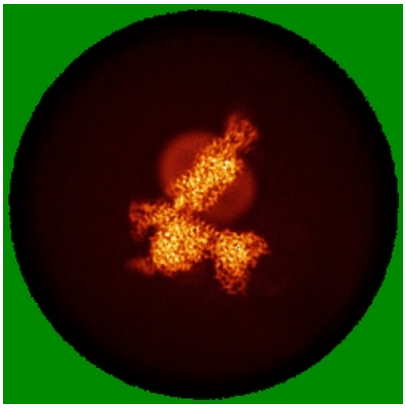


Z Index: 109

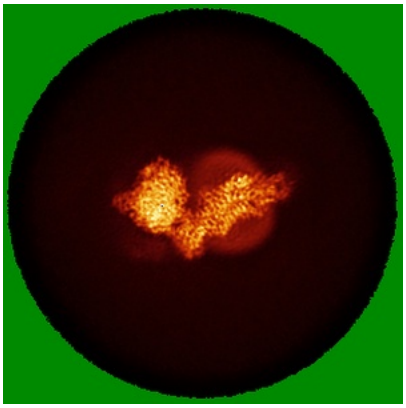
The images above show the largest variance slices of the map in three orthogonal directions.

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

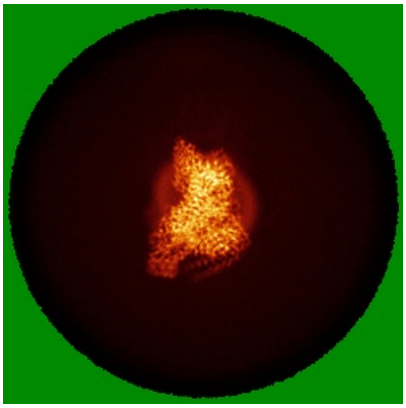
6.4.1 Primary map



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 8.33. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

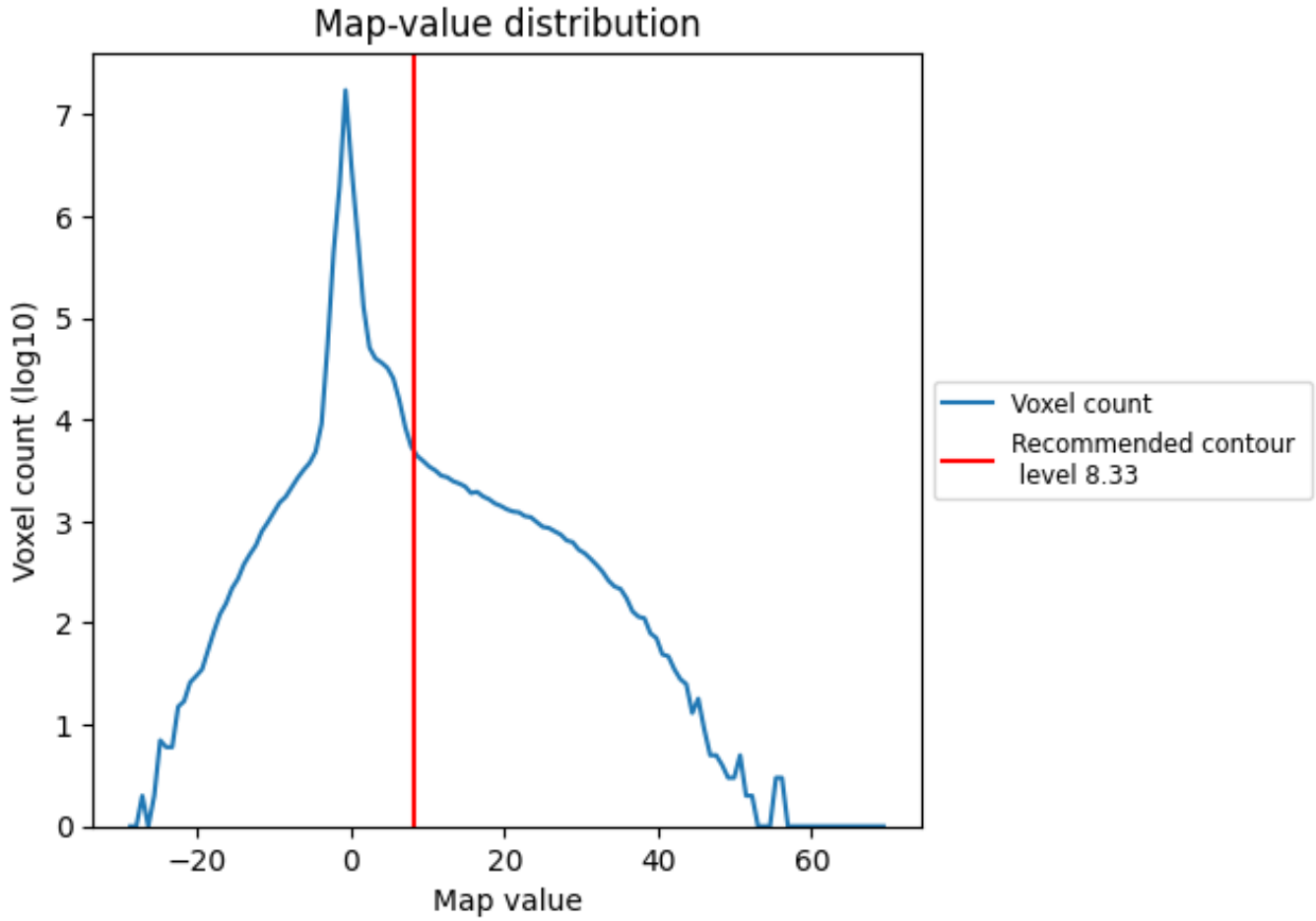
6.6 Mask visualisation (i)

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

7 Map analysis

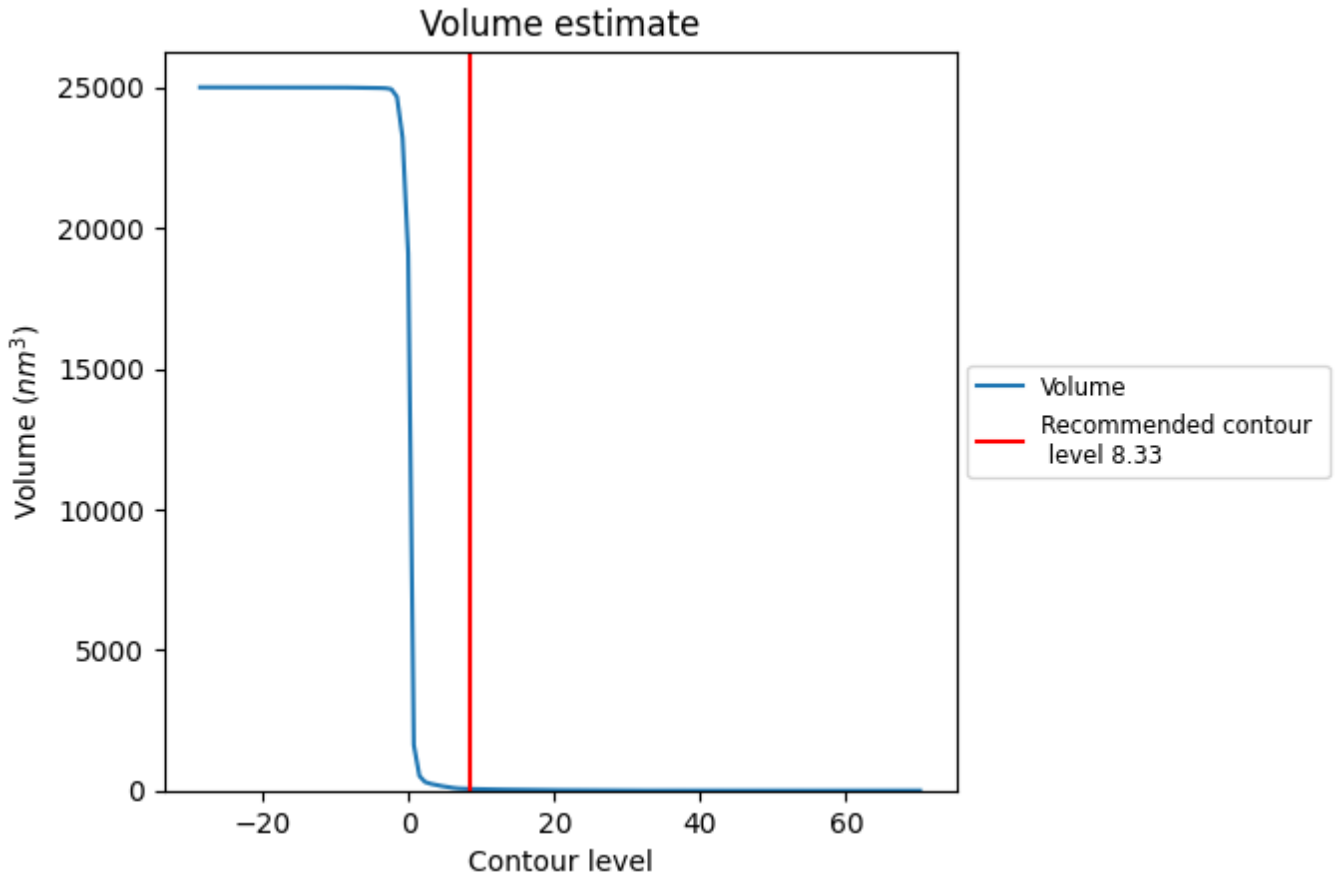
This section contains the results of statistical analysis of the map.

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.

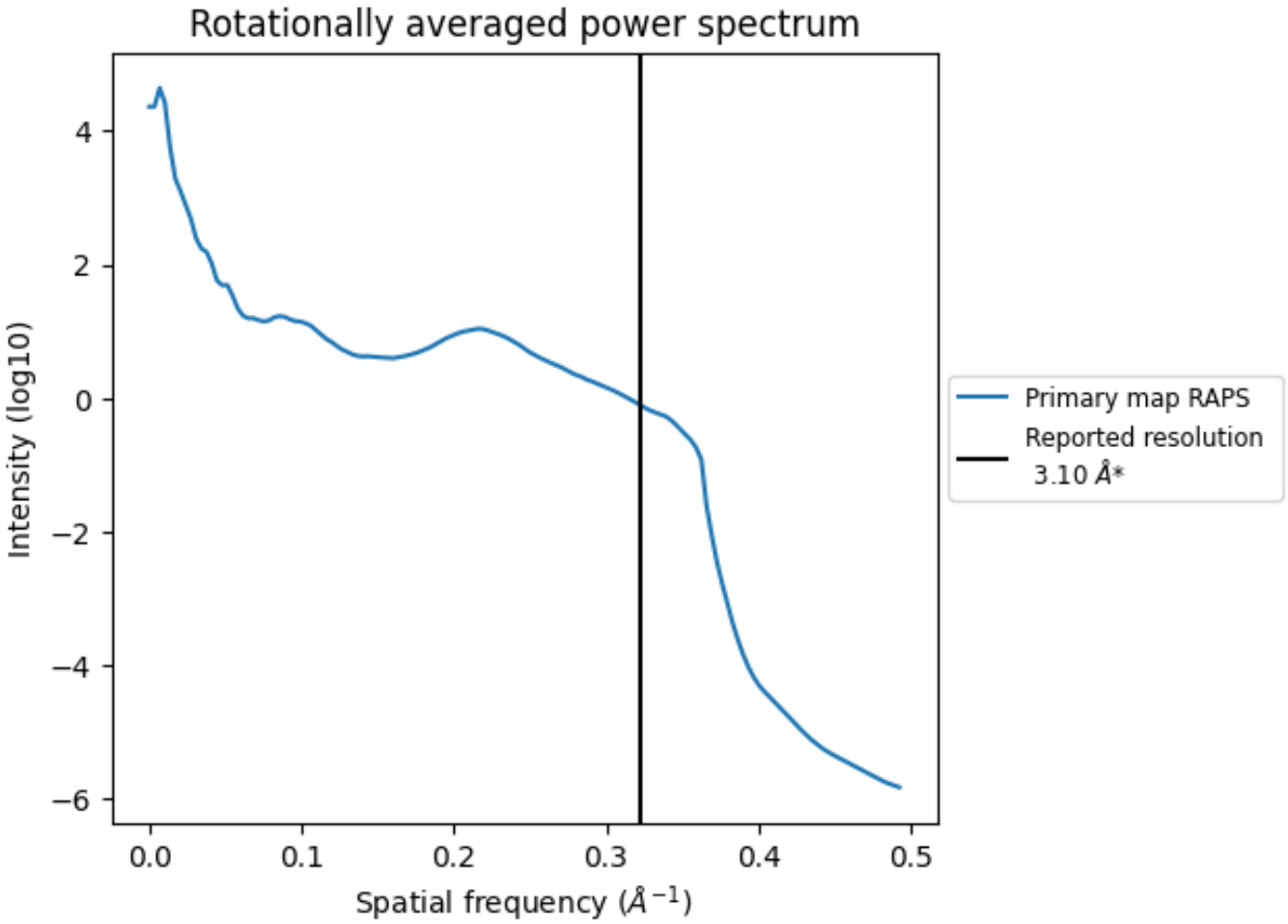
7.2 Volume estimate



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 0.323 Å^{-1}

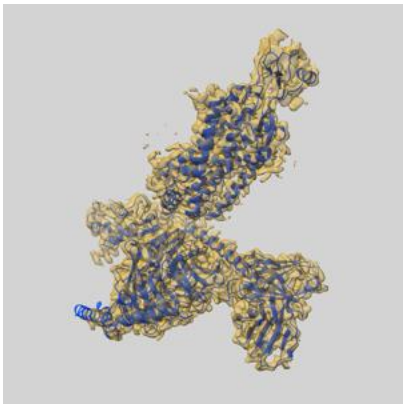
8 Fourier-Shell correlation (i)

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

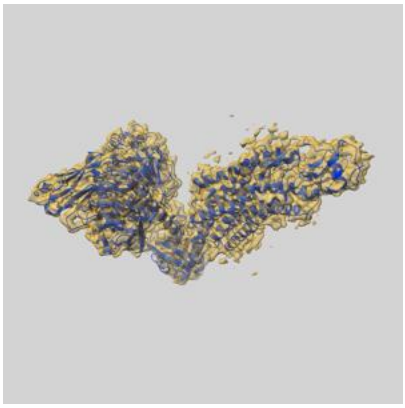
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41829 and PDB model 8U1U. Per-residue inclusion information can be found in section 3 on page 8.

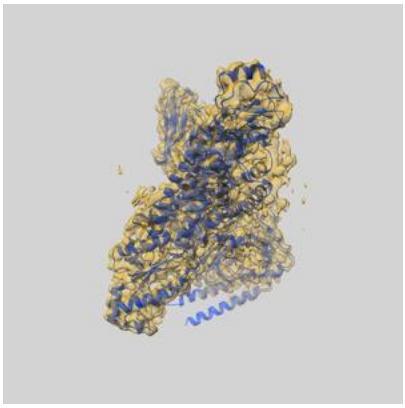
9.1 Map-model overlay



X



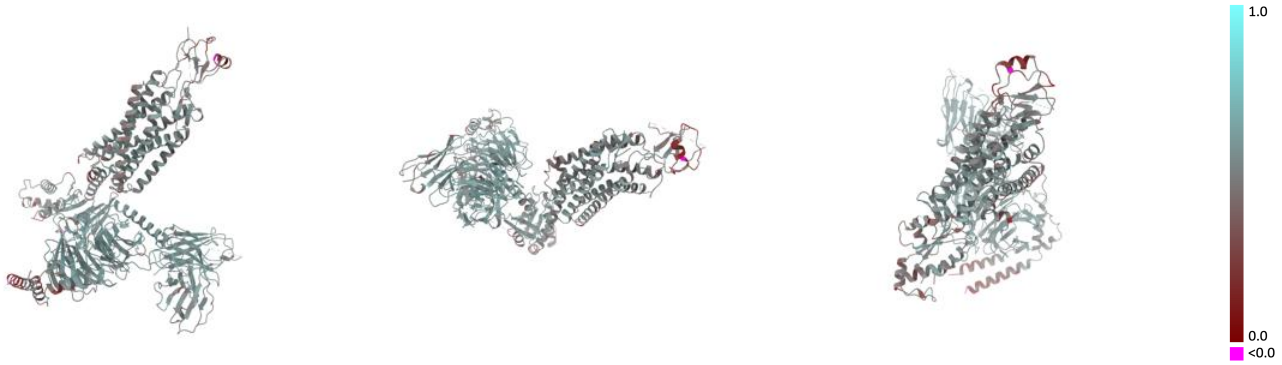
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.33 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.

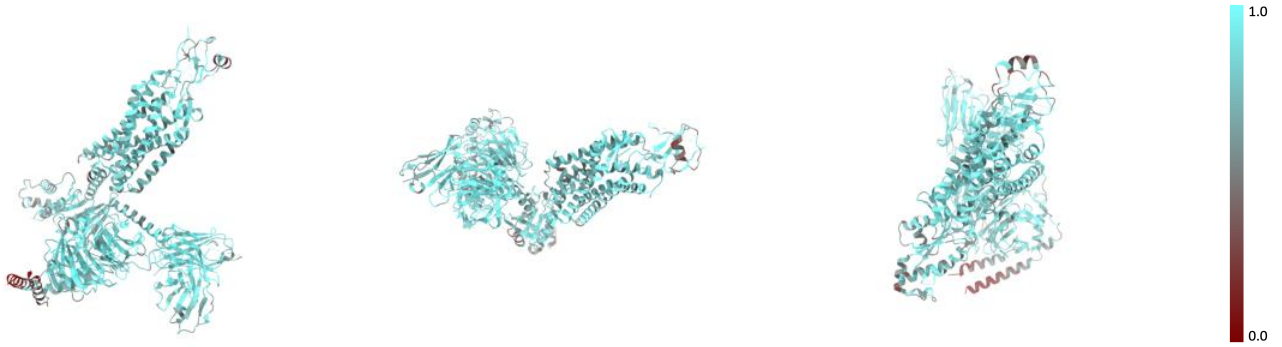
9.2 Q-score mapped to coordinate model (i)



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.

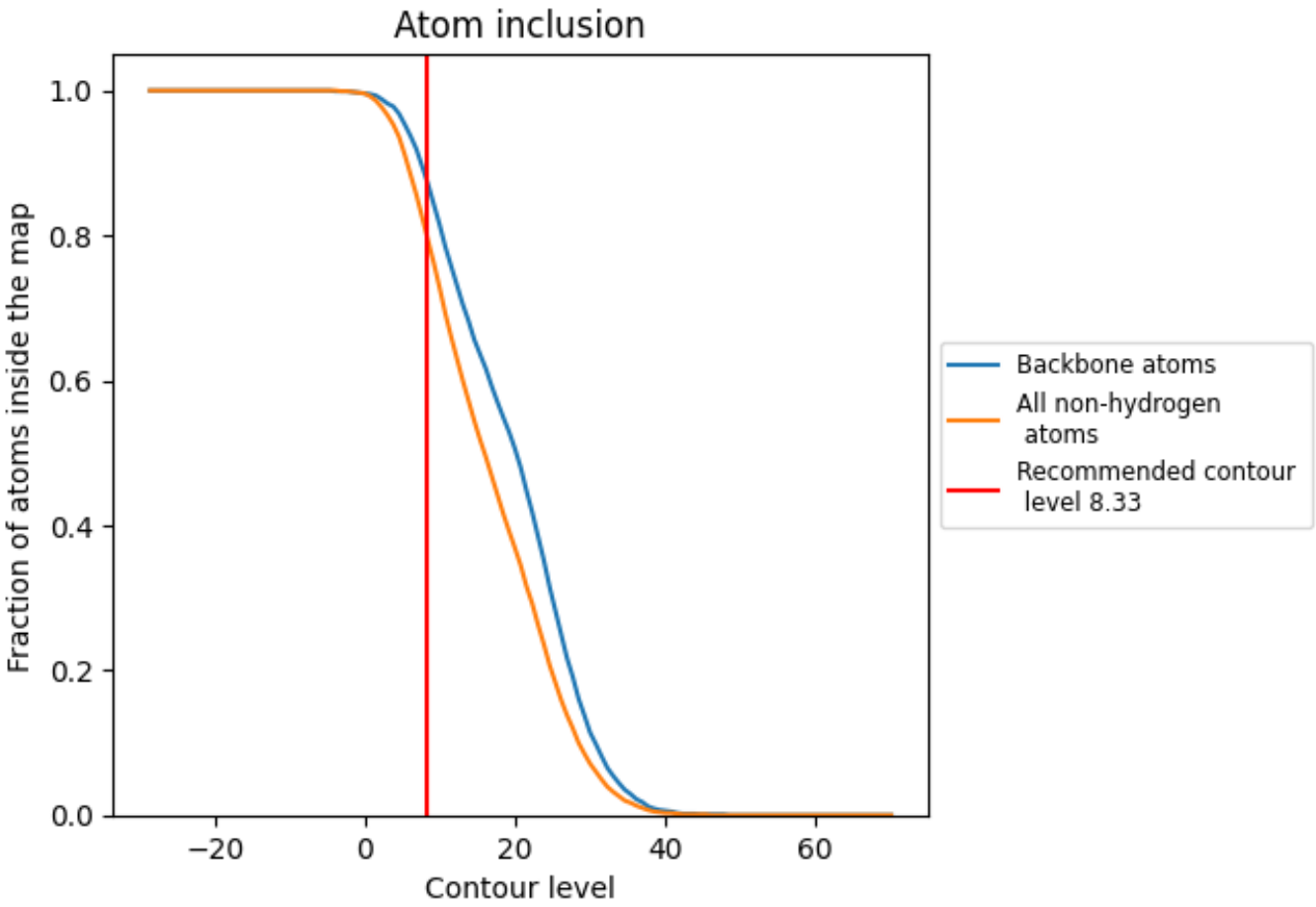
9.3 Atom inclusion mapped to coordinate model (i)



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 (8.33).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 80% 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 (8.33) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7960	0.5150
A	0.7890	0.4790
B	0.7490	0.5020
C	0.8260	0.5490
D	0.6020	0.4370
E	0.8600	0.5560