



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 05:23 AM UTC

PDB ID : 5U0P / pdb_00005u0p
EMDB ID : EMD-8479
Title : Cryo-EM structure of the transcriptional Mediator
Authors : Tsai, K.-L.; Yu, X.; Gopalan, S.; Chao, T.-C.; Zhang, Y.; Florens, L.; Washburn, M.P.; Murakami, K.; Conaway, R.C.; Conaway, J.W.; Asturias, F.
Deposited on : 2016-11-26
Resolution : 4.40 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:

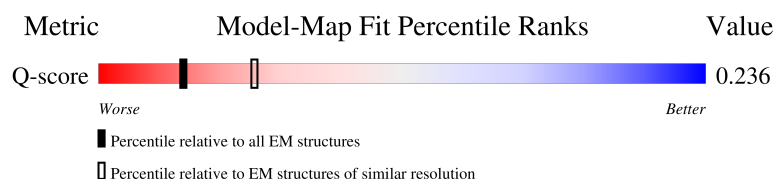
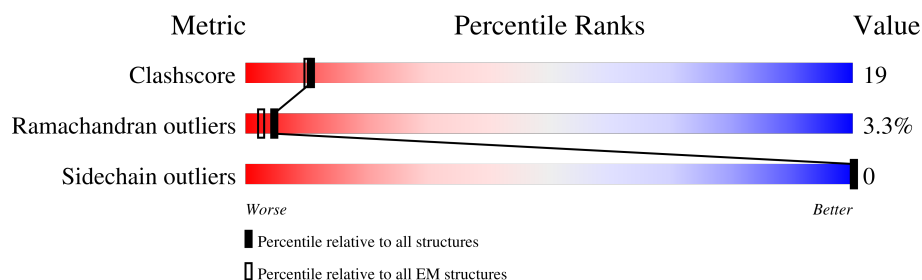
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.40 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.



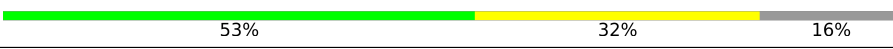
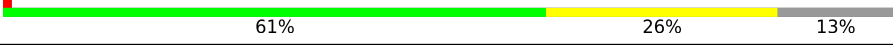
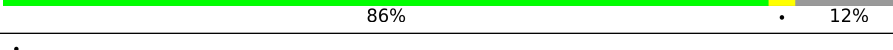
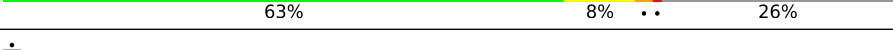
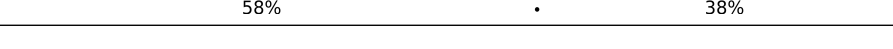
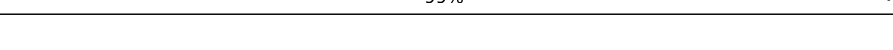
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 (3.91 - 4.90)

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	N	931	
2	F	216	
3	H	200	
4	Q	545	

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Mol	Chain	Length	Quality of chain
5	R	207	
6	T	193	
7	K	116	
8	V	136	
9	D	239	
10	G	376	
11	U	138	
12	3	139	
13	I	121	
14	2	273	
15	S	139	
16	J	132	

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 20268 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 Mediator complex subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	520	Total	C	N	O	S	0	0
			3887	2498	683	698	8		

- Molecule 2 is a protein called Mediator complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	195	Total	C	N	O	S	0	0
			1590	1014	266	301	9		

- Molecule 3 is a protein called Mediator complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	182	Total	C	N	O	S	0	0
			1493	941	257	292	3		

- Molecule 4 is a protein called Mediator complex subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	508	Total	C	N	O	S	0	0
			3831	2419	659	734	19		

- Molecule 5 is a protein called Mediator complex subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	207	Total	C	N	O	S	0	0
			1694	1082	288	316	8		

- Molecule 6 is a protein called Mediator complex subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	179	Total	C	N	O	S	0	0
			1455	950	237	263	5		

- Molecule 7 is a protein called Mediator complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	98	Total	C	N	O	S	0	0
			769	486	128	154	1		

- Molecule 8 is a protein called Mediator complex subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	118	Total	C	N	O	S	0	0
			949	599	161	187	2		

- Molecule 9 is a protein called Mediator complex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	D	96	Total	C	N	O	0	0
			480	288	96	96		

- Molecule 10 is a protein called Mediator complex subunit 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	G	194	Total	C	N	O	0	0
			965	577	194	194		

- Molecule 11 is a protein called Mediator complex subunit 21.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	U	122	Total	C	N	O	0	0
			608	364	122	122		

- Molecule 12 is a protein called Mediator complex subunit 31.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	3	103	Total	C	N	O	0	0
			515	309	103	103		

- Molecule 13 is a protein called Mediator complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	I	75	Total	C	N	O	0	0
			374	224	75	75		

- Molecule 14 is a protein called Mediator complex subunit 27.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	2	78	Total	C	N	O	0	0
			388	232	78	78		

- Molecule 15 is a protein called Mediator complex subunit 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	S	122	Total	C	N	O	0	0
			610	366	122	122		

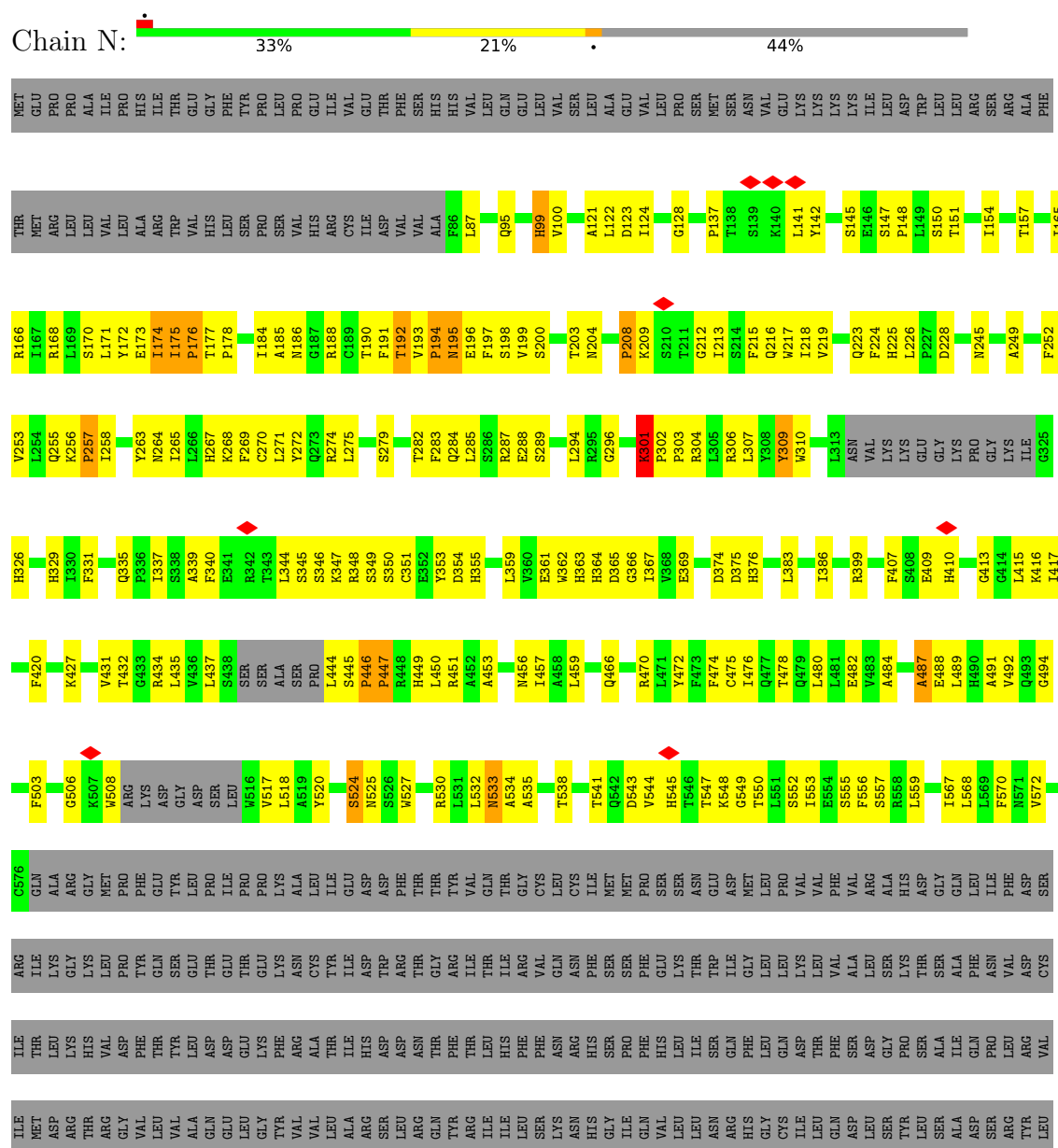
- Molecule 16 is a protein called Mediator complex subunit 10.

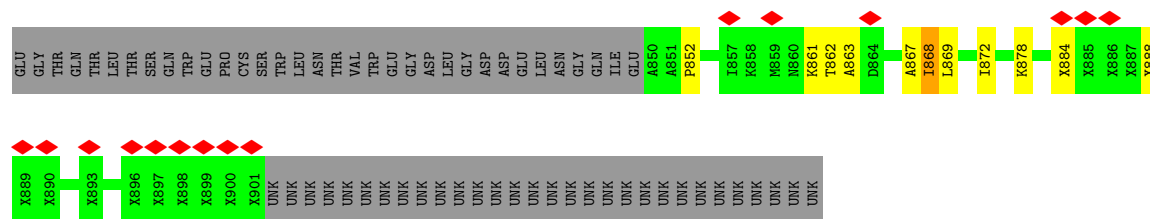
Mol	Chain	Residues	Atoms				AltConf	Trace
16	J	132	Total	C	N	O	0	0
			660	396	132	132		

3 Residue-property plots

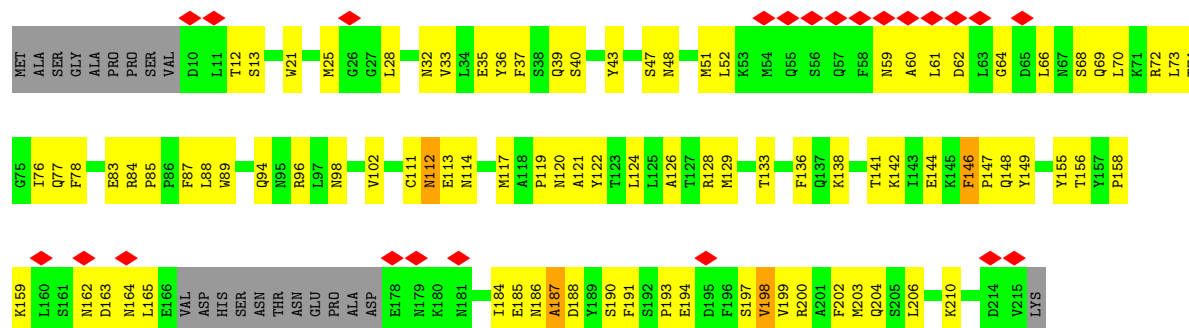
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Mediator complex subunit 14

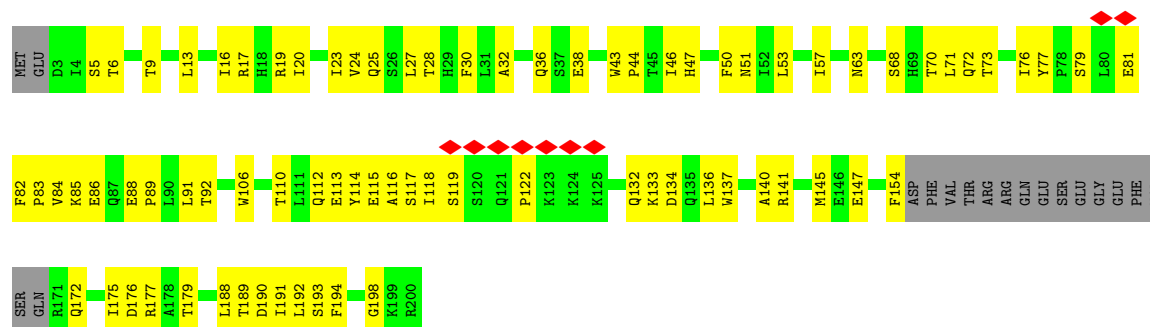




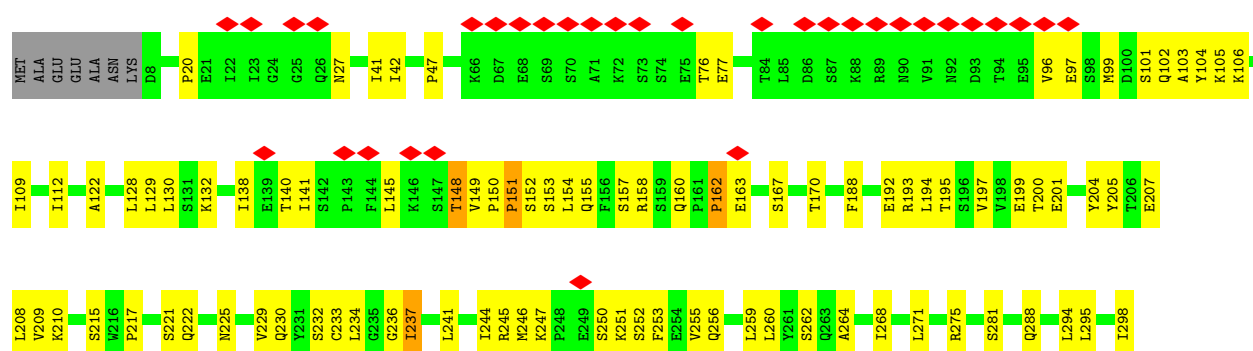
• Molecule 2: Mediator complex subunit 6

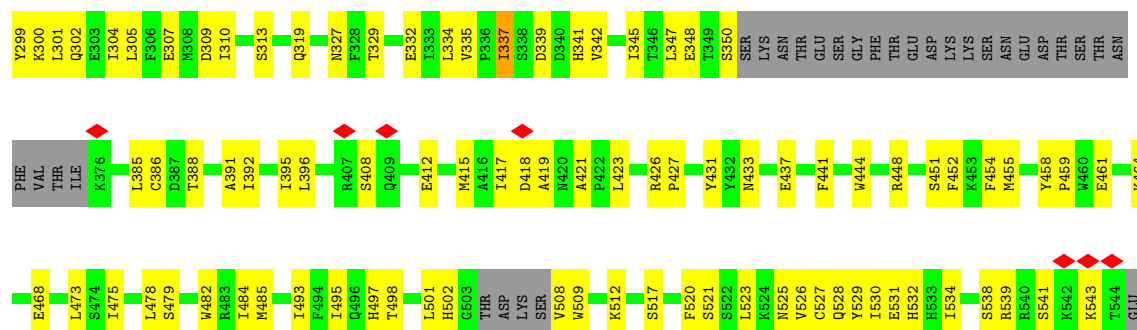


• Molecule 3: Mediator complex subunit 8

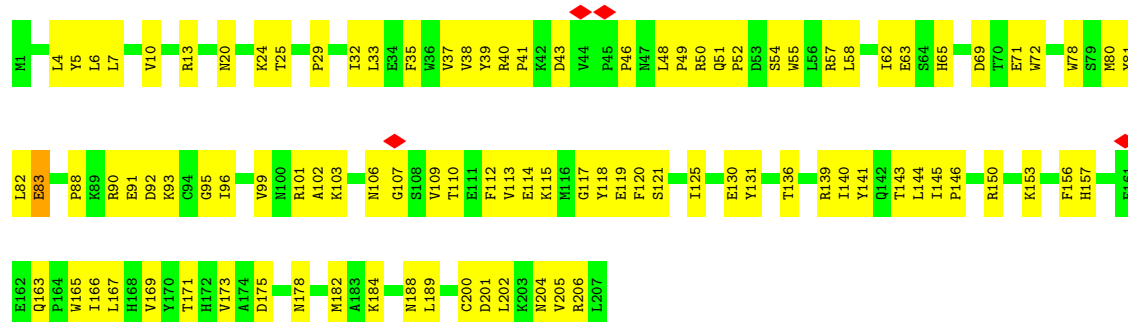


• Molecule 4: Mediator complex subunit 17

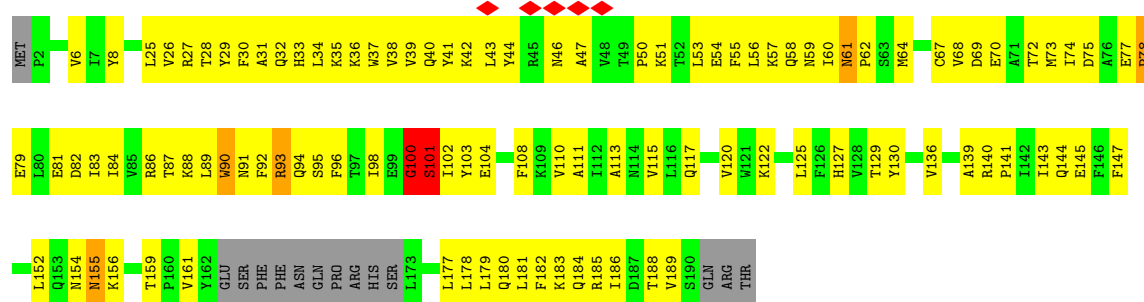




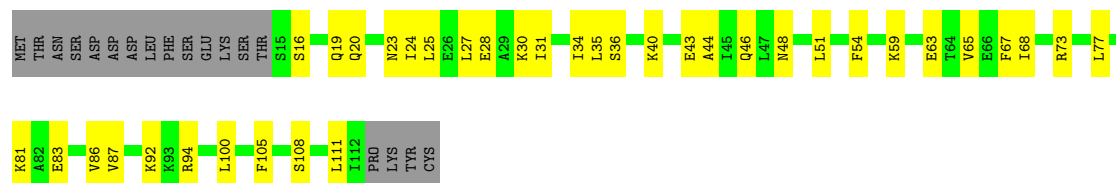
• Molecule 5: Mediator complex subunit 18



• Molecule 6: Mediator complex subunit 20

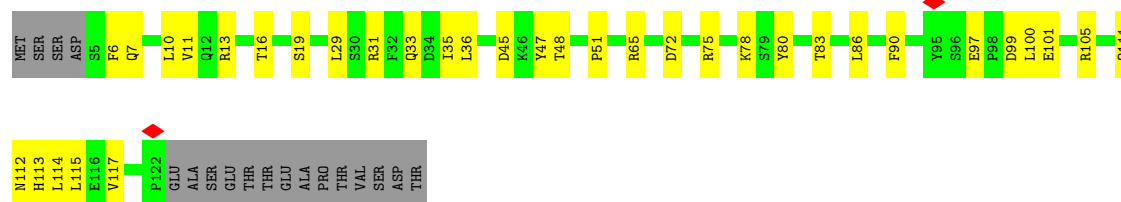


• Molecule 7: Mediator complex subunit 11



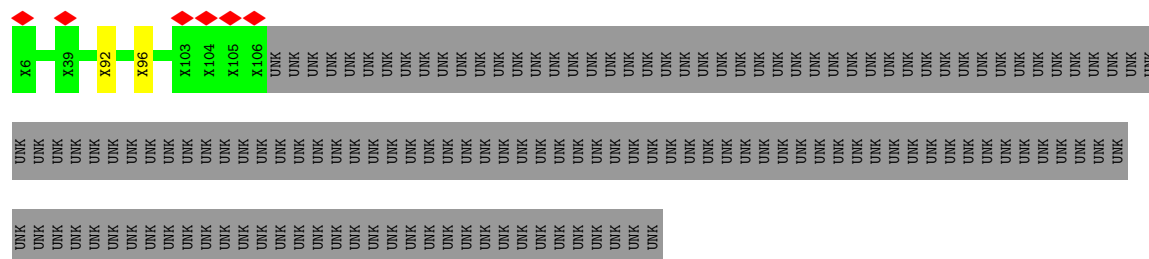
• Molecule 8: Mediator complex subunit 22

Chain V: 



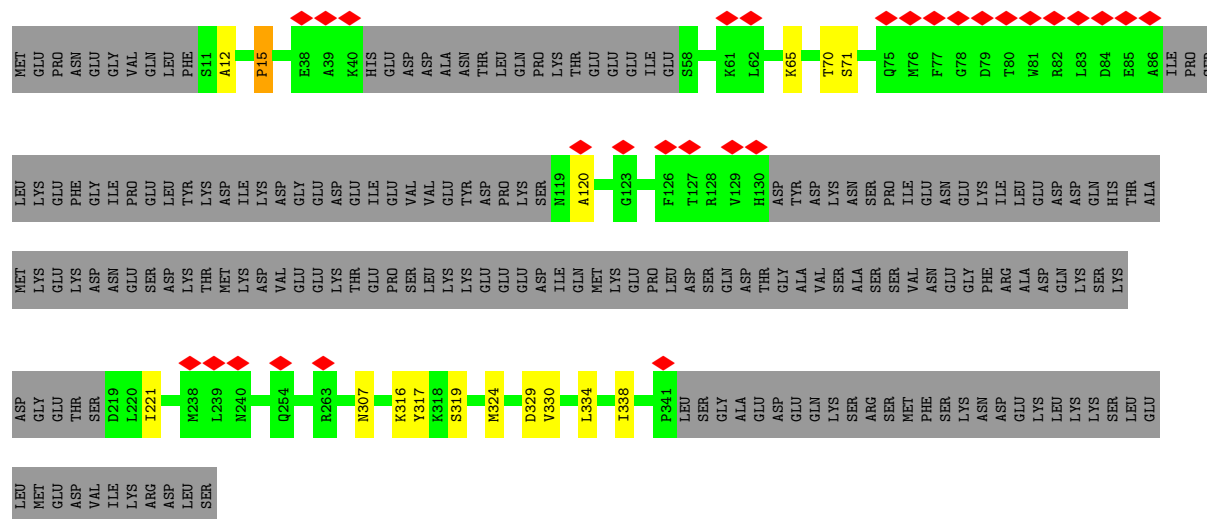
• Molecule 9: Mediator complex subunit 4

Chain D: 



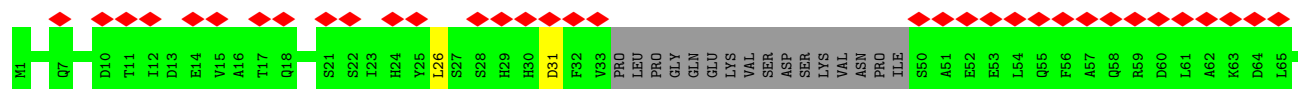
• Molecule 10: Mediator complex subunit 7

Chain G: 



• Molecule 11: Mediator complex subunit 21

Chain U: 



X1	X2	X6	X7	X8	X13	X14	X17	X18	X19	X20	X21	X27	X30	X31	X38	X39	X42	X45	X46	X47	X48	X49	X50	X51	X52	X53	X54	X55	X56	X60	X61	X62	X63	X64	X65	X66	X67	X68	X69	X71	X72	X73	X74	X75	X76	X77	X78	X79	X80	X81	X82	X83	X84	X85	X86	X87	X88	X89	X90	X91	X92	X93	X94	X95	X96	X97	X98	X99	X100	X101	X102	X103	X104	X109	X110	X111	X112	X113	X114	X115	X116	X117	X118	X119	X120	X121	X122	X123	X124	X125	X126	X127	X128	X129	X130	X131	X132	X133	X134	X135	X136	X137	X138	X139	X140	X141	X142	X143	X144	X145	X146	X147	X148	X149	X150	X151	X152	X153	X154	X155	X156	X157	X158	X159	X160	X161	X162	X163	X164	X165	X166	X167	X168	X169	X170	X171	X172	X173	X174	X175	X176	X177	X178	X179	X180	X181	X182	X183	X184	X185	X186	X187	X188	X189	X190	X191	X192	X193	X194	X195	X196	X197	X198	X199	X200	X201	X202	X203	X204	X209	X210	X211	X212	X213	X214	X215	X216	X217	X218	X219	X220	X221	X222	X223	X224	X225	X226	X227	X228	X229	X230	X231	X232	X233	X234	X235	X236	X237	X238	X239	X240	X241	X242	X243	X244	X245	X246	X247	X248	X249	X250	X251	X252	X253	X254	X255	X256	X257	X258	X259	X260	X261	X262	X263	X264	X265	X266	X267	X268	X269	X270	X271	X272	X273	X274	X275	X276	X277	X278	X279	X280	X281	X282	X283	X284	X285	X286	X287	X288	X289	X290	X291	X292	X293	X294	X295	X296	X297	X298	X299	X300	X301	X302	X303	X304	X305	X306	X307	X308	X309	X310	X311	X312	X313	X314	X315	X316	X317	X318	X319	X320	X321	X322	X323	X324	X325	X326	X327	X328	X329	X330	X331	X332	X333	X334	X335	X336	X337	X338	X339	X340	X341	X342	X343	X344	X345	X346	X347	X348	X349	X350	X351	X352	X353	X354	X355	X356	X357	X358	X359	X360	X361	X362	X363	X364	X365	X366	X367	X368	X369	X370	X371	X372	X373	X374	X375	X376	X377	X378	X379	X380	X381	X382	X383	X384	X385	X386	X387	X388	X389	X390	X391	X392	X393	X394	X395	X396	X397	X398	X399	X400	X401	X402	X403	X404	X405	X406	X407	X408	X409	X410	X411	X412	X413	X414	X415	X416	X417	X418	X419	X420	X421	X422	X423	X424	X425	X426	X427	X428	X429	X430	X431	X432	X433	X434	X435	X436	X437	X438	X439	X440	X441	X442	X443	X444	X445	X446	X447	X448	X449	X450	X451	X452	X453	X454	X455	X456	X457	X458	X459	X460	X461	X462	X463	X464	X465	X466	X467	X468	X469	X470	X471	X472	X473	X474	X475	X476	X477	X478	X479	X480	X481	X482	X483	X484	X485	X486	X487	X488	X489	X490	X491	X492	X493	X494	X495	X496	X497	X498	X499	X500	X501	X502	X503	X504	X505	X506	X507	X508	X509	X510	X511	X512	X513	X514	X515	X516	X517	X518	X519	X520	X521	X522	X523	X524	X525	X526	X527	X528	X529	X530	X531	X532	X533	X534	X535	X536	X537	X538	X539	X540	X541	X542	X543	X544	X545	X546	X547	X548	X549	X550	X551	X552	X553	X554	X555	X556	X557	X558
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	42484	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	9.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.075	Depositor
Minimum map value	-0.017	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	461.12, 461.12, 461.12	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	Depositor

5 Model quality

5.1 Standard geometry

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	N	0.43	0/3865	0.93	20/5275 (0.4%)
2	F	0.34	0/1629	0.73	0/2209
3	H	0.37	0/1523	0.73	0/2063
4	Q	0.41	0/3901	0.75	5/5286 (0.1%)
5	R	0.36	0/1739	0.84	2/2362 (0.1%)
6	T	0.86	4/1489 (0.3%)	0.99	7/2020 (0.3%)
7	K	0.41	0/778	0.81	1/1049 (0.1%)
8	V	0.39	0/963	0.77	2/1309 (0.2%)
10	G	0.44	0/961	0.89	5/1336 (0.4%)
11	U	0.37	0/606	0.87	0/844
12	3	0.41	0/514	0.99	3/718 (0.4%)
13	I	0.40	0/373	0.85	0/520
14	2	0.38	0/382	0.77	0/524
All	All	0.45	4/18723 (0.0%)	0.84	45/25515 (0.2%)

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
6	T	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	T	100	GLY	C-O	22.98	1.54	1.23
6	T	100	GLY	C-N	17.41	1.58	1.33
6	T	101	SER	N-CA	6.76	1.54	1.46
6	T	100	GLY	CA-C	5.46	1.59	1.51

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	100	GLY	O-C-N	-15.16	102.99	122.70
1	N	301	LYS	CA-C-N	-12.03	107.99	120.38
1	N	301	LYS	C-N-CA	-12.03	107.99	120.38
5	R	153	LYS	CA-C-N	9.23	126.31	119.66
5	R	153	LYS	C-N-CA	9.23	126.31	119.66
1	N	194	PRO	CA-N-CD	-9.08	99.28	112.00
6	T	100	GLY	CA-C-O	-8.12	106.43	120.57
6	T	101	SER	N-CA-CB	-8.00	96.97	110.49
1	N	148	PRO	N-CA-CB	7.11	109.95	103.34
1	N	868	ILE	N-CA-C	6.82	117.58	110.62
4	Q	20	PRO	N-CA-CB	6.77	110.69	103.52
12	3	11	PRO	N-CA-CB	6.75	110.34	103.25
1	N	852	PRO	N-CA-CB	6.75	110.02	102.60
4	Q	47	PRO	N-CA-CB	6.58	110.49	103.52
4	Q	455	MET	CA-C-N	6.57	126.48	119.85
4	Q	455	MET	C-N-CA	6.57	126.48	119.85
10	G	15	PRO	CA-C-N	-6.34	113.85	120.38
10	G	15	PRO	C-N-CA	-6.34	113.85	120.38
6	T	78	PRO	CA-C-O	-6.33	114.13	121.34
1	N	445	SER	CA-C-N	6.26	126.82	120.38
1	N	445	SER	C-N-CA	6.26	126.82	120.38
1	N	137	PRO	N-CA-CB	6.22	110.11	103.39
10	G	65	LYS	CA-C-N	6.19	126.16	119.78
10	G	65	LYS	C-N-CA	6.19	126.16	119.78
1	N	365	ASP	N-CA-C	-6.04	107.74	114.62
8	V	97	GLU	CA-C-N	6.04	125.98	119.76
8	V	97	GLU	C-N-CA	6.04	125.98	119.76
1	N	533	ASN	CA-C-N	5.83	132.20	121.70
1	N	533	ASN	C-N-CA	5.83	132.20	121.70
1	N	99	HIS	CA-C-N	5.81	132.16	121.70
1	N	99	HIS	C-N-CA	5.81	132.16	121.70
1	N	366	GLY	N-CA-C	-5.64	107.86	115.36
4	Q	27	ASN	CB-CA-C	-5.63	110.06	116.54
1	N	524	SER	N-CA-C	5.63	118.18	111.71
1	N	309	TYR	N-CA-C	5.61	115.81	108.07
1	N	195	ASN	N-CA-C	5.59	117.35	108.79
10	G	15	PRO	N-CA-C	5.52	117.43	110.70
6	T	78	PRO	CA-C-N	5.36	131.34	121.70
6	T	78	PRO	C-N-CA	5.36	131.34	121.70
6	T	155	ASN	N-CA-C	5.30	117.12	109.07
1	N	446	PRO	CA-C-N	5.28	126.43	119.84
1	N	446	PRO	C-N-CA	5.28	126.43	119.84
7	K	31	ILE	CB-CA-C	-5.24	107.14	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	3	67	ILE	CA-C-N	5.22	126.27	120.06
12	3	67	ILE	C-N-CA	5.22	126.27	120.06

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	T	100	GLY	Mainchain,Peptide

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	N	3887	0	3543	222	0
2	F	1590	0	1527	75	0
3	H	1493	0	1467	69	0
4	Q	3831	0	3571	126	0
5	R	1694	0	1670	85	0
6	T	1455	0	1476	94	0
7	K	769	0	783	33	0
8	V	949	0	961	31	0
9	D	480	0	100	1	0
10	G	965	0	402	7	0
11	U	608	0	265	4	0
12	3	515	0	209	10	0
13	I	374	0	163	2	0
14	2	388	0	155	2	0
15	S	610	0	138	0	0
16	J	660	0	141	1	0
All	All	20268	0	16571	686	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 19.

All (686) 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:N:191:PHE:CB	1:N:194:PRO:HG2	1.56	1.35
6:T:30:PHE:O	6:T:100:GLY:O	1.54	1.24
6:T:6:VAL:O	6:T:159:THR:HG22	1.39	1.20
1:N:191:PHE:HB3	1:N:194:PRO:CG	1.75	1.16
1:N:195:ASN:CG	1:N:224:PHE:HB2	1.71	1.14
1:N:191:PHE:HB3	1:N:194:PRO:HG2	1.15	1.12
1:N:199:VAL:CG1	1:N:217:TRP:CE3	2.39	1.05
1:N:199:VAL:HG12	1:N:217:TRP:HE3	1.16	1.05
1:N:192:THR:C	1:N:194:PRO:HD3	1.88	0.98
1:N:362:TRP:HZ3	1:N:367:ILE:HD12	1.28	0.98
1:N:199:VAL:CG1	1:N:217:TRP:HE3	1.73	0.98
1:N:195:ASN:ND2	1:N:224:PHE:HB2	1.78	0.97
1:N:199:VAL:HG12	1:N:217:TRP:CE3	1.98	0.96
1:N:197:PHE:HE2	1:N:199:VAL:CG2	1.79	0.95
1:N:191:PHE:CB	1:N:194:PRO:CG	2.41	0.95
1:N:197:PHE:HE2	1:N:199:VAL:HG22	1.32	0.94
6:T:64:MET:SD	6:T:77:GLU:HG3	2.07	0.94
1:N:199:VAL:HG11	1:N:217:TRP:CE3	2.01	0.93
1:N:195:ASN:CG	1:N:224:PHE:CB	2.43	0.90
10:G:12:ALA:HB3	10:G:15:PRO:HA	1.55	0.88
1:N:194:PRO:O	1:N:195:ASN:OD1	1.90	0.88
1:N:195:ASN:OD1	1:N:224:PHE:HB2	1.74	0.87
1:N:197:PHE:CE1	1:N:219:VAL:HG13	2.08	0.87
6:T:78:PRO:HA	6:T:79:GLU:HB2	1.57	0.86
4:Q:281:SER:HB2	4:Q:386:CYS:HB3	1.55	0.86
1:N:197:PHE:CE2	1:N:199:VAL:CG2	2.59	0.85
4:Q:441:PHE:HB2	4:Q:523:LEU:HD11	1.58	0.85
1:N:197:PHE:CE2	1:N:199:VAL:HG22	2.10	0.85
6:T:6:VAL:O	6:T:159:THR:CG2	2.24	0.84
1:N:195:ASN:ND2	1:N:270:CYS:SG	2.50	0.84
5:R:88:PRO:HA	5:R:206:ARG:HH22	1.43	0.83
1:N:362:TRP:HZ3	1:N:367:ILE:CD1	1.92	0.83
1:N:197:PHE:CZ	1:N:219:VAL:HG22	2.13	0.82
1:N:191:PHE:CG	1:N:194:PRO:HG2	2.14	0.82
5:R:141:TYR:HB2	5:R:166:ILE:HB	1.59	0.82
1:N:362:TRP:CZ3	1:N:367:ILE:HD12	2.13	0.82
4:Q:444:TRP:O	4:Q:448:ARG:NH1	2.14	0.81
1:N:191:PHE:HB2	1:N:194:PRO:HG2	1.59	0.80
1:N:192:THR:C	1:N:194:PRO:CD	2.57	0.78
1:N:337:ILE:HG22	1:N:339:ALA:H	1.49	0.78
1:N:195:ASN:ND2	1:N:224:PHE:CB	2.45	0.77
6:T:64:MET:SD	6:T:77:GLU:CG	2.73	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:255:VAL:HG23	4:Q:294:LEU:HD11	1.65	0.77
5:R:46:PRO:HA	5:R:48:LEU:H	1.51	0.76
1:N:174:ILE:HA	1:N:175:ILE:HG13	1.67	0.76
4:Q:335:VAL:H	4:Q:342:VAL:HG13	1.51	0.76
1:N:264:ASN:HD21	1:N:354:ASP:H	1.33	0.75
1:N:491:ALA:HA	1:N:503:PHE:HA	1.67	0.74
1:N:195:ASN:OD1	1:N:225:HIS:N	2.19	0.74
1:N:172:TYR:HA	1:N:173:GLU:HB3	1.68	0.74
6:T:96:PHE:HB2	6:T:117:GLN:HG2	1.69	0.74
1:N:193:VAL:N	1:N:194:PRO:HD3	2.03	0.73
1:N:269:PHE:HB2	2:F:206:LEU:HD11	1.70	0.73
1:N:197:PHE:CE1	1:N:219:VAL:HG22	2.24	0.73
5:R:81:TYR:OH	5:R:101:ARG:NH1	2.22	0.72
4:Q:339:ASP:OD2	4:Q:341:HIS:NE2	2.22	0.72
3:H:177:ARG:NH2	7:K:83:GLU:OE2	2.23	0.72
3:H:134:ASP:HA	3:H:137:TRP:HD1	1.54	0.71
1:N:326:HIS:HA	1:N:364:HIS:CD2	2.26	0.71
5:R:43:ASP:HB2	5:R:48:LEU:HD21	1.70	0.71
1:N:362:TRP:HE1	1:N:386:ILE:HG23	1.56	0.71
5:R:33:LEU:HB3	5:R:63:GLU:HB2	1.73	0.71
5:R:103:LYS:H	6:T:78:PRO:HG3	1.55	0.70
1:N:197:PHE:HE1	1:N:219:VAL:HG13	1.53	0.70
4:Q:327:ASN:HB2	4:Q:334:LEU:HB2	1.72	0.70
4:Q:484:ILE:HD11	4:Q:493:ILE:HB	1.73	0.70
5:R:106:ASN:HD22	6:T:74:ILE:HA	1.56	0.70
1:N:544:VAL:HG12	1:N:545:HIS:H	1.57	0.70
4:Q:497:HIS:ND1	4:Q:508:VAL:O	2.25	0.70
1:N:331:PHE:HB2	1:N:359:LEU:HD12	1.73	0.69
2:F:84:ARG:HB2	2:F:88:LEU:HB3	1.74	0.69
1:N:196:GLU:OE2	1:N:223:GLN:HB2	1.93	0.69
1:N:191:PHE:HB3	1:N:194:PRO:CD	2.23	0.68
1:N:309:TYR:OH	1:N:383:LEU:HG	1.93	0.68
2:F:120:ASN:ND2	3:H:72:GLN:O	2.27	0.68
4:Q:138:ILE:HD13	4:Q:151:PRO:HG3	1.74	0.68
1:N:99:HIS:H	1:N:100:VAL:C	2.02	0.68
1:N:165:ILE:HG23	1:N:217:TRP:HH2	1.58	0.67
5:R:93:LYS:O	5:R:204:ASN:ND2	2.28	0.67
6:T:29:TYR:HA	6:T:101:SER:HA	1.77	0.67
1:N:306:ARG:HG2	1:N:329:HIS:CE1	2.30	0.67
5:R:4:LEU:HG	5:R:96:ILE:HG12	1.77	0.67
4:Q:132:LYS:HA	4:Q:152:SER:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:6:VAL:HG21	6:T:184:GLN:HE22	1.58	0.67
6:T:185:ARG:NH1	6:T:188:THR:OG1	2.28	0.67
2:F:119:PRO:HG2	3:H:76:ILE:HB	1.76	0.66
4:Q:217:PRO:HB2	4:Q:230:GLN:HB3	1.76	0.66
12:3:41:TYR:CB	12:3:46:ALA:HB1	2.25	0.66
2:F:124:LEU:HD21	3:H:76:ILE:HD13	1.76	0.66
5:R:37:VAL:HG23	5:R:58:LEU:HB2	1.77	0.66
6:T:144:GLN:HA	6:T:147:PHE:HD2	1.59	0.66
1:N:533:ASN:HB2	1:N:534:ALA:HB3	1.77	0.66
4:Q:129:LEU:HB2	4:Q:154:LEU:HD12	1.77	0.66
6:T:27:ARG:HG2	6:T:28:THR:H	1.59	0.66
6:T:100:GLY:HA3	6:T:113:ALA:HA	1.78	0.66
2:F:28:LEU:HD13	2:F:33:VAL:HG23	1.77	0.65
8:V:101:GLU:HB3	8:V:105:ARG:HH12	1.62	0.65
6:T:127:HIS:HE1	6:T:129:THR:HG23	1.60	0.65
1:N:492:VAL:HG12	1:N:494:GLY:H	1.61	0.65
5:R:39:TYR:OH	5:R:150:ARG:NH2	2.30	0.65
1:N:533:ASN:H	1:N:534:ALA:C	2.04	0.65
5:R:24:LYS:HB3	7:K:94:ARG:HH21	1.62	0.65
4:Q:412:GLU:HA	4:Q:415:MET:HE3	1.79	0.65
4:Q:225:ASN:OD1	8:V:75:ARG:NH2	2.30	0.64
6:T:38:VAL:HB	6:T:93:ARG:HH22	1.62	0.64
3:H:76:ILE:HG23	4:Q:154:LEU:HD22	1.80	0.64
4:Q:167:SER:O	4:Q:170:THR:OG1	2.12	0.64
2:F:203:MET:HA	2:F:206:LEU:HD12	1.78	0.64
7:K:30:LYS:HE2	7:K:67:PHE:HD2	1.62	0.64
2:F:28:LEU:HD22	2:F:33:VAL:HA	1.80	0.64
4:Q:201:GLU:OE2	8:V:78:LYS:NZ	2.30	0.64
4:Q:233:CYS:SG	7:K:94:ARG:NH1	2.71	0.64
5:R:49:PRO:HG3	6:T:88:LYS:HG3	1.80	0.64
8:V:112:ASN:HA	8:V:115:LEU:HD12	1.81	0.64
3:H:147:GLU:OE2	7:K:59:LYS:NZ	2.28	0.63
5:R:6:LEU:HB2	5:R:169:VAL:HB	1.80	0.63
5:R:184:LYS:O	5:R:188:ASN:ND2	2.31	0.63
4:Q:268:ILE:HG22	4:Q:345:ILE:HG12	1.80	0.63
1:N:367:ILE:HG22	1:N:369:GLU:HB2	1.81	0.63
2:F:163:ASP:HA	2:F:164:ASN:HB2	1.81	0.63
2:F:190:SER:OG	2:F:191:PHE:N	2.31	0.63
1:N:226:LEU:HD23	1:N:228:ASP:H	1.64	0.63
6:T:31:ALA:HB3	6:T:59:ASN:HD22	1.63	0.63
4:Q:531:GLU:HA	4:Q:534:ILE:HG22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:192:THR:N	1:N:194:PRO:HD3	2.14	0.62
5:R:139:ARG:HE	5:R:141:TYR:HE1	1.47	0.62
12:3:42:PHE:H	12:3:46:ALA:HB3	1.65	0.62
6:T:89:LEU:HB3	6:T:90:TRP:CD1	2.34	0.62
6:T:108:PHE:HB3	6:T:130:TYR:HD1	1.64	0.62
1:N:218:ILE:HG23	1:N:245:ASN:OD1	1.99	0.62
1:N:191:PHE:HB2	1:N:195:ASN:H	1.65	0.62
2:F:146:PHE:H	2:F:147:PRO:HD2	1.65	0.61
3:H:176:ASP:O	3:H:179:THR:OG1	2.18	0.61
5:R:35:PHE:HB2	5:R:62:ILE:HD13	1.81	0.61
5:R:65:HIS:HE1	5:R:69:ASP:HB3	1.65	0.61
5:R:145:ILE:HB	5:R:157:HIS:HB2	1.81	0.61
1:N:306:ARG:HG2	1:N:329:HIS:HE1	1.64	0.61
7:K:43:GLU:HA	7:K:46:GLN:HB3	1.83	0.61
1:N:172:TYR:HB2	1:N:213:ILE:HA	1.83	0.61
4:Q:237:ILE:HD12	4:Q:309:ASP:HB3	1.81	0.61
1:N:197:PHE:HZ	1:N:219:VAL:HG22	1.64	0.61
1:N:399:ARG:NH2	1:N:409:GLU:O	2.33	0.61
1:N:331:PHE:O	1:N:359:LEU:N	2.29	0.61
4:Q:482:TRP:HB2	4:Q:495:ILE:HB	1.82	0.61
5:R:106:ASN:OD1	5:R:107:GLY:N	2.33	0.61
5:R:144:LEU:HD23	5:R:156:PHE:HB2	1.81	0.61
4:Q:221:SER:OG	4:Q:222:GLN:OE1	2.19	0.60
2:F:47:SER:HA	2:F:76:ILE:HB	1.82	0.60
1:N:294:LEU:HD21	1:N:383:LEU:CD1	2.32	0.60
2:F:74:THR:HA	2:F:96:ARG:HB2	1.82	0.60
9:D:92:UNK:O	9:D:96:UNK:CB	2.49	0.60
12:3:41:TYR:HA	12:3:46:ALA:HB2	1.82	0.60
1:N:868:ILE:N	1:N:869:LEU:HA	2.15	0.60
1:N:527:TRP:CD1	1:N:543:ASP:H	2.18	0.60
5:R:39:TYR:HD1	5:R:120:PHE:HA	1.66	0.60
6:T:78:PRO:HB2	6:T:81:GLU:H	1.67	0.60
7:K:86:VAL:HG23	8:V:13:ARG:HD3	1.84	0.59
7:K:86:VAL:HG13	7:K:87:VAL:HG23	1.83	0.59
1:N:188:ARG:NH1	1:N:198:SER:OG	2.35	0.59
1:N:166:ARG:O	1:N:170:SER:N	2.35	0.59
1:N:347:LYS:HG2	1:N:348:ARG:H	1.67	0.59
1:N:301:LYS:HB2	1:N:302:PRO:HD2	1.84	0.59
5:R:80:MET:HE3	6:T:84:ILE:HG21	1.84	0.59
1:N:269:PHE:N	2:F:206:LEU:HD21	2.18	0.59
1:N:451:ARG:NH2	4:Q:415:MET:O	2.25	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:234:LEU:HB3	7:K:100:LEU:HB2	1.85	0.59
12:3:41:TYR:CB	12:3:46:ALA:CB	2.81	0.58
3:H:70:THR:O	3:H:73:THR:OG1	2.19	0.58
3:H:77:TYR:HE2	4:Q:157:SER:HB2	1.66	0.58
5:R:143:THR:H	5:R:163:GLN:HE22	1.51	0.58
6:T:144:GLN:HA	6:T:147:PHE:CD2	2.38	0.58
3:H:6:THR:O	3:H:9:THR:OG1	2.19	0.58
5:R:112:PHE:HA	5:R:115:LYS:HD2	1.86	0.58
1:N:175:ILE:HB	1:N:176:PRO:HA	1.84	0.58
1:N:884:UNK:O	1:N:888:UNK:N	2.35	0.58
5:R:20:ASN:ND2	8:V:86:LEU:O	2.32	0.58
7:K:65:VAL:HG21	8:V:29:LEU:HD21	1.86	0.58
10:G:70:THR:N	10:G:71:SER:HA	2.19	0.58
1:N:196:GLU:HG2	1:N:223:GLN:O	2.04	0.58
1:N:367:ILE:CG2	1:N:369:GLU:HB2	2.33	0.58
2:F:165:LEU:HD11	3:H:38:GLU:HB3	1.86	0.58
1:N:193:VAL:N	1:N:194:PRO:CD	2.68	0.57
2:F:52:LEU:HD21	2:F:73:LEU:HD13	1.86	0.57
2:F:111:CYS:N	2:F:114:ASN:O	2.32	0.57
4:Q:464:LYS:N	4:Q:468:GLU:OE1	2.31	0.57
1:N:191:PHE:CD2	1:N:194:PRO:HG2	2.39	0.57
3:H:140:ALA:HB1	7:K:54:PHE:CE2	2.39	0.57
4:Q:103:ALA:HA	4:Q:106:LYS:HB3	1.86	0.57
2:F:186:ASN:O	2:F:188:ASP:N	2.35	0.57
5:R:110:THR:O	5:R:113:VAL:HG22	2.05	0.57
1:N:541:THR:HB	1:N:867:ALA:HB3	1.85	0.57
1:N:872:ILE:HA	1:N:878:LYS:H	1.69	0.57
3:H:194:PHE:O	3:H:198:GLY:N	2.31	0.57
4:Q:538:SER:O	4:Q:541:SER:OG	2.19	0.57
7:K:34:ILE:HD11	7:K:68:ILE:HD12	1.87	0.57
5:R:46:PRO:HA	5:R:48:LEU:N	2.20	0.56
6:T:35:LYS:HA	6:T:95:SER:HA	1.86	0.56
6:T:61:ASN:H	6:T:62:PRO:HD2	1.70	0.56
4:Q:221:SER:HG	4:Q:222:GLN:H	1.53	0.56
6:T:98:ILE:HG12	6:T:115:VAL:HG13	1.86	0.56
7:K:44:ALA:HA	7:K:48:ASN:HB2	1.86	0.56
1:N:191:PHE:CB	1:N:194:PRO:CD	2.83	0.56
1:N:192:THR:CA	1:N:194:PRO:HD3	2.35	0.56
1:N:447:PRO:HG2	1:N:449:HIS:CD2	2.40	0.56
6:T:89:LEU:HB3	6:T:90:TRP:HD1	1.70	0.56
6:T:127:HIS:CE1	6:T:129:THR:HG23	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:524:SER:N	1:N:525:ASN:HA	2.20	0.56
4:Q:421:ALA:HB3	4:Q:426:ARG:HH22	1.71	0.56
1:N:213:ILE:HD13	1:N:256:LYS:HE3	1.87	0.56
1:N:487:ALA:O	1:N:489:LEU:N	2.39	0.56
1:N:508:TRP:HH2	1:N:518:LEU:H	1.52	0.56
5:R:32:ILE:HG13	5:R:130:GLU:HG3	1.87	0.55
1:N:475:CYS:O	1:N:478:THR:OG1	2.15	0.55
6:T:62:PRO:HB2	6:T:64:MET:HG2	1.89	0.55
1:N:197:PHE:CE2	1:N:199:VAL:HG23	2.38	0.55
6:T:8:TYR:HB3	6:T:156:LYS:HB3	1.87	0.55
12:3:79:LYS:O	12:3:81:PRO:N	2.39	0.55
1:N:154:ILE:O	1:N:157:THR:OG1	2.21	0.55
7:K:65:VAL:HG11	8:V:29:LEU:HD11	1.88	0.55
1:N:353:TYR:HB2	1:N:354:ASP:HA	1.88	0.55
8:V:10:LEU:HD22	8:V:13:ARG:HH21	1.71	0.55
1:N:216:GLN:HG3	1:N:252:PHE:HE2	1.72	0.55
2:F:148:GLN:O	2:F:156:THR:OG1	2.21	0.55
5:R:52:PRO:HA	5:R:55:TRP:CD1	2.42	0.55
1:N:268:LYS:O	1:N:272:TYR:N	2.29	0.55
7:K:77:LEU:HG	7:K:81:LYS:HE3	1.89	0.55
1:N:553:ILE:HA	1:N:556:PHE:HD2	1.73	0.54
3:H:114:TYR:O	3:H:117:SER:OG	2.18	0.54
1:N:173:GLU:HG3	1:N:174:ILE:H	1.72	0.54
1:N:453:ALA:O	1:N:457:ILE:N	2.39	0.54
1:N:552:SER:O	1:N:555:SER:OG	2.15	0.54
1:N:353:TYR:N	1:N:354:ASP:HB2	2.23	0.54
2:F:37:PHE:O	2:F:40:SER:OG	2.21	0.54
2:F:158:PRO:O	2:F:159:LYS:HD2	2.07	0.54
5:R:140:ILE:HD11	5:R:165:TRP:HB3	1.90	0.54
5:R:29:PRO:HB3	5:R:131:TYR:HE1	1.72	0.54
6:T:69:ASP:N	6:T:72:THR:OG1	2.36	0.54
1:N:301:LYS:HG3	1:N:302:PRO:O	2.08	0.54
1:N:480:LEU:O	1:N:484:ALA:N	2.40	0.54
6:T:25:LEU:HD22	6:T:104:GLU:HB2	1.90	0.54
1:N:567:ILE:HA	1:N:570:PHE:HD2	1.72	0.54
14:2:104:THR:O	14:2:114:GLY:N	2.41	0.54
5:R:39:TYR:CD1	5:R:120:PHE:HA	2.43	0.54
1:N:506:GLY:HA2	1:N:508:TRP:H	1.71	0.53
2:F:21:TRP:CZ3	2:F:36:TYR:HB2	2.43	0.53
5:R:82:LEU:HD21	6:T:84:ILE:HG23	1.89	0.53
1:N:527:TRP:HB2	1:N:541:THR:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:87:PHE:HE2	3:H:85:LYS:HG2	1.72	0.53
4:Q:246:MET:HA	4:Q:253:PHE:HD1	1.74	0.53
6:T:35:LYS:NZ	6:T:55:PHE:O	2.37	0.53
6:T:39:VAL:HG12	6:T:41:TYR:H	1.74	0.53
1:N:283:PHE:HB3	1:N:287:ARG:NH1	2.23	0.53
1:N:329:HIS:HB3	1:N:331:PHE:CE2	2.43	0.53
2:F:155:TYR:HE2	3:H:44:PRO:HG3	1.73	0.53
10:G:334:LEU:O	10:G:338:ILE:N	2.41	0.53
3:H:68:SER:HA	3:H:71:LEU:HD12	1.91	0.53
1:N:294:LEU:HD21	1:N:383:LEU:HD11	1.91	0.53
1:N:335:GLN:H	1:N:355:HIS:CD2	2.26	0.53
6:T:42:LYS:HA	6:T:51:LYS:HE2	1.91	0.53
6:T:58:GLN:HE22	6:T:178:LEU:HB2	1.73	0.53
6:T:64:MET:HB3	6:T:75:ASP:HB3	1.90	0.53
1:N:446:PRO:HG2	1:N:450:LEU:HD11	1.91	0.53
2:F:184:ILE:HD12	4:Q:241:LEU:HD21	1.91	0.53
5:R:145:ILE:O	5:R:157:HIS:N	2.38	0.53
4:Q:310:ILE:O	4:Q:313:SER:OG	2.20	0.53
6:T:82:ASP:O	6:T:86:ARG:HG3	2.09	0.53
1:N:354:ASP:CG	1:N:355:HIS:HB2	2.34	0.52
8:V:113:HIS:CE1	8:V:114:LEU:HG	2.44	0.52
1:N:177:THR:HG21	1:N:348:ARG:O	2.09	0.52
3:H:53:LEU:O	3:H:57:ILE:HD12	2.08	0.52
3:H:145:MET:HG2	8:V:33:GLN:HE21	1.74	0.52
1:N:399:ARG:HH22	1:N:410:HIS:HA	1.74	0.52
3:H:79:SER:N	4:Q:153:SER:O	2.42	0.52
4:Q:520:PHE:HD2	4:Q:526:VAL:HG22	1.75	0.52
6:T:39:VAL:HG23	6:T:51:LYS:HA	1.91	0.52
1:N:559:LEU:HB3	1:N:862:THR:H	1.74	0.52
7:K:36:SER:O	7:K:40:LYS:N	2.43	0.52
12:3:59:GLU:O	12:3:60:PRO:CB	2.57	0.52
1:N:197:PHE:HE1	1:N:219:VAL:CG1	2.19	0.52
1:N:399:ARG:HH12	1:N:410:HIS:HA	1.73	0.52
1:N:166:ARG:NH2	11:U:126:GLU:HA	2.25	0.52
2:F:70:LEU:O	2:F:77:GLN:NE2	2.41	0.52
6:T:177:LEU:O	6:T:181:LEU:HG	2.10	0.52
1:N:559:LEU:HD13	1:N:863:ALA:H	1.75	0.52
4:Q:160:GLN:HB3	4:Q:162:PRO:HA	1.92	0.52
4:Q:415:MET:O	4:Q:502:HIS:ND1	2.43	0.52
1:N:354:ASP:OD1	1:N:355:HIS:HB2	2.10	0.52
1:N:527:TRP:NE1	1:N:543:ASP:O	2.32	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:218:ILE:HG22	1:N:219:VAL:O	2.10	0.52
1:N:407:PHE:CE2	1:N:416:LYS:HD2	2.45	0.52
1:N:530:ARG:HA	1:N:538:THR:HG22	1.90	0.51
3:H:17:ARG:HD2	4:Q:130:LEU:HD22	1.91	0.51
4:Q:105:LYS:O	4:Q:109:ILE:HG12	2.10	0.51
4:Q:145:LEU:O	4:Q:148:THR:OG1	2.22	0.51
7:K:16:SER:N	7:K:19:GLN:OE1	2.42	0.51
6:T:180:GLN:HA	6:T:183:LYS:HD2	1.91	0.51
2:F:193:PRO:HA	2:F:194:GLU:HB3	1.91	0.51
4:Q:149:VAL:HG12	4:Q:150:PRO:O	2.11	0.51
4:Q:215:SER:HB2	8:V:90:PHE:HB3	1.92	0.51
5:R:40:ARG:HB3	5:R:121:SER:HB2	1.92	0.51
5:R:143:THR:H	5:R:163:GLN:NE2	2.08	0.51
6:T:26:VAL:HG13	6:T:103:TYR:CE1	2.45	0.51
1:N:172:TYR:HB3	1:N:213:ILE:HG23	1.93	0.51
3:H:77:TYR:CE1	4:Q:155:GLN:HB3	2.46	0.51
4:Q:259:LEU:HD12	4:Q:301:LEU:HD12	1.92	0.51
4:Q:452:PHE:HA	4:Q:484:ILE:HA	1.92	0.51
6:T:39:VAL:HG21	6:T:44:TYR:HB2	1.92	0.51
6:T:41:TYR:CE2	6:T:43:LEU:HB2	2.46	0.51
6:T:108:PHE:HB3	6:T:130:TYR:CD1	2.45	0.51
1:N:264:ASN:ND2	1:N:354:ASP:H	2.05	0.50
2:F:199:VAL:HA	2:F:202:PHE:CE2	2.46	0.50
3:H:115:GLU:HA	3:H:118:ILE:HD12	1.93	0.50
3:H:154:PHE:HD2	7:K:73:ARG:HE	1.57	0.50
4:Q:99:MET:HB3	4:Q:104:TYR:OH	2.11	0.50
4:Q:431:TYR:HE2	4:Q:473:LEU:HD22	1.76	0.50
5:R:91:GLU:O	5:R:93:LYS:N	2.44	0.50
6:T:33:HIS:HD2	6:T:57:LYS:HB2	1.74	0.50
1:N:265:ILE:HG23	2:F:206:LEU:HB3	1.93	0.50
3:H:136:LEU:HD22	7:K:51:LEU:HD22	1.92	0.50
4:Q:264:ALA:HB1	4:Q:347:LEU:HD11	1.93	0.50
5:R:37:VAL:CG2	5:R:58:LEU:HB2	2.41	0.50
6:T:37:TRP:CZ3	6:T:92:PHE:HE1	2.29	0.50
14:2:112:ILE:HA	14:2:126:SER:HA	1.93	0.50
1:N:362:TRP:NE1	1:N:386:ILE:HG23	2.23	0.50
6:T:36:LYS:HE3	6:T:96:PHE:CE2	2.45	0.50
6:T:73:MET:HE2	6:T:179:LEU:HD23	1.93	0.50
6:T:186:ILE:HA	6:T:189:VAL:HG23	1.93	0.50
1:N:197:PHE:CZ	1:N:219:VAL:HA	2.47	0.50
1:N:199:VAL:HG11	1:N:217:TRP:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:175:ILE:HG21	1:N:349:SER:C	2.37	0.50
1:N:503:PHE:HB2	1:N:520:TYR:O	2.12	0.50
4:Q:423:LEU:HD11	4:Q:501:LEU:HD21	1.93	0.50
1:N:375:ASP:HA	1:N:376:HIS:C	2.37	0.50
1:N:166:ARG:HH22	11:U:126:GLU:HA	1.77	0.50
3:H:116:ALA:O	3:H:119:SER:OG	2.18	0.50
1:N:175:ILE:HD13	1:N:351:CYS:H	1.77	0.49
4:Q:103:ALA:HA	4:Q:106:LYS:HE2	1.94	0.49
6:T:178:LEU:HD12	6:T:181:LEU:HD12	1.93	0.49
8:V:13:ARG:O	8:V:16:THR:OG1	2.22	0.49
1:N:427:LYS:HG3	1:N:434:ARG:HE	1.77	0.49
1:N:532:LEU:HB2	1:N:534:ALA:O	2.12	0.49
4:Q:234:LEU:HB2	4:Q:302:GLN:NE2	2.27	0.49
8:V:99:ASP:OD1	8:V:100:LEU:N	2.45	0.49
1:N:427:LYS:HA	1:N:434:ARG:HE	1.77	0.49
2:F:141:THR:O	2:F:144:GLU:HG2	2.12	0.49
3:H:145:MET:HG2	8:V:33:GLN:NE2	2.27	0.49
5:R:7:LEU:HD12	5:R:205:VAL:HB	1.93	0.49
5:R:10:VAL:HB	5:R:165:TRP:HB2	1.93	0.49
8:V:101:GLU:HB3	8:V:105:ARG:NH1	2.25	0.49
4:Q:392:ILE:HD13	4:Q:395:ILE:HD12	1.94	0.49
4:Q:458:TYR:HB2	4:Q:461:GLU:HG2	1.94	0.49
6:T:46:ASN:HA	6:T:50:PRO:HA	1.94	0.49
6:T:64:MET:SD	6:T:77:GLU:HG2	2.52	0.49
6:T:83:ILE:HA	6:T:86:ARG:HD2	1.95	0.49
1:N:177:THR:OG1	1:N:350:SER:N	2.37	0.49
1:N:304:ARG:HG3	1:N:331:PHE:CZ	2.47	0.49
2:F:59:ASN:O	2:F:61:LEU:N	2.46	0.49
2:F:96:ARG:NH2	2:F:98:ASN:O	2.45	0.49
5:R:38:VAL:HG22	5:R:57:ARG:HG2	1.94	0.49
5:R:40:ARG:N	5:R:119:GLU:O	2.42	0.49
6:T:40:GLN:HG3	6:T:90:TRP:N	2.27	0.49
1:N:257:PRO:HD2	1:N:258:ILE:HA	1.93	0.49
2:F:48:ASN:HA	2:F:51:MET:HE3	1.94	0.49
3:H:188:LEU:HD23	3:H:192:LEU:HD23	1.95	0.49
6:T:68:VAL:HG13	6:T:72:THR:H	1.78	0.49
1:N:544:VAL:HG12	1:N:545:HIS:N	2.25	0.49
2:F:96:ARG:HD2	2:F:102:VAL:HB	1.94	0.49
7:K:63:GLU:OE1	7:K:63:GLU:N	2.44	0.49
12:3:11:PRO:O	12:3:13:ASP:N	2.46	0.49
3:H:30:PHE:HE2	4:Q:112:ILE:HG13	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:65:HIS:CE1	5:R:72:TRP:HB3	2.48	0.49
5:R:130:GLU:HG2	5:R:139:ARG:HB2	1.95	0.49
1:N:444:LEU:HD23	4:Q:433:ASN:HD21	1.77	0.49
4:Q:207:GLU:OE1	4:Q:210:LYS:HD2	2.13	0.49
6:T:108:PHE:HB2	6:T:129:THR:O	2.13	0.49
13:I:106:GLU:O	13:I:110:GLU:N	2.45	0.49
1:N:275:LEU:O	1:N:279:SER:N	2.32	0.48
2:F:12:THR:HA	2:F:117:MET:HE2	1.95	0.48
5:R:83:GLU:HG2	5:R:99:VAL:HG22	1.94	0.48
6:T:32:GLN:NE2	6:T:58:GLN:HG2	2.28	0.48
4:Q:197:VAL:O	4:Q:200:THR:OG1	2.20	0.48
5:R:33:LEU:HD23	5:R:63:GLU:HA	1.94	0.48
5:R:101:ARG:HE	5:R:103:LYS:NZ	2.11	0.48
1:N:195:ASN:OD1	1:N:224:PHE:CB	2.52	0.48
3:H:23:ILE:O	3:H:27:LEU:HG	2.13	0.48
4:Q:250:SER:O	4:Q:252:SER:N	2.43	0.48
6:T:54:GLU:HB2	6:T:182:PHE:HE1	1.78	0.48
1:N:345:SER:OG	1:N:346:SER:N	2.45	0.48
3:H:172:GLN:HA	3:H:175:ILE:HD12	1.96	0.48
4:Q:162:PRO:HB2	4:Q:163:GLU:OE1	2.14	0.48
7:K:30:LYS:HE2	7:K:67:PHE:CD2	2.47	0.48
1:N:175:ILE:HG22	1:N:177:THR:HG23	1.94	0.48
3:H:47:HIS:CE1	3:H:51:ASN:HD21	2.32	0.48
1:N:203:THR:OG1	1:N:204:ASN:N	2.46	0.48
5:R:82:LEU:HD11	6:T:84:ILE:HA	1.96	0.48
1:N:447:PRO:HG2	1:N:449:HIS:HD2	1.79	0.48
5:R:52:PRO:O	5:R:55:TRP:HD1	1.97	0.48
1:N:213:ILE:HB	1:N:256:LYS:CE	2.44	0.47
4:Q:221:SER:OG	4:Q:222:GLN:N	2.45	0.47
1:N:435:LEU:HD21	1:N:453:ALA:HB1	1.96	0.47
4:Q:451:SER:HB3	4:Q:485:MET:HB2	1.96	0.47
2:F:111:CYS:O	2:F:114:ASN:HB2	2.15	0.47
5:R:41:PRO:HA	5:R:118:TYR:CD1	2.50	0.47
5:R:143:THR:N	5:R:163:GLN:HE22	2.12	0.47
10:G:317:TYR:HA	13:I:120:ALA:HA	1.96	0.47
4:Q:508:VAL:HG23	4:Q:509:TRP:HD1	1.79	0.47
5:R:90:ARG:HG2	5:R:95:GLY:HA2	1.97	0.47
5:R:167:LEU:HD22	5:R:202:LEU:HD11	1.96	0.47
1:N:296:GLY:HA3	1:N:307:LEU:HD23	1.96	0.47
4:Q:526:VAL:O	4:Q:530:ILE:HG12	2.14	0.47
6:T:136:VAL:HG11	6:T:161:VAL:HG13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:168:ARG:HH21	1:N:215:PHE:N	2.13	0.47
3:H:88:GLU:HB3	3:H:89:PRO:HD3	1.96	0.47
4:Q:132:LYS:HG2	4:Q:152:SER:HA	1.97	0.47
4:Q:268:ILE:HG13	4:Q:281:SER:HB3	1.97	0.47
4:Q:475:ILE:HG22	4:Q:501:LEU:HD23	1.97	0.47
5:R:171:THR:HG22	5:R:189:LEU:HD11	1.97	0.47
6:T:33:HIS:CD2	6:T:57:LYS:HB2	2.50	0.47
6:T:58:GLN:NE2	6:T:178:LEU:HB2	2.30	0.47
6:T:185:ARG:HD2	6:T:188:THR:OG1	2.15	0.47
1:N:194:PRO:O	1:N:195:ASN:CG	2.58	0.47
5:R:40:ARG:NH1	5:R:119:GLU:OE1	2.48	0.47
5:R:201:ASP:CG	8:V:6:PHE:H	2.23	0.47
6:T:37:TRP:HB2	6:T:53:LEU:O	2.15	0.47
1:N:272:TYR:CD1	1:N:303:PRO:HG3	2.49	0.47
1:N:335:GLN:H	1:N:355:HIS:HD2	1.62	0.47
4:Q:459:PRO:HD3	4:Q:478:LEU:HD13	1.97	0.47
4:Q:479:SER:HA	4:Q:498:THR:HG22	1.97	0.47
1:N:361:GLU:OE1	1:N:363:HIS:NE2	2.46	0.46
2:F:28:LEU:HB3	2:F:33:VAL:HB	1.97	0.46
3:H:190:ASP:O	3:H:193:SER:OG	2.21	0.46
4:Q:300:LYS:O	4:Q:304:ILE:HG12	2.15	0.46
4:Q:391:ALA:HB2	7:K:111:LEU:HD12	1.96	0.46
3:H:19:ARG:HG3	3:H:63:ASN:HD22	1.80	0.46
7:K:24:ILE:O	7:K:28:GLU:HG3	2.15	0.46
1:N:171:LEU:HD13	1:N:209:LYS:HA	1.98	0.46
2:F:119:PRO:HB2	2:F:124:LEU:HD23	1.98	0.46
3:H:82:PHE:CE2	3:H:91:LEU:HD13	2.50	0.46
6:T:136:VAL:HG21	6:T:161:VAL:HG13	1.97	0.46
4:Q:539:ARG:O	4:Q:543:LYS:HG3	2.15	0.46
3:H:44:PRO:HB3	8:V:65:ARG:NH2	2.31	0.46
3:H:141:ARG:HA	8:V:36:LEU:HD13	1.96	0.46
5:R:113:VAL:O	5:R:118:TYR:N	2.44	0.46
1:N:255:GLN:O	1:N:257:PRO:HD3	2.16	0.46
1:N:437:LEU:HD11	1:N:449:HIS:HB2	1.96	0.46
6:T:117:GLN:CD	6:T:122:LYS:HB2	2.40	0.46
2:F:200:ARG:CZ	2:F:204:GLN:HE22	2.28	0.46
4:Q:247:LYS:O	4:Q:251:LYS:N	2.49	0.46
1:N:184:ILE:O	1:N:186:ASN:N	2.48	0.46
1:N:449:HIS:O	1:N:453:ALA:N	2.49	0.46
2:F:186:ASN:OD1	2:F:187:ALA:N	2.49	0.46
5:R:78:TRP:CD1	5:R:109:VAL:HG11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:81:TYR:HE1	5:R:101:ARG:HG3	1.81	0.46
8:V:80:TYR:O	8:V:83:THR:HG22	2.16	0.46
1:N:175:ILE:HD13	1:N:350:SER:HA	1.98	0.46
2:F:138:LYS:HZ3	2:F:142:LYS:HD2	1.79	0.46
4:Q:454:PHE:HD2	8:V:117:VAL:HA	1.80	0.46
5:R:69:ASP:OD1	5:R:71:GLU:HG2	2.16	0.46
1:N:337:ILE:HB	1:N:340:PHE:CE2	2.50	0.45
2:F:85:PRO:HG3	2:F:89:TRP:HE1	1.81	0.45
3:H:32:ALA:O	3:H:36:GLN:HG2	2.16	0.45
6:T:102:ILE:HG13	6:T:110:VAL:O	2.15	0.45
2:F:129:MET:HE2	8:V:51:PRO:HG3	1.97	0.45
6:T:67:CYS:HB2	6:T:74:ILE:HB	1.99	0.45
12:3:41:TYR:CA	12:3:46:ALA:HB2	2.47	0.45
2:F:37:PHE:O	2:F:43:TYR:HB2	2.17	0.45
5:R:35:PHE:HD1	5:R:125:ILE:HG12	1.82	0.45
6:T:50:PRO:HD2	6:T:69:ASP:HB3	1.98	0.45
10:G:324:MET:O	10:G:329:ASP:N	2.49	0.45
1:N:199:VAL:HG12	1:N:200:SER:N	2.31	0.45
2:F:77:GLN:OE1	2:F:94:GLN:NE2	2.36	0.45
4:Q:385:LEU:O	4:Q:388:THR:OG1	2.28	0.45
5:R:51:GLN:O	5:R:54:SER:OG	2.28	0.45
1:N:257:PRO:HB2	1:N:258:ILE:HA	1.97	0.45
1:N:268:LYS:HA	1:N:271:LEU:HB2	1.99	0.45
2:F:83:GLU:HB2	2:F:89:TRP:CD1	2.51	0.45
3:H:17:ARG:HH22	4:Q:140:THR:HG21	1.81	0.45
4:Q:148:THR:OG1	4:Q:149:VAL:N	2.49	0.45
4:Q:262:SER:N	4:Q:350:SER:O	2.48	0.45
5:R:106:ASN:ND2	6:T:73:MET:O	2.50	0.45
1:N:215:PHE:CZ	1:N:256:LYS:HD2	2.52	0.45
4:Q:96:VAL:HA	4:Q:97:GLU:HA	1.79	0.45
4:Q:437:GLU:OE2	4:Q:509:TRP:NE1	2.41	0.45
5:R:80:MET:HB3	5:R:102:ALA:HB3	1.98	0.45
6:T:34:LEU:HD23	6:T:56:LEU:HD21	1.97	0.45
1:N:195:ASN:CG	1:N:224:PHE:CA	2.89	0.45
8:V:16:THR:O	8:V:19:SER:OG	2.30	0.45
4:Q:525:ASN:HA	4:Q:528:GLN:HG2	1.98	0.45
5:R:40:ARG:HG2	5:R:119:GLU:O	2.17	0.45
3:H:13:LEU:HD23	3:H:16:ILE:HD12	1.99	0.45
1:N:532:LEU:HB2	1:N:535:ALA:HA	1.99	0.44
2:F:122:TYR:OH	8:V:45:ASP:OD2	2.29	0.44
4:Q:194:LEU:HD12	7:K:35:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:28:LEU:HD12	2:F:89:TRP:CZ3	2.52	0.44
2:F:197:SER:C	2:F:199:VAL:H	2.25	0.44
3:H:188:LEU:HA	3:H:191:ILE:HG22	1.99	0.44
6:T:141:PRO:O	6:T:145:GLU:HG3	2.16	0.44
1:N:173:GLU:CG	1:N:174:ILE:H	2.30	0.44
1:N:271:LEU:O	1:N:274:ARG:HB3	2.17	0.44
4:Q:132:LYS:NZ	4:Q:154:LEU:O	2.38	0.44
6:T:40:GLN:HG2	6:T:91:ASN:OD1	2.18	0.44
6:T:181:LEU:O	6:T:185:ARG:N	2.48	0.44
1:N:177:THR:HG21	1:N:348:ARG:C	2.43	0.44
3:H:189:THR:O	3:H:192:LEU:HG	2.17	0.44
4:Q:229:VAL:HG23	4:Q:244:ILE:HD11	2.00	0.44
4:Q:288:GLN:HG3	4:Q:299:TYR:CD2	2.52	0.44
2:F:112:ASN:O	2:F:113:GLU:HG2	2.17	0.44
3:H:86:GLU:O	3:H:89:PRO:HD2	2.18	0.44
1:N:284:GLN:O	1:N:288:GLU:HB2	2.18	0.44
2:F:59:ASN:HB3	2:F:62:ASP:HB2	2.00	0.44
3:H:82:PHE:HA	3:H:83:PRO:HD2	1.92	0.44
4:Q:234:LEU:HB2	4:Q:302:GLN:HE22	1.83	0.44
5:R:39:TYR:HD2	5:R:113:VAL:HG11	1.82	0.44
1:N:166:ARG:NH2	11:U:129:GLY:HA3	2.32	0.44
1:N:195:ASN:HD21	1:N:224:PHE:HB2	1.72	0.44
1:N:283:PHE:HB3	1:N:287:ARG:HH12	1.83	0.44
1:N:427:LYS:NZ	4:Q:319:GLN:HB3	2.33	0.44
1:N:547:THR:OG1	1:N:548:LYS:N	2.49	0.44
4:Q:426:ARG:N	4:Q:427:PRO:HD2	2.33	0.44
1:N:279:SER:O	1:N:282:THR:OG1	2.26	0.44
4:Q:232:SER:HB3	4:Q:305:LEU:HD23	2.00	0.44
1:N:178:PRO:HD2	1:N:263:TYR:OH	2.18	0.44
1:N:374:ASP:N	1:N:374:ASP:OD1	2.51	0.44
2:F:21:TRP:CH2	2:F:25:MET:HG3	2.53	0.44
4:Q:101:SER:C	4:Q:103:ALA:H	2.26	0.44
4:Q:102:GLN:OE1	4:Q:105:LYS:HE3	2.17	0.44
5:R:178:ASN:O	5:R:182:MET:HG2	2.18	0.44
6:T:111:ALA:HB3	6:T:127:HIS:HB3	2.00	0.44
1:N:168:ARG:HH21	1:N:215:PHE:H	1.66	0.43
1:N:417:ILE:O	1:N:420:PHE:N	2.51	0.43
2:F:64:GLY:O	2:F:68:SER:OG	2.35	0.43
4:Q:41:ILE:HA	4:Q:42:ILE:HA	1.60	0.43
7:K:27:LEU:HD11	7:K:68:ILE:HG12	2.00	0.43
3:H:46:ILE:HG22	3:H:50:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:147:PHE:HD1	6:T:152:LEU:HD12	1.82	0.43
1:N:431:VAL:HG12	1:N:432:THR:N	2.34	0.43
2:F:87:PHE:CE2	3:H:85:LYS:HG2	2.51	0.43
3:H:88:GLU:O	3:H:92:THR:HG23	2.18	0.43
7:K:20:GLN:O	7:K:24:ILE:HG12	2.18	0.43
12:3:42:PHE:H	12:3:46:ALA:CB	2.30	0.43
1:N:568:LEU:O	1:N:572:VAL:HG23	2.17	0.43
2:F:12:THR:OG1	2:F:13:SER:N	2.48	0.43
2:F:200:ARG:NH2	2:F:204:GLN:HE22	2.17	0.43
3:H:25:GLN:O	3:H:28:THR:OG1	2.30	0.43
3:H:82:PHE:HE2	3:H:84:VAL:HG12	1.84	0.43
1:N:195:ASN:ND2	1:N:224:PHE:HB3	2.31	0.43
1:N:208:PRO:C	1:N:212:GLY:HA3	2.44	0.43
1:N:265:ILE:HD11	2:F:210:LYS:HD3	2.00	0.43
1:N:413:GLY:O	1:N:415:LEU:N	2.51	0.43
1:N:427:LYS:HZ1	4:Q:319:GLN:HB3	1.83	0.43
7:K:92:LYS:HE2	7:K:94:ARG:HA	2.00	0.43
2:F:121:ALA:HA	3:H:76:ILE:HD11	2.00	0.43
4:Q:337:ILE:HD11	4:Q:341:HIS:HB2	2.00	0.43
6:T:8:TYR:HA	6:T:125:LEU:HD23	2.01	0.43
6:T:84:ILE:O	6:T:87:THR:HG22	2.19	0.43
6:T:140:ARG:N	6:T:141:PRO:HD2	2.33	0.43
1:N:190:THR:HA	1:N:196:GLU:HA	2.01	0.43
4:Q:245:ARG:HE	4:Q:256:GLN:CD	2.27	0.43
4:Q:307:GLU:O	4:Q:310:ILE:HG22	2.18	0.43
5:R:173:VAL:HG12	5:R:175:ASP:H	1.83	0.43
1:N:508:TRP:HZ3	1:N:517:VAL:HA	1.84	0.43
1:N:532:LEU:CB	1:N:535:ALA:HA	2.49	0.43
4:Q:295:LEU:HD23	4:Q:298:ILE:HD12	2.01	0.43
4:Q:307:GLU:HA	4:Q:310:ILE:HG22	2.01	0.43
5:R:25:THR:C	7:K:92:LYS:HB3	2.43	0.43
8:V:7:GLN:O	8:V:11:VAL:HG23	2.18	0.43
2:F:197:SER:O	2:F:199:VAL:N	2.52	0.43
3:H:77:TYR:CZ	4:Q:155:GLN:HB3	2.54	0.43
3:H:112:GLN:HG3	3:H:113:GLU:HG3	2.00	0.43
6:T:139:ALA:O	6:T:143:ILE:HG12	2.18	0.43
7:K:92:LYS:NZ	7:K:94:ARG:HG2	2.34	0.43
3:H:20:ILE:HA	3:H:23:ILE:HG22	2.01	0.42
4:Q:271:LEU:HB3	4:Q:275:ARG:HA	2.00	0.42
4:Q:431:TYR:HB3	8:V:111:GLN:OE1	2.19	0.42
5:R:5:TYR:OH	5:R:205:VAL:O	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:43:ASP:O	5:R:48:LEU:HD22	2.19	0.42
11:U:26:LEU:O	16:J:186:UNK:HA	2.18	0.42
2:F:149:TYR:OH	8:V:72:ASP:OD1	2.27	0.42
6:T:47:ALA:O	6:T:50:PRO:HD3	2.18	0.42
7:K:25:LEU:HD23	7:K:28:GLU:OE2	2.18	0.42
2:F:128:ARG:HD2	4:Q:122:ALA:HB2	2.00	0.42
4:Q:193:ARG:O	4:Q:197:VAL:HG23	2.19	0.42
4:Q:327:ASN:O	4:Q:334:LEU:N	2.52	0.42
5:R:90:ARG:HG3	5:R:204:ASN:HD21	1.84	0.42
6:T:36:LYS:HD2	6:T:94:GLN:HB3	2.02	0.42
1:N:173:GLU:HG3	1:N:174:ILE:N	2.34	0.42
3:H:177:ARG:HH22	5:R:13:ARG:NH1	2.17	0.42
4:Q:205:TYR:O	4:Q:209:VAL:HG23	2.19	0.42
6:T:8:TYR:O	6:T:155:ASN:HB2	2.20	0.42
1:N:353:TYR:H	1:N:354:ASP:HB2	1.82	0.42
5:R:51:GLN:N	5:R:54:SER:OG	2.52	0.42
10:G:324:MET:HA	10:G:329:ASP:CB	2.49	0.42
1:N:150:SER:HA	1:N:151:THR:HA	1.83	0.42
1:N:249:ALA:O	1:N:253:VAL:HG23	2.20	0.42
5:R:39:TYR:HE1	5:R:120:PHE:HD1	1.68	0.42
5:R:136:THR:HG22	5:R:171:THR:HB	2.02	0.42
6:T:78:PRO:HA	6:T:79:GLU:CB	2.39	0.42
1:N:309:TYR:HB3	1:N:310:TRP:H	1.62	0.42
4:Q:138:ILE:O	4:Q:141:ILE:HG12	2.20	0.42
4:Q:329:THR:OG1	4:Q:332:GLU:HG2	2.20	0.42
5:R:146:PRO:HA	5:R:156:PHE:HD1	1.85	0.42
1:N:344:LEU:HB3	1:N:345:SER:H	1.51	0.42
1:N:345:SER:HA	1:N:349:SER:O	2.20	0.42
2:F:120:ASN:OD1	2:F:121:ALA:N	2.53	0.42
3:H:133:LYS:O	3:H:136:LEU:HB2	2.20	0.42
4:Q:188:PHE:O	4:Q:192:GLU:HG2	2.20	0.42
1:N:285:LEU:HA	1:N:289:SER:O	2.20	0.42
3:H:44:PRO:HB3	8:V:65:ARG:HH22	1.85	0.42
3:H:132:GLN:O	3:H:136:LEU:HG	2.20	0.42
4:Q:195:THR:O	4:Q:199:GLU:HG3	2.20	0.42
4:Q:527:CYS:O	4:Q:531:GLU:HG3	2.19	0.42
6:T:35:LYS:O	6:T:54:GLU:HG2	2.19	0.42
7:K:20:GLN:HA	7:K:23:ASN:ND2	2.35	0.42
4:Q:76:THR:HA	4:Q:77:GLU:HA	1.63	0.41
6:T:117:GLN:NE2	6:T:122:LYS:HB2	2.35	0.41
7:K:25:LEU:HA	7:K:28:GLU:CD	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:172:TYR:CD2	1:N:213:ILE:HG13	2.55	0.41
1:N:347:LYS:HG2	1:N:348:ARG:N	2.33	0.41
2:F:155:TYR:CD2	3:H:43:TRP:HB3	2.54	0.41
7:K:105:PHE:O	7:K:108:SER:OG	2.17	0.41
1:N:267:HIS:O	1:N:271:LEU:N	2.49	0.41
2:F:32:ASN:O	2:F:35:GLU:HB3	2.21	0.41
1:N:168:ARG:NH2	1:N:215:PHE:H	2.18	0.41
1:N:456:ASN:O	1:N:459:LEU:HB3	2.20	0.41
2:F:21:TRP:O	2:F:25:MET:HG2	2.19	0.41
2:F:126:ALA:HB1	8:V:47:TYR:CG	2.54	0.41
2:F:163:ASP:HB2	2:F:164:ASN:O	2.20	0.41
4:Q:204:TYR:CE2	4:Q:208:LEU:HD11	2.56	0.41
2:F:66:LEU:O	2:F:70:LEU:N	2.52	0.41
4:Q:128:LEU:HD22	4:Q:151:PRO:HB3	2.03	0.41
4:Q:529:TYR:HA	4:Q:532:HIS:HD2	1.85	0.41
12:3:41:TYR:CA	12:3:46:ALA:CB	2.99	0.41
1:N:472:TYR:CZ	1:N:476:ILE:HD11	2.56	0.41
2:F:199:VAL:HA	2:F:202:PHE:CD2	2.55	0.41
1:N:192:THR:OG1	1:N:193:VAL:N	2.52	0.41
1:N:256:LYS:HG3	1:N:258:ILE:HG13	2.02	0.41
1:N:257:PRO:CB	1:N:258:ILE:HA	2.51	0.41
1:N:527:TRP:HZ3	1:N:557:SER:HB3	1.86	0.41
2:F:69:GLN:OE1	2:F:72:ARG:NH2	2.54	0.41
5:R:52:PRO:HA	5:R:55:TRP:NE1	2.36	0.41
5:R:114:GLU:C	5:R:117:GLY:H	2.29	0.41
8:V:31:ARG:O	8:V:35:ILE:HG13	2.19	0.41
1:N:172:TYR:CB	1:N:213:ILE:HA	2.51	0.41
1:N:177:THR:N	1:N:350:SER:HB3	2.35	0.41
1:N:196:GLU:CD	1:N:225:HIS:NE2	2.78	0.41
1:N:466:GLN:O	1:N:470:ARG:HG3	2.21	0.41
2:F:133:THR:HA	2:F:136:PHE:CD2	2.56	0.41
5:R:80:MET:HE3	6:T:84:ILE:HD13	2.03	0.41
6:T:38:VAL:O	6:T:91:ASN:N	2.53	0.41
1:N:199:VAL:CG1	1:N:200:SER:N	2.83	0.41
1:N:215:PHE:HA	1:N:258:ILE:HD13	2.03	0.41
1:N:549:GLY:HA3	1:N:550:THR:HA	1.50	0.41
3:H:25:GLN:NE2	3:H:28:THR:OG1	2.54	0.41
3:H:30:PHE:CE2	4:Q:112:ILE:HG13	2.55	0.41
3:H:68:SER:O	3:H:72:GLN:HG3	2.21	0.41
3:H:177:ARG:HH22	5:R:13:ARG:CZ	2.33	0.41
4:Q:304:ILE:HD13	4:Q:304:ILE:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:396:LEU:HD21	4:Q:473:LEU:HD12	2.03	0.41
6:T:94:GLN:NE2	6:T:96:PHE:HB3	2.36	0.41
6:T:117:GLN:NE2	6:T:122:LYS:HD3	2.36	0.41
10:G:324:MET:CB	10:G:329:ASP:CB	2.98	0.41
1:N:217:TRP:O	1:N:218:ILE:HG13	2.21	0.41
1:N:544:VAL:CG1	1:N:545:HIS:H	2.31	0.41
2:F:47:SER:HB3	2:F:78:PHE:HE2	1.86	0.41
3:H:5:SER:OG	4:Q:158:ARG:NH2	2.49	0.41
3:H:24:VAL:O	3:H:28:THR:HG23	2.21	0.40
4:Q:508:VAL:HG23	4:Q:509:TRP:CD1	2.56	0.40
4:Q:512:LYS:HZ3	4:Q:517:SER:HB2	1.87	0.40
1:N:861:LYS:HA	1:N:862:THR:HA	1.84	0.40
2:F:164:ASN:HB3	2:F:165:LEU:H	1.65	0.40
4:Q:221:SER:HG	4:Q:222:GLN:N	2.18	0.40
4:Q:264:ALA:HA	4:Q:348:GLU:HB2	2.03	0.40
1:N:474:PHE:O	1:N:478:THR:HG23	2.22	0.40
3:H:81:GLU:OE1	4:Q:152:SER:HB3	2.21	0.40
5:R:29:PRO:HB3	5:R:131:TYR:CE1	2.54	0.40
5:R:200:CYS:SG	5:R:201:ASP:N	2.94	0.40
1:N:123:ASP:HA	1:N:124:ILE:HA	1.82	0.40
2:F:36:TYR:O	2:F:39:GLN:HB2	2.21	0.40
3:H:106:TRP:O	3:H:110:THR:HG23	2.21	0.40
4:Q:418:ASP:HA	4:Q:419:ALA:HA	1.86	0.40
6:T:30:PHE:O	6:T:100:GLY:C	2.61	0.40
8:V:45:ASP:HB3	8:V:48:THR:HG23	2.04	0.40
1:N:197:PHE:CE1	1:N:219:VAL:CG2	3.02	0.40
1:N:482:GLU:OE2	4:Q:521:SER:OG	2.33	0.40
2:F:198:VAL:HG12	2:F:202:PHE:CE1	2.57	0.40
3:H:89:PRO:O	3:H:92:THR:OG1	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	N	271/931 (29%)	216 (80%)	35 (13%)	20 (7%)	1	10
2	F	187/216 (87%)	163 (87%)	17 (9%)	7 (4%)	2	19
3	H	155/200 (78%)	149 (96%)	5 (3%)	1 (1%)	21	58
4	Q	337/545 (62%)	301 (89%)	27 (8%)	9 (3%)	4	25
5	R	205/207 (99%)	191 (93%)	11 (5%)	3 (2%)	8	38
6	T	175/193 (91%)	153 (87%)	14 (8%)	8 (5%)	2	17
7	K	96/116 (83%)	90 (94%)	6 (6%)	0	100	100
8	V	116/136 (85%)	108 (93%)	8 (7%)	0	100	100
10	G	186/376 (50%)	165 (89%)	15 (8%)	6 (3%)	3	21
11	U	118/138 (86%)	112 (95%)	5 (4%)	1 (1%)	16	52
12	3	101/139 (73%)	80 (79%)	12 (12%)	9 (9%)	0	8
13	I	73/121 (60%)	64 (88%)	7 (10%)	2 (3%)	4	25
14	2	66/273 (24%)	63 (96%)	1 (2%)	2 (3%)	3	22
All	All	2086/3591 (58%)	1855 (89%)	163 (8%)	68 (3%)	5	21

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	257	PRO
2	F	198	VAL
4	Q	162	PRO
6	T	101	SER
12	3	60	PRO
13	I	94	ALA
14	2	123	PRO
1	N	95	GLN
1	N	121	ALA
1	N	141	LEU
1	N	142	TYR
1	N	208	PRO
1	N	488	GLU
2	F	162	ASN
2	F	185	GLU
3	H	122	PRO
4	Q	260	LEU
10	G	221	ILE
10	G	330	VAL
11	U	31	ASP

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Mol	Chain	Res	Type
12	3	12	ASP
12	3	44	ASP
1	N	87	LEU
1	N	122	LEU
1	N	145	SER
1	N	175	ILE
1	N	301	LYS
1	N	487	ALA
2	F	60	ALA
2	F	187	ALA
4	Q	151	PRO
4	Q	417	ILE
5	R	92	ASP
6	T	61	ASN
6	T	70	GLU
6	T	120	VAL
10	G	120	ALA
10	G	307	ASN
12	3	11	PRO
12	3	16	ARG
12	3	41	TYR
12	3	42	PHE
12	3	80	ASN
12	3	87	ILE
13	I	62	LYS
14	2	108	GLU
1	N	176	PRO
1	N	185	ALA
1	N	192	THR
2	F	112	ASN
5	R	50	ARG
5	R	83	GLU
6	T	60	ILE
6	T	90	TRP
6	T	93	ARG
6	T	154	ASN
10	G	319	SER
2	F	146	PHE
10	G	316	LYS
1	N	147	SER
4	Q	148	THR
4	Q	408	SER

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Mol	Chain	Res	Type
1	N	174	ILE
1	N	447	PRO
4	Q	237	ILE
4	Q	337	ILE
4	Q	236	GLY
1	N	128	GLY

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	N	369/799 (46%)	369 (100%)	0	100	100
2	F	177/198 (89%)	177 (100%)	0	100	100
3	H	168/185 (91%)	168 (100%)	0	100	100
4	Q	391/509 (77%)	391 (100%)	0	100	100
5	R	191/191 (100%)	191 (100%)	0	100	100
6	T	164/178 (92%)	164 (100%)	0	100	100
7	K	88/108 (82%)	88 (100%)	0	100	100
8	V	112/129 (87%)	112 (100%)	0	100	100
All	All	1660/2297 (72%)	1660 (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 (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	159	HIS
1	N	355	HIS
1	N	364	HIS
1	N	381	HIS
1	N	403	HIS
1	N	449	HIS
1	N	469	ASN

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Mol	Chain	Res	Type
2	F	49	ASN
2	F	100	ASN
2	F	112	ASN
3	H	18	HIS
3	H	25	GLN
3	H	51	ASN
3	H	62	ASN
3	H	63	ASN
3	H	67	HIS
3	H	150	ASN
3	H	182	GLN
4	Q	111	GLN
4	Q	202	HIS
4	Q	226	HIS
4	Q	319	GLN
4	Q	433	ASN
4	Q	518	ASN
5	R	65	HIS
5	R	77	GLN
5	R	85	ASN
5	R	163	GLN
6	T	33	HIS
6	T	59	ASN
6	T	94	GLN
6	T	127	HIS
6	T	144	GLN
6	T	184	GLN
7	K	75	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
15	S	6
16	J	3
9	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	56:UNK	C	160:UNK	N	37.47
1	J	204:UNK	C	310:UNK	N	31.08
1	S	265:UNK	C	271:UNK	N	28.46
1	S	366:UNK	C	381:UNK	N	26.50
1	S	287:UNK	C	301:UNK	N	18.90
1	S	349:UNK	C	351:UNK	N	15.79
1	S	82:UNK	C	251:UNK	N	12.59
1	D	27:UNK	C	33:UNK	N	10.41
1	S	322:UNK	C	331:UNK	N	7.78
1	J	22:UNK	C	25:UNK	N	5.85

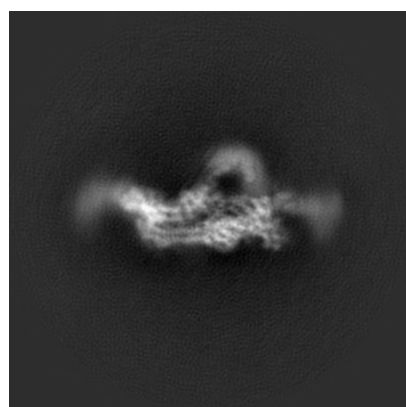
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8479. These allow visual inspection of the internal detail of the map and identification of artifacts.

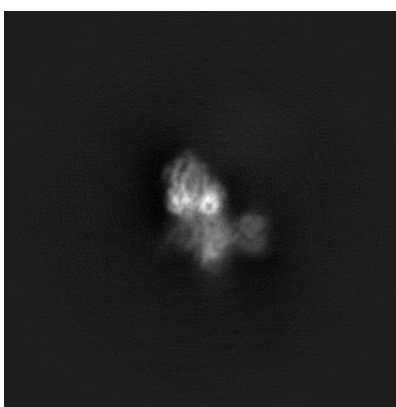
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

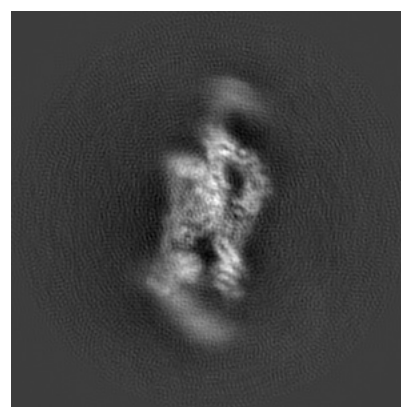
6.1.1 Primary map



X



Y

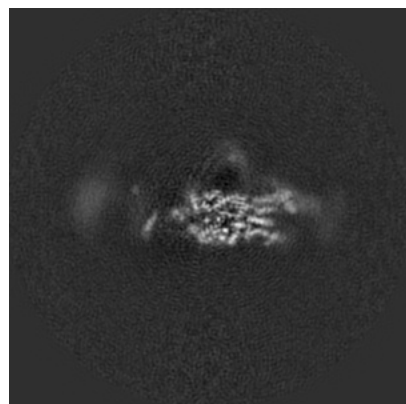


Z

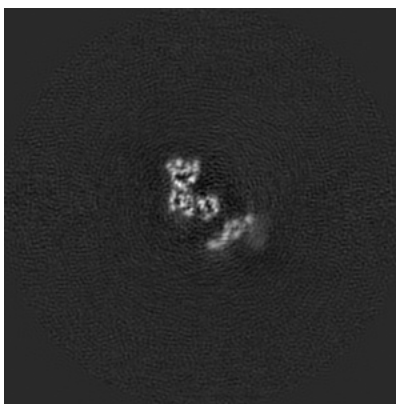
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 176



Y Index: 176

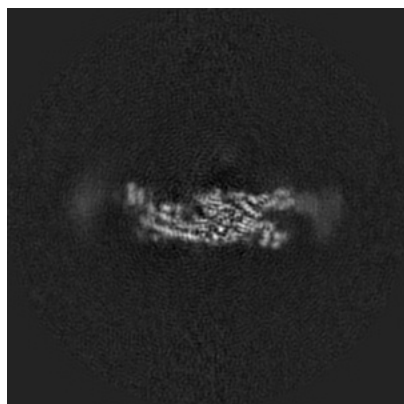


Z Index: 176

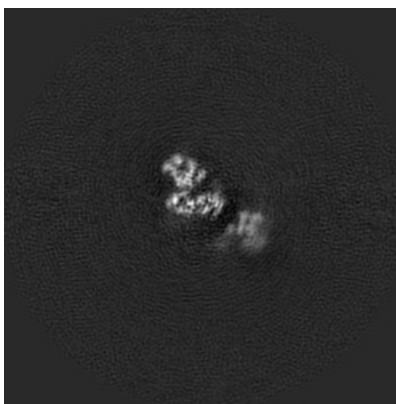
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

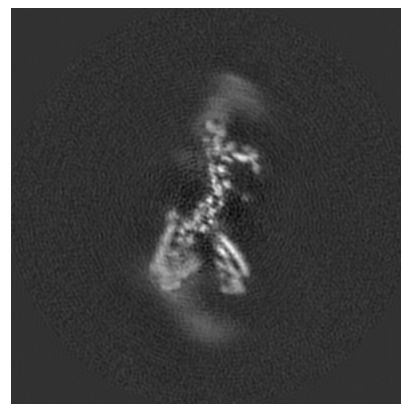
6.3.1 Primary map



X Index: 183



Y Index: 183

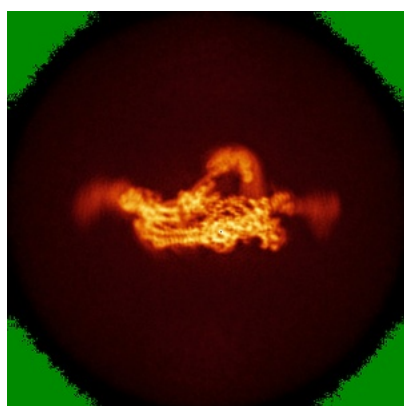


Z Index: 177

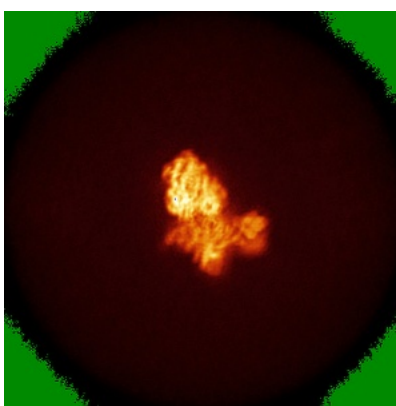
The images above show the largest variance slices of the map in three orthogonal directions.

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

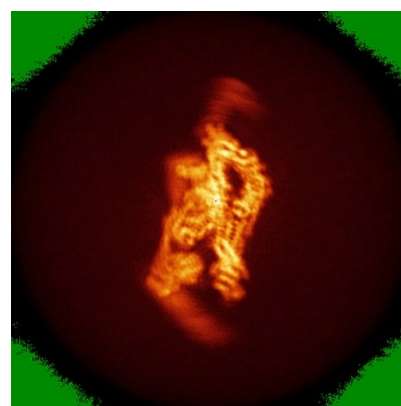
6.4.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

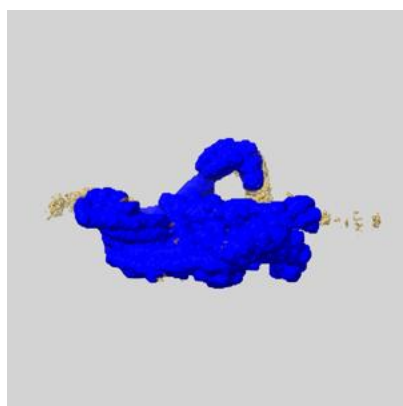
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

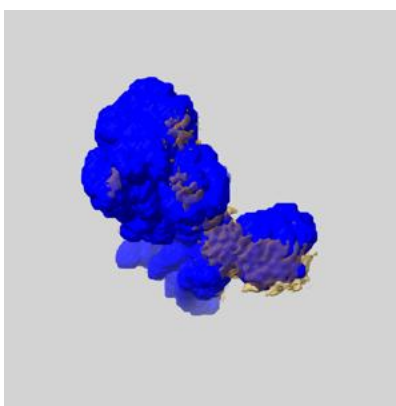
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

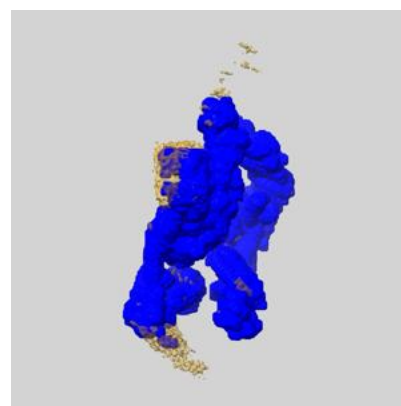
6.6.1 emd_8479_msk_1.map [i](#)



X



Y

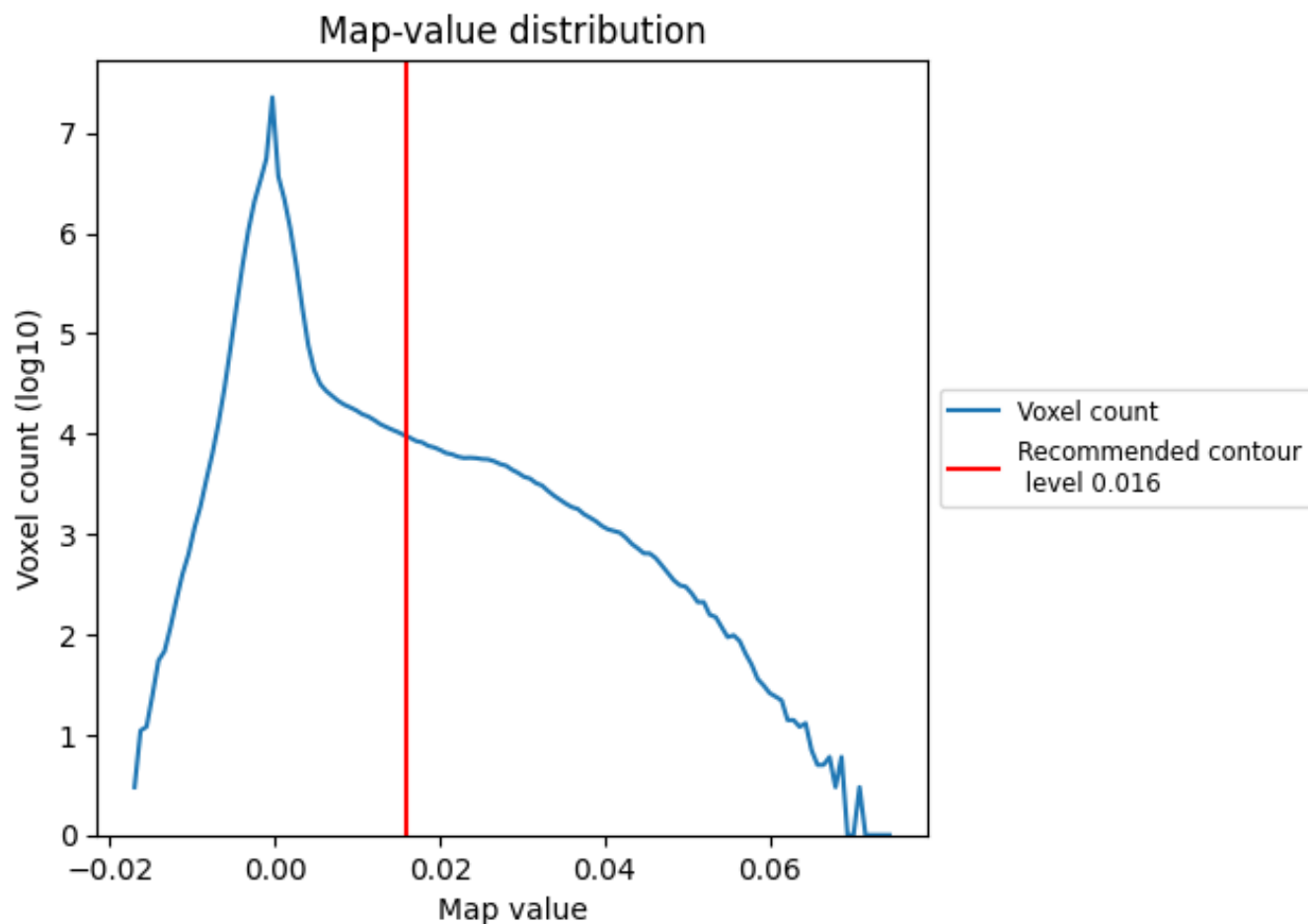


Z

7 Map analysis [i](#)

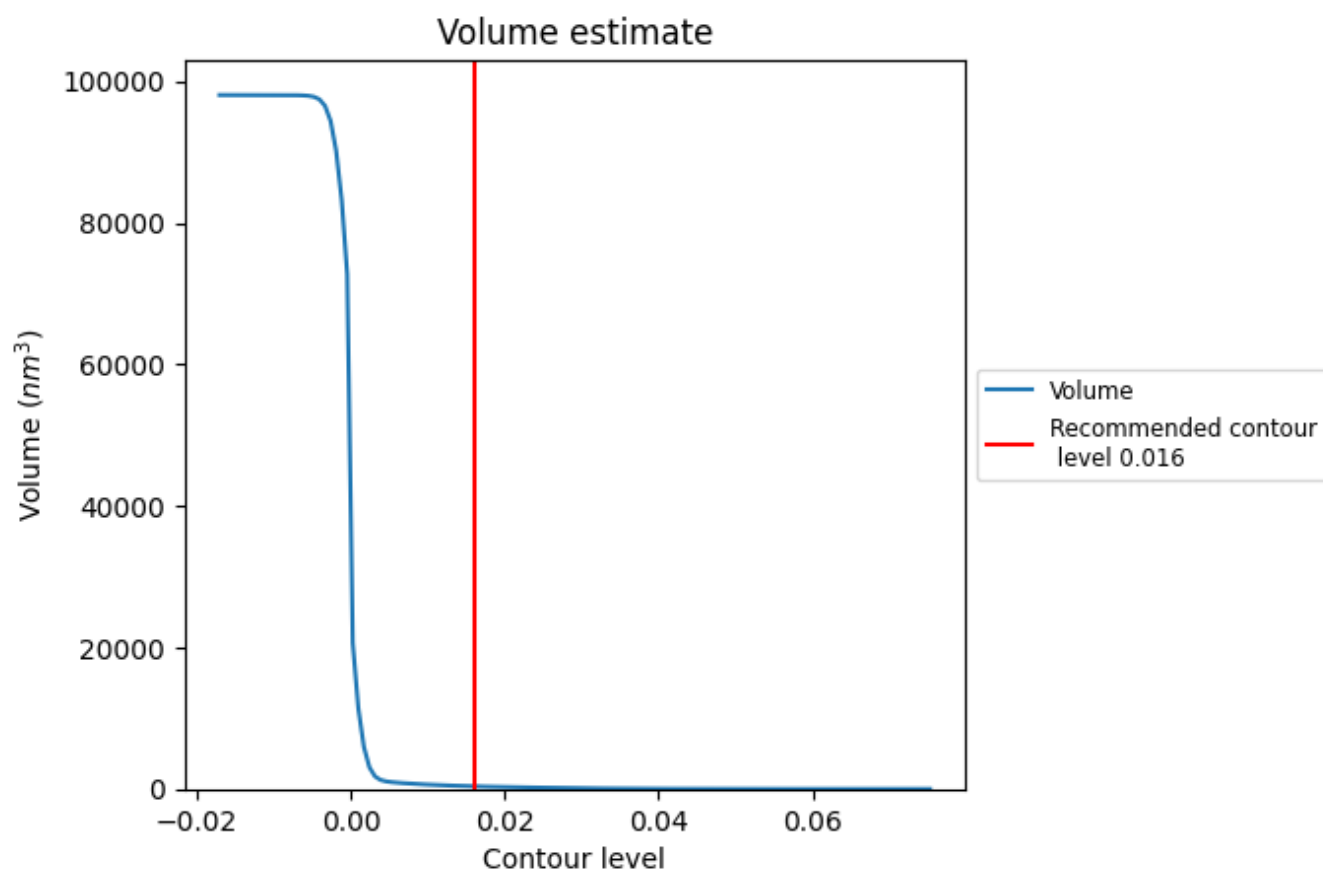
This section contains the results of statistical analysis of the map.

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.

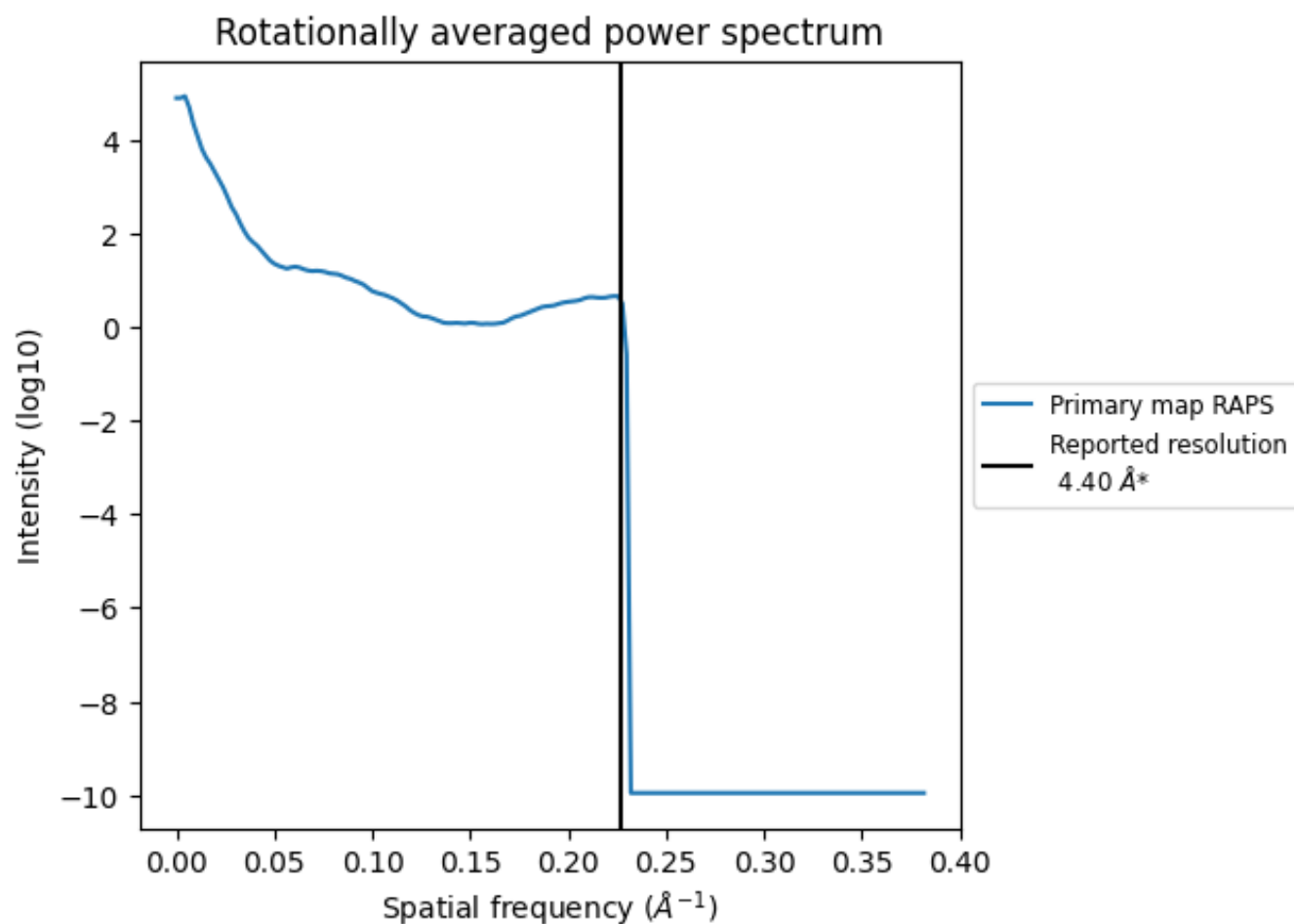
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 375 nm^3 ; this corresponds to an approximate mass of 339 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 ⓘ

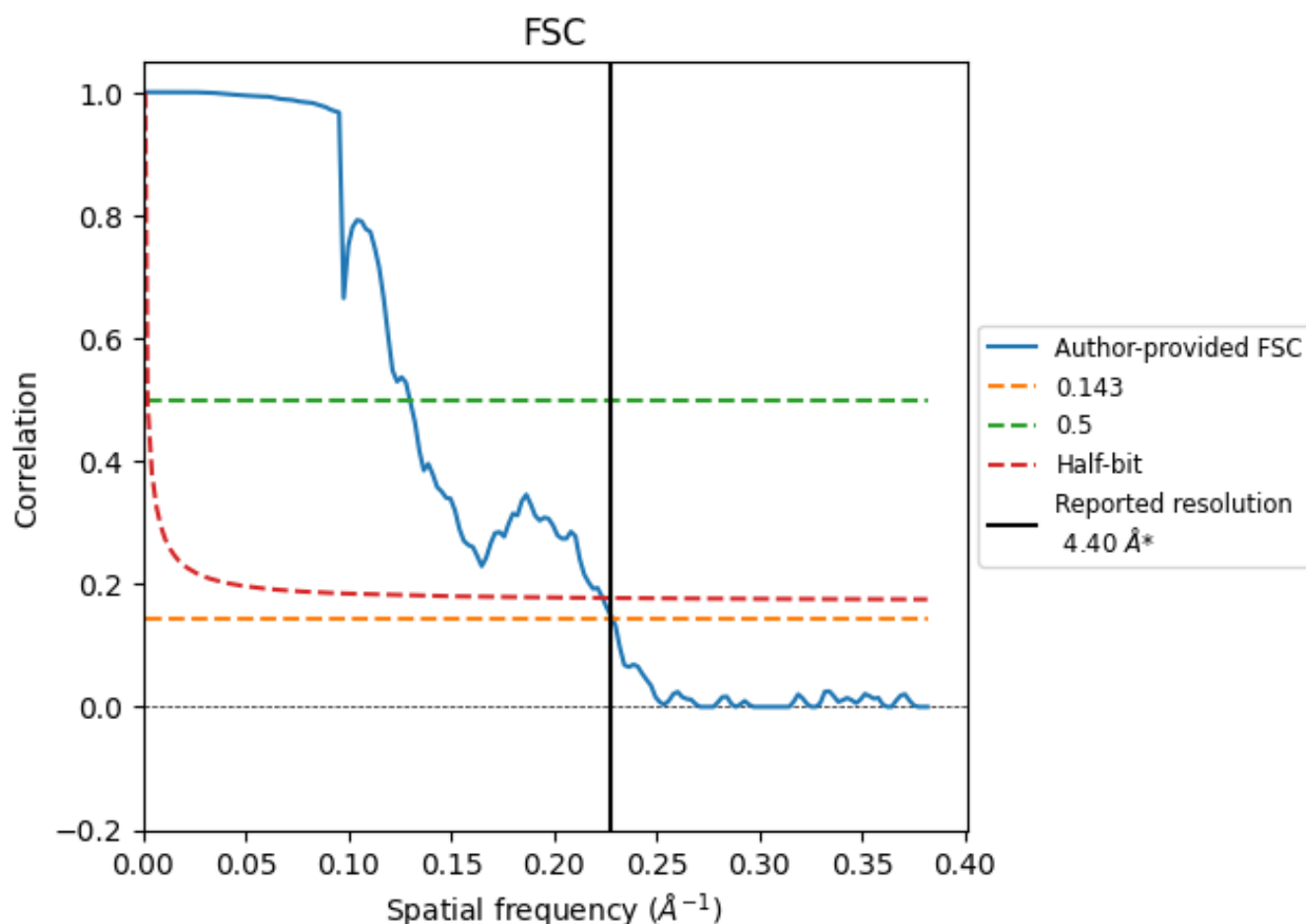


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

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 0.227 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.38	7.70	4.47
Unmasked-calculated*	-	-	-

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

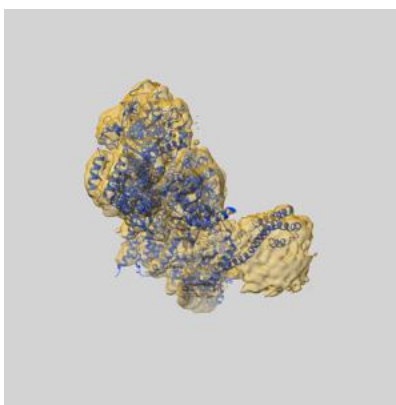
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8479 and PDB model 5U0P. Per-residue inclusion information can be found in section [3](#) on page [7](#).

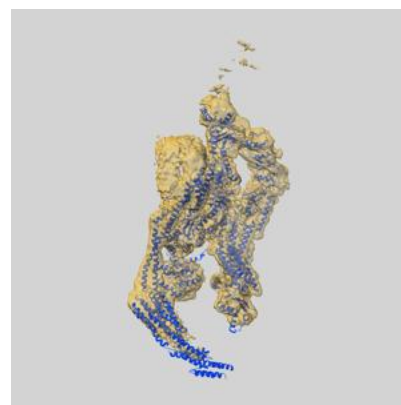
9.1 Map-model overlay [i](#)



X



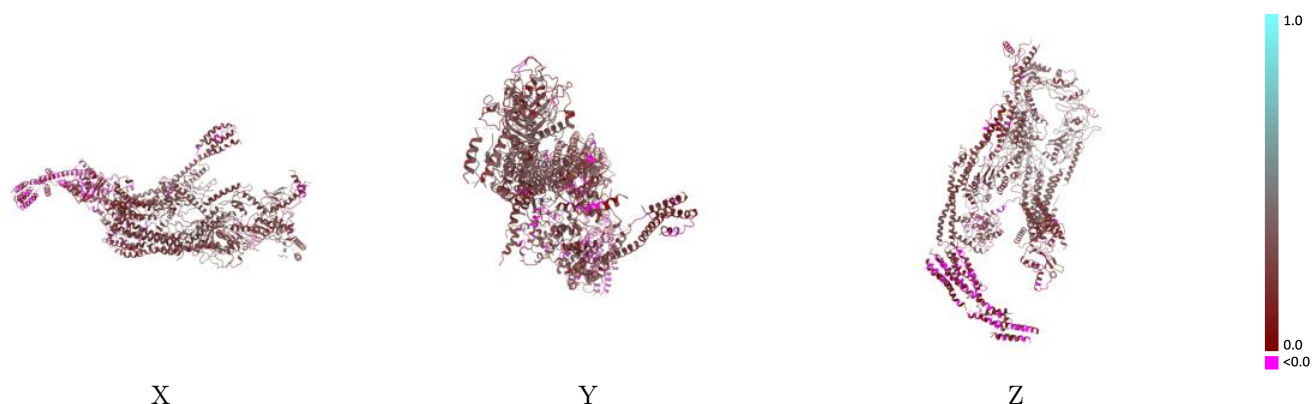
Y



Z

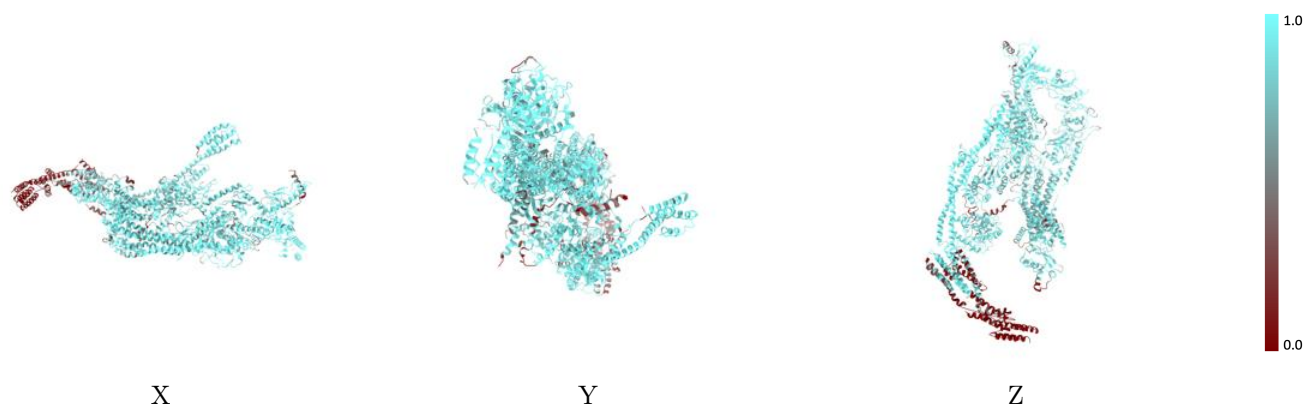
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



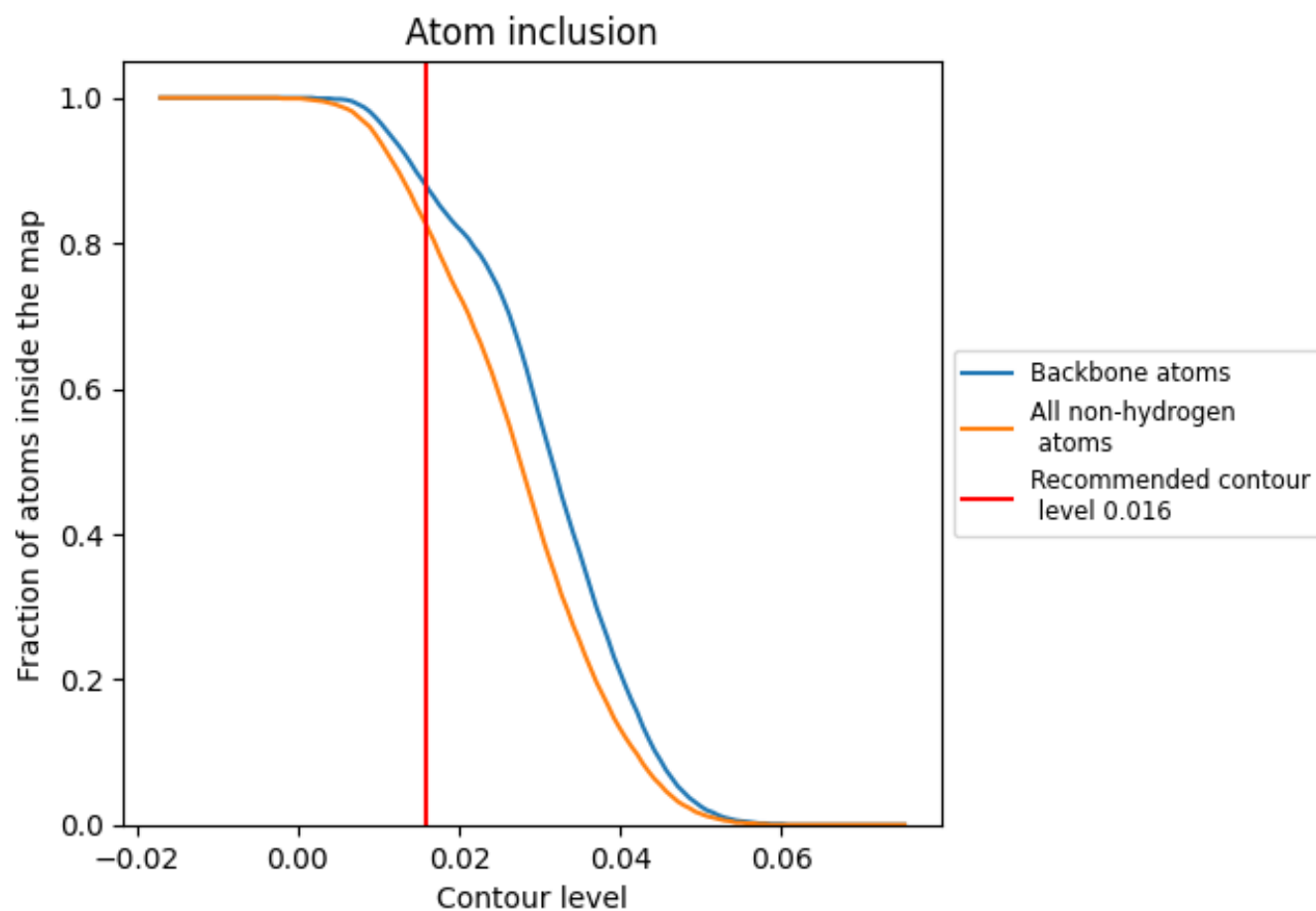
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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 (0.016).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 82% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8240	 0.2360
2	 0.9850	 0.3370
3	 0.9440	 0.1970
D	 0.9170	 0.2030
F	 0.7730	 0.2050
G	 0.8530	 0.1470
H	 0.8500	 0.2330
I	 0.9470	 0.2020
J	 0.5010	 0.0640
K	 0.9010	 0.2780
N	 0.8710	 0.2620
Q	 0.8370	 0.2720
R	 0.8900	 0.2900
S	 0.0390	 0.0540
T	 0.9030	 0.2510
U	 0.7040	 0.1750
V	 0.8850	 0.2750

