Full wwPDB EM Validation Report (i)

May 19, 2025 – 02:29 PM EDT

PDB ID	:	7T3C / pdb_00007t3c
EMDB ID	:	EMD-25654
Title	:	GATOR1-RAG-RAGULATOR - Dual Complex
Authors	:	Egri, S.B.; Shen, K.
Deposited on	:	2021-12-07
Resolution	:	4.00 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 (i) 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 (1)) were used in the production of this report:

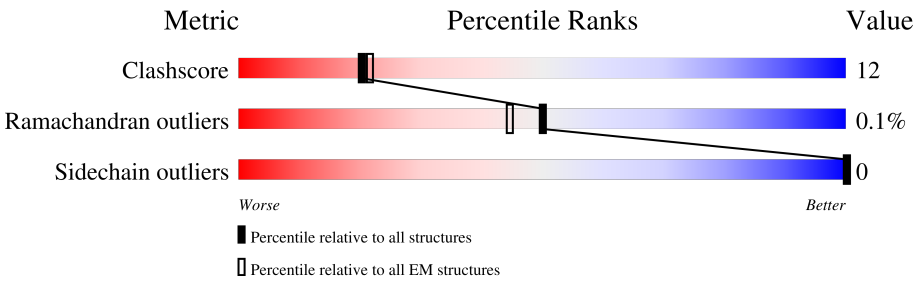
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	B	380	67% 26% • 5%
2	A	1603	• 45% 17% 38%
3	H	124	7% 70% 27% •
3	O	124	• 73% 23% •
4	G	125	• 56% 44%
4	N	125	58% 40% • •
5	J	91	11% 79% 21%
5	Q	91	5% 78% 22%

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Mol	Chain	Length	Quality of chain
6	I	99	30% 66% 20% 14%
6	P	99	27% 70% 28%
7	F	161	12% 56% 13% 31%
7	M	161	11% 52% 19% 29%
8	C	569	56% 15% 29%
9	D	313	59% 34% 5%
9	K	313	61% 34%
10	E	399	6% 51% 26% 23%
11	L	399	48% 28% 23%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	AF3	K	502	-	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 32452 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 GATOR complex protein NPRL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	362	2918	1868	486	546	18	0	0

- Molecule 2 is a protein called GATOR complex protein DEPDC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	990	8120	5243	1347	1485	45	0	0

- Molecule 3 is a protein called Ragulator complex protein LAMTOR3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	121	939	604	158	176	1	0	0
3	O	120	934	601	157	175	1	0	0

- Molecule 4 is a protein called Ragulator complex protein LAMTOR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	125	944	593	162	182	7	0	0
4	N	124	936	588	161	181	6	0	0

- Molecule 5 is a protein called Ragulator complex protein LAMTOR5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	J	91	672	409	116	139	8	1	0
5	Q	91	666	406	115	138	7	0	0

- Molecule 6 is a protein called Ragulator complex protein LAMTOR4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	I	85	647	407	116	123	1	0	0
6	P	97	738	460	135	140	3	0	0

- Molecule 7 is a protein called Ragulator complex protein LAMTOR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	F	111	861	541	148	170	2	0	0
7	M	115	892	560	155	175	2	0	0

- Molecule 8 is a protein called GATOR complex protein NPRL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	C	406	3242	2087	568	568	19	0	0

- Molecule 9 is a protein called Ras-related GTP-binding protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	D	296	2429	1543	423	446	17	0	0
9	K	300	2459	1561	428	452	18	0	0

- Molecule 10 is a protein called Ras-related GTP-binding protein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	E	306	2471	1590	398	469	14	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	92	ALA	PHE	engineered mutation	UNP Q9HB90

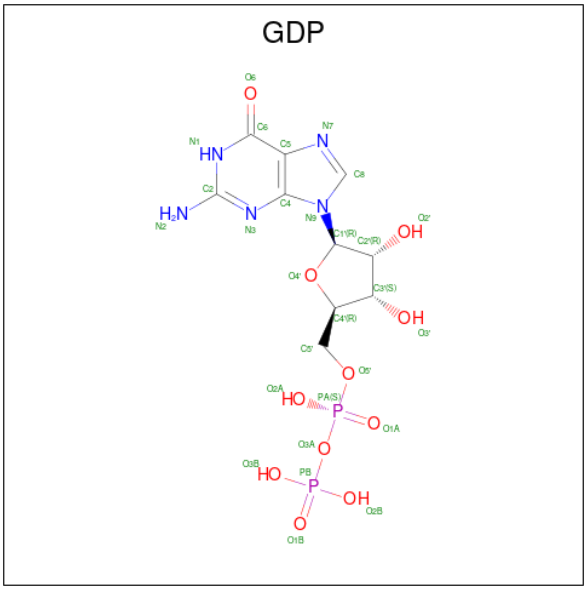
- Molecule 11 is a protein called Ras-related GTP-binding protein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	307	2488	1603	401	470	14	0	0

There is a discrepancy between the modelled and reference sequences:

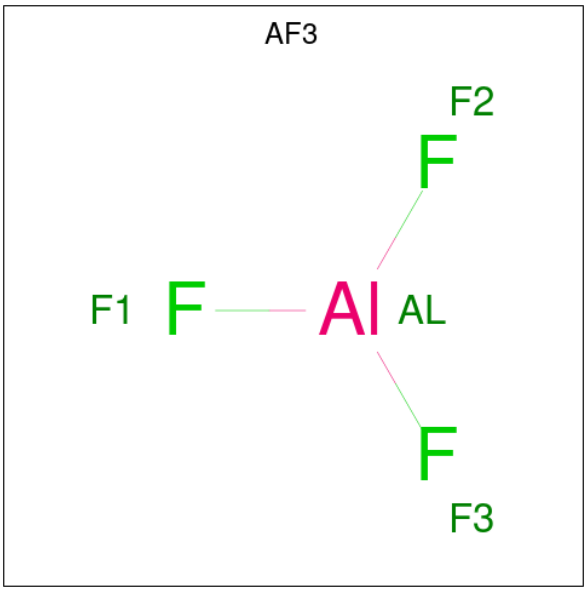
Chain	Residue	Modelled	Actual	Comment	Reference
L	75	ASN	SER	engineered mutation	UNP Q9HB90

- Molecule 12 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
12	D	1	28	10	5	11	2	0
			Total	C	N	O	P	
12	E	1	28	10	5	11	2	0
			Total	C	N	O	P	
12	K	1	28	10	5	11	2	0

- Molecule 13 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3) (labeled as "Ligand of Interest" by depositor).



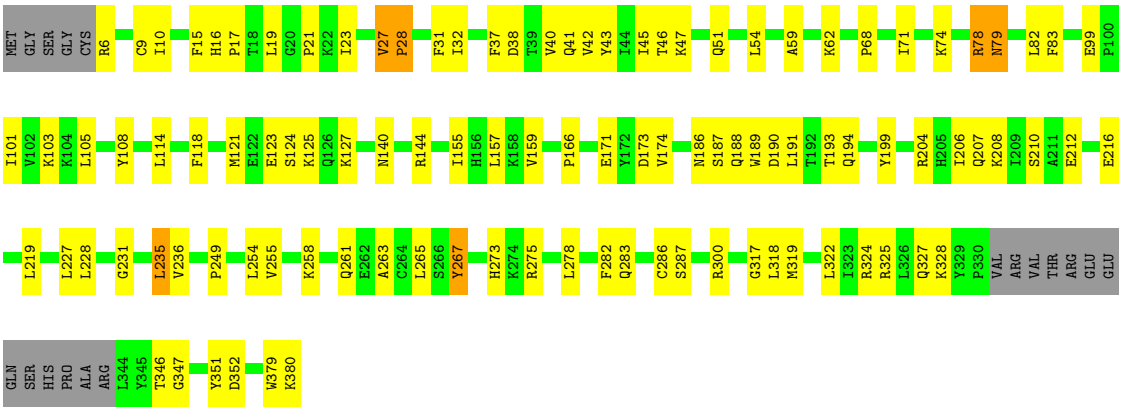
Mol	Chain	Residues	Atoms			AltConf
			Total	Al	F	
13	D	1	4	1	3	0
13	E	1	4	1	3	0
13	K	1	4	1	3	0

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.

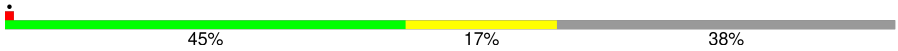
- Molecule 1: GATOR complex protein NPRL2

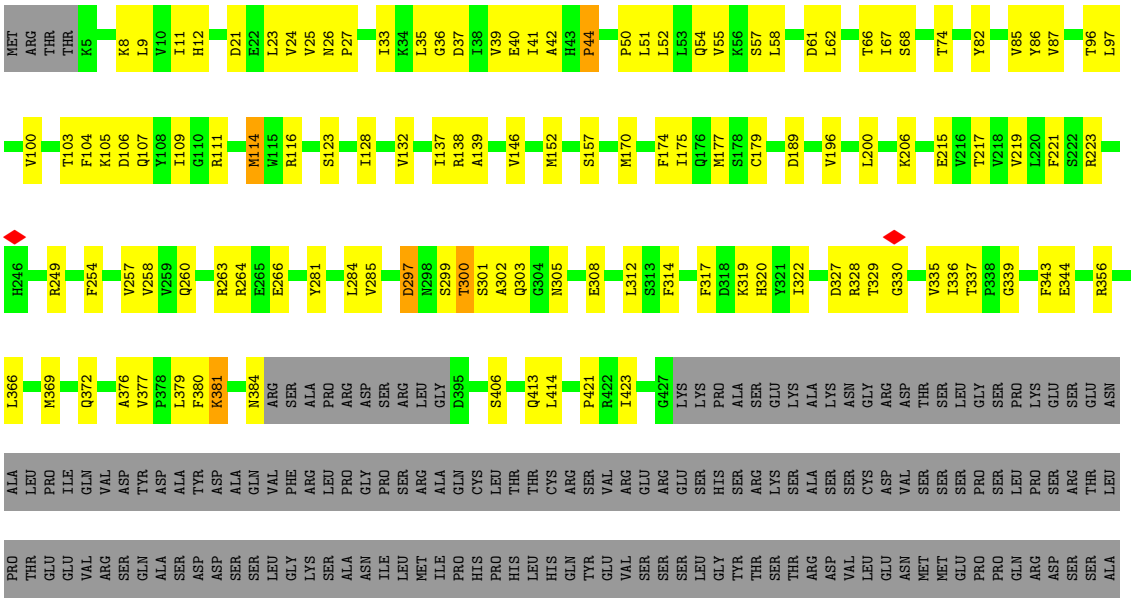
Chain B:

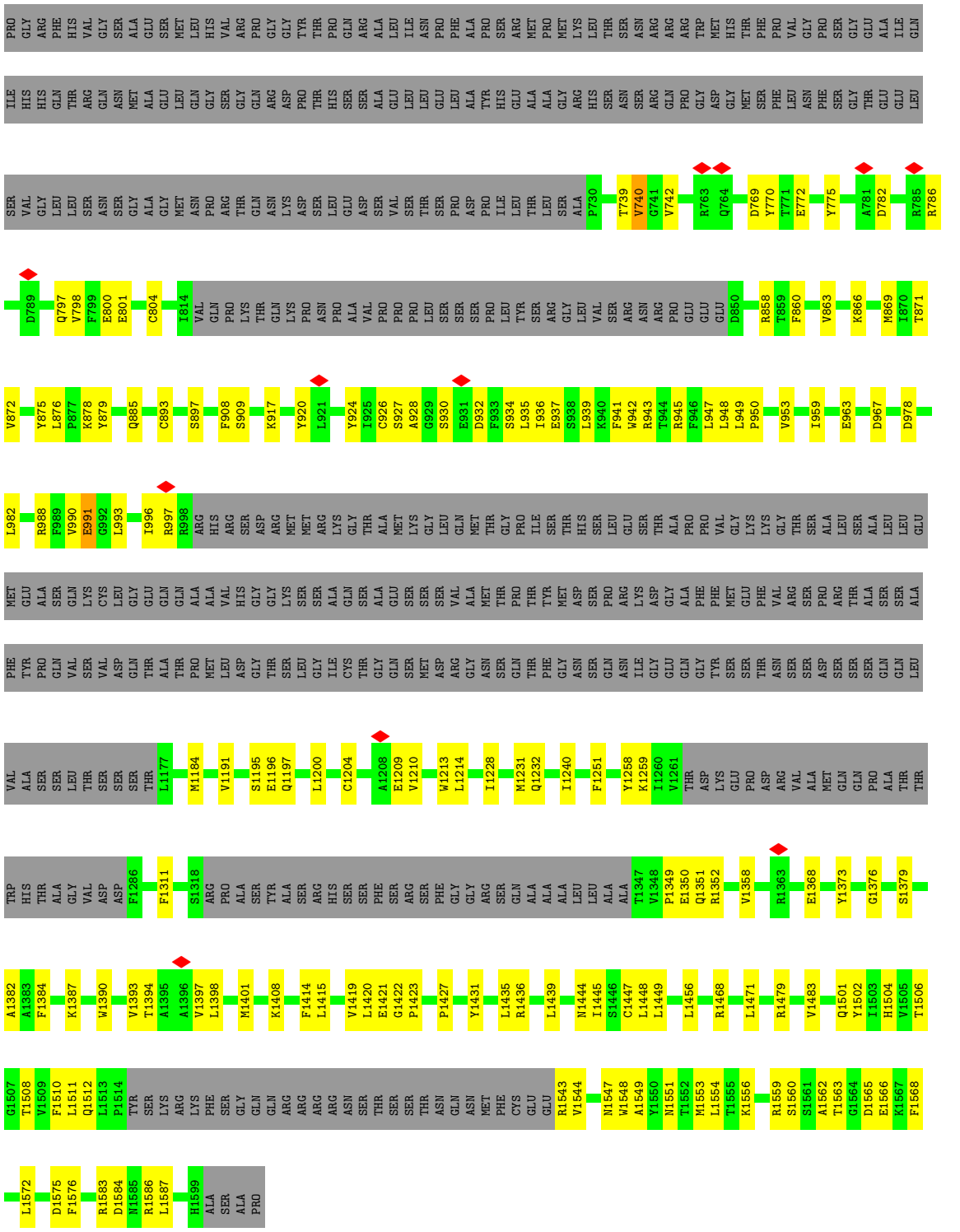


- Molecule 2: GATOR complex protein DEPDC5

Chain A:

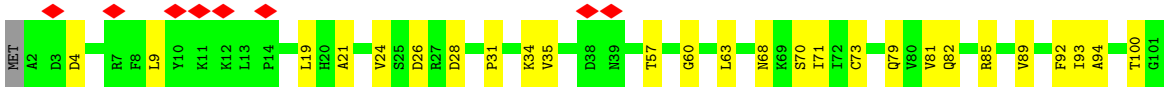






• Molecule 3: Ragulator complex protein LAMTOR3

Chain H:

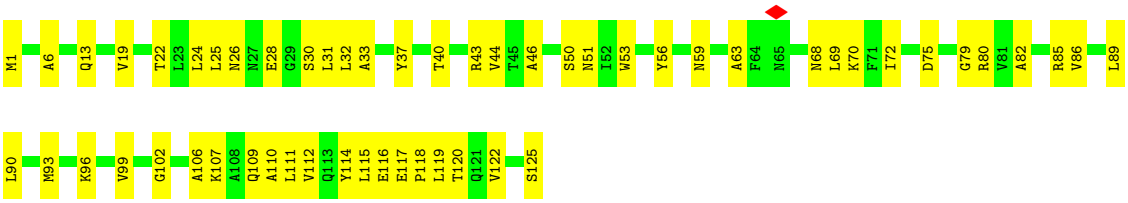


• Molecule 3: Ragulator complex protein LAMTOR3

Chain O:

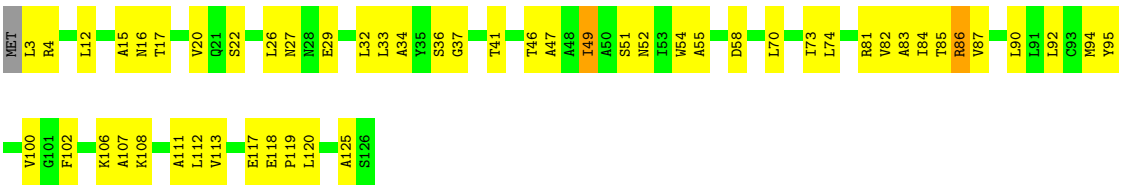
• Molecule 4: Ragulator complex protein LAMTOR2

Chain G:



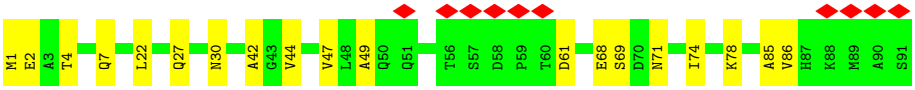
• Molecule 4: Ragulator complex protein LAMTOR2

Chain N:



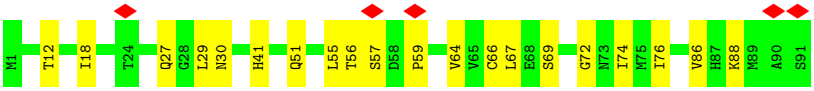
• Molecule 5: Ragulator complex protein LAMTOR5

Chain J:



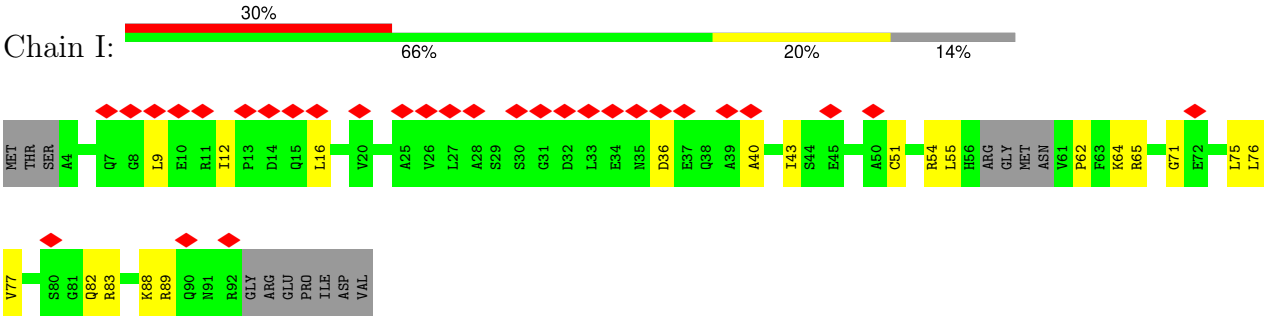
• Molecule 5: Ragulator complex protein LAMTOR5

Chain Q:



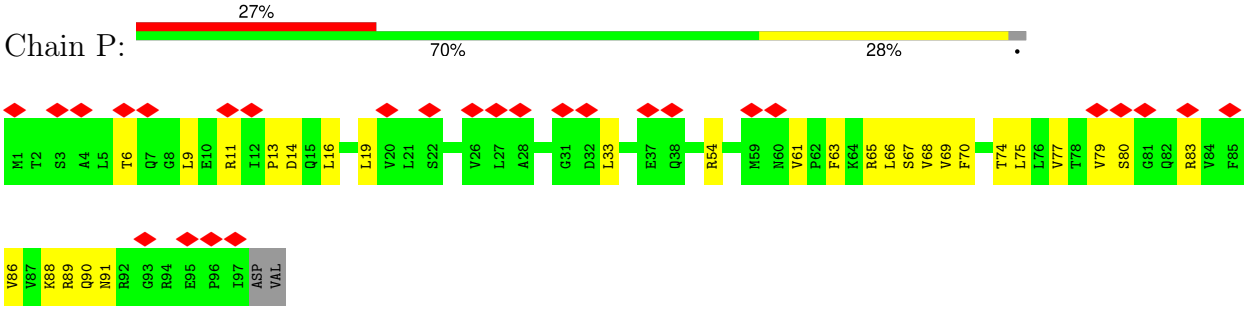
• Molecule 6: Ragulator complex protein LAMTOR4

Chain I:



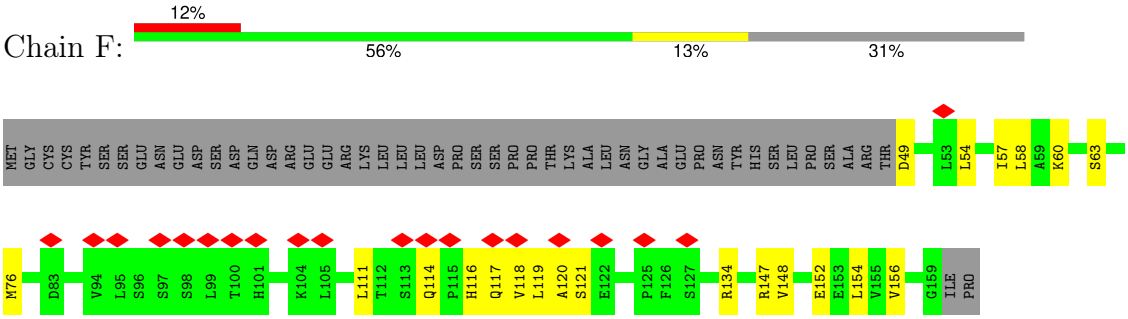
- Molecule 6: Ragulator complex protein LAMTOR4

Chain P:



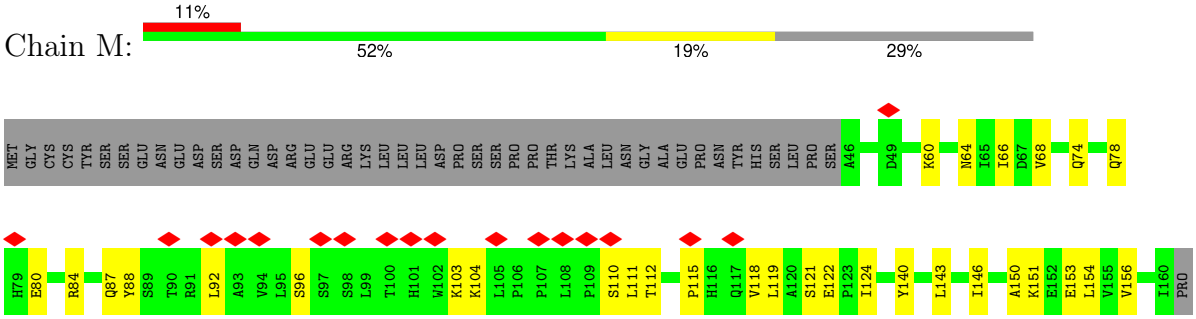
- Molecule 7: Ragulator complex protein LAMTOR1

Chain F:



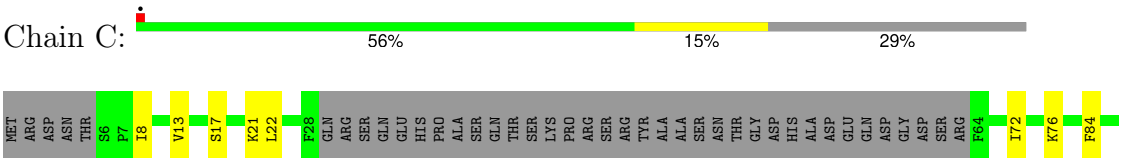
- Molecule 7: Ragulator complex protein LAMTOR1

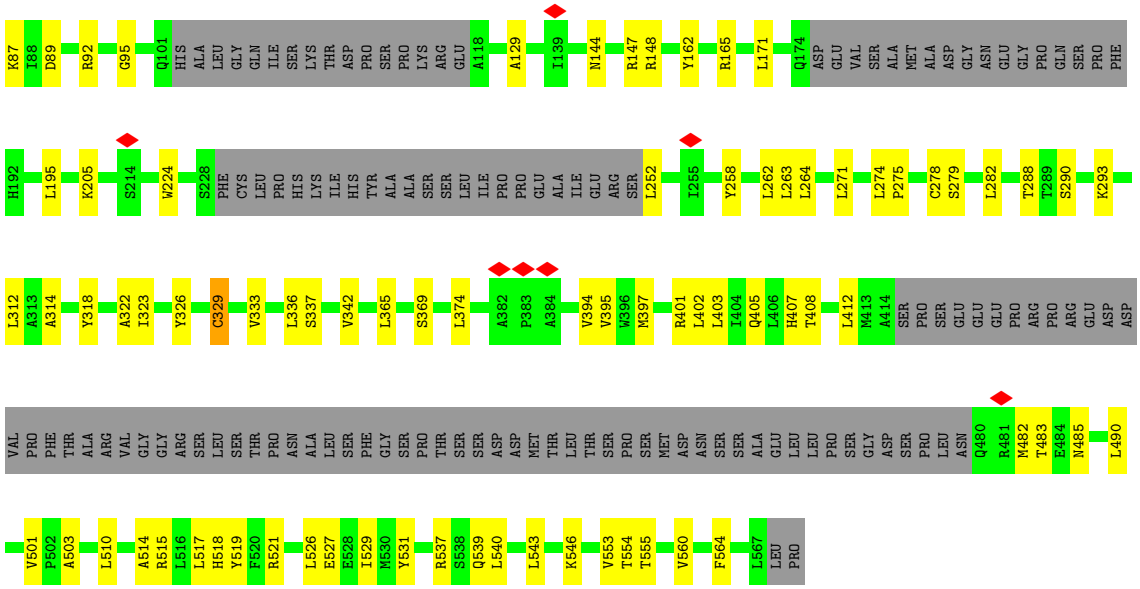
Chain M:



- Molecule 8: GATOR complex protein NPRL3

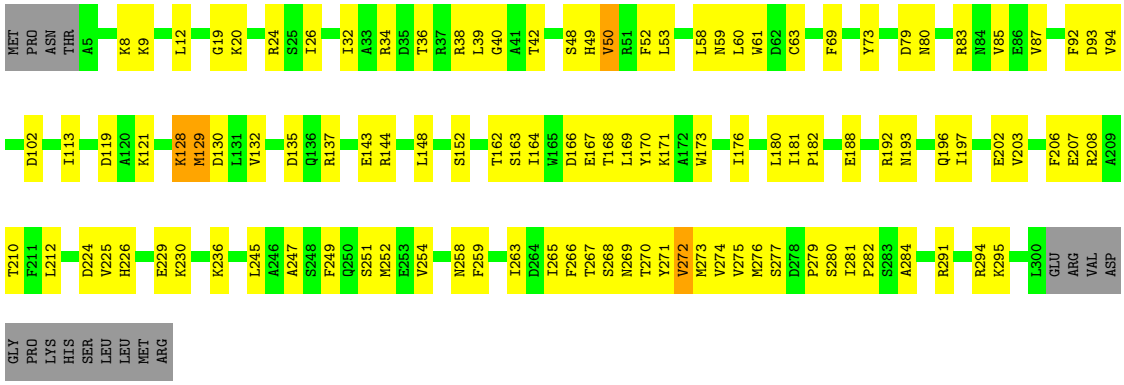
Chain C:





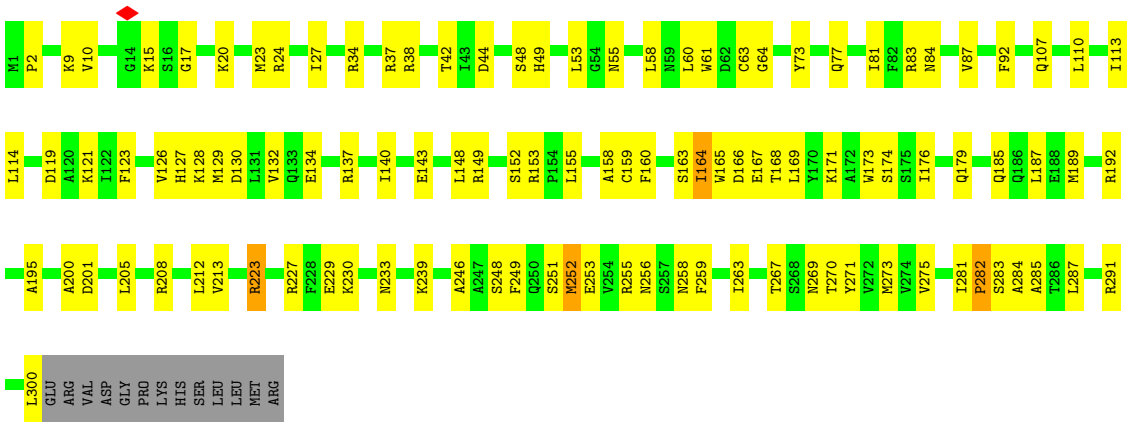
- Molecule 9: Ras-related GTP-binding protein A

Chain D:



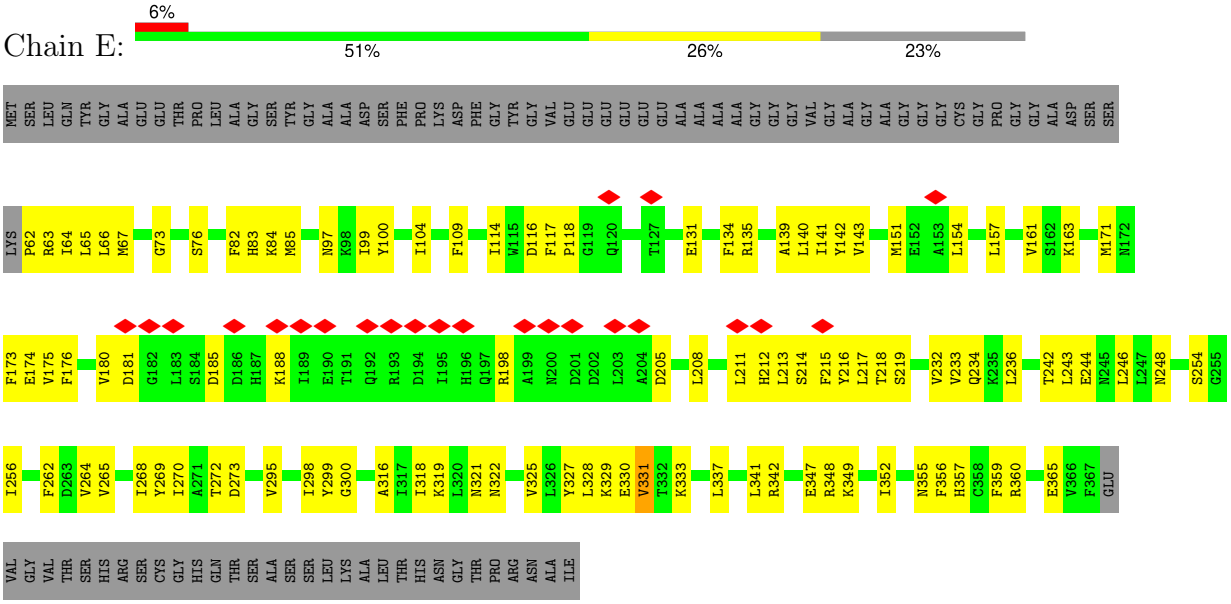
- Molecule 9: Ras-related GTP-binding protein A

Chain K:



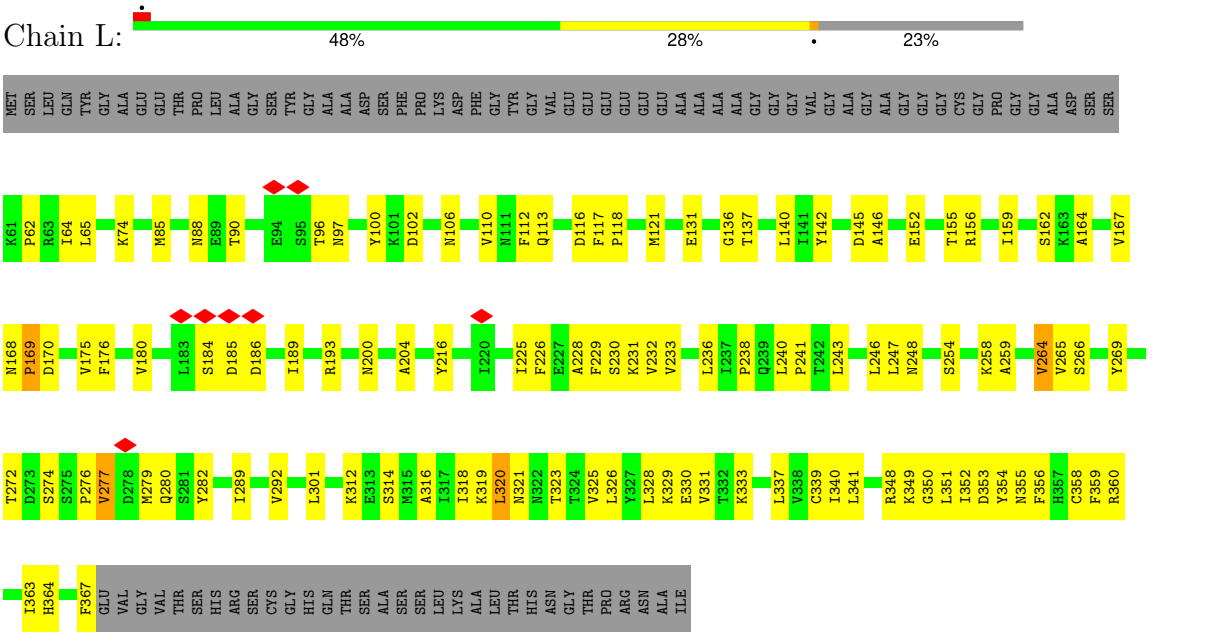
• Molecule 10: Ras-related GTP-binding protein C

Chain E:



• Molecule 11: Ras-related GTP-binding protein C

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56117	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 ($e^-/Å^2$)	52.6	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.763	Depositor
Minimum map value	-0.291	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	381.8, 381.8, 381.8	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, AF3

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	B	0.36	0/2977	0.81	4/4034 (0.1%)
2	A	0.39	0/8337	0.81	13/11305 (0.1%)
3	H	0.29	0/956	0.72	0/1297
3	O	0.28	0/951	0.70	0/1290
4	G	0.35	0/955	0.90	0/1293
4	N	0.34	0/947	0.83	1/1283 (0.1%)
5	J	0.29	0/678	0.76	0/919
5	Q	0.28	0/672	0.68	2/911 (0.2%)
6	I	0.29	0/654	0.71	0/883
6	P	0.25	0/747	0.65	2/1008 (0.2%)
7	F	0.26	0/877	0.63	0/1192
7	M	0.24	0/908	0.59	0/1234
8	C	0.29	0/3306	0.69	0/4483
9	D	0.37	0/2474	0.88	4/3331 (0.1%)
9	K	0.37	0/2505	0.86	3/3374 (0.1%)
10	E	0.36	0/2523	0.87	0/3407
11	L	0.36	0/2541	0.89	2/3431 (0.1%)
All	All	0.35	0/33008	0.80	31/44675 (0.1%)

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
1	B	0	7
2	A	0	6
4	N	0	2
5	J	0	1
7	M	0	1
8	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	D	0	3
9	K	0	3
10	E	0	5
11	L	0	7
All	All	0	36

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	413	GLN	CA-C-N	7.48	135.82	121.54
2	A	413	GLN	C-N-CA	7.48	135.82	121.54
2	A	369	MET	CB-CG-SD	6.58	132.45	112.70
2	A	266	GLU	CA-CB-CG	6.42	126.95	114.10
2	A	114	MET	CB-CG-SD	6.14	131.11	112.70
9	D	93	ASP	CA-C-N	-6.01	116.83	122.66
9	D	93	ASP	C-N-CA	-6.01	116.83	122.66
9	K	53	LEU	CA-CB-CG	6.00	137.29	116.30
5	Q	59	PRO	N-CD-CG	-5.97	94.24	103.20
2	A	414	LEU	N-CA-C	5.89	123.35	110.80
4	N	49	ILE	CG1-CB-CG2	-5.84	93.19	110.70
5	Q	59	PRO	CA-N-CD	-5.62	104.14	112.00
1	B	319	MET	CA-CB-CG	5.58	125.25	114.10
9	D	128	LYS	CA-C-N	-5.38	113.31	122.56
9	D	128	LYS	C-N-CA	-5.38	113.31	122.56
9	K	164	ILE	CB-CA-C	5.32	119.17	111.88
6	P	13	PRO	CA-C-N	5.31	131.69	121.54
6	P	13	PRO	C-N-CA	5.31	131.69	121.54
2	A	128	ILE	CA-C-N	5.30	129.93	122.46
2	A	128	ILE	C-N-CA	5.30	129.93	122.46
2	A	44	PRO	CA-C-N	5.27	129.82	122.08
2	A	44	PRO	C-N-CA	5.27	129.82	122.08
11	L	277	VAL	CA-C-N	5.25	131.57	121.54
11	L	277	VAL	C-N-CA	5.25	131.57	121.54
2	A	1214	LEU	CA-CB-CG	5.15	134.32	116.30
1	B	319	MET	CB-CG-SD	5.08	127.94	112.70
1	B	17	PRO	CA-C-N	5.08	131.24	121.54
1	B	17	PRO	C-N-CA	5.08	131.24	121.54
2	A	991	GLU	N-CA-CB	5.05	118.62	110.40
2	A	177	MET	CB-CG-SD	-5.02	97.65	112.70
9	K	252	MET	CB-CG-SD	5.00	127.71	112.70

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	258	VAL	Peptide
2	A	264	ARG	Peptide
2	A	297	ASP	Peptide
2	A	377	VAL	Peptide
2	A	381	LYS	Peptide
2	A	740	VAL	Peptide
1	B	23	ILE	Peptide
1	B	235	LEU	Peptide
1	B	267	TYR	Peptide
1	B	27	VAL	Peptide
1	B	28	PRO	Peptide
1	B	78	ARG	Peptide
1	B	79	ASN	Peptide
8	C	329	CYS	Peptide
9	D	129	MET	Peptide
9	D	272	VAL	Peptide
9	D	50	VAL	Peptide
10	E	171	MET	Peptide
10	E	269	TYR	Peptide
10	E	330	GLU	Peptide
10	E	331	VAL	Peptide
10	E	342	ARG	Peptide
5	J	2	GLU	Peptide
9	K	223	ARG	Peptide
9	K	249	PHE	Peptide
9	K	258	ASN	Peptide
11	L	117	PHE	Peptide
11	L	169	PRO	Peptide
11	L	170	ASP	Peptide
11	L	226	PHE	Peptide
11	L	264	VAL	Peptide
11	L	320	LEU	Peptide
11	L	333	LYS	Peptide
7	M	151	LYS	Peptide
4	N	86	ARG	Peptide
4	N	87	VAL	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	B	2918	0	2945	74	0
2	A	8120	0	7898	159	0
3	H	939	0	963	24	0
3	O	934	0	958	21	0
4	G	944	0	955	42	0
4	N	936	0	943	41	0
5	J	672	0	670	14	0
5	Q	666	0	666	17	0
6	I	647	0	657	19	0
6	P	738	0	753	23	0
7	F	861	0	858	21	0
7	M	892	0	894	22	0
8	C	3242	0	3342	56	0
9	D	2429	0	2423	91	0
9	K	2459	0	2458	80	0
10	E	2471	0	2444	78	0
11	L	2488	0	2461	80	0
12	D	28	0	10	3	0
12	E	28	0	12	2	0
12	K	28	0	12	3	0
13	D	4	0	0	0	0
13	E	4	0	0	0	0
13	K	4	0	0	2	0
All	All	32452	0	32322	774	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 12.

All (774) 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)
2:A:9:LEU:O	2:A:82:TYR:HA	1.10	1.25
2:A:9:LEU:O	2:A:82:TYR:CA	2.07	1.02
11:L:152:GLU:O	11:L:156:ARG:HB2	1.62	0.99
9:K:255:ARG:O	11:L:314:SER:HA	1.63	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1508:THR:O	2:A:1551:ASN:HB2	1.66	0.95
2:A:1204:CYS:HA	2:A:1258:TYR:O	1.67	0.93
2:A:942:TRP:HB2	2:A:1390:TRP:O	1.71	0.90
10:E:66:LEU:HA	10:E:141:ILE:O	1.73	0.89
2:A:866:LYS:O	2:A:869:MET:HB2	1.75	0.85
11:L:102:ASP:O	11:L:106:ASN:HB2	1.77	0.85
11:L:164:ALA:O	11:L:168:ASN:HB2	1.77	0.84
4:N:113:VAL:O	4:N:117:GLU:HB2	1.79	0.83
8:C:84:PHE:HB3	8:C:95:GLY:O	1.80	0.81
8:C:539:GLN:O	8:C:543:LEU:HB2	1.81	0.81
2:A:1483:VAL:O	2:A:1502:TYR:HA	1.82	0.79
10:E:212:HIS:HE2	10:E:214:SER:HG	1.28	0.78
10:E:356:PHE:O	10:E:360:ARG:HB2	1.84	0.78
8:C:408:THR:HA	8:C:554:THR:O	1.85	0.77
5:Q:64:VAL:HA	5:Q:76:ILE:O	1.86	0.75
10:E:141:ILE:HA	10:E:174:GLU:O	1.88	0.73
2:A:343:PHE:O	2:A:380:PHE:HA	1.89	0.73
10:E:176:PHE:HA	10:E:216:TYR:O	1.89	0.72
9:D:69:PHE:O	9:D:73:TYR:HB2	1.89	0.72
7:M:92:LEU:O	7:M:96:SER:HB3	1.89	0.71
2:A:41:ILE:HA	2:A:86:TYR:O	1.91	0.70
3:H:24:VAL:HA	3:H:89:VAL:O	1.92	0.70
5:Q:74:ILE:HA	5:Q:86:VAL:O	1.92	0.70
2:A:1373:TYR:HB2	2:A:1387:LYS:O	1.91	0.69
2:A:215:GLU:HG3	2:A:328:ARG:HE	1.57	0.69
2:A:1572:LEU:O	2:A:1576:PHE:HB2	1.92	0.68
8:C:252:LEU:N	8:C:318:TYR:HH	1.93	0.67
9:K:283:SER:O	9:K:287:LEU:HB2	1.95	0.67
2:A:1439:LEU:O	2:A:1548:TRP:HB3	1.94	0.66
3:O:99:ASN:HB3	3:O:102:LEU:HB2	1.77	0.66
2:A:1565:ASP:H	2:A:1568:PHE:HB3	1.59	0.66
4:G:25:LEU:HD13	4:G:50:SER:HB2	1.76	0.66
11:L:258:LYS:HB2	11:L:340:ILE:HG12	1.78	0.66
9:D:247:ALA:HA	10:E:321:ASN:HB2	1.78	0.66
10:E:355:ASN:O	10:E:359:PHE:HB3	1.96	0.66
4:N:81:ARG:HH12	4:N:102:PHE:HA	1.60	0.66
11:L:316:ALA:HB3	11:L:328:LEU:HB3	1.78	0.65
9:D:230:LYS:HD2	10:E:298:ILE:HD13	1.79	0.65
4:N:49:ILE:HA	11:L:350:GLY:HA3	1.79	0.64
9:K:205:LEU:HA	9:K:271:TYR:O	1.97	0.64
8:C:87:LYS:HB2	8:C:92:ARG:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:252:MET:HB2	9:K:263:ILE:HB	1.80	0.64
9:K:83:ARG:HD2	9:K:84:ASN:HB2	1.78	0.64
1:B:227:LEU:O	1:B:231:GLY:N	2.32	0.63
4:G:6:ALA:HB1	7:F:154:LEU:HD22	1.81	0.63
2:A:1390:TRP:HB2	2:A:1393:VAL:HG21	1.79	0.63
9:D:254:VAL:HG11	10:E:295:VAL:HG11	1.79	0.63
10:E:175:VAL:O	10:E:215:PHE:HA	1.98	0.63
4:N:22:SER:HB3	4:N:95:TYR:HB2	1.80	0.62
9:K:256:ASN:HB3	9:K:259:PHE:HB3	1.79	0.62
1:B:51:GLN:HA	1:B:68:PRO:HG2	1.81	0.62
9:D:251:SER:HB2	10:E:319:LYS:HB2	1.82	0.62
2:A:24:VAL:HB	2:A:68:SER:HB3	1.82	0.62
2:A:111:ARG:HA	2:A:114:MET:HE2	1.81	0.62
10:E:180:VAL:HG11	10:E:217:LEU:HB2	1.80	0.62
2:A:860:PHE:HB2	2:A:875:TYR:HB2	1.82	0.62
10:E:349:LYS:HA	10:E:352:ILE:HB	1.82	0.61
9:D:203:VAL:HG22	9:D:274:VAL:HG12	1.82	0.61
9:D:206:PHE:O	9:D:270:THR:OG1	2.17	0.61
11:L:320:LEU:O	11:L:323:THR:N	2.34	0.61
2:A:770:TYR:HA	2:A:876:LEU:O	2.01	0.61
3:H:24:VAL:HG11	3:H:117:LEU:HD21	1.82	0.61
8:C:275:PRO:HG2	8:C:278:CYS:HB2	1.83	0.61
8:C:543:LEU:HA	8:C:546:LYS:HD2	1.81	0.61
11:L:247:LEU:HD12	11:L:363:ILE:HG21	1.82	0.61
3:H:102:LEU:HD22	5:J:47:VAL:HG21	1.83	0.60
2:A:303:GLN:O	2:A:305:ASN:ND2	2.35	0.60
4:N:17:THR:O	4:N:108:LYS:NZ	2.34	0.60
2:A:775:TYR:HB2	2:A:872:VAL:HB	1.83	0.60
2:A:107:GLN:NE2	2:A:138:ARG:O	2.34	0.60
8:C:195:LEU:HD22	8:C:205:LYS:HD2	1.83	0.60
2:A:945:ARG:NH2	2:A:1501:GLN:OE1	2.34	0.60
8:C:501:VAL:HG12	8:C:503:ALA:H	1.64	0.60
3:H:21:ALA:HB3	3:H:93:ILE:HB	1.82	0.60
11:L:259:ALA:HA	11:L:339:CYS:HA	1.83	0.60
9:D:87:VAL:HG12	9:D:121:LYS:HG3	1.82	0.60
3:H:28:ASP:HB2	7:F:76:MET:HE3	1.84	0.60
11:L:274:SER:HA	11:L:277:VAL:HB	1.84	0.60
4:N:51:SER:OG	11:L:349:LYS:N	2.34	0.60
5:Q:64:VAL:HB	6:P:69:VAL:HB	1.84	0.60
9:K:27:ILE:HD11	9:K:212:LEU:HD21	1.83	0.59
4:N:118:GLU:HG2	4:N:119:PRO:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:289:ILE:HA	11:L:292:VAL:HG12	1.83	0.59
2:A:260:GLN:NE2	2:A:1435:LEU:O	2.36	0.59
8:C:329:CYS:SG	8:C:537:ARG:NH1	2.75	0.59
2:A:406:SER:HB2	2:A:742:VAL:HA	1.84	0.59
2:A:106:ASP:OD1	2:A:328:ARG:NH1	2.36	0.59
4:N:16:ASN:ND2	4:N:36:SER:O	2.35	0.59
9:D:266:PHE:HB2	9:D:272:VAL:HG22	1.85	0.58
2:A:885:GLN:HA	2:A:908:PHE:O	2.02	0.58
9:D:245:LEU:O	10:E:322:ASN:ND2	2.36	0.58
9:D:270:THR:OG1	9:D:271:TYR:N	2.35	0.58
9:K:248:SER:H	11:L:321:ASN:HB3	1.68	0.58
4:G:13:GLN:O	5:J:1:MET:N	2.36	0.58
9:D:49:HIS:HA	9:D:58:LEU:O	2.04	0.58
9:D:291:ARG:O	9:D:295:LYS:NZ	2.37	0.58
9:K:129:MET:HB3	9:K:137:ARG:HG2	1.84	0.58
8:C:515:ARG:O	8:C:518:HIS:NE2	2.37	0.58
4:N:102:PHE:HB2	5:Q:30:ASN:H	1.68	0.58
11:L:228:ALA:HA	11:L:231:LYS:HD2	1.86	0.57
9:D:32:ILE:HG21	9:D:34:ARG:HH21	1.70	0.57
9:K:223:ARG:HD3	9:K:227:ARG:HE	1.69	0.57
11:L:318:ILE:HB	11:L:326:LEU:HB2	1.85	0.57
10:E:84:LYS:HG3	10:E:264:VAL:HG12	1.86	0.57
3:O:72:ILE:HG23	3:O:81:VAL:HG22	1.87	0.57
4:N:73:ILE:HD12	4:N:84:ILE:HB	1.85	0.57
2:A:772:GLU:OE2	9:K:38:ARG:NH1	2.38	0.57
1:B:174:VAL:HB	1:B:235:LEU:O	2.05	0.57
10:E:141:ILE:HG12	10:E:174:GLU:HB3	1.86	0.57
2:A:44:PRO:HD3	2:A:85:VAL:HG12	1.86	0.57
10:E:185:ASP:HA	10:E:188:LYS:HD2	1.87	0.57
6:P:77:VAL:HG13	6:P:86:VAL:HG22	1.87	0.57
2:A:41:ILE:HG12	2:A:87:VAL:HG22	1.87	0.57
9:D:276:MET:HG3	9:D:279:PRO:HD2	1.87	0.57
1:B:121:MET:O	1:B:125:LYS:NZ	2.38	0.56
2:A:1583:ARG:NH1	2:A:1584:ASP:OD2	2.37	0.56
4:G:93:MET:HE1	4:G:107:LYS:HB3	1.86	0.56
9:D:266:PHE:H	9:D:271:TYR:HA	1.70	0.56
3:O:75:TYR:HA	4:N:70:LEU:HA	1.86	0.56
11:L:258:LYS:HE3	11:L:274:SER:HB2	1.87	0.56
1:B:379:TRP:HB2	8:C:369:SER:HB2	1.86	0.56
2:A:356:ARG:NH1	2:A:909:SER:O	2.39	0.56
11:L:352:ILE:O	11:L:356:PHE:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:LEU:HB2	1:B:318:LEU:HD13	1.87	0.56
2:A:308:GLU:O	2:A:312:LEU:HB2	2.05	0.56
2:A:319:LYS:NZ	2:A:1427:PRO:O	2.38	0.56
6:I:76:LEU:HB2	6:I:89:ARG:HH21	1.71	0.56
8:C:560:VAL:O	8:C:564:PHE:HB2	2.04	0.56
9:D:258:ASN:ND2	10:E:299:TYR:O	2.39	0.56
6:P:89:ARG:NH1	7:M:119:LEU:O	2.37	0.56
9:D:252:MET:HG3	9:D:263:ILE:HD13	1.87	0.56
2:A:170:MET:HG2	2:A:215:GLU:HB2	1.88	0.56
2:A:782:ASP:HB3	2:A:786:ARG:HH12	1.70	0.56
10:E:254:SER:OG	10:E:355:ASN:ND2	2.33	0.56
8:C:483:THR:HG23	8:C:510:LEU:HD22	1.87	0.56
9:K:121:LYS:NZ	9:K:179:GLN:O	2.34	0.56
3:O:96:SER:O	5:Q:27:GLN:NE2	2.39	0.56
1:B:6:ARG:N	1:B:140:ASN:OD1	2.39	0.56
11:L:247:LEU:HG	11:L:359:PHE:HE2	1.71	0.56
1:B:263:ALA:O	1:B:267:TYR:HB3	2.05	0.55
4:G:80:ARG:NH1	4:G:99:VAL:O	2.39	0.55
1:B:278:LEU:O	1:B:282:PHE:HB2	2.06	0.55
2:A:317:PHE:O	2:A:320:HIS:ND1	2.40	0.55
4:G:43:ARG:HH22	9:D:280:SER:HB2	1.70	0.55
9:K:49:HIS:HA	9:K:60:LEU:H	1.72	0.55
9:K:44:ASP:O	9:K:73:TYR:OH	2.23	0.55
9:D:265:ILE:O	9:D:294:ARG:NH2	2.40	0.55
6:P:19:LEU:HB2	6:P:33:LEU:HB3	1.87	0.55
1:B:46:THR:OG1	1:B:47:LYS:N	2.38	0.55
3:H:73:CYS:O	3:H:79:GLN:HA	2.06	0.55
6:I:36:ASP:O	6:I:40:ALA:HB2	2.07	0.55
2:A:8:LYS:HB2	2:A:66:THR:HG22	1.87	0.55
9:D:8:LYS:NZ	9:D:180:LEU:O	2.40	0.55
5:Q:66:CYS:HA	5:Q:74:ILE:O	2.05	0.55
9:K:148:LEU:O	9:K:152:SER:HB3	2.06	0.55
2:A:786:ARG:HE	2:A:928:ALA:HB3	1.70	0.55
2:A:1358:VAL:HG22	2:A:1401:MET:HE2	1.88	0.55
7:F:116:HIS:HA	7:F:119:LEU:HB2	1.87	0.55
10:E:331:VAL:HB	10:E:360:ARG:HE	1.71	0.55
9:K:17:GLY:N	12:K:501:GDP:O3B	2.40	0.55
9:K:149:ARG:NH2	9:K:159:CYS:SG	2.80	0.55
1:B:21:PRO:HG2	1:B:41:GLN:HG3	1.87	0.55
2:A:991:GLU:HB2	2:A:996:ILE:HB	1.89	0.55
9:D:166:ASP:HB2	9:D:168:THR:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:65:ARG:NH1	7:M:121:SER:OG	2.40	0.55
2:A:219:VAL:HA	2:A:257:VAL:HA	1.88	0.55
10:E:328:LEU:HA	10:E:337:LEU:O	2.07	0.55
11:L:229:PHE:HA	11:L:232:VAL:HG22	1.89	0.55
2:A:1420:LEU:HB3	2:A:1423:PRO:HB3	1.89	0.54
8:C:408:THR:HG23	8:C:553:VAL:HG13	1.90	0.54
9:D:208:ARG:NH1	9:D:268:SER:O	2.41	0.54
10:E:97:ASN:HA	10:E:118:PRO:HG3	1.90	0.54
11:L:64:ILE:HB	11:L:112:PHE:HE1	1.73	0.54
2:A:27:PRO:HB3	2:A:58:LEU:HD13	1.90	0.54
2:A:249:ARG:NH2	2:A:302:ALA:O	2.40	0.54
3:O:17:GLU:OE2	5:Q:51:GLN:NE2	2.40	0.54
2:A:42:ALA:HB3	2:A:86:TYR:HB2	1.89	0.54
2:A:949:LEU:O	2:A:1415:LEU:N	2.39	0.54
9:K:166:ASP:OD2	9:K:168:THR:OG1	2.25	0.54
5:J:68:GLU:O	6:I:64:LYS:N	2.40	0.54
8:C:290:SER:HB3	8:C:293:LYS:HB2	1.90	0.54
9:D:24:ARG:HH21	9:D:42:THR:HG21	1.72	0.54
9:D:53:LEU:HD12	9:D:181:ILE:HG12	1.89	0.54
8:C:526:LEU:HD11	8:C:540:LEU:HD22	1.90	0.54
9:K:2:PRO:O	9:K:55:ASN:ND2	2.40	0.54
4:G:31:LEU:HD23	9:D:282:PRO:HG3	1.90	0.54
6:I:65:ARG:HH12	7:F:121:SER:HB2	1.73	0.54
9:D:166:ASP:OD1	9:D:166:ASP:N	2.36	0.53
9:D:171:LYS:HE3	9:D:225:VAL:HG11	1.90	0.53
7:M:60:LYS:NZ	7:M:64:ASN:OD1	2.41	0.53
9:K:189:MET:HA	9:K:192:ARG:HB3	1.90	0.53
2:A:97:LEU:HD21	2:A:100:VAL:HB	1.89	0.53
8:C:374:LEU:HD11	8:C:394:VAL:HG21	1.90	0.53
6:P:70:PHE:O	6:P:91:ASN:ND2	2.41	0.53
9:K:283:SER:O	9:K:287:LEU:CB	2.57	0.53
2:A:175:ILE:HD13	2:A:336:ILE:HG13	1.90	0.53
2:A:920:TYR:HE1	2:A:932:ASP:HB2	1.73	0.53
4:N:27:ASN:ND2	4:N:29:GLU:OE1	2.41	0.53
5:Q:55:LEU:HD22	6:P:75:LEU:HD12	1.90	0.53
9:K:48:SER:OG	9:K:49:HIS:N	2.41	0.53
9:K:121:LYS:HD3	9:K:179:GLN:HG3	1.90	0.53
9:K:208:ARG:HG3	9:K:269:ASN:HA	1.89	0.53
1:B:190:ASP:HB2	2:A:421:PRO:HD2	1.89	0.53
1:B:199:TYR:O	1:B:204:ARG:NH1	2.42	0.53
2:A:1510:PHE:HB2	2:A:1549:ALA:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:19:GLY:HA2	12:D:501:GDP:H5"	1.89	0.53
9:D:69:PHE:O	9:D:73:TYR:CB	2.56	0.53
9:K:134:GLU:HA	9:K:137:ARG:HD2	1.91	0.53
10:E:234:GLN:HG3	10:E:268:ILE:HD11	1.90	0.53
2:A:11:ILE:HG12	2:A:74:THR:HG21	1.90	0.53
2:A:1209:GLU:O	2:A:1213:TRP:HB2	2.09	0.53
2:A:103:THR:O	2:A:105:LYS:NZ	2.42	0.53
4:N:33:LEU:HA	9:K:284:ALA:HB3	1.90	0.53
7:M:150:ALA:HB1	7:M:153:GLU:HG2	1.91	0.53
9:K:187:LEU:HD22	9:K:300:LEU:HD23	1.91	0.53
11:L:329:LYS:O	11:L:337:LEU:HB3	2.08	0.53
10:E:298:ILE:HG23	10:E:299:TYR:HD1	1.72	0.53
3:O:72:ILE:HB	4:N:74:LEU:HB2	1.90	0.53
1:B:380:LYS:HE2	8:C:342:VAL:H	1.74	0.52
9:K:126:VAL:HG13	9:K:129:MET:HE1	1.91	0.52
9:D:162:THR:HG23	9:D:169:LEU:HB3	1.91	0.52
3:O:13:LEU:HA	3:O:19:LEU:HD23	1.91	0.52
8:C:288:THR:O	8:C:293:LYS:NZ	2.40	0.52
6:P:65:ARG:NH2	7:M:122:GLU:O	2.42	0.52
9:K:130:ASP:OD1	9:K:130:ASP:N	2.38	0.52
2:A:36:GLY:N	2:A:55:VAL:O	2.40	0.52
2:A:299:SER:O	2:A:301:SER:N	2.42	0.52
9:D:63:CYS:HG	9:D:73:TYR:HH	1.56	0.52
9:D:166:ASP:OD2	9:D:168:THR:OG1	2.23	0.52
10:E:268:ILE:HG12	10:E:270:ILE:HG13	1.90	0.52
2:A:1556:LYS:NZ	2:A:1566:GLU:OE1	2.43	0.52
9:D:148:LEU:O	9:D:152:SER:HB3	2.10	0.52
10:E:316:ALA:HB3	10:E:328:LEU:HG	1.92	0.52
9:D:188:GLU:O	9:D:192:ARG:HB3	2.10	0.52
10:E:63:ARG:HB2	10:E:114:ILE:HG23	1.91	0.52
7:M:78:GLN:NE2	7:M:80:GLU:OE2	2.43	0.52
1:B:43:TYR:OH	8:C:72:ILE:O	2.25	0.52
5:J:22:LEU:HB3	5:J:85:ALA:HB3	1.92	0.52
9:D:48:SER:OG	9:D:49:HIS:N	2.41	0.52
11:L:88:ASN:ND2	11:L:265:VAL:O	2.42	0.52
2:A:1554:LEU:O	2:A:1559:ARG:NH1	2.43	0.52
10:E:131:GLU:HA	10:E:134:PHE:HB2	1.92	0.52
2:A:384:ASN:OD1	2:A:384:ASN:N	2.41	0.51
2:A:858:ARG:NH2	2:A:879:TYR:O	2.42	0.51
4:G:51:ASN:OD1	10:E:348:ARG:NH1	2.42	0.51
8:C:412:LEU:HB3	8:C:521:ARG:HH21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:56:TYR:HB3	4:G:69:LEU:HD11	1.93	0.51
9:D:12:LEU:HD11	9:D:60:LEU:HD12	1.92	0.51
10:E:318:ILE:O	10:E:325:VAL:HA	2.10	0.51
6:P:14:ASP:OD1	6:P:89:ARG:NE	2.43	0.51
2:A:12:HIS:NE2	2:A:21:ASP:O	2.36	0.51
2:A:1422:GLY:HA3	2:A:1431:TYR:HB3	1.92	0.51
2:A:1512:GLN:HB3	2:A:1547:ASN:HB2	1.92	0.51
10:E:273:ASP:OD1	10:E:273:ASP:N	2.44	0.51
3:O:19:LEU:HD11	3:O:92:PHE:HB3	1.92	0.51
2:A:284:LEU:HD12	2:A:285:VAL:HG23	1.92	0.51
9:D:163:SER:HB3	9:D:166:ASP:HB3	1.92	0.51
10:E:208:LEU:HD13	10:E:211:LEU:HD13	1.92	0.51
4:N:119:PRO:HG2	7:M:154:LEU:HD22	1.92	0.51
5:Q:69:SER:HB3	6:P:63:PHE:HA	1.91	0.51
1:B:144:ARG:NH2	1:B:159:VAL:O	2.44	0.51
2:A:937:GLU:HA	2:A:941:PHE:HE1	1.76	0.51
2:A:1240:ILE:HA	2:A:1259:LYS:O	2.10	0.51
1:B:327:GLN:HE22	1:B:351:TYR:HB2	1.74	0.51
1:B:327:GLN:NE2	1:B:328:LYS:O	2.39	0.51
2:A:1349:PRO:HD2	2:A:1352:ARG:HH21	1.75	0.51
8:C:8:ILE:N	8:C:129:ALA:O	2.44	0.51
11:L:230:SER:OG	11:L:269:TYR:O	2.28	0.51
1:B:283:GLN:HA	1:B:286:CYS:HB2	1.92	0.51
2:A:322:ILE:HG23	2:A:943:ARG:HH21	1.75	0.51
2:A:769:ASP:OD1	2:A:878:LYS:NZ	2.44	0.51
4:G:1:MET:N	9:D:197:ILE:O	2.44	0.51
4:N:55:ALA:HB3	11:L:348:ARG:HE	1.76	0.51
9:K:123:PHE:HD1	9:K:158:ALA:HB3	1.76	0.51
9:K:148:LEU:O	9:K:152:SER:CB	2.59	0.51
1:B:59:ALA:HB3	1:B:62:LYS:H	1.76	0.51
2:A:1311:PHE:HB3	2:A:1471:LEU:HB2	1.93	0.51
7:F:60:LYS:NZ	10:E:365:GLU:OE2	2.44	0.51
9:D:129:MET:SD	9:D:129:MET:N	2.84	0.51
10:E:234:GLN:HG2	10:E:270:ILE:HG23	1.92	0.51
7:M:74:GLN:NE2	7:M:80:GLU:OE2	2.43	0.51
11:L:142:TYR:HB2	11:L:175:VAL:HA	1.92	0.51
1:B:273:HIS:O	1:B:275:ARG:NH1	2.44	0.51
2:A:263:ARG:NH2	2:A:327:ASP:OD2	2.44	0.51
2:A:997:ARG:NH1	10:E:205:ASP:OD1	2.43	0.51
3:H:26:ASP:OD1	3:H:26:ASP:N	2.44	0.51
4:N:16:ASN:HA	4:N:20:VAL:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:115:PRO:HA	7:M:118:VAL:HG12	1.92	0.51
9:K:42:THR:N	12:K:501:GDP:O1B	2.41	0.51
9:K:256:ASN:HD21	11:L:312:LYS:HD2	1.76	0.51
3:H:85:ARG:NE	3:H:107:GLU:OE2	2.44	0.50
4:G:114:TYR:OH	7:F:152:GLU:O	2.30	0.50
2:A:372:GLN:NE2	2:A:739:THR:O	2.45	0.50
9:D:36:THR:HA	9:D:39:LEU:HD23	1.93	0.50
9:K:263:ILE:HG23	9:K:273:MET:HB3	1.91	0.50
2:A:281:TYR:HA	2:A:284:LEU:HG	1.92	0.50
1:B:171:GLU:HA	1:B:206:ILE:HD13	1.93	0.50
9:D:181:ILE:HD12	9:D:182:PRO:HD2	1.93	0.50
7:M:143:LEU:HA	7:M:146:ILE:HG13	1.93	0.50
3:H:85:ARG:HH11	3:H:118:ARG:HH22	1.59	0.50
4:G:72:ILE:O	4:G:82:ALA:HA	2.11	0.50
8:C:407:HIS:O	8:C:555:THR:HA	2.12	0.50
10:E:65:LEU:HA	10:E:67:MET:HE3	1.94	0.50
4:G:26:ASN:OD1	4:G:30:SER:N	2.45	0.50
6:I:51:CYS:O	6:I:54:ARG:NH2	2.44	0.50
7:F:116:HIS:O	7:F:120:ALA:HB2	2.12	0.50
1:B:54:LEU:HD11	1:B:99:GLU:HB3	1.94	0.50
2:A:1393:VAL:HG11	2:A:1398:LEU:HD22	1.94	0.50
10:E:329:LYS:O	10:E:360:ARG:NH2	2.45	0.50
11:L:258:LYS:HD3	11:L:340:ILE:HD11	1.93	0.50
2:A:132:VAL:N	2:A:139:ALA:O	2.45	0.50
2:A:174:PHE:O	2:A:335:VAL:HA	2.12	0.50
3:H:4:ASP:OD1	3:H:4:ASP:N	2.43	0.50
8:C:162:TYR:HD1	8:C:165:ARG:HD2	1.76	0.50
2:A:179:CYS:HB3	2:A:297:ASP:HB2	1.94	0.49
2:A:934:SER:OG	2:A:935:LEU:N	2.43	0.49
2:A:959:ILE:HA	2:A:963:GLU:H	1.77	0.49
3:H:102:LEU:HD12	5:J:44:VAL:HG22	1.93	0.49
8:C:397:MET:O	8:C:402:LEU:N	2.43	0.49
10:E:233:VAL:HG23	10:E:236:LEU:HD12	1.92	0.49
2:A:221:PHE:HA	2:A:254:PHE:O	2.12	0.49
2:A:254:PHE:HD2	2:A:285:VAL:HG22	1.77	0.49
9:D:207:GLU:OE1	9:D:210:THR:N	2.45	0.49
11:L:74:LYS:NZ	11:L:145:ASP:OD1	2.45	0.49
1:B:71:ILE:HD11	1:B:83:PHE:HE1	1.78	0.49
1:B:255:VAL:HG22	1:B:278:LEU:HD21	1.93	0.49
2:A:1449:LEU:HA	2:A:1456:LEU:HD13	1.93	0.49
4:G:32:LEU:HA	9:D:284:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:36:ASP:O	6:I:40:ALA:CB	2.60	0.49
9:K:61:TRP:HZ3	9:K:81:ILE:HG22	1.77	0.49
7:F:54:LEU:HA	7:F:57:ILE:HD12	1.94	0.49
4:N:83:ALA:HB3	4:N:94:MET:HB2	1.94	0.49
9:D:202:GLU:HB3	9:D:275:VAL:HB	1.93	0.49
10:E:82:PHE:HA	10:E:265:VAL:HG13	1.94	0.49
11:L:96:THR:OG1	11:L:97:ASN:N	2.46	0.49
5:J:61:ASP:OD1	6:I:71:GLY:N	2.44	0.49
2:A:948:LEU:HB3	2:A:1384:PHE:HB3	1.93	0.49
8:C:278:CYS:SG	8:C:279:SER:N	2.83	0.49
9:D:58:LEU:HD11	9:D:180:LEU:HD21	1.94	0.49
10:E:104:ILE:HG21	10:E:265:VAL:HG21	1.95	0.49
11:L:240:LEU:HB2	11:L:243:LEU:HB3	1.94	0.49
9:K:10:VAL:HG11	9:K:58:LEU:HD23	1.95	0.49
9:K:23:MET:HB2	9:K:169:LEU:HD11	1.95	0.49
1:B:123:GLU:O	1:B:127:LYS:NZ	2.44	0.49
1:B:173:ASP:HA	1:B:236:VAL:HA	1.95	0.49
2:A:35:LEU:HD22	2:A:57:SER:HA	1.94	0.49
2:A:61:ASP:OD1	2:A:61:ASP:N	2.46	0.49
9:D:94:VAL:HG22	9:D:128:LYS:HB2	1.93	0.49
2:A:920:TYR:O	2:A:924:TYR:HB2	2.13	0.49
7:F:49:ASP:OD1	7:F:49:ASP:N	2.45	0.49
9:D:143:GLU:OE1	9:D:144:ARG:NE	2.44	0.49
9:K:205:LEU:HD11	9:K:270:THR:HB	1.94	0.49
11:L:331:VAL:HG11	11:L:364:HIS:HB2	1.95	0.49
9:D:26:ILE:O	9:D:236:LYS:NZ	2.42	0.48
2:A:26:ASN:HB2	2:A:62:LEU:HD12	1.95	0.48
2:A:337:THR:OG1	2:A:366:LEU:O	2.30	0.48
4:G:68:ASN:OD1	4:G:70:LYS:NZ	2.47	0.48
6:I:76:LEU:HD13	6:I:89:ARG:HE	1.78	0.48
2:A:23:LEU:HD21	2:A:67:ILE:HD11	1.95	0.48
9:D:275:VAL:HG12	9:D:277:SER:HB3	1.95	0.48
2:A:1350:GLU:O	2:A:1376:GLY:N	2.47	0.48
9:D:32:ILE:O	9:D:36:THR:OG1	2.25	0.48
4:N:54:TRP:O	4:N:58:ASP:N	2.46	0.48
1:B:346:THR:OG1	1:B:347:GLY:N	2.46	0.48
8:C:264:LEU:HD11	8:C:323:ILE:HG12	1.95	0.48
9:D:119:ASP:OD1	9:D:119:ASP:N	2.45	0.48
2:A:930:SER:OG	2:A:932:ASP:OD1	2.31	0.48
2:A:1228:ILE:HA	2:A:1231:MET:HG2	1.96	0.48
9:K:107:GLN:OE1	9:K:153:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:21:ASP:OD2	2:A:57:SER:OG	2.32	0.48
2:A:104:PHE:HB3	2:A:329:THR:HG21	1.94	0.48
4:G:86:VAL:HG23	4:G:89:LEU:HB2	1.95	0.48
7:F:116:HIS:O	7:F:120:ALA:CB	2.62	0.48
9:D:167:GLU:HG3	9:D:226:HIS:HB3	1.94	0.48
12:K:501:GDP:O2B	13:K:502:AF3:F3	2.22	0.48
11:L:360:ARG:HA	11:L:363:ILE:HG12	1.96	0.48
2:A:217:THR:O	2:A:217:THR:OG1	2.31	0.48
10:E:85:MET:SD	10:E:85:MET:N	2.87	0.48
2:A:1448:LEU:HD21	2:A:1587:LEU:HG	1.95	0.48
9:K:223:ARG:HB3	9:K:227:ARG:HG2	1.96	0.48
11:L:216:TYR:CG	11:L:225:ILE:HG23	2.49	0.48
3:H:115:GLU:OE2	3:H:118:ARG:NH2	2.47	0.47
4:G:119:LEU:HA	4:G:122:VAL:HG12	1.96	0.47
9:D:129:MET:HA	9:D:132:VAL:HG22	1.95	0.47
7:M:92:LEU:O	7:M:96:SER:CB	2.61	0.47
9:D:173:TRP:HA	9:D:176:ILE:HB	1.96	0.47
5:Q:41:HIS:NE2	6:P:54:ARG:O	2.43	0.47
6:P:79:VAL:H	7:M:111:LEU:HB2	1.78	0.47
9:K:119:ASP:OD1	9:K:119:ASP:N	2.47	0.47
2:A:863:VAL:HA	2:A:871:THR:O	2.14	0.47
2:A:978:ASP:O	2:A:982:LEU:HB2	2.14	0.47
4:N:106:LYS:HD2	5:Q:29:LEU:HD12	1.96	0.47
11:L:314:SER:OG	11:L:330:GLU:OE2	2.32	0.47
1:B:166:PRO:HB3	1:B:228:LEU:HD22	1.96	0.47
1:B:287:SER:O	1:B:300:ARG:NH1	2.46	0.47
2:A:376:ALA:HB3	2:A:379:LEU:HD23	1.96	0.47
2:A:1445:ILE:HD12	2:A:1448:LEU:HD12	1.96	0.47
4:G:33:ALA:HB1	9:D:281:ILE:HD12	1.97	0.47
5:J:74:ILE:HA	5:J:86:VAL:O	2.14	0.47
11:L:325:VAL:O	11:L:341:LEU:N	2.47	0.47
1:B:263:ALA:O	1:B:267:TYR:CB	2.63	0.47
2:A:1436:ARG:HA	2:A:1436:ARG:HD2	1.71	0.47
3:H:31:PRO:HB3	3:H:34:LYS:HE3	1.96	0.47
4:G:106:ALA:O	7:F:147:ARG:NH1	2.47	0.47
8:C:258:TYR:HB2	8:C:326:TYR:HE1	1.79	0.47
9:D:279:PRO:HG2	9:D:281:ILE:HG12	1.96	0.47
3:O:66:SER:OG	3:O:67:LYS:N	2.47	0.47
9:K:110:LEU:HA	9:K:113:ILE:HG22	1.96	0.47
1:B:105:LEU:HD13	1:B:157:LEU:HD21	1.97	0.47
1:B:191:LEU:HA	1:B:194:GLN:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:GLY:HA2	1:B:322:LEU:HD12	1.97	0.47
2:A:189:ASP:OD1	2:A:189:ASP:N	2.48	0.47
2:A:215:GLU:OE2	2:A:263:ARG:NH2	2.48	0.47
10:E:142:TYR:HB2	10:E:175:VAL:HG22	1.96	0.47
10:E:244:GLU:O	10:E:248:ASN:ND2	2.47	0.47
5:Q:66:CYS:HB2	6:P:67:SER:HB2	1.96	0.47
9:K:34:ARG:O	9:K:37:ARG:NH1	2.48	0.47
2:A:196:VAL:HA	2:A:200:LEU:HB2	1.96	0.47
9:D:79:ASP:OD1	9:D:79:ASP:N	2.47	0.47
9:D:273:MET:HE3	9:D:273:MET:HB3	1.72	0.47
10:E:243:LEU:HD12	10:E:246:LEU:HD22	1.97	0.47
4:N:32:LEU:HB3	9:K:282:PRO:HG2	1.97	0.47
6:P:16:LEU:HB2	6:P:88:LYS:HB3	1.96	0.47
1:B:208:LYS:O	1:B:212:GLU:CB	2.62	0.47
2:A:1575:ASP:OD1	2:A:1586:ARG:NH1	2.48	0.47
6:I:16:LEU:HB2	6:I:88:LYS:HB2	1.95	0.47
3:O:23:VAL:HG22	3:O:34:LYS:HG3	1.96	0.47
9:K:9:LYS:NZ	9:K:81:ILE:O	2.48	0.47
2:A:223:ARG:HH22	2:A:302:ALA:HB3	1.80	0.47
7:F:60:LYS:HA	7:F:63:SER:HB3	1.96	0.47
10:E:337:LEU:HB2	10:E:360:ARG:HH12	1.80	0.47
9:K:132:VAL:HG23	9:K:137:ARG:HG3	1.97	0.47
10:E:272:THR:OG1	10:E:273:ASP:N	2.48	0.46
9:K:123:PHE:CG	9:K:176:ILE:HG12	2.50	0.46
11:L:118:PRO:HB2	11:L:121:MET:HE1	1.97	0.46
1:B:32:ILE:HD12	1:B:37:PHE:HE2	1.80	0.46
2:A:36:GLY:HA2	2:A:54:GLN:HE21	1.80	0.46
2:A:1351:GLN:HE22	2:A:1387:LYS:HD2	1.81	0.46
4:G:102:GLY:N	5:J:30:ASN:O	2.47	0.46
9:D:92:PHE:HE1	9:D:102:ASP:HB3	1.80	0.46
4:N:3:LEU:HD21	4:N:119:PRO:HB3	1.95	0.46
4:N:52:ASN:HD21	7:M:66:ILE:HG21	1.80	0.46
11:L:65:LEU:HD11	11:L:113:GLN:HG2	1.97	0.46
11:L:137:THR:O	11:L:168:ASN:ND2	2.40	0.46
1:B:15:PHE:HB2	1:B:45:ILE:HG21	1.97	0.46
1:B:101:ILE:HG23	1:B:157:LEU:HD12	1.97	0.46
1:B:249:PRO:HD2	1:B:324:ARG:HH12	1.79	0.46
2:A:1232:GLN:OE1	2:A:1251:PHE:N	2.40	0.46
4:G:44:VAL:HG21	10:E:357:HIS:CG	2.51	0.46
4:G:116:GLU:O	4:G:120:THR:N	2.41	0.46
9:K:185:GLN:HB2	9:K:189:MET:HE1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:VAL:O	1:B:258:LYS:NZ	2.47	0.46
2:A:1543:ARG:NH1	2:A:1544:VAL:O	2.48	0.46
6:I:65:ARG:HD3	7:F:118:VAL:HB	1.97	0.46
11:L:159:ILE:O	11:L:162:SER:OG	2.32	0.46
11:L:353:ASP:OD1	11:L:353:ASP:N	2.47	0.46
1:B:37:PHE:HA	1:B:40:VAL:HG12	1.97	0.46
1:B:78:ARG:NH2	12:D:501:GDP:O3A	2.47	0.46
4:G:19:VAL:O	4:G:37:TYR:OH	2.29	0.46
10:E:140:LEU:HB3	10:E:173:PHE:HD1	1.79	0.46
11:L:100:TYR:HE1	11:L:367:PHE:HB3	1.81	0.46
10:E:331:VAL:H	10:E:360:ARG:HH21	1.64	0.46
5:Q:56:THR:OG1	5:Q:57:SER:N	2.49	0.46
1:B:207:GLN:HA	1:B:210:SER:HB3	1.97	0.46
2:A:1191:VAL:HG21	2:A:1210:VAL:HG22	1.98	0.46
6:I:89:ARG:NH1	7:F:119:LEU:O	2.49	0.46
10:E:151:MET:HE2	10:E:198:ARG:HH12	1.80	0.46
11:L:62:PRO:HG3	11:L:233:VAL:HG22	1.98	0.46
11:L:276:PRO:HA	11:L:280:GLN:HE22	1.81	0.46
2:A:97:LEU:HA	2:A:146:VAL:HG13	1.98	0.46
8:C:264:LEU:HG	8:C:322:ALA:HA	1.98	0.46
9:K:10:VAL:HG12	9:K:87:VAL:HB	1.97	0.46
9:K:253:GLU:OE2	9:K:283:SER:OG	2.29	0.46
1:B:186:ASN:OD1	1:B:194:GLN:NE2	2.41	0.46
2:A:314:PHE:HA	2:A:317:PHE:HB2	1.97	0.46
2:A:927:SER:O	2:A:930:SER:OG	2.29	0.46
2:A:1379:SER:HB3	2:A:1382:ALA:HB3	1.97	0.46
9:K:24:ARG:HA	9:K:27:ILE:HG22	1.98	0.46
9:K:201:ASP:N	9:K:275:VAL:O	2.49	0.46
9:D:207:GLU:HB3	9:D:212:LEU:H	1.82	0.45
3:O:16:VAL:HB	3:O:19:LEU:HD22	1.96	0.45
2:A:40:GLU:HB2	2:A:50:PRO:HB3	1.96	0.45
9:D:129:MET:HB2	9:D:137:ARG:HG2	1.97	0.45
3:O:32:VAL:HA	7:M:88:TYR:HB3	1.98	0.45
2:A:51:LEU:HB3	2:A:152:MET:HE3	1.97	0.45
2:A:300:THR:HG21	2:A:339:GLY:HA3	1.98	0.45
2:A:1444:ASN:OD1	2:A:1447:CYS:N	2.50	0.45
8:C:514:ALA:HA	8:C:517:LEU:HB2	1.98	0.45
5:J:69:SER:OG	5:J:71:ASN:OD1	2.29	0.45
8:C:365:LEU:O	8:C:369:SER:N	2.50	0.45
9:D:249:PHE:CZ	9:D:252:MET:HB2	2.51	0.45
9:K:63:CYS:O	13:K:502:AF3:F1	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:248:ASN:HD21	11:L:272:THR:HB	1.82	0.45
2:A:105:LYS:HB2	2:A:105:LYS:HE2	1.78	0.45
4:G:24:LEU:HD11	4:G:115:LEU:HD22	1.99	0.45
9:D:170:TYR:HB2	9:D:229:GLU:HB3	1.99	0.45
9:D:208:ARG:NH1	9:D:269:ASN:O	2.49	0.45
4:N:4:ARG:HH21	7:M:156:VAL:HG23	1.81	0.45
6:P:80:SER:O	6:P:83:ARG:HB2	2.16	0.45
7:M:110:SER:OG	7:M:112:THR:O	2.35	0.45
6:I:9:LEU:HD23	6:I:12:ILE:HD13	1.99	0.45
10:E:333:LYS:HB3	10:E:333:LYS:HE3	1.77	0.45
4:N:81:ARG:NH2	4:N:100:VAL:O	2.49	0.45
6:P:11:ARG:O	6:P:11:ARG:NH1	2.49	0.45
9:K:15:LYS:HA	9:K:15:LYS:HD3	1.80	0.45
11:L:146:ALA:HB2	11:L:180:VAL:HA	1.97	0.45
2:A:329:THR:OG1	2:A:330:GLY:N	2.49	0.45
2:A:967:ASP:OD1	2:A:967:ASP:N	2.43	0.45
7:F:114:GLN:HG3	7:F:117:GLN:H	1.81	0.45
9:D:193:ASN:OD1	9:D:196:GLN:NE2	2.50	0.45
10:E:99:ILE:HG23	10:E:117:PHE:HE1	1.82	0.45
10:E:161:VAL:HG21	10:E:213:LEU:HD21	1.98	0.45
3:O:113:LEU:HA	3:O:116:GLU:HG2	1.99	0.45
11:L:116:ASP:OD1	11:L:116:ASP:N	2.46	0.45
4:G:79:GLY:HA2	4:G:96:LYS:HA	1.99	0.45
5:J:22:LEU:HD11	5:J:42:ALA:HB2	1.99	0.45
10:E:62:PRO:HG2	10:E:109:PHE:HD1	1.82	0.45
10:E:73:GLY:N	12:E:501:GDP:O3B	2.49	0.45
3:O:12:LYS:O	3:O:15:SER:OG	2.33	0.45
4:G:122:VAL:HA	4:G:125:SER:HB3	1.99	0.45
8:C:17:SER:OG	9:D:80:ASN:O	2.35	0.45
8:C:21:LYS:HD2	8:C:171:LEU:HD13	1.99	0.45
9:D:79:ASP:O	9:D:83:ARG:HB2	2.17	0.45
10:E:262:PHE:HB3	10:E:268:ILE:O	2.17	0.45
5:Q:12:THR:HG22	5:Q:18:ILE:HG21	1.99	0.45
11:L:136:GLY:HA2	11:L:169:PRO:HG2	1.98	0.45
2:A:1368:GLU:OE2	2:A:1394:THR:N	2.44	0.44
4:G:93:MET:HE3	4:G:111:LEU:HD12	1.99	0.44
4:N:33:LEU:HG	9:K:285:ALA:HB2	1.99	0.44
6:P:6:THR:HA	6:P:9:LEU:HB2	1.99	0.44
11:L:184:SER:OG	11:L:185:ASP:N	2.47	0.44
1:B:121:MET:O	1:B:124:SER:OG	2.34	0.44
8:C:17:SER:OG	9:D:80:ASN:OD1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:100:TYR:HB3	10:E:116:ASP:HB3	2.00	0.44
10:E:131:GLU:O	10:E:135:ARG:NH1	2.50	0.44
4:N:113:VAL:O	4:N:117:GLU:CB	2.56	0.44
11:L:269:TYR:O	11:L:282:TYR:OH	2.35	0.44
1:B:16:HIS:CE1	1:B:19:LEU:HB2	2.52	0.44
7:F:134:ARG:HA	7:F:134:ARG:HD2	1.86	0.44
7:F:156:VAL:HG21	9:D:197:ILE:HB	1.98	0.44
8:C:262:LEU:HD11	8:C:395:VAL:HG13	1.99	0.44
9:D:224:ASP:OD2	9:D:226:HIS:ND1	2.47	0.44
4:N:90:LEU:HD12	4:N:120:LEU:HD23	1.98	0.44
11:L:243:LEU:HA	11:L:246:LEU:HG	1.97	0.44
1:B:254:LEU:O	1:B:261:GLN:NE2	2.42	0.44
2:A:1502:TYR:HB2	2:A:1511:LEU:HB3	2.00	0.44
3:H:81:VAL:HB	3:H:92:PHE:HB2	1.99	0.44
1:B:118:PHE:O	1:B:124:SER:OG	2.35	0.44
1:B:325:ARG:NH2	1:B:327:GLN:OE1	2.47	0.44
2:A:990:VAL:HG13	2:A:993:LEU:HD12	2.00	0.44
9:D:20:LYS:N	12:D:501:GDP:O2A	2.50	0.44
10:E:254:SER:HG	10:E:355:ASN:HD22	1.60	0.44
10:E:316:ALA:O	10:E:327:TYR:HA	2.18	0.44
4:N:125:ALA:HA	9:K:291:ARG:HD2	2.00	0.44
9:K:246:ALA:O	11:L:321:ASN:ND2	2.50	0.44
11:L:189:ILE:HG23	11:L:193:ARG:HH11	1.82	0.44
1:B:101:ILE:HG13	1:B:159:VAL:HG22	1.99	0.44
4:G:1:MET:HE2	7:F:156:VAL:HG23	1.99	0.44
5:J:49:ALA:HB1	5:J:78:LYS:HB3	1.99	0.44
6:I:55:LEU:HD13	6:I:62:PRO:HA	2.00	0.44
10:E:64:ILE:HB	10:E:140:LEU:HA	2.00	0.44
9:K:140:ILE:HA	9:K:143:GLU:HB3	2.00	0.44
11:L:85:MET:HE3	11:L:225:ILE:HD11	2.00	0.44
2:A:1184:MET:HE1	2:A:1191:VAL:H	1.82	0.44
3:H:114:PHE:HB3	3:H:118:ARG:HH21	1.81	0.44
9:D:59:ASN:HB3	9:D:61:TRP:HE1	1.83	0.44
4:N:41:THR:HG22	4:N:47:ALA:HB2	1.99	0.44
11:L:121:MET:SD	11:L:121:MET:N	2.91	0.44
11:L:131:GLU:HG2	11:L:167:VAL:HG11	1.98	0.44
2:A:25:VAL:HG21	2:A:33:ILE:HG21	2.00	0.44
9:K:171:LYS:HB2	9:K:229:GLU:HG2	1.99	0.44
2:A:96:THR:HG23	2:A:157:SER:HB3	2.00	0.43
2:A:798:VAL:HA	2:A:801:GLU:HG3	2.00	0.43
3:H:9:LEU:HB3	3:H:35:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:26:ASN:HA	4:G:89:LEU:HD22	2.00	0.43
4:G:44:VAL:HG11	10:E:357:HIS:HB2	2.00	0.43
10:E:355:ASN:O	10:E:359:PHE:CB	2.65	0.43
4:N:15:ALA:HB2	4:N:112:LEU:HD11	2.00	0.43
1:B:216:GLU:HB2	1:B:219:LEU:HD23	2.00	0.43
2:A:123:SER:O	2:A:123:SER:OG	2.32	0.43
9:D:130:ASP:OD1	9:D:130:ASP:N	2.43	0.43
9:K:163:SER:OG	9:K:164:ILE:N	2.51	0.43
1:B:37:PHE:O	1:B:41:GLN:NE2	2.51	0.43
1:B:189:TRP:CD1	2:A:423:ILE:HD11	2.53	0.43
1:B:208:LYS:O	1:B:212:GLU:HB3	2.18	0.43
2:A:893:CYS:SG	2:A:897:SER:OG	2.77	0.43
8:C:336:LEU:HD11	8:C:365:LEU:HD13	2.00	0.43
10:E:143:VAL:HA	10:E:176:PHE:O	2.19	0.43
10:E:256:ILE:HG13	10:E:341:LEU:HB3	2.00	0.43
4:N:22:SER:HA	4:N:37:GLY:HA3	1.99	0.43
11:L:62:PRO:HD2	11:L:236:LEU:HB2	2.00	0.43
4:G:59:ASN:O	4:G:63:ALA:N	2.52	0.43
6:I:82:GLN:HG3	6:I:83:ARG:HG3	2.00	0.43
9:D:259:PHE:HE2	10:E:300:GLY:HA2	1.82	0.43
3:O:12:LYS:HD2	3:O:12:LYS:HA	1.83	0.43
4:N:107:ALA:O	4:N:111:ALA:HB2	2.18	0.43
2:A:1504:HIS:ND1	2:A:1506:THR:OG1	2.37	0.43
5:J:4:THR:HA	5:J:7:GLN:HB2	1.99	0.43
9:D:266:PHE:O	9:D:294:ARG:NE	2.33	0.43
2:A:116:ARG:NH2	2:A:804:CYS:SG	2.77	0.43
3:H:117:LEU:HD12	3:H:120:VAL:HG21	2.00	0.43
8:C:13:VAL:HG22	8:C:22:LEU:HG	2.01	0.43
8:C:89:ASP:OD1	8:C:89:ASP:N	2.49	0.43
9:D:20:LYS:HG3	9:D:24:ARG:HH22	1.83	0.43
9:D:148:LEU:O	9:D:152:SER:CB	2.65	0.43
10:E:154:LEU:HD23	10:E:157:LEU:HD21	2.01	0.43
4:N:85:THR:OG1	4:N:86:ARG:N	2.52	0.43
1:B:9:CYS:SG	1:B:10:ILE:N	2.91	0.43
2:A:936:ILE:H	2:A:939:LEU:HD12	1.83	0.43
3:H:57:THR:HA	3:H:68:ASN:HD22	1.84	0.43
3:H:100:THR:N	5:J:27:GLN:O	2.51	0.43
8:C:337:SER:OG	8:C:401:ARG:O	2.35	0.43
10:E:63:ARG:HH22	10:E:232:VAL:HG12	1.84	0.43
9:K:251:SER:HB2	11:L:319:LYS:HB2	2.00	0.43
2:A:39:VAL:O	2:A:52:LEU:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:117:GLU:HG2	4:G:118:PRO:HD3	2.01	0.43
5:Q:67:LEU:HD12	5:Q:74:ILE:HD12	2.01	0.43
11:L:301:LEU:HD13	11:L:312:LYS:HE2	2.00	0.43
11:L:319:LYS:HD3	11:L:323:THR:HB	2.01	0.43
11:L:325:VAL:HG13	11:L:341:LEU:HB3	2.01	0.43
1:B:103:LYS:HA	1:B:103:LYS:HD2	1.84	0.43
1:B:124:SER:HA	1:B:127:LYS:HE2	2.00	0.43
2:A:947:LEU:HD23	2:A:1419:VAL:HG21	2.01	0.43
4:G:33:ALA:HA	9:D:281:ILE:HG23	2.01	0.43
6:I:54:ARG:HA	6:I:62:PRO:HG3	2.00	0.43
8:C:263:LEU:HD23	8:C:322:ALA:HB2	2.01	0.43
4:N:102:PHE:HB3	5:Q:29:LEU:HD22	2.00	0.43
6:P:54:ARG:HH22	6:P:61:VAL:HA	1.84	0.43
6:P:68:VAL:O	6:P:74:THR:HA	2.19	0.43
9:K:92:PHE:O	9:K:127:HIS:ND1	2.50	0.43
2:A:37:ASP:O	2:A:54:GLN:HA	2.19	0.42
2:A:950:PRO:HA	2:A:1414:PHE:HA	2.00	0.42
3:H:70:SER:O	4:G:75:ASP:HB3	2.18	0.42
8:C:333:VAL:O	8:C:405:GLN:HA	2.19	0.42
8:C:252:LEU:HG	8:C:314:ALA:HB1	2.01	0.42
8:C:258:TYR:HB3	8:C:531:TYR:CG	2.54	0.42
9:K:239:LYS:HA	9:K:239:LYS:HD2	1.78	0.42
4:G:22:THR:HG21	4:G:111:LEU:HD13	2.01	0.42
4:G:28:GLU:HG2	10:E:347:GLU:HG3	2.01	0.42
8:C:482:MET:HA	8:C:485:ASN:HB2	2.00	0.42
9:D:9:LYS:HE2	9:D:85:VAL:HG22	2.00	0.42
9:D:267:THR:OG1	9:D:270:THR:N	2.43	0.42
3:O:115:GLU:HA	3:O:118:ARG:HG2	2.00	0.42
9:K:263:ILE:HG23	9:K:273:MET:HE3	2.01	0.42
11:L:65:LEU:HD12	11:L:65:LEU:HA	1.92	0.42
2:A:1560:SER:N	2:A:1563:THR:OG1	2.53	0.42
11:L:100:TYR:HD2	11:L:102:ASP:H	1.66	0.42
11:L:186:ASP:OD1	11:L:186:ASP:N	2.51	0.42
2:A:797:GLN:HA	2:A:800:GLU:HB2	2.00	0.42
7:F:58:LEU:HD11	10:E:242:THR:HA	2.01	0.42
7:M:84:ARG:HA	7:M:87:GLN:HG2	2.02	0.42
11:L:90:THR:HA	11:L:110:VAL:HG22	2.01	0.42
2:A:344:GLU:HB2	2:A:381:LYS:HE3	2.02	0.42
2:A:953:VAL:HG22	2:A:1562:ALA:HB2	2.02	0.42
2:A:967:ASP:HB2	2:A:1479:ARG:NE	2.34	0.42
4:G:85:ARG:HA	4:G:89:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:75:LEU:HG	6:I:88:LYS:HD3	2.02	0.42
9:D:163:SER:OG	9:D:164:ILE:N	2.53	0.42
11:L:254:SER:HB2	11:L:356:PHE:HZ	1.84	0.42
11:L:325:VAL:N	11:L:341:LEU:O	2.53	0.42
1:B:82:LEU:HD12	1:B:82:LEU:HA	1.89	0.42
10:E:163:LYS:HE3	10:E:163:LYS:HB3	1.88	0.42
10:E:272:THR:OG1	10:E:273:ASP:OD1	2.37	0.42
7:M:103:LYS:HG3	7:M:104:LYS:HG3	2.01	0.42
9:K:114:LEU:HD21	9:K:155:LEU:HD22	2.02	0.42
1:B:74:LYS:HE3	9:D:38:ARG:HG2	2.02	0.42
6:I:43:ILE:HG23	6:I:77:VAL:HG21	2.02	0.42
8:C:148:ARG:HB3	8:C:224:TRP:HH2	1.84	0.42
6:P:66:LEU:HD12	6:P:66:LEU:HA	1.93	0.42
9:K:127:HIS:CD2	9:K:128:LYS:HB2	2.55	0.42
9:K:132:VAL:O	9:K:137:ARG:NE	2.53	0.42
9:K:227:ARG:HA	9:K:230:LYS:HD2	2.02	0.42
4:G:53:TRP:CG	4:G:90:LEU:HD11	2.55	0.42
3:O:23:VAL:HB	3:O:91:SER:O	2.20	0.42
11:L:355:ASN:HA	11:L:358:CYS:HB2	2.02	0.42
2:A:786:ARG:NH2	2:A:926:CYS:O	2.52	0.41
6:I:65:ARG:HA	7:F:111:LEU:HD23	2.01	0.41
8:C:527:GLU:O	8:C:531:TYR:HB2	2.20	0.41
9:D:85:VAL:HG11	9:D:113:ILE:HD11	2.01	0.41
9:K:130:ASP:OD2	9:K:165:TRP:NE1	2.49	0.41
1:B:42:VAL:O	1:B:47:LYS:NZ	2.45	0.41
2:A:109:ILE:HD13	2:A:137:ILE:HG23	2.02	0.41
3:H:71:ILE:HB	3:H:82:GLN:HB2	2.03	0.41
4:G:110:ALA:HB1	7:F:148:VAL:HG23	2.03	0.41
8:C:540:LEU:HD23	8:C:543:LEU:HD23	2.02	0.41
3:O:5:LEU:HD13	3:O:113:LEU:HD21	2.00	0.41
9:K:167:GLU:HB3	9:K:233:ASN:HB2	2.02	0.41
9:K:173:TRP:HA	9:K:176:ILE:HD12	2.02	0.41
9:K:195:ALA:O	9:K:200:ALA:N	2.53	0.41
11:L:102:ASP:O	11:L:106:ASN:CB	2.60	0.41
1:B:187:SER:OG	1:B:188:GLN:OE1	2.37	0.41
1:B:265:LEU:HD12	1:B:265:LEU:HA	1.92	0.41
2:A:945:ARG:HD3	2:A:1421:GLU:HA	2.03	0.41
3:H:60:GLY:HA2	3:H:63:LEU:HD12	2.02	0.41
6:I:54:ARG:HA	6:I:54:ARG:HD3	1.85	0.41
8:C:519:TYR:CG	8:C:529:ILE:HG12	2.55	0.41
9:D:50:VAL:HG22	9:D:58:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:63:LEU:HD13	4:N:82:VAL:HG21	2.01	0.41
6:P:16:LEU:HD12	6:P:88:LYS:HG2	2.02	0.41
6:P:69:VAL:HG11	7:M:124:ILE:HD13	2.01	0.41
4:G:37:TYR:O	4:G:40:THR:OG1	2.36	0.41
8:C:394:VAL:HA	8:C:403:LEU:HD12	2.02	0.41
10:E:181:ASP:OD1	10:E:181:ASP:N	2.51	0.41
1:B:108:TYR:CD2	1:B:155:ILE:HD13	2.55	0.41
3:H:19:LEU:HB2	3:H:103:ILE:HD11	2.02	0.41
9:D:263:ILE:HG23	9:D:273:MET:HB3	2.02	0.41
1:B:28:PRO:HG2	1:B:31:PHE:HZ	1.85	0.41
1:B:114:LEU:HD12	1:B:114:LEU:HA	1.91	0.41
1:B:255:VAL:HA	1:B:278:LEU:HD11	2.02	0.41
4:N:12:LEU:HB2	4:N:36:SER:HB3	2.02	0.41
4:N:34:ALA:HB2	9:K:281:ILE:HG23	2.02	0.41
10:E:76:SER:OG	12:E:501:GDP:O2A	2.35	0.41
10:E:135:ARG:HA	10:E:135:ARG:HD3	1.89	0.41
11:L:140:LEU:HB3	11:L:142:TYR:CZ	2.56	0.41
11:L:152:GLU:HA	11:L:155:THR:HG22	2.02	0.41
1:B:254:LEU:HD11	1:B:322:LEU:HD13	2.02	0.41
1:B:325:ARG:NH2	1:B:352:ASP:OD2	2.54	0.41
5:J:78:LYS:HB2	5:J:78:LYS:HE3	1.82	0.41
8:C:144:ASN:HA	8:C:147:ARG:HG2	2.03	0.41
4:N:26:LEU:HD22	11:L:349:LYS:HD3	2.03	0.41
9:K:174:SER:HB2	9:K:213:VAL:H	1.86	0.41
11:L:142:TYR:O	11:L:176:PHE:N	2.52	0.41
2:A:372:GLN:HE22	2:A:740:VAL:HG22	1.86	0.41
2:A:917:LYS:HB3	2:A:917:LYS:HE3	1.84	0.41
2:A:1195:SER:OG	2:A:1196:GLU:N	2.52	0.41
2:A:1394:THR:HB	2:A:1397:VAL:HG22	2.03	0.41
3:H:79:GLN:HG3	3:H:94:ALA:HB3	2.02	0.41
8:C:271:LEU:HD23	8:C:274:LEU:HD12	2.03	0.41
9:D:135:ASP:OD1	9:D:135:ASP:N	2.53	0.41
10:E:139:ALA:HB2	10:E:236:LEU:HD21	2.03	0.41
3:O:21:ALA:HB3	3:O:93:ILE:HD12	2.02	0.41
5:Q:72:GLY:HA2	5:Q:88:LYS:O	2.21	0.41
9:K:163:SER:H	9:K:166:ASP:CG	2.29	0.41
11:L:243:LEU:HD12	11:L:246:LEU:HD11	2.02	0.41
1:B:54:LEU:HD22	8:C:89:ASP:HA	2.03	0.41
1:B:318:LEU:HD23	1:B:318:LEU:HA	1.92	0.41
8:C:282:LEU:HD13	8:C:312:LEU:HD22	2.02	0.41
10:E:83:HIS:HB2	10:E:85:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:267:THR:OG1	9:K:270:THR:OG1	2.31	0.41
2:A:1551:ASN:OD1	2:A:1553:MET:N	2.54	0.40
8:C:490:LEU:HD21	8:C:517:LEU:HD21	2.03	0.40
9:K:160:PHE:HB3	9:K:171:LYS:HZ2	1.85	0.40
9:K:282:PRO:HB2	9:K:283:SER:H	1.68	0.40
1:B:10:ILE:H	1:B:27:VAL:HG12	1.85	0.40
9:D:249:PHE:HZ	9:D:252:MET:HB2	1.85	0.40
10:E:218:THR:OG1	10:E:219:SER:N	2.54	0.40
3:O:46:ARG:HG3	3:O:48:GLY:H	1.86	0.40
4:N:46:THR:HA	11:L:354:TYR:HE1	1.86	0.40
1:B:190:ASP:O	1:B:193:THR:OG1	2.34	0.40
4:G:25:LEU:HD11	4:G:46:ALA:HB1	2.03	0.40
9:D:208:ARG:HG3	9:D:271:TYR:HE2	1.87	0.40
7:M:140:TYR:HA	7:M:143:LEU:HD12	2.04	0.40
9:K:64:GLY:N	9:K:73:TYR:OH	2.45	0.40
1:B:79:ASN:ND2	9:D:40:GLY:HA3	2.37	0.40
2:A:988:ARG:O	2:A:1408:LYS:NZ	2.40	0.40
2:A:1197:GLN:HE21	2:A:1200:LEU:HB2	1.86	0.40
2:A:1311:PHE:O	2:A:1468:ARG:NH1	2.55	0.40
4:N:92:LEU:HD21	4:N:112:LEU:HB2	2.04	0.40
6:P:16:LEU:HD11	6:P:90:GLN:HG2	2.02	0.40
7:M:68:VAL:HG12	11:L:351:LEU:HD21	2.03	0.40
9:K:20:LYS:HB2	9:K:20:LYS:HE3	1.80	0.40
11:L:200:ASN:O	11:L:204:ALA:N	2.55	0.40
11:L:258:LYS:NZ	11:L:279:MET:SD	2.91	0.40
1:B:38:ASP:O	8:C:76:LYS:NZ	2.37	0.40
2:A:97:LEU:HG	2:A:146:VAL:HG22	2.02	0.40
2:A:206:LYS:HD3	2:A:206:LYS:HA	1.93	0.40
4:G:109:GLN:HA	4:G:112:VAL:HG22	2.02	0.40
9:D:52:PHE:HE2	9:D:181:ILE:HB	1.87	0.40
11:L:238:PRO:HB2	11:L:241:PRO:HD3	2.04	0.40
11:L:264:VAL:O	11:L:266:SER:OG	2.33	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	B	358/380 (94%)	303 (85%)	55 (15%)	0	100	100
2	A	974/1603 (61%)	876 (90%)	97 (10%)	1 (0%)	48	81
3	H	119/124 (96%)	108 (91%)	11 (9%)	0	100	100
3	O	118/124 (95%)	107 (91%)	11 (9%)	0	100	100
4	G	123/125 (98%)	107 (87%)	16 (13%)	0	100	100
4	N	122/125 (98%)	107 (88%)	15 (12%)	0	100	100
5	J	90/91 (99%)	84 (93%)	6 (7%)	0	100	100
5	Q	89/91 (98%)	80 (90%)	9 (10%)	0	100	100
6	I	81/99 (82%)	68 (84%)	13 (16%)	0	100	100
6	P	95/99 (96%)	90 (95%)	5 (5%)	0	100	100
7	F	109/161 (68%)	100 (92%)	9 (8%)	0	100	100
7	M	113/161 (70%)	105 (93%)	8 (7%)	0	100	100
8	C	394/569 (69%)	367 (93%)	27 (7%)	0	100	100
9	D	294/313 (94%)	260 (88%)	34 (12%)	0	100	100
9	K	298/313 (95%)	264 (89%)	32 (11%)	2 (1%)	19	55
10	E	304/399 (76%)	263 (86%)	41 (14%)	0	100	100
11	L	305/399 (76%)	253 (83%)	52 (17%)	0	100	100
All	All	3986/5176 (77%)	3542 (89%)	441 (11%)	3 (0%)	50	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	300	THR
9	K	77	GLN
9	K	282	PRO

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	B	334/351 (95%)	334 (100%)	0	100	100
2	A	891/1412 (63%)	891 (100%)	0	100	100
3	H	105/108 (97%)	105 (100%)	0	100	100
3	O	105/108 (97%)	105 (100%)	0	100	100
4	G	98/98 (100%)	98 (100%)	0	100	100
4	N	97/98 (99%)	97 (100%)	0	100	100
5	J	78/77 (101%)	78 (100%)	0	100	100
5	Q	77/77 (100%)	77 (100%)	0	100	100
6	I	71/83 (86%)	71 (100%)	0	100	100
6	P	81/83 (98%)	81 (100%)	0	100	100
7	F	96/141 (68%)	96 (100%)	0	100	100
7	M	99/141 (70%)	99 (100%)	0	100	100
8	C	363/504 (72%)	363 (100%)	0	100	100
9	D	271/287 (94%)	271 (100%)	0	100	100
9	K	275/287 (96%)	275 (100%)	0	100	100
10	E	279/339 (82%)	279 (100%)	0	100	100
11	L	281/340 (83%)	281 (100%)	0	100	100
All	All	3601/4534 (79%)	3601 (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 (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	41	GLN
1	B	226	ASN
1	B	371	ASN
2	A	107	GLN
2	A	197	ASN
2	A	401	HIS
2	A	405	HIS
2	A	809	GLN
2	A	923	GLN
2	A	1212	HIS
2	A	1377	ASN

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Mol	Chain	Res	Type
2	A	1484	GLN
2	A	1512	GLN
3	H	68	ASN
3	H	82	GLN
4	G	65	ASN
5	J	8	HIS
5	J	79	HIS
8	C	133	ASN
8	C	140	ASN
8	C	339	ASN
8	C	392	GLN
8	C	485	ASN
9	D	30	ASN
9	D	116	ASN
9	D	196	GLN
10	E	97	ASN
10	E	106	ASN
10	E	355	ASN
3	O	84	ASN
4	N	114	GLN
5	Q	73	ASN
6	P	60	ASN
9	K	30	ASN
9	K	115	GLN
9	K	222	GLN
11	L	111	ASN
11	L	158	HIS
11	L	168	ASN
11	L	248	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	GDP	K	501	-	25,30,30	1.02	1 (4%)	30,47,47	1.25	4 (13%)
13	AF3	D	502	-	0,3,3	-	-	-		
13	AF3	E	502	-	0,3,3	-	-	-		
12	GDP	D	501	-	25,30,30	1.15	2 (8%)	30,47,47	1.26	6 (20%)
13	AF3	K	502	-	0,3,3	-	-	-		
12	GDP	E	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.22	4 (13%)

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
12	GDP	K	501	-	-	3/12/32/32	0/3/3/3
12	GDP	D	501	-	-	5/12/32/32	0/3/3/3
12	GDP	E	501	-	-	2/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	501	GDP	C6-N1	-3.59	1.32	1.37
12	K	501	GDP	C6-N1	-3.02	1.33	1.37
12	E	501	GDP	C6-N1	-2.47	1.34	1.37
12	D	501	GDP	O4'-C1'	2.34	1.44	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	K	501	GDP	C8-N7-C5	3.35	108.25	102.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	D	501	GDP	O4'-C1'-N9	3.28	113.10	108.75
12	E	501	GDP	C8-N7-C5	2.77	107.27	102.55
12	D	501	GDP	C8-N7-C5	2.69	107.13	102.55
12	K	501	GDP	C4'-O4'-C1'	2.49	112.20	109.92
12	D	501	GDP	C5-C6-N1	2.48	118.80	114.07
12	E	501	GDP	O4'-C1'-N9	2.35	111.86	108.75
12	D	501	GDP	O2A-PA-O3A	-2.23	101.24	107.27
12	K	501	GDP	C5-C6-N1	2.22	118.31	114.07
12	E	501	GDP	O5'-C5'-C4'	2.16	116.34	108.99
12	K	501	GDP	C2'-C3'-C4'	2.14	106.75	102.61
12	D	501	GDP	C2'-C3'-C4'	2.14	106.75	102.61
12	D	501	GDP	C2-N1-C6	-2.07	121.32	125.11
12	E	501	GDP	C5-C6-N1	2.04	117.97	114.07

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	D	501	GDP	C5'-O5'-PA-O3A
12	D	501	GDP	C5'-O5'-PA-O1A
12	D	501	GDP	C3'-C4'-C5'-O5'
12	D	501	GDP	O4'-C4'-C5'-O5'
12	K	501	GDP	O4'-C4'-C5'-O5'
12	K	501	GDP	C3'-C4'-C5'-O5'
12	E	501	GDP	PB-O3A-PA-O1A
12	E	501	GDP	PB-O3A-PA-O2A
12	K	501	GDP	PB-O3A-PA-O2A
12	D	501	GDP	PB-O3A-PA-O2A

There are no ring outliers.

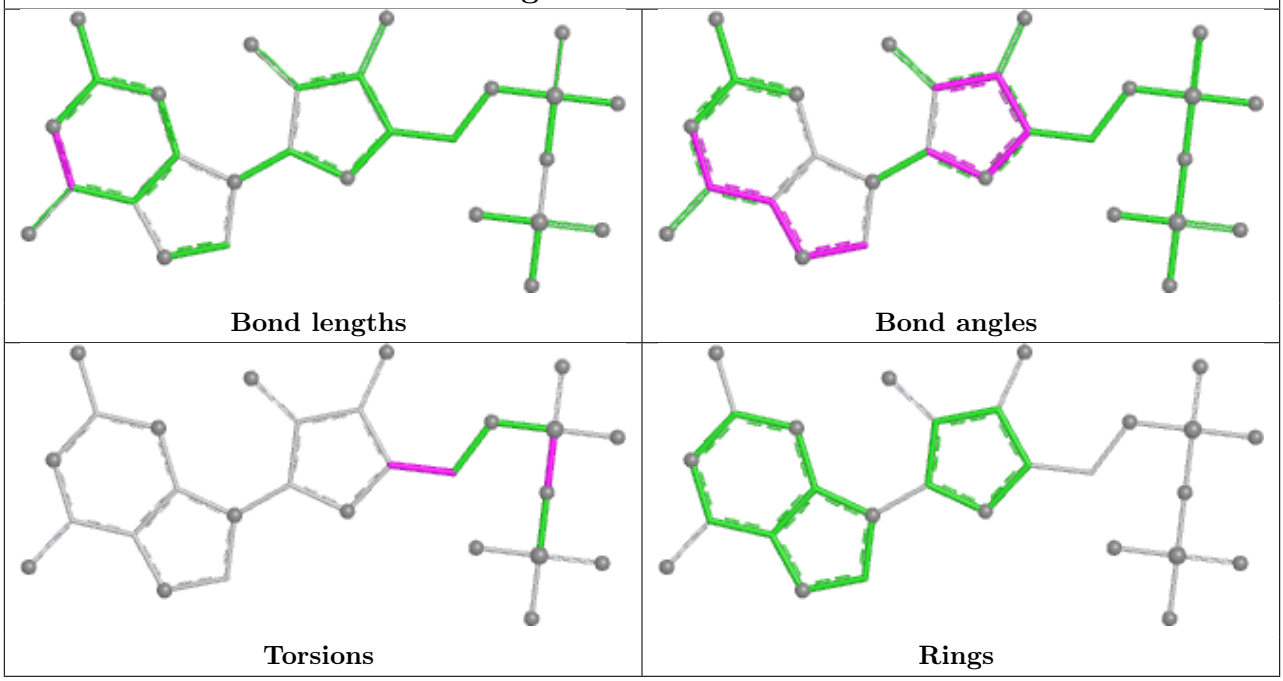
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	K	501	GDP	3	0
12	D	501	GDP	3	0
13	K	502	AF3	2	0
12	E	501	GDP	2	0

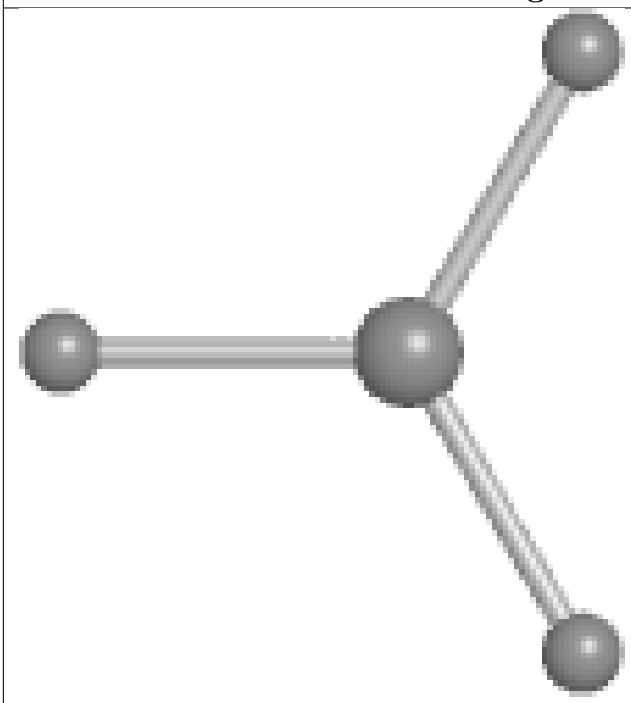
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

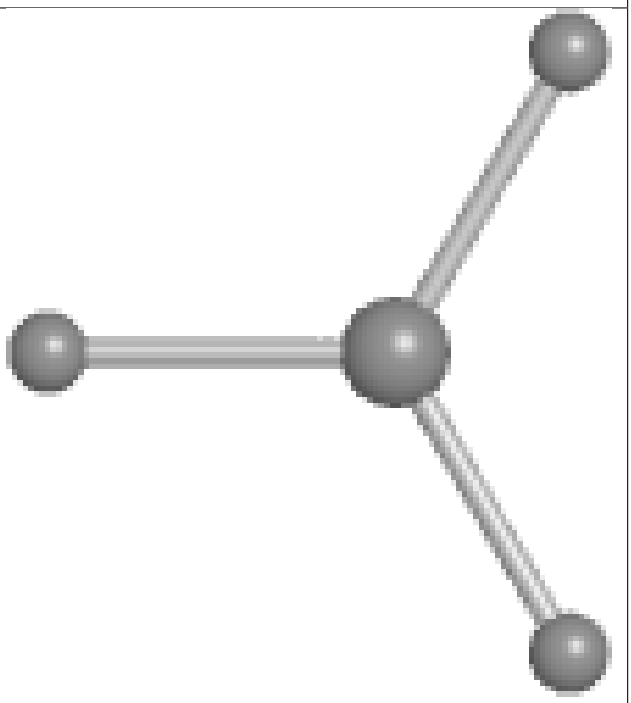
Ligand GDP K 501



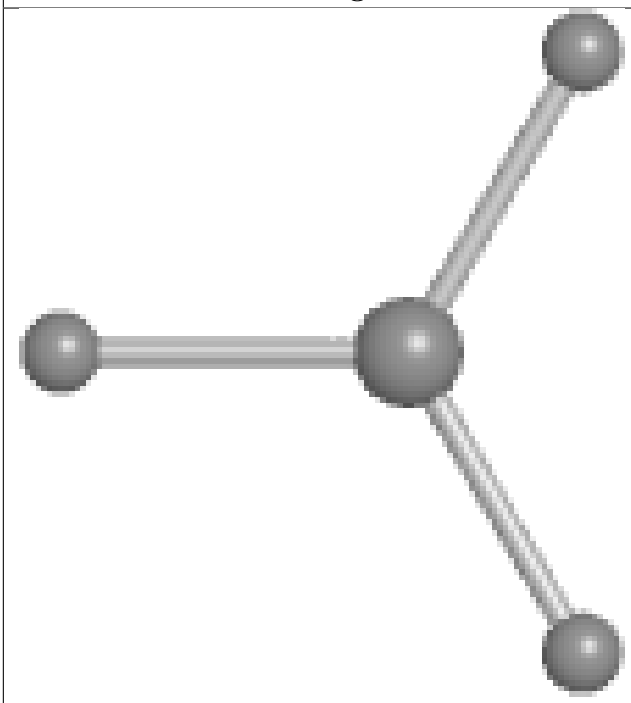
Ligand AF3 D 502



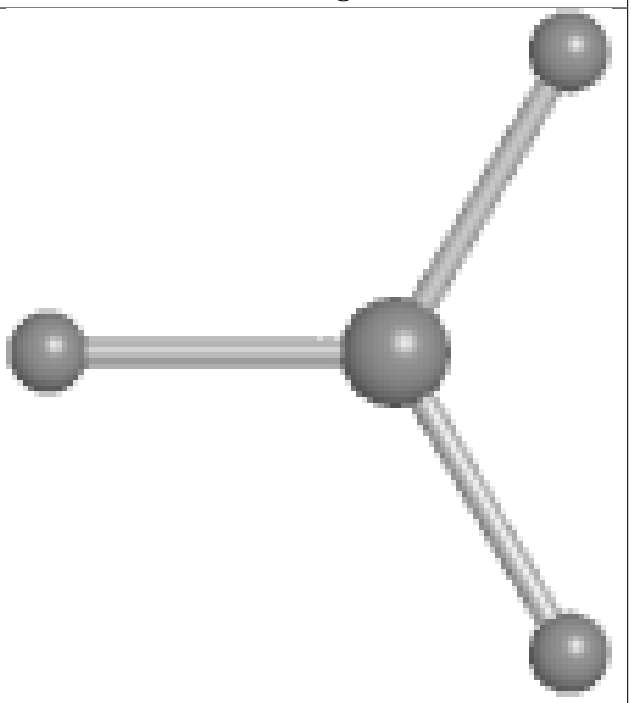
Bond lengths



Bond angles

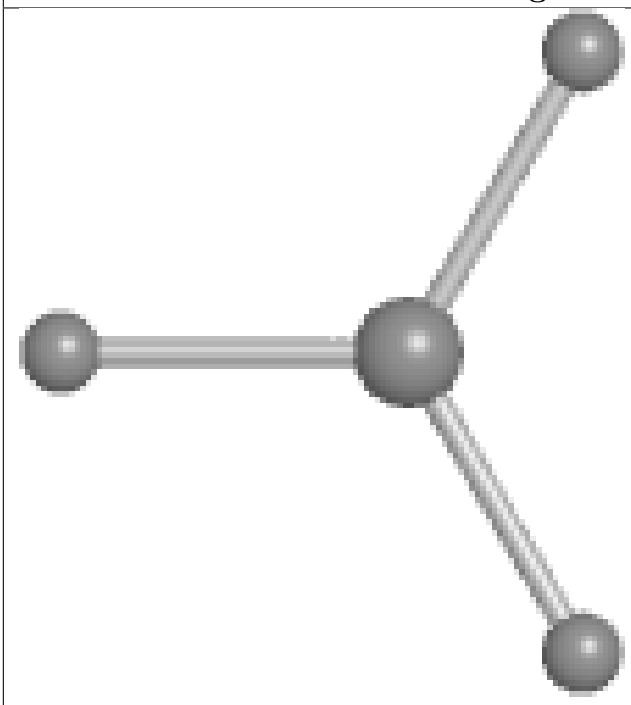


Torsions

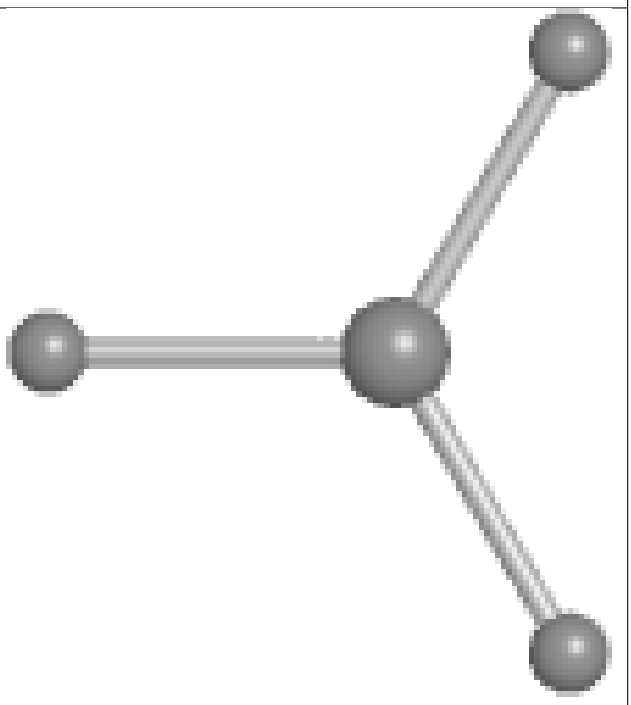


Rings

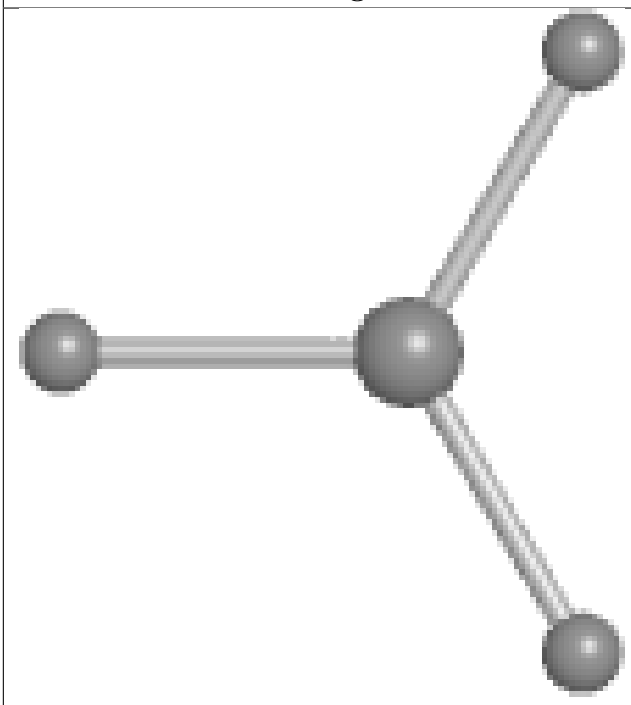
Ligand AF3 E 502



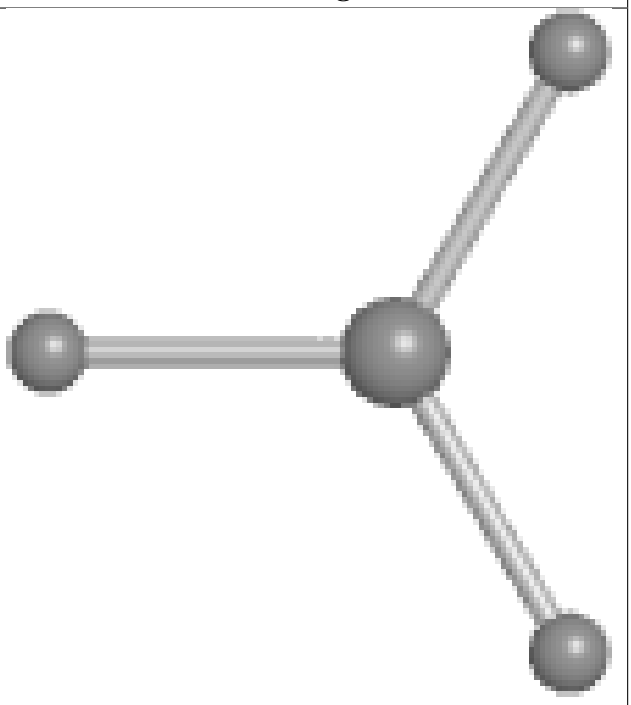
Bond lengths



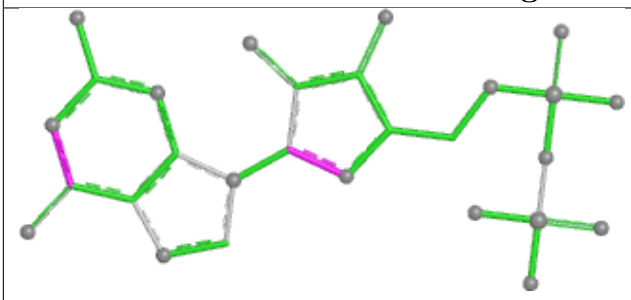
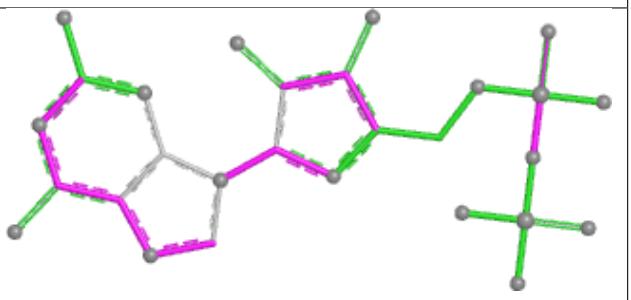
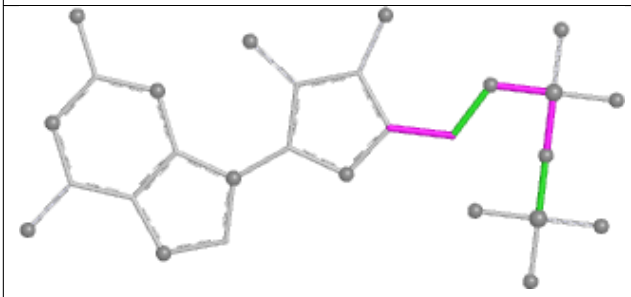
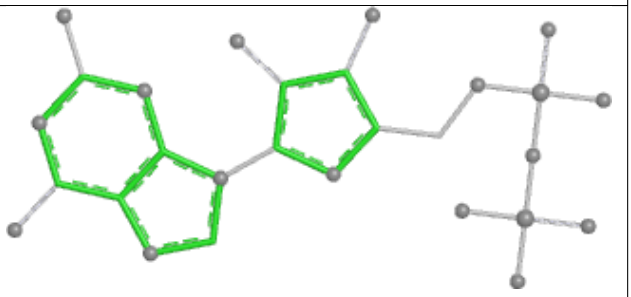
Bond angles



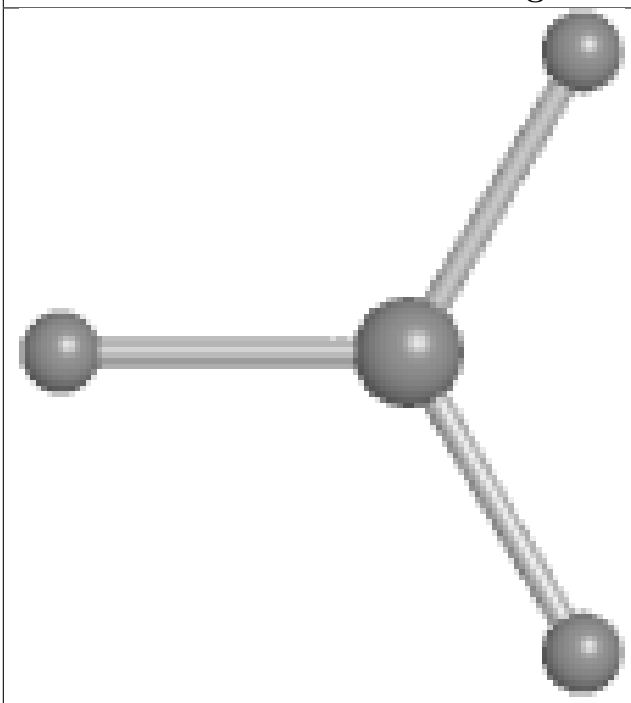
Torsions



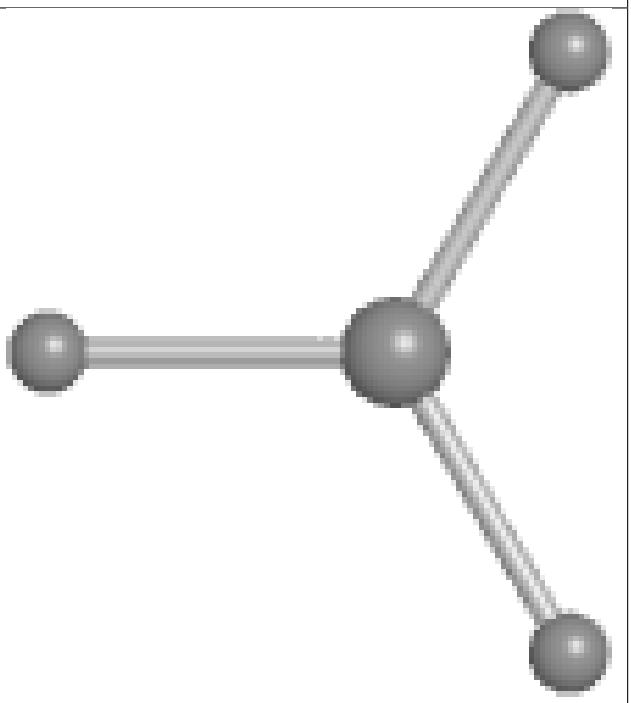
Rings

Ligand GDP D 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

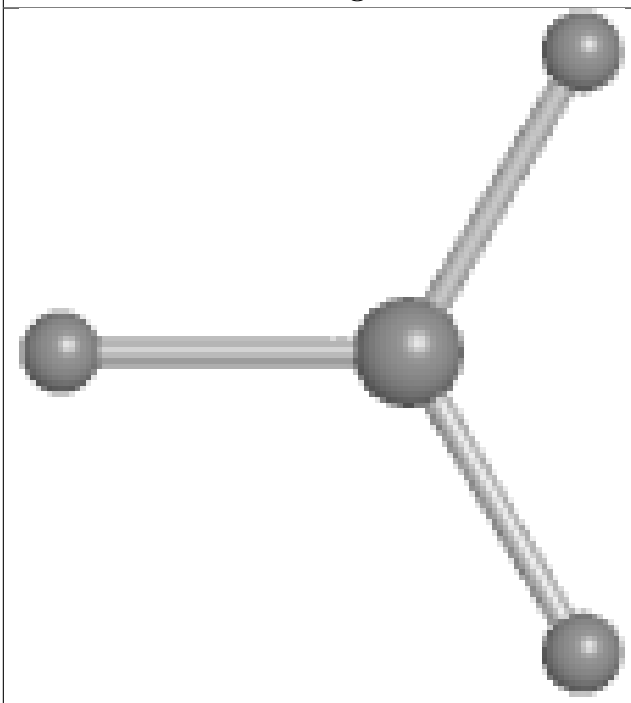
Ligand AF3 K 502



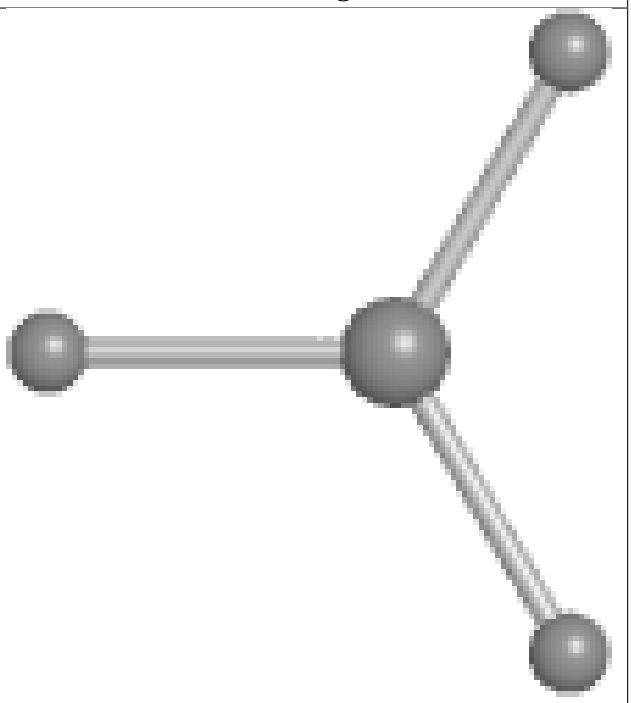
Bond lengths



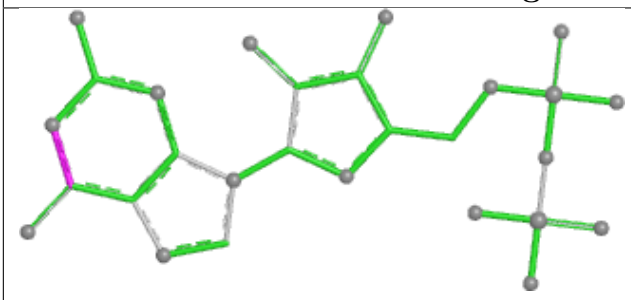
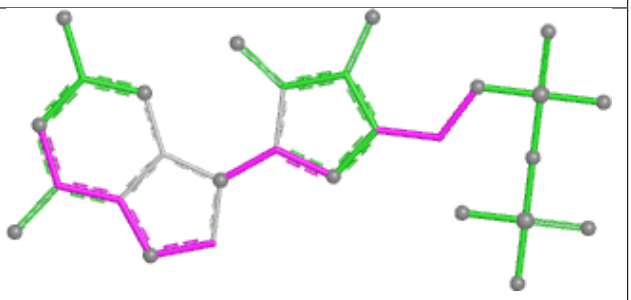
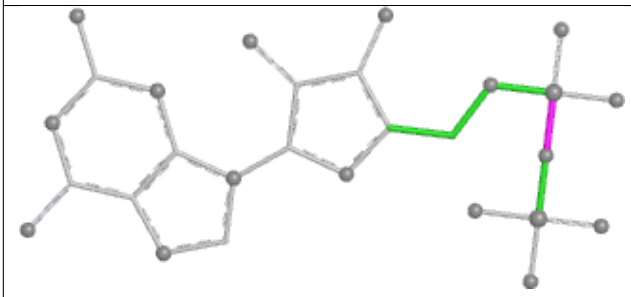
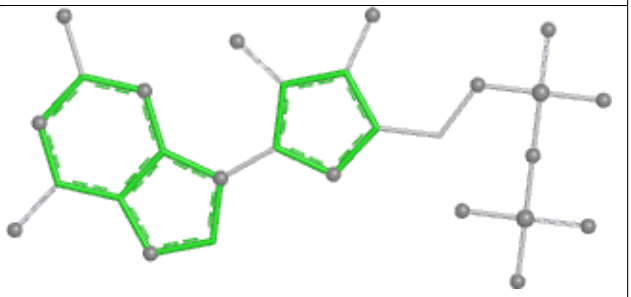
Bond angles



Torsions



Rings

Ligand GDP E 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

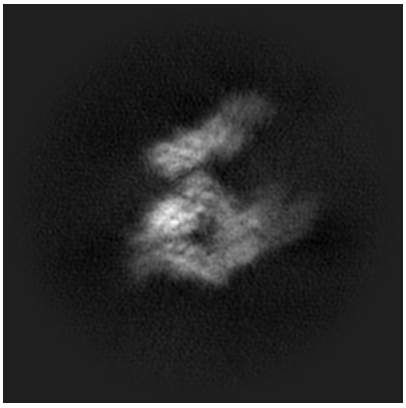
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-25654. These allow visual inspection of the internal detail of the map and identification of artifacts.

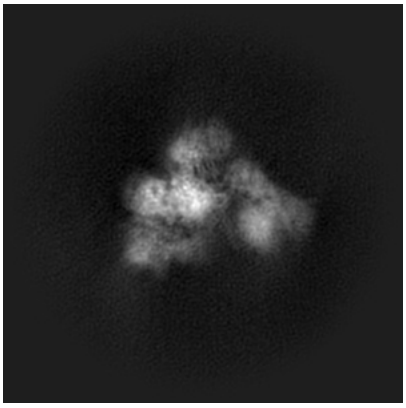
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

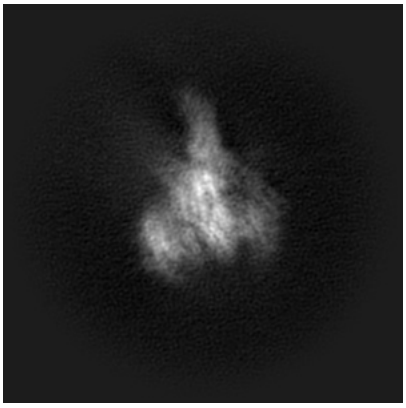
6.1.1 Primary map



X



Y

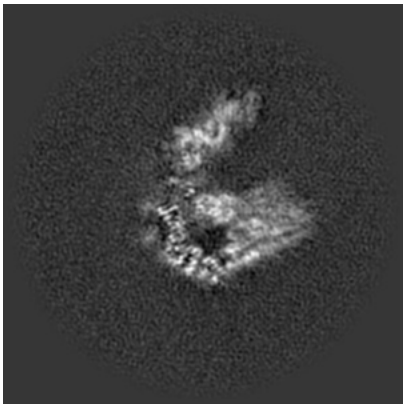


Z

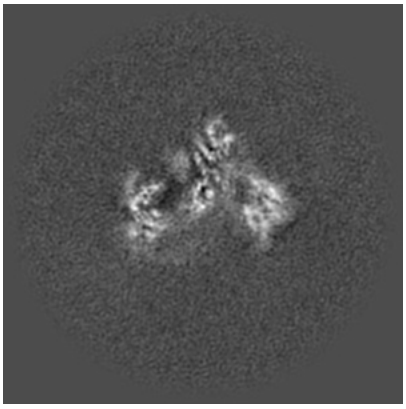
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

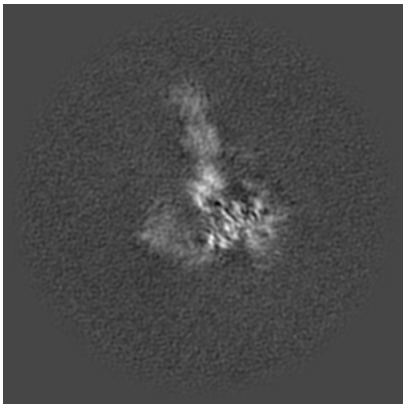
6.2.1 Primary map



X Index: 230



Y Index: 230

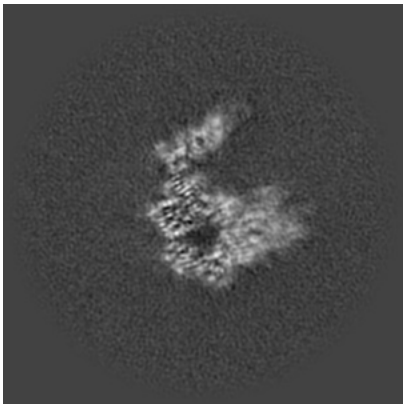


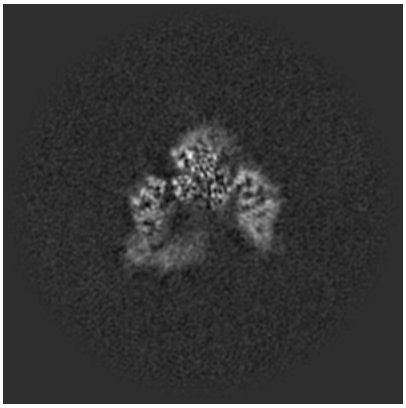
Z Index: 230

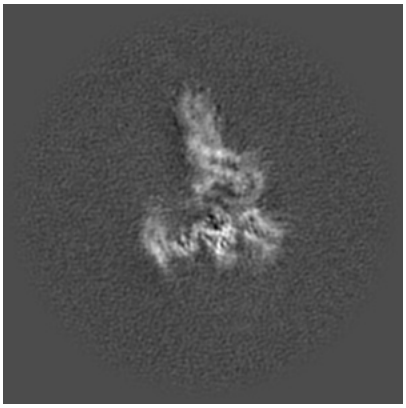
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 239

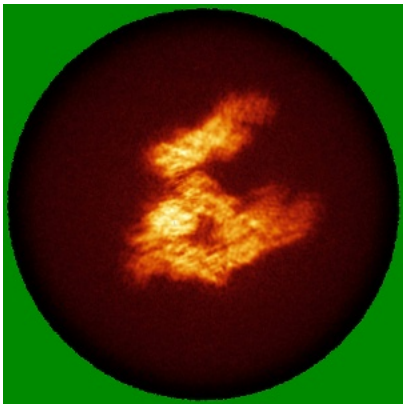

Y Index: 211

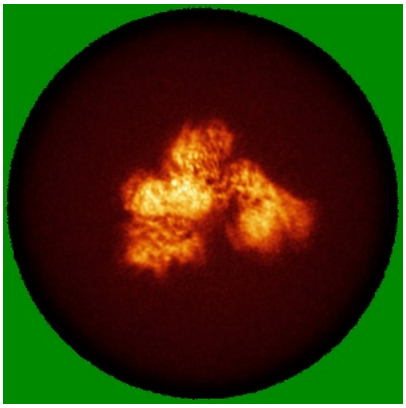

Z Index: 208

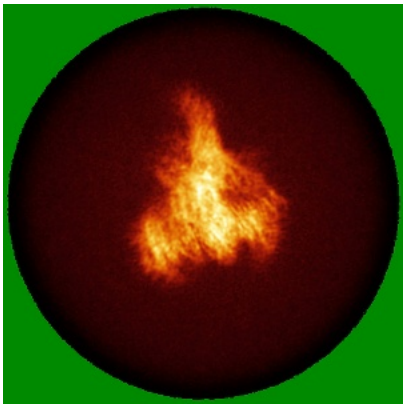
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

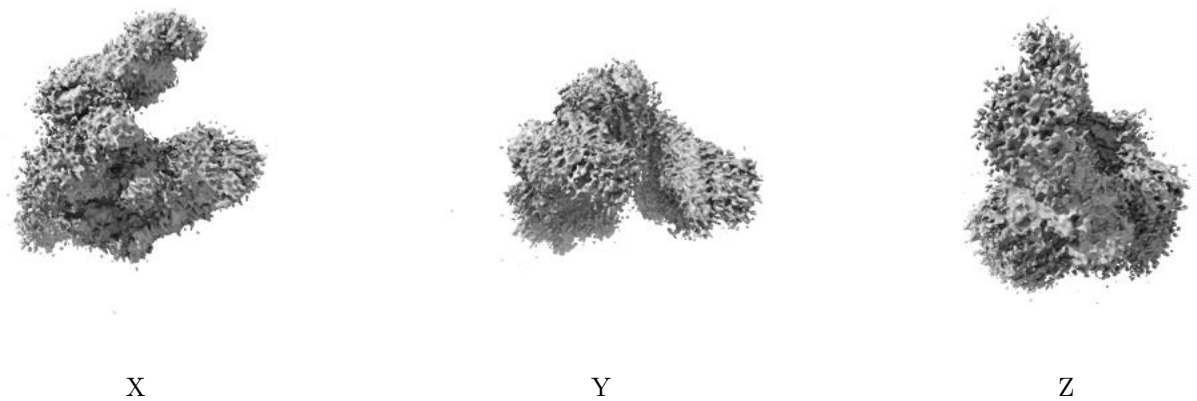

Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

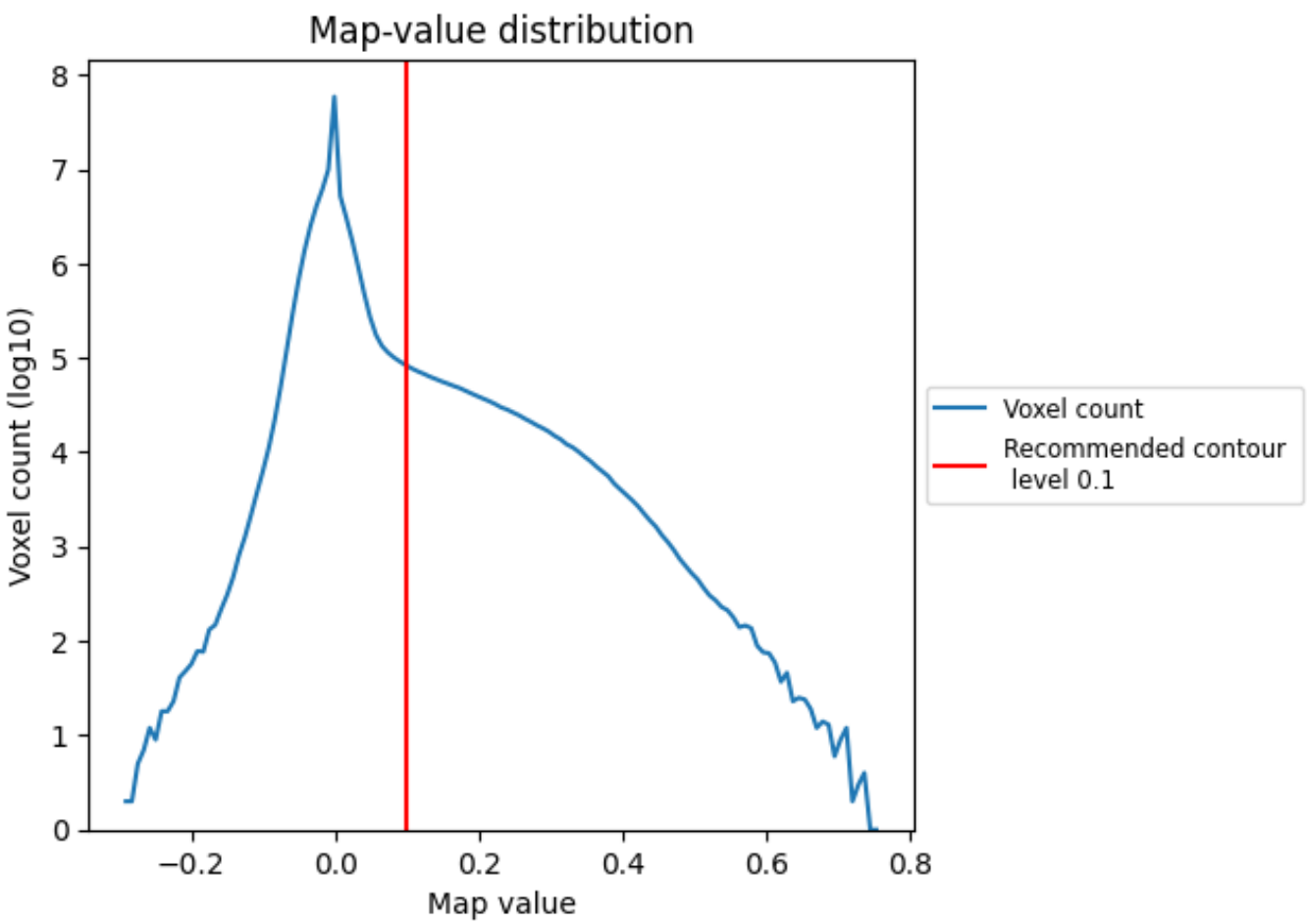
6.6 Mask visualisation (i)

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

7 Map analysis (i)

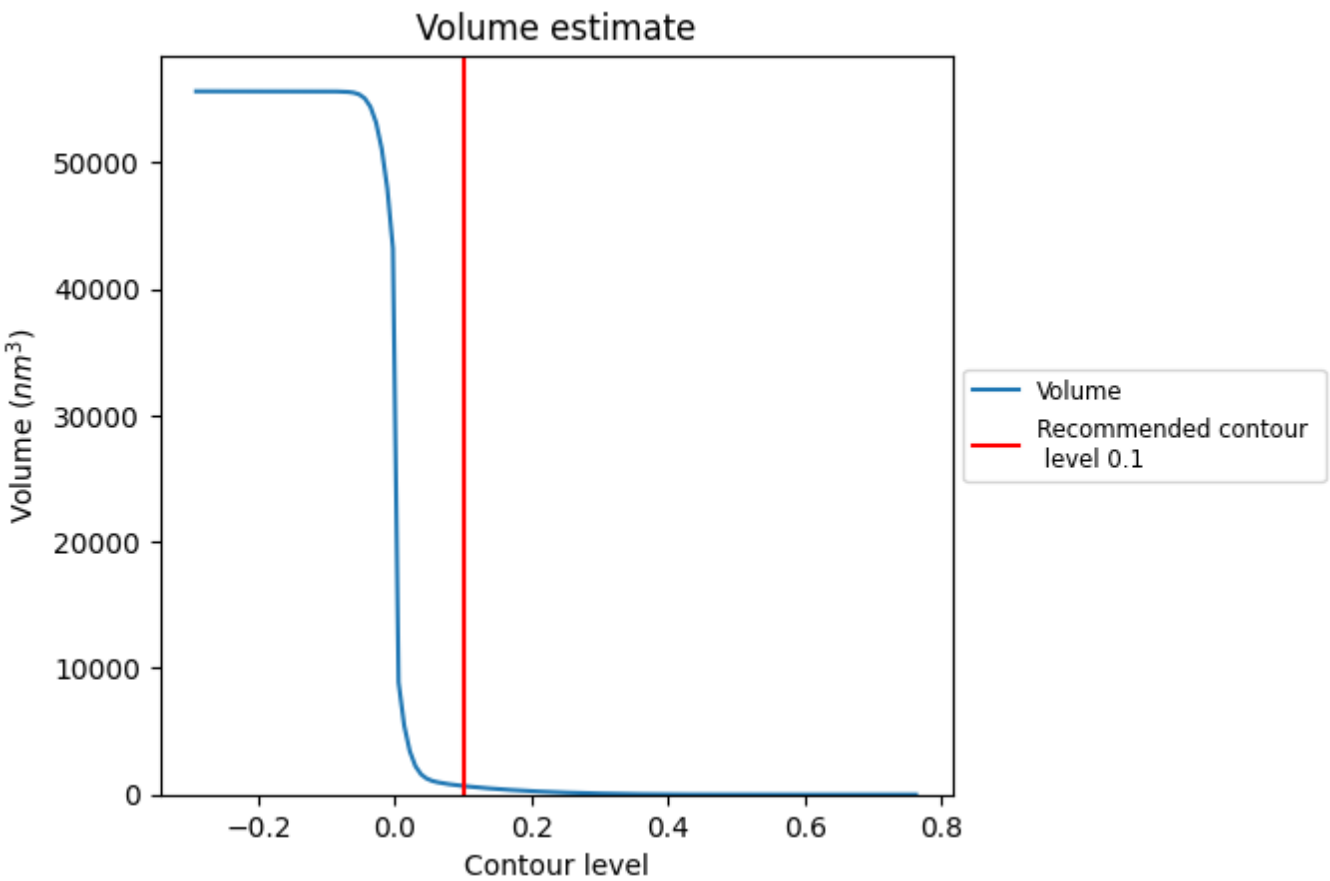
This section contains the results of statistical analysis of the map.

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.

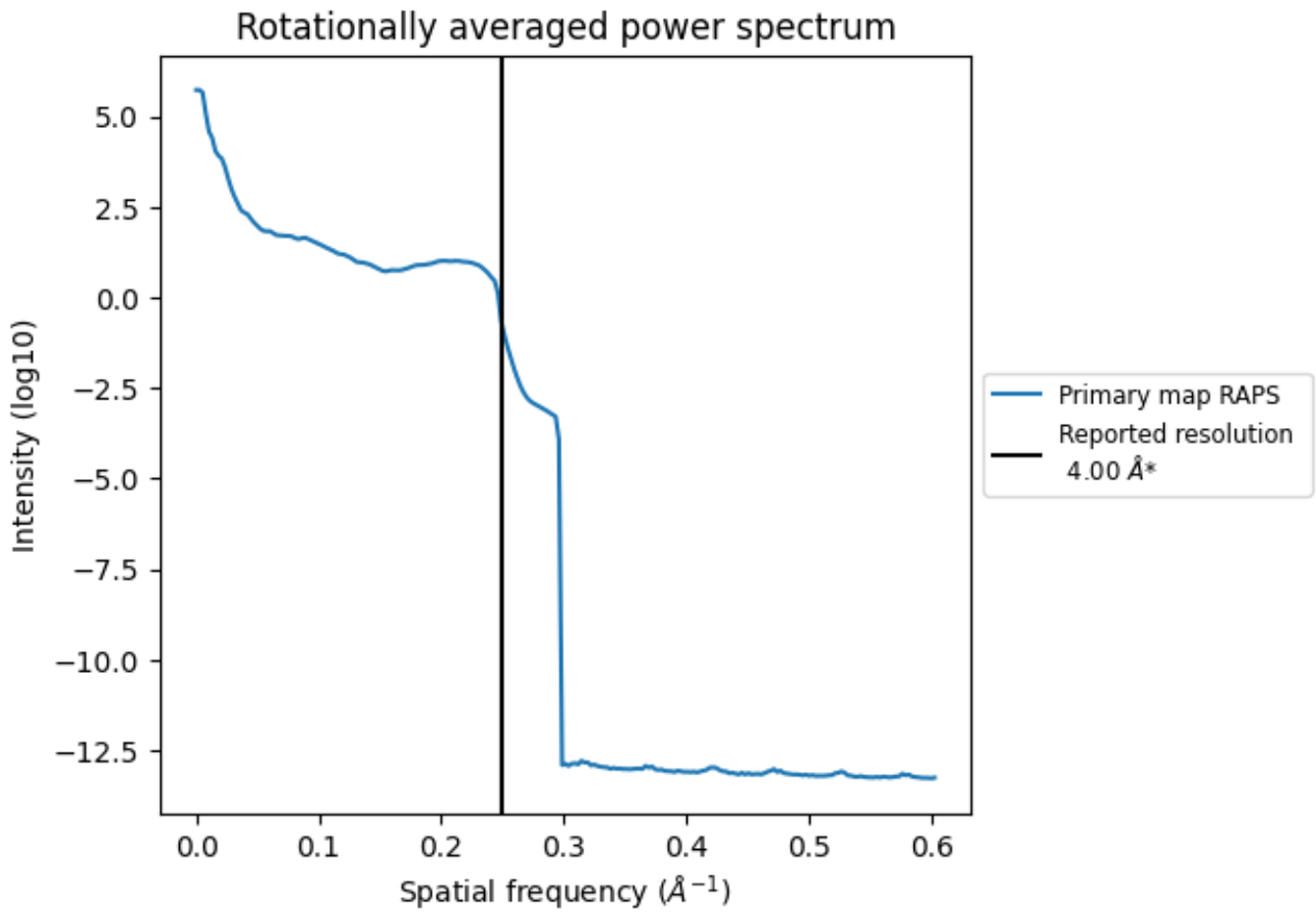
7.2 Volume estimate (i)



The volume at the recommended contour level is 680 nm^3; this corresponds to an approximate mass of 614 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 0.250 Å^{-1}

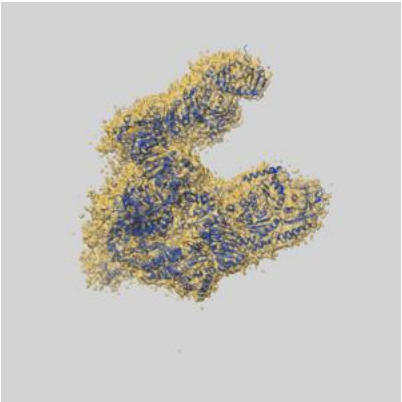
8 Fourier-Shell correlation (i)

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

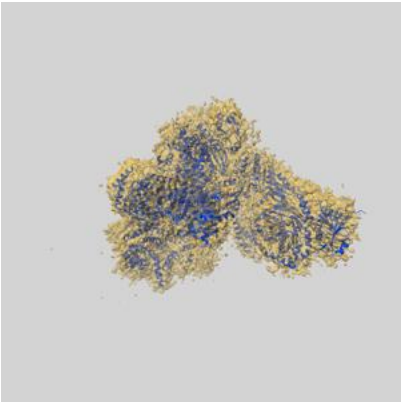
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-25654 and PDB model 7T3C. Per-residue inclusion information can be found in section 3 on page 8.

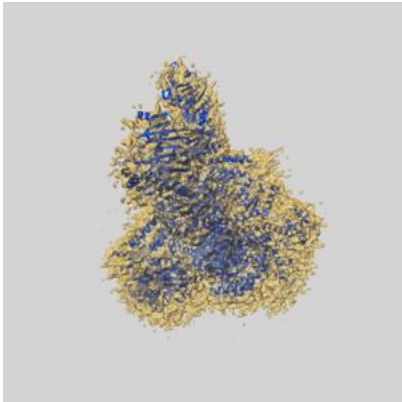
9.1 Map-model overlay (i)



X



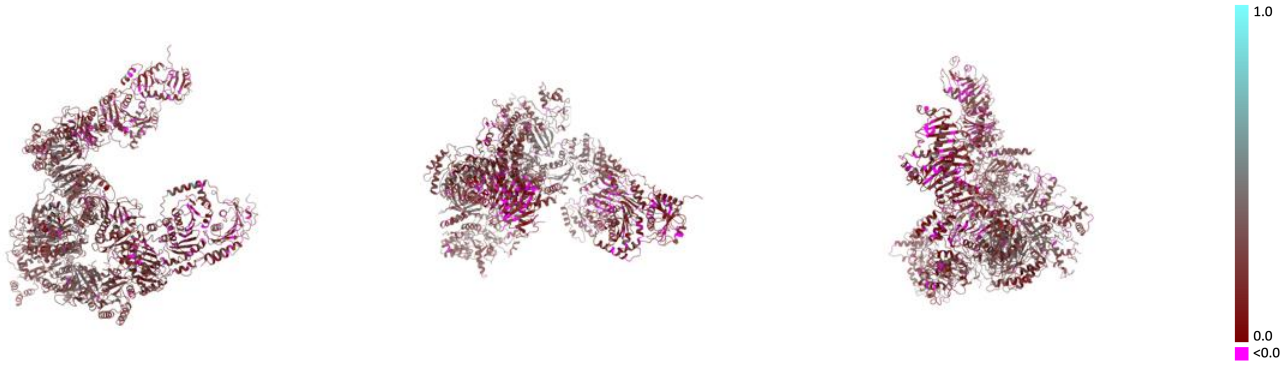
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

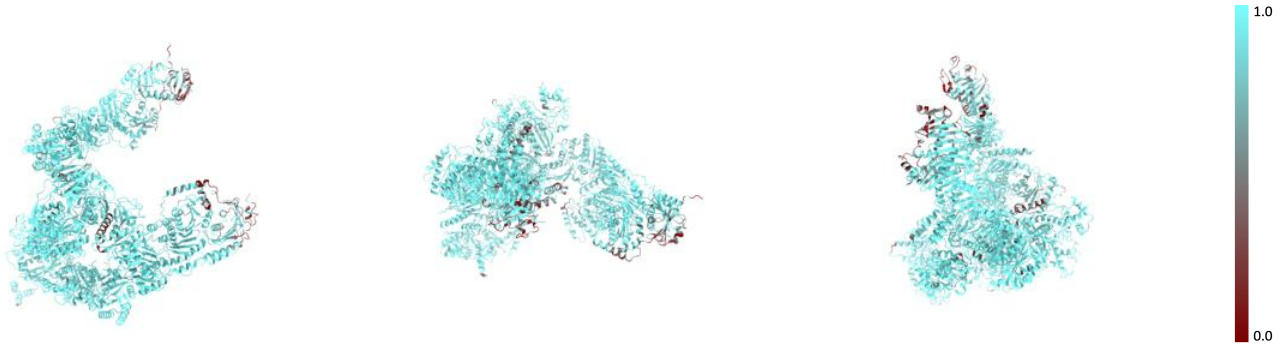
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

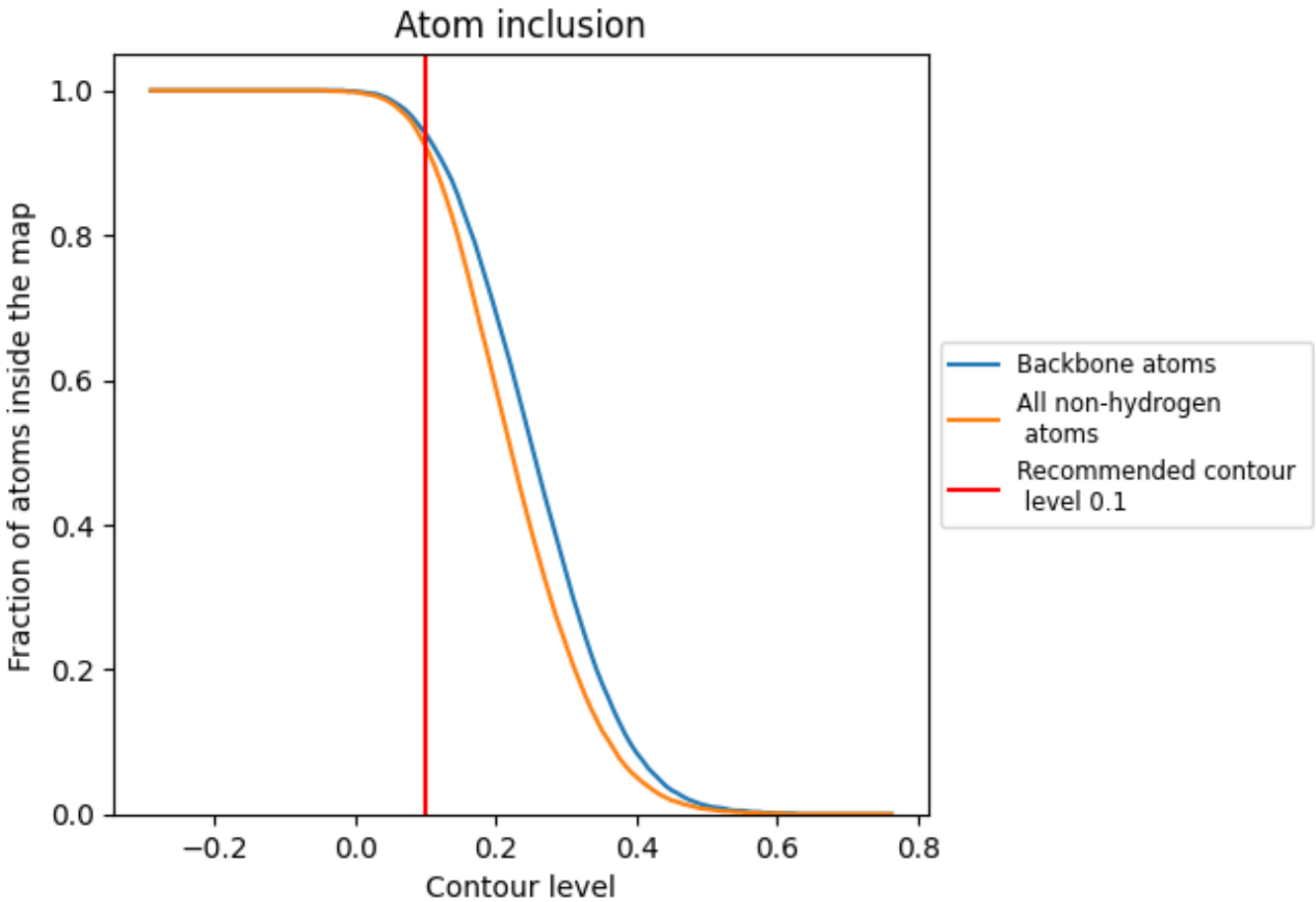
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9220	0.2420
A	0.9480	0.3030
B	0.9800	0.3120
C	0.9640	0.2540
D	0.9790	0.2660
E	0.8840	0.2160
F	0.7560	0.2170
G	0.9820	0.1600
H	0.8610	0.1410
I	0.5950	0.1580
J	0.8310	0.1600
K	0.9760	0.2480
L	0.9500	0.1820
M	0.7790	0.1560
N	0.9900	0.1740
O	0.9120	0.1770
P	0.5800	0.1820
Q	0.9080	0.1600