WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Jan 25, 2025 – 01:05 PM EST

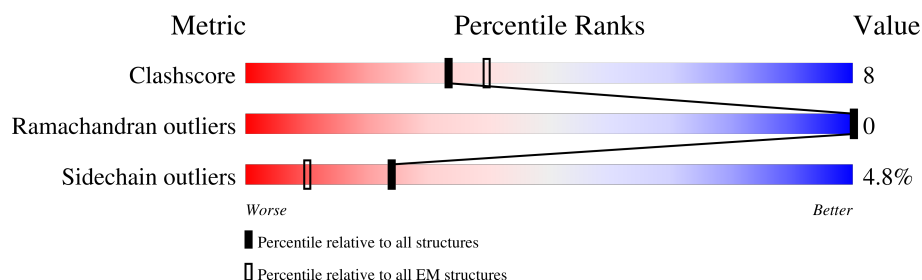|		
PDB ID	:	9CU1
EMDB ID	:	EMD-45925
Title	:	Azotobacter vinelandii filamentous 2:2:1 MoFeP:FeP:FeSII-Complex (termini; C1 symmetry)
Authors	:	Narehood, S.M.; Cook, B.D.; Srisantitham, S.; Eng, V.H.; Shiau, A.; Britt, R.D.; Herzik, M.A.; Tezcan, F.A.
Deposited on	:	2024-07-25
Resolution	:	2.83 Å(reported)
Based on initial model	:	7UT7

1   Overall quality at a glance   ⓘ

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

The reported resolution of this entry is 2.83 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	Percentile Ranks	Value
Clashscore		8
Ramachandran outliers		0
Sidechain outliers		4.8%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

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	A	492	29% / 77% / 19% ••
1	C	492	76% / 66% / 28% ••
1	H	492	28% / 76% / 21% •
1	J	492	31% / 76% / 19% ••
2	B	523	33% / 81% / 18% •
2	D	523	50% / 83% / 16% •
2	I	523	16% / 81% / 18% •
2	K	523	23% / 80% / 19% •

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Mol	Chain	Length	Quality of chain
3	E	290	84% 63% 28% 6%
3	F	290	79% 73% 22%
3	L	290	76% 63% 29% 6%
3	M	290	71% 67% 27%
4	G	122	31% 83% 15%
5	N	122	23% 81% 17%

2 Entry composition ⓘ

There are 14 unique types of molecules in this entry. The entry contains 43507 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 Nitrogenase molybdenum-iron protein alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	477	Total 3790	C 2410	N 646	O 709	S 25	1	0
1	C	477	Total 3793	C 2412	N 646	O 709	S 26	1	0
1	H	477	Total 3790	C 2410	N 646	O 709	S 25	1	0
1	J	477	Total 3793	C 2412	N 646	O 709	S 26	1	0

- Molecule 2 is a protein called Nitrogenase molybdenum-iron protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	522	Total 4174	C 2666	N 705	O 775	S 28	0	0
2	D	522	Total 4174	C 2666	N 705	O 775	S 28	0	0
2	I	522	Total 4174	C 2666	N 705	O 775	S 28	0	0
2	K	522	Total 4174	C 2666	N 705	O 775	S 28	0	0

- Molecule 3 is a protein called Nitrogenase iron protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	274	Total 2077	C 1298	N 353	O 405	S 21	0	0
3	F	283	Total 2145	C 1340	N 363	O 421	S 21	0	0
3	L	272	Total 2060	C 1288	N 351	O 401	S 20	0	0
3	M	280	Total 2121	C 1323	N 359	O 418	S 21	0	0

- Molecule 4 is a protein called Protein FeSII.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	121	918	574	161	177	6	0	0

- Molecule 5 is a protein called Protein FeSII.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	N	121	920	574	163	177	6	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	27	LYS	LEU	conflict	UNP Q44501
N	28	LYS	LEU	conflict	UNP Q44501

- Molecule 6 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: $C_7H_{10}O_7$) (labeled as "Ligand of Interest" by depositor).
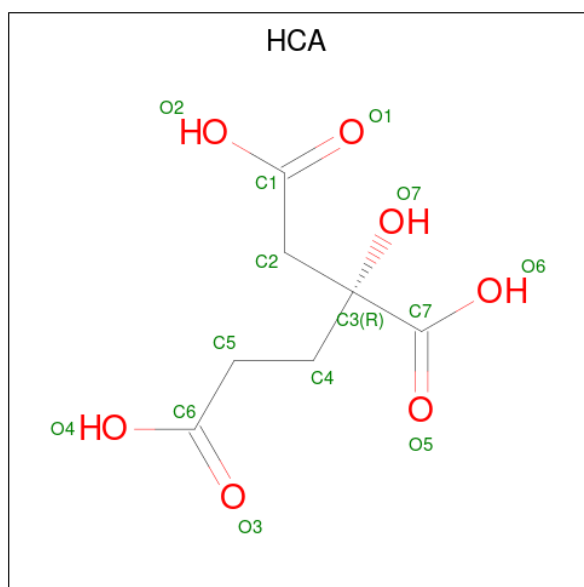
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
6	A	1	14	7	7	0
6	C	1	14	7	7	0
6	H	1	14	7	7	0
6	J	1	14	7	7	0

- Molecule 7 is iron-sulfur-molybdenum cluster with interstitial carbon (three-letter code: ICS) (formula: CFe_7MoS_9) (labeled as "Ligand of Interest" by depositor).
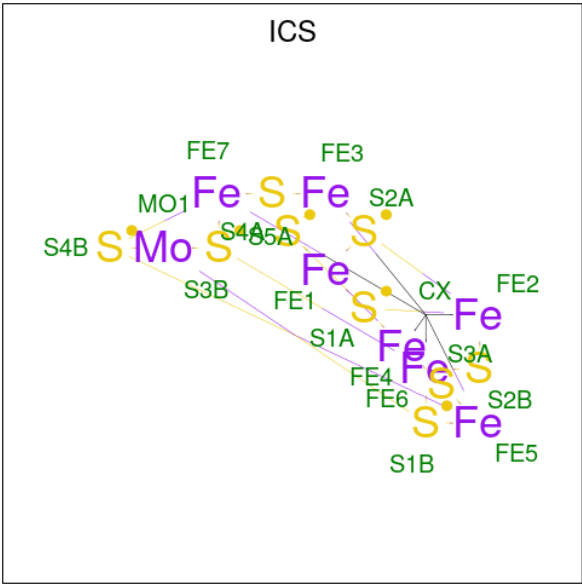
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	Fe	Mo	S	0
			18	1	7	1	9	
7	C	1	Total	C	Fe	Mo	S	0
			18	1	7	1	9	
7	H	1	Total	C	Fe	Mo	S	0
			18	1	7	1	9	
7	J	1	Total	C	Fe	Mo	S	0
			18	1	7	1	9	

- Molecule 8 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe_8S_7) (labeled as "Ligand of Interest" by depositor).
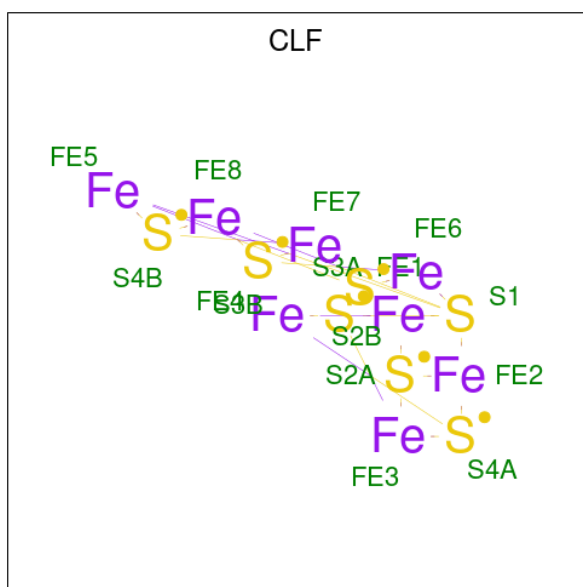
Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total 15	Fe 8	S 7	0
8	D	1	Total 15	Fe 8	S 7	0
8	H	1	Total 15	Fe 8	S 7	0
8	K	1	Total 15	Fe 8	S 7	0

- Molecule 9 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	B	1	Total 1	Fe 1	0
9	D	1	Total 1	Fe 1	0
9	I	1	Total 1	Fe 1	0
9	K	1	Total 1	Fe 1	0

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).
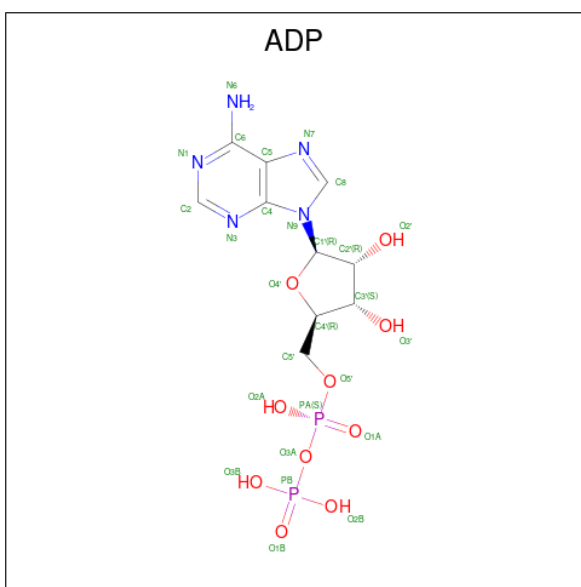
Mol	Chain	Residues	Atoms					AltConf
10	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	L	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	M	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	E	1	Total	Mg	0
			1	1	
11	F	1	Total	Mg	0
			1	1	
11	L	1	Total	Mg	0
			1	1	
11	M	1	Total	Mg	0
			1	1	

- Molecule 12 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).
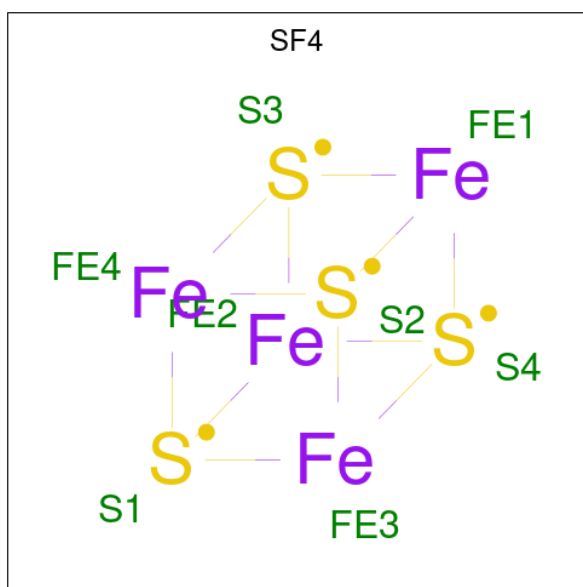
Mol	Chain	Residues	Atoms			AltConf
12	F	1	Total	Fe	S	0
			8	4	4	
12	L	1	Total	Fe	S	0
			8	4	4	

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).
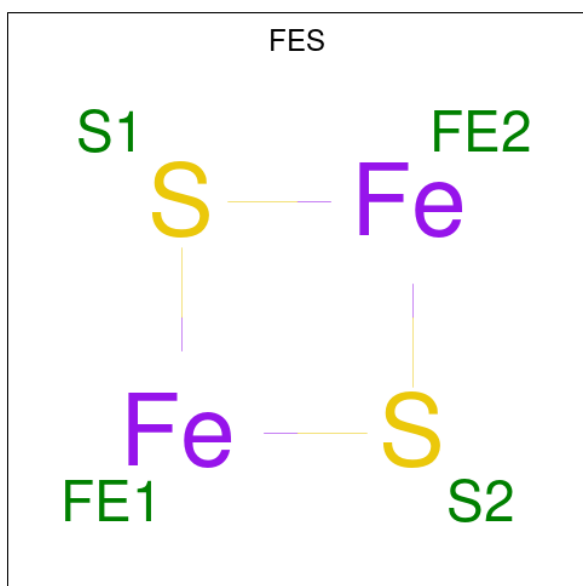
Mol	Chain	Residues	Atoms			AltConf
13	G	1	Total	Fe	S	0
			4	2	2	

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Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
13	N	1	4	2	2	0

- Molecule 14 is water.

| Mol	Chain	Residues	Atoms		AltConf
14	A	73	Total	O	0
			73	73	
14	B	86	Total	O	0
			86	86	
14	C	97	Total	O	0
			97	97	
14	D	73	Total	O	0
			73	73	
14	E	78	Total	O	0
			78	78	
14	F	88	Total	O	0
			88	88	
14	G	26	Total	O	0
			26	26	
14	H	83	Total	O	0
			83	83	
14	I	108	Total	O	0
			108	108	
14	J	74	Total	O	0
			74	74	
14	K	100	Total	O	0
			100	100	
14	L	77	Total	O	0
			77	77	
14	M	94	Total	O	0
			94	94	
14	N	19	Total	O	0
			19	19	

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: Nitrogenase molybdenum-iron protein alpha chain
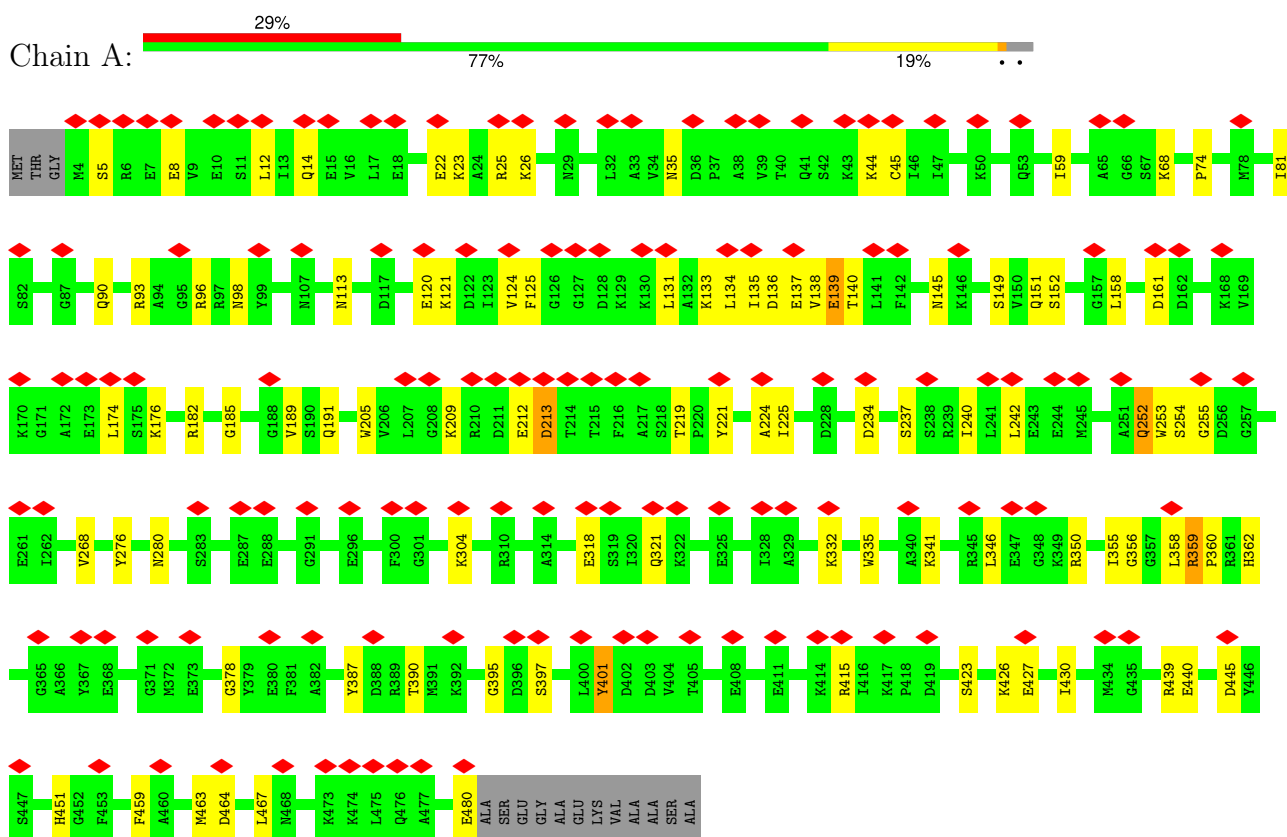
Chain A:

• Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

Chain C:

• Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

Chain H:

• Molecule 1: Nitrogenase molybdenum-iron protein alpha chain
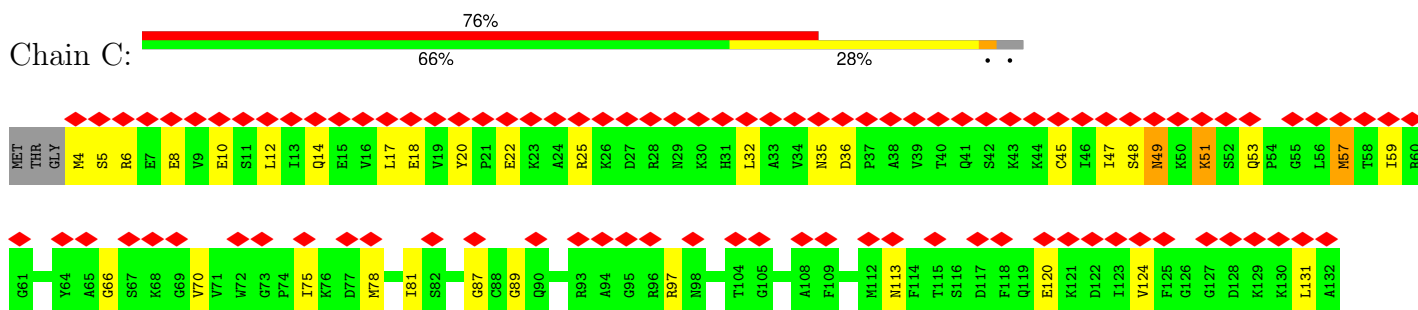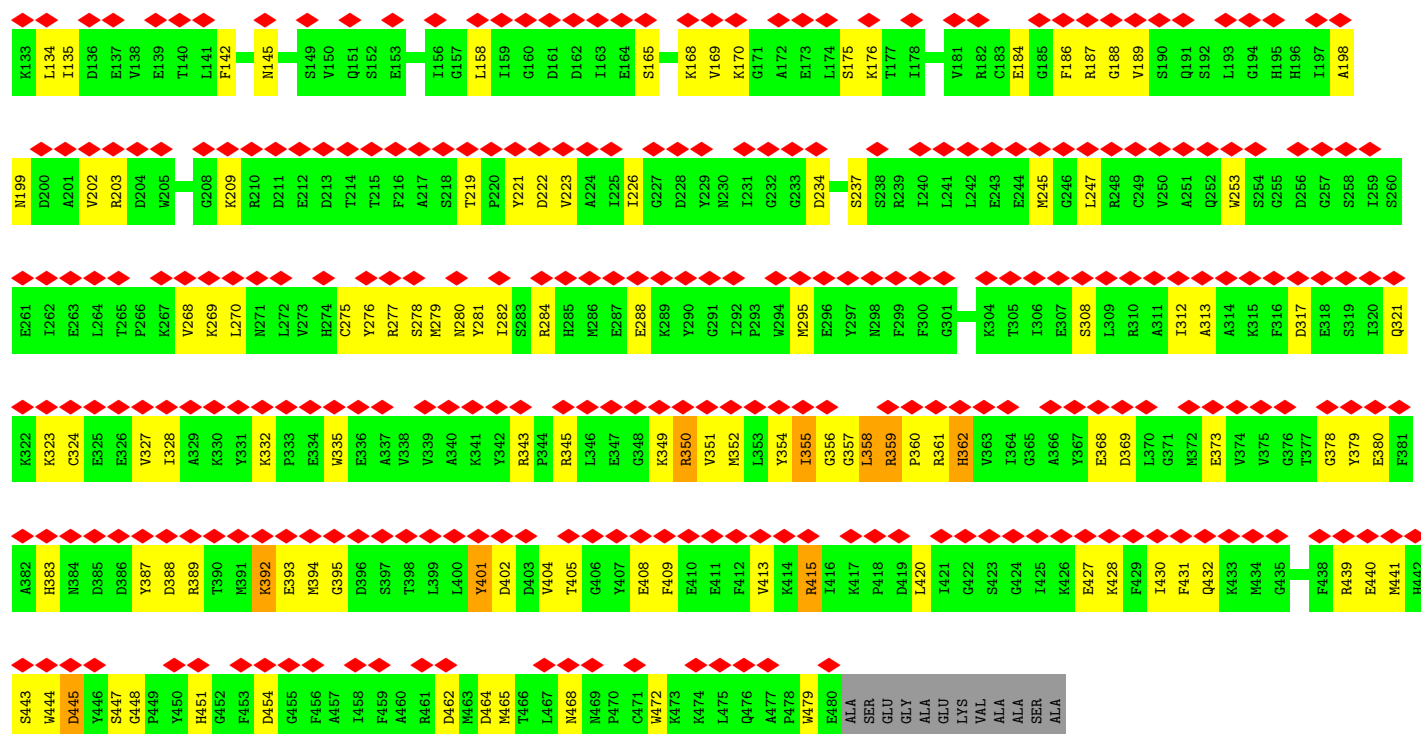
Chain J:

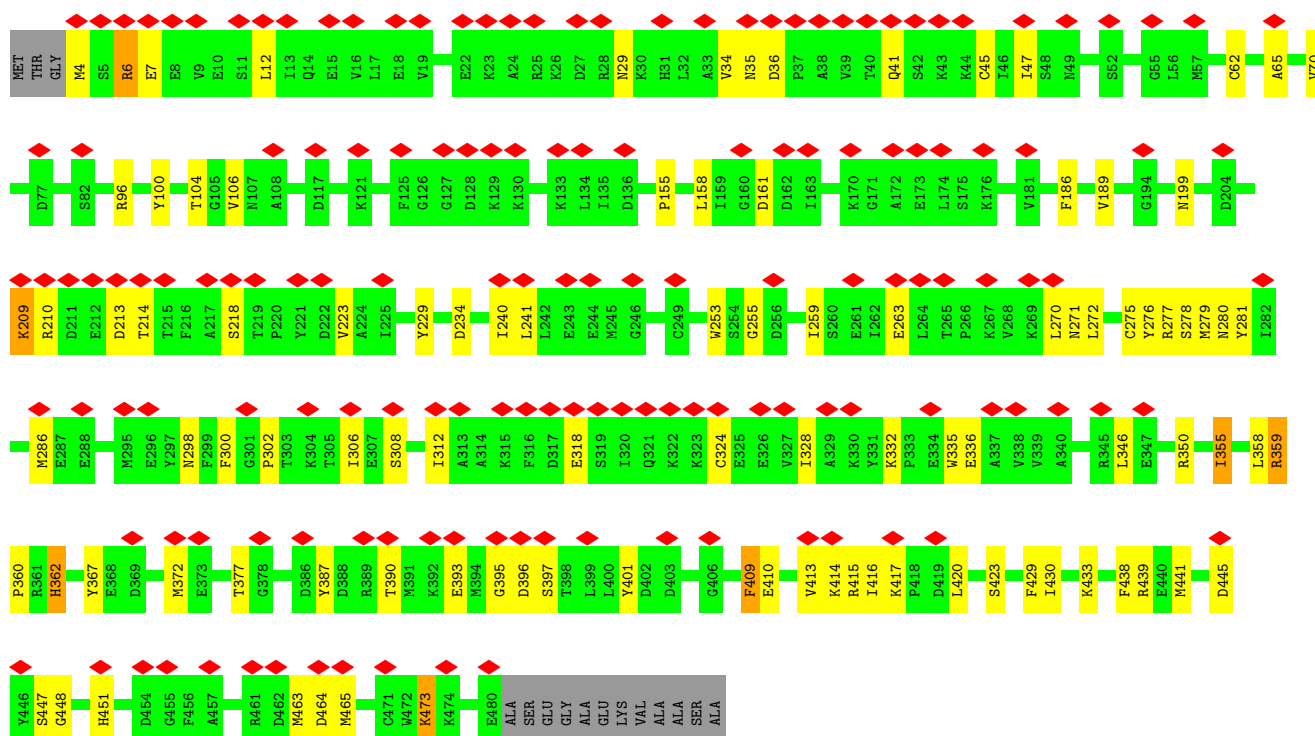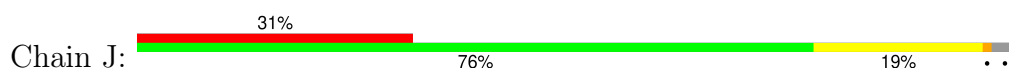• Molecule 2: Nitrogenase molybdenum-iron protein beta chain
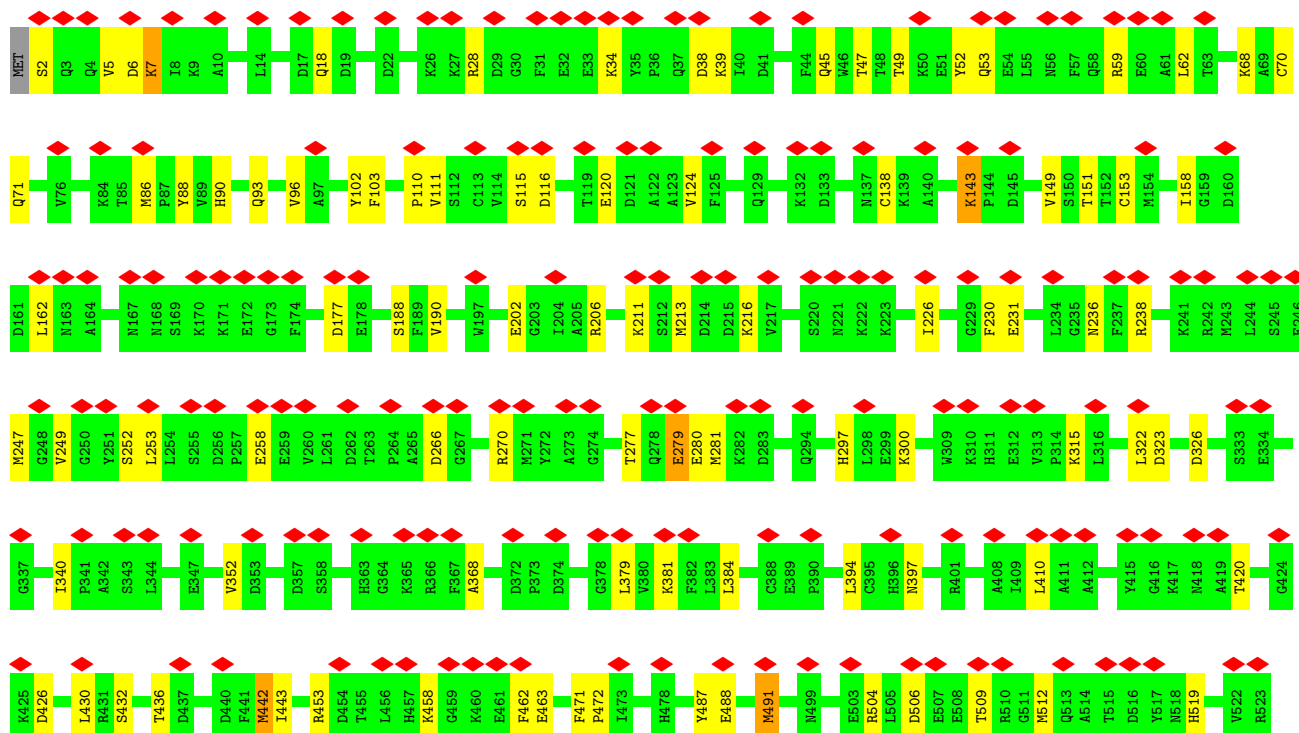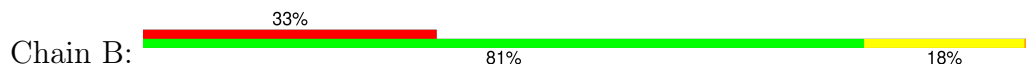
Chain B:

• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain D:

• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain I:

• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain K:

• Molecule 3: Nitrogenase iron protein 1

Chain E:

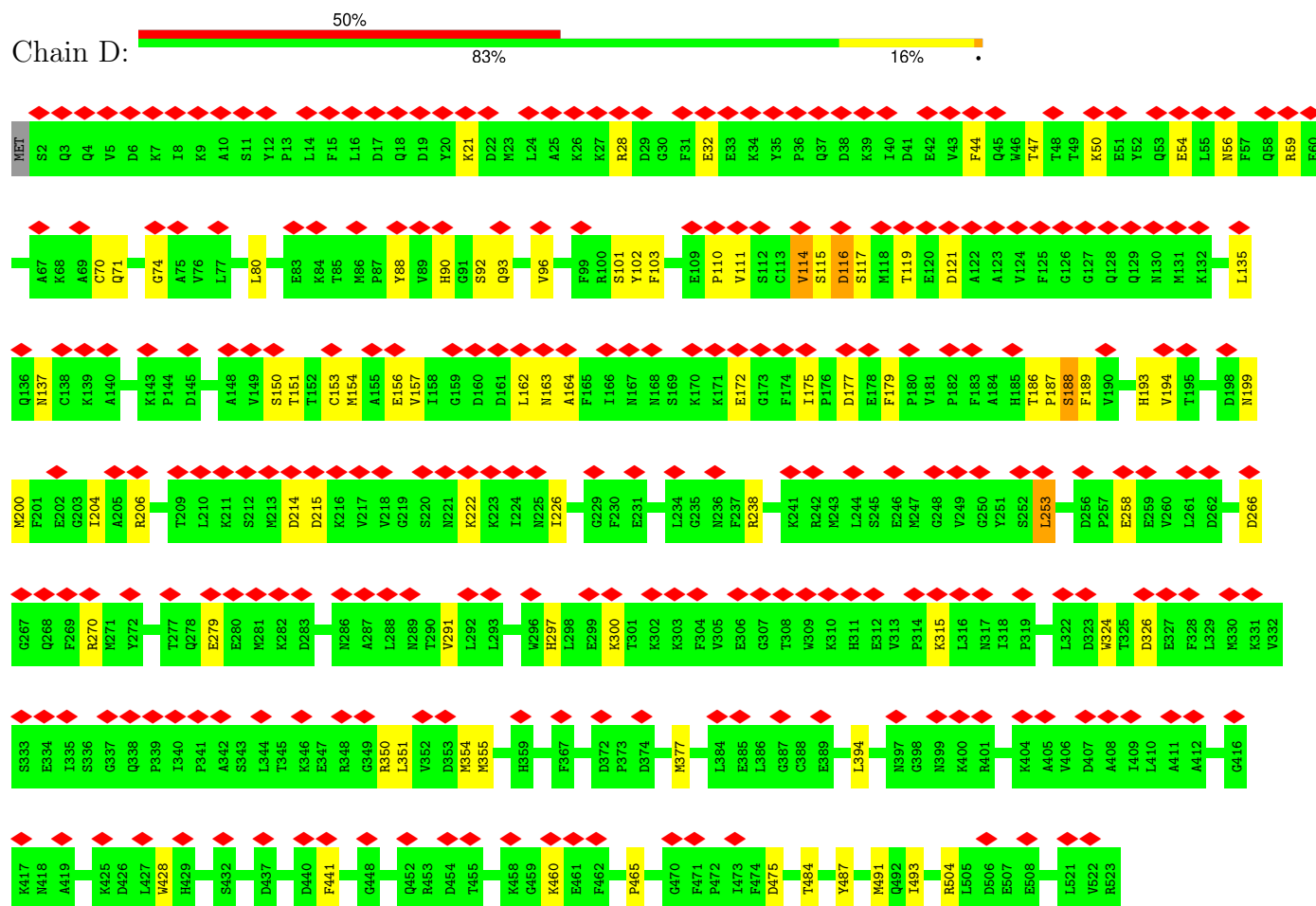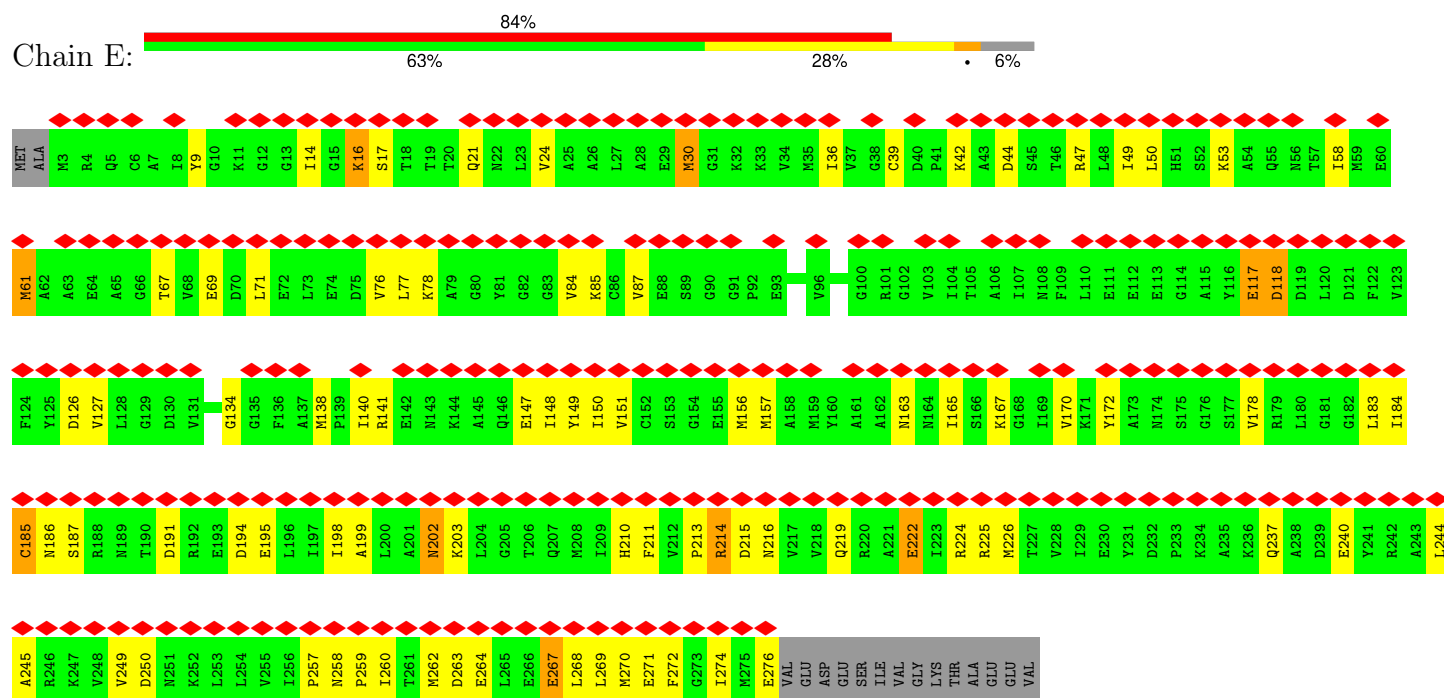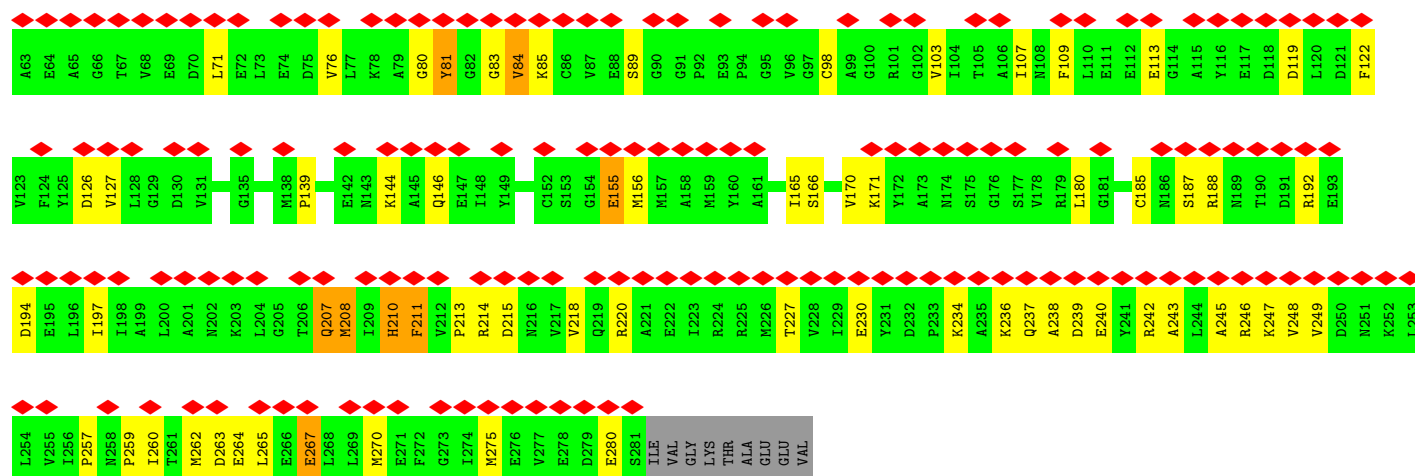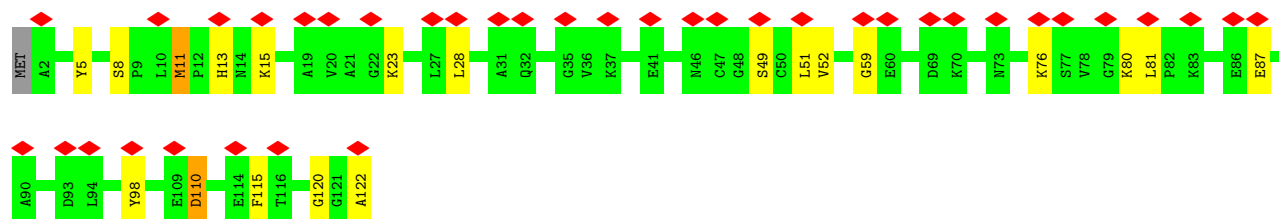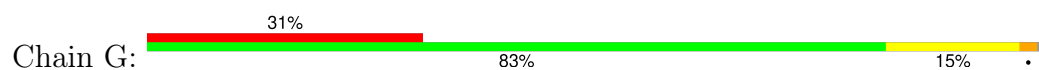• Molecule 3: Nitrogenase iron protein 1

Chain F:

• Molecule 3: Nitrogenase iron protein 1

Chain L:

• Molecule 3: Nitrogenase iron protein 1

Chain M:

A63 E64 A65 G66 T67 V68 E69 D70 L71 E72 L73 E74 D75 V76 L77 K78 A79 G80 Y81 G82 G83 V84 K85 C86 V87 E88 S89 G90 G91 P92 E93 P94 G95 V96 G97 C98 A99 G100 R101 G102 V103 I104 T105 A106 I107 N108 F109 L110 E111 E112 E113 G114 A115 Y116 E117 D118 D119 L120 D121 F122

V123 F124 Y125 D126 V127 L128 G129 D130 V131 G135 M138 P139 E142 N143 K144 A145 Q146 E147 I148 Y149 C152 S153 G154 E155 M156 M157 A158 M159 Y160 A161 I165 S166 V170 K171 Y172 A173 N174 S175 G176 S177 V178 R179 L180 G181 C185 N186 S187 R188 T190 N189 D191 R192 E193

D194 E195 L196 I197 I198 A199 L200 A201 N202 K203 L204 G205 T206 Q207 M208 I209 H210 F211 V212 P213 R214 D215 N216 V217 V218 Q219 R220 A221 E222 I223 R224 R225 M226 T227 V228 I229 E230 Y231 D232 P233 K234 A235 K236 Q237 A238 D239 E240 Y241 R242 A243 L244 A245 R246 K247 V248 V249 D250 N251 K252 L253

L254 V255 I256 P257 N258 P259 I260 T261 M262 D263 E264 L265 E266 E267 L268 L269 M270 E271 F272 G273 I274 M275 E276 V277 E278 D279 E280 S281 ILE VAL GLY LYS THR ALA GLU GLU VAL

• Molecule 4: Protein FeSII

Chain G:

31%
83% 15%

MET A2 Y5 S8 P9 L10 M11 P12 H13 N14 K15 A19 V20 A21 G22 K23 L27 L28 A31 Q32 G35 V36 K37 E41 N46 C47 G48 S49 C50 L51 V52 G59 E60 D69 K70 N73 K76 S77 V78 G79 K80 L81 P82 K83 E86 E87

A90 D93 L94 Y98 E109 D110 E114 F115 T116 G120 G121 A122

• Molecule 5: Protein FeSII

Chain N:

23%
81% 17%

MET A2 Y5 L10 M11 P12 H13 A19 V20 K23 K27 K28 K37 F40 D44 G45 N46 C47 G48 S49 C50 L51 V52 L57 D58 G59 E60 R61 D69 K70 E71 R72 V78 G79 K83 S84 E85 E86 E87 R92 D93 L94 L100 A101 C102 Q103

T107 D108 E109 D110 V113 E114 F115 T116 G117 E118 A122
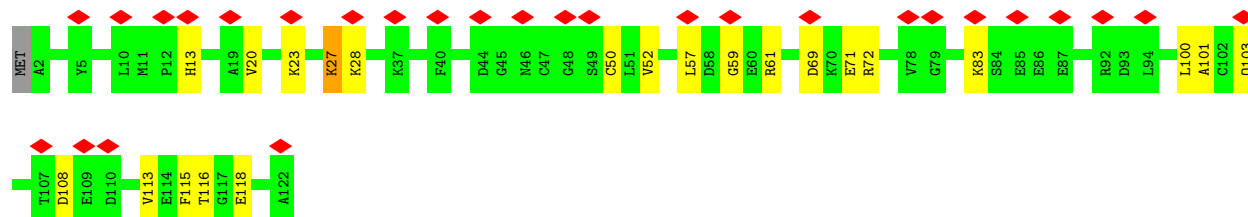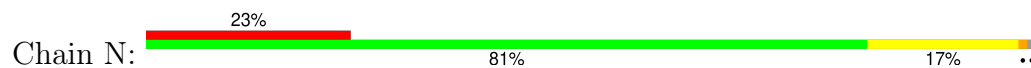
4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30209	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	60	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.704	Depositor
Minimum map value	-0.536	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.221	Depositor
Map size (Å)	563.2, 563.2, 563.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FE, ADP, FES, SF4, CLF, MG, ICS, HCA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.26	0/3881	0.48	1/5234 (0.0%)
1	C	0.27	0/3884	0.50	0/5237
1	H	0.30	0/3881	0.52	0/5234
1	J	0.32	0/3884	0.53	0/5237
2	B	0.26	0/4280	0.46	0/5786
2	D	0.25	0/4280	0.46	0/5786
2	I	0.26	0/4280	0.46	0/5786
2	K	0.25	0/4280	0.47	1/5786 (0.0%)
3	E	0.26	0/2101	0.54	1/2829 (0.0%)
3	F	0.28	0/2169	0.51	0/2921
3	L	0.26	0/2084	0.51	0/2807
3	M	0.27	0/2145	0.55	0/2889
4	G	0.29	0/931	0.50	0/1256
5	N	0.30	0/933	0.51	0/1256
All	All	0.27	0/43013	0.49	3/58044 (0.0%)

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	H	0	1
3	E	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	256	ASP	CB-CG-OD1	7.51	125.06	118.30
1	A	213	ASP	CB-CG-OD2	5.44	123.20	118.30
3	E	118	ASP	CB-CG-OD2	5.40	123.16	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	117	GLU	Peptide
1	H	357	GLY	Mainchain

5.2   Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3790	0	3727	56	0
1	C	3793	0	3735	89	0
1	H	3790	0	3727	58	0
1	J	3793	0	3734	64	0
2	B	4174	0	4088	50	0
2	D	4174	0	4088	53	0
2	I	4174	0	4088	55	0
2	K	4174	0	4089	64	0
3	E	2077	0	2089	54	0
3	F	2145	0	2157	40	0
3	L	2060	0	2074	56	0
3	M	2121	0	2124	56	0
4	G	918	0	936	12	0
5	N	920	0	940	13	0
6	A	14	0	7	1	0
6	C	14	0	7	0	0
6	H	14	0	6	0	0
6	J	14	0	6	0	0
7	A	18	0	0	3	0
7	C	18	0	0	1	0
7	H	18	0	0	2	0
7	J	18	0	0	2	0
8	A	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	15	0	0	0	0
8	H	15	0	0	0	0
8	K	15	0	0	0	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
9	I	1	0	0	0	0
9	K	1	0	0	0	0
10	E	27	0	12	1	0
10	F	27	0	12	1	0
10	L	27	0	12	2	0
10	M	27	0	12	4	0
11	E	1	0	0	0	0
11	F	1	0	0	0	0
11	L	1	0	0	0	0
11	M	1	0	0	0	0
12	F	8	0	0	0	0
12	L	8	0	0	1	0
13	G	4	0	0	0	0
13	N	4	0	0	0	0
14	A	73	0	0	1	0
14	B	86	0	0	2	0
14	C	97	0	0	4	0
14	D	73	0	0	1	0
14	E	78	0	0	1	0
14	F	88	0	0	3	0
14	G	26	0	0	0	0
14	H	83	0	0	1	0
14	I	108	0	0	1	0
14	J	74	0	0	1	0
14	K	100	0	0	5	0
14	L	77	0	0	2	0
14	M	94	0	0	4	0
14	N	19	0	0	0	0
All	All	43507	0	41670	677	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 8.

All (677) 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)
3:L:24:VAL:HG21	3:L:36:ILE:HD11	1.54	0.87
1:C:81:ILE:HG12	1:C:134:LEU:HD21	1.59	0.83
3:E:9:TYR:HB3	3:E:165:ILE:HD13	1.61	0.81
1:C:199:ASN:HD21	1:C:279:MET:HA	1.46	0.80
1:C:223:VAL:HG12	1:C:270:LEU:HB3	1.65	0.78
3:F:224:ARG:HB3	3:F:226:MET:HG3	1.66	0.77
1:C:219:THR:HG22	1:C:221:TYR:H	1.51	0.74
1:J:158:LEU:HD22	2:K:158:ILE:HD11	1.70	0.74
1:C:226:ILE:HG22	1:C:279:MET:HG2	1.69	0.74
1:C:142:PHE:O	1:C:145:ASN:ND2	2.23	0.72
3:F:16:LYS:N	10:F:302:ADP:O1B	2.22	0.71
1:C:22:GLU:OE2	1:C:22:GLU:N	2.21	0.71
1:C:275:CYS:HA	1:C:358:LEU:HD13	1.73	0.71
1:J:6:ARG:HH22	1:J:36:ASP:HB3	1.56	0.71
3:L:157:MET:SD	3:M:42:LYS:NZ	2.63	0.71
3:F:33:LYS:HG3	3:F:120:LEU:HA	1.72	0.69
3:E:185:CYS:HB3	3:E:211:PHE:HA	1.74	0.69
1:A:387:TYR:HA	1:A:390:THR:HG22	1.73	0.69
1:C:186:PHE:O	14:C:601:HOH:O	2.11	0.69
1:C:276:TYR:O	1:C:280:ASN:HB3	1.93	0.68
1:C:188:GLY:O	14:C:601:HOH:O	2.10	0.68
3:L:198:ILE:HD12	3:L:208:MET:HB2	1.75	0.68
1:J:308:SER:O	1:J:312:ILE:HG12	1.93	0.68
1:A:219:THR:HG22	1:A:221:TYR:H	1.60	0.67
2:B:509:THR:O	2:B:519:HIS:ND1	2.27	0.67
2:I:104:ASN:ND2	2:I:109:GLU:O	2.27	0.67
1:H:64:TYR:HH	1:H:82:SER:HG	1.42	0.67
1:A:96:ARG:NH2	7:A:502:ICS:S5A	2.66	0.66
2:B:90:HIS:ND1	2:B:116:ASP:OD2	2.28	0.66
1:C:275:CYS:SG	1:C:278:SER:OG	2.52	0.66
1:H:459:PHE:O	1:H:463:MET:HG2	1.94	0.66
1:H:142:PHE:O	1:H:145:ASN:ND2	2.29	0.66
1:H:251:ALA:HA	1:H:261:GLU:HB3	1.77	0.66
3:L:210:HIS:HB3	3:L:244:LEU:HD23	1.77	0.66
3:E:203:LYS:NZ	3:E:264:GLU:OE2	2.29	0.66
2:I:294:GLN:HG2	2:I:318:ILE:HD12	1.76	0.66
1:A:139:GLU:HG3	1:A:174:LEU:HD22	1.77	0.65
2:D:103:PHE:HB3	2:D:111:VAL:HG21	1.77	0.65
3:E:187:SER:HB3	3:E:213:PRO:HA	1.78	0.65
1:J:276:TYR:O	1:J:280:ASN:HB3	1.96	0.65
1:A:5:SER:HB3	1:A:8:GLU:HB3	1.77	0.65
1:C:12:LEU:HD13	1:C:415:ARG:HD3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:56:ASN:HD21	2:D:59:ARG:HH21	1.44	0.65
3:E:77:LEU:HD11	3:E:85:LYS:HB3	1.79	0.65
2:I:213:MET:HE1	2:I:216:LYS:HG3	1.77	0.65
1:J:433:LYS:NZ	2:K:263:THR:O	2.30	0.65
3:F:190:THR:HB	3:F:193:GLU:HB3	1.79	0.64
3:M:207:GLN:OE1	3:M:208:MET:N	2.30	0.64
2:K:103:PHE:HB3	2:K:111:VAL:HG21	1.80	0.64
3:L:24:VAL:HG12	3:L:34:VAL:HG21	1.79	0.64
1:A:318:GLU:HA	1:A:321:GLN:HG3	1.78	0.64
3:F:159:MET:HG2	3:F:200:LEU:HD22	1.79	0.64
1:H:226:ILE:HA	1:H:253:TRP:HB2	1.80	0.64
1:A:12:LEU:HD13	1:A:415:ARG:HE	1.64	0.63
3:F:101:ARG:HA	3:F:104:ILE:HD12	1.81	0.63
1:C:158:LEU:HD11	2:D:154:MET:HG3	1.81	0.63
3:M:260:ILE:HD11	3:M:265:LEU:HD13	1.81	0.63
1:A:212:GLU:OE2	1:A:212:GLU:N	2.29	0.62
1:C:284:ARG:NH2	14:C:603:HOH:O	2.31	0.62
3:M:23:LEU:HD11	3:M:248:VAL:HG21	1.82	0.62
1:C:53:GLN:OE1	2:D:137:ASN:ND2	2.33	0.61
1:C:308:SER:O	1:C:312:ILE:HD12	2.00	0.61
1:C:447:SER:OG	1:C:448:GLY:N	2.34	0.61
3:E:225:ARG:O	14:E:401:HOH:O	2.16	0.61
2:D:279:GLU:OE2	2:D:279:GLU:N	2.30	0.61
1:C:35:ASN:ND2	1:C:395:GLY:O	2.31	0.61
2:K:80:LEU:HD11	2:K:111:VAL:HG13	1.83	0.61
1:C:47:ILE:HD12	1:C:48:SER:H	1.65	0.60
2:K:266:ASP:OD2	2:K:270:ARG:NH2	2.34	0.60
1:H:11:SER:O	1:H:15:GLU:HG2	2.01	0.60
2:D:90:HIS:ND1	2:D:116:ASP:OD2	2.35	0.60
3:E:44:ASP:OD2	3:E:47:ARG:NH2	2.34	0.60
3:F:138:MET:HG2	3:F:142:GLU:HG3	1.83	0.60
1:J:189:VAL:O	2:K:93:GLN:NE2	2.34	0.60
3:L:195:GLU:HG2	3:L:272:PHE:HE2	1.65	0.60
3:F:171:LYS:HD3	3:F:172:TYR:CE2	2.37	0.60
2:I:56:ASN:OD1	2:I:59:ARG:NH1	2.34	0.60
3:L:185:CYS:SG	14:L:454:HOH:O	2.56	0.60
2:B:247:MET:HG2	2:B:249:VAL:HG23	1.84	0.60
3:L:4:ARG:NH1	3:L:147:GLU:OE2	2.35	0.60
3:F:238:ALA:HB1	3:F:242:ARG:HH21	1.66	0.60
1:H:359:ARG:HD2	1:H:444:TRP:HH2	1.66	0.60
1:J:359:ARG:HB2	7:J:502:ICS:S3A	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:484:THR:HG23	2:D:493:ILE:HD11	1.84	0.60
4:G:52:VAL:HG12	4:G:115:PHE:HB3	1.84	0.59
1:J:387:TYR:HA	1:J:390:THR:HG22	1.84	0.59
2:K:96:VAL:HG21	2:K:115:SER:HB2	1.84	0.59
2:K:121:ASP:OD1	2:K:122:ALA:N	2.35	0.59
3:E:194:ASP:OD1	3:E:194:ASP:N	2.35	0.59
2:I:322:LEU:HD22	2:I:355:MET:HE1	1.84	0.59
1:J:429:PHE:HB3	2:K:110:PRO:HD3	1.83	0.59
4:G:8:SER:HB3	4:G:11:MET:HG3	1.84	0.59
2:I:90:HIS:ND1	2:I:116:ASP:OD2	2.36	0.59
2:B:488:GLU:HA	2:B:491:MET:HG3	1.83	0.59
3:E:24:VAL:HG11	3:E:36:ILE:HD11	1.84	0.59
3:M:39:CYS:HB2	3:M:127:VAL:HG12	1.85	0.59
1:C:358:LEU:HD21	1:C:362:HIS:CD2	2.38	0.59
1:H:134:LEU:HG	2:I:62:LEU:HB2	1.84	0.59
3:M:29:GLU:OE1	3:M:242:ARG:NH1	2.36	0.59
3:M:243:ALA:HA	3:M:246:ARG:HD2	1.85	0.59
1:H:356:GLY:HA3	1:H:380:GLU:HG2	1.85	0.59
1:C:184:GLU:HB2	1:C:187:ARG:HG3	1.84	0.58
2:I:255:SER:H	2:I:276:THR:HG21	1.68	0.58
2:K:84:LYS:NZ	14:K:704:HOH:O	2.34	0.58
2:D:350:ARG:O	2:D:354:MET:HG3	2.02	0.58
1:J:306:ILE:HD12	1:J:328:ILE:HD13	1.84	0.58
1:J:275:CYS:HA	1:J:358:LEU:HD13	1.85	0.58
1:H:387:TYR:HA	1:H:390:THR:HG22	1.85	0.58
1:C:345:ARG:O	1:C:349:LYS:NZ	2.36	0.58
1:J:390:THR:HA	1:J:393:GLU:HB2	1.86	0.58
1:J:199:ASN:HD22	1:J:281:TYR:HD1	1.49	0.58
2:D:354:MET:SD	2:D:491:MET:HG2	2.43	0.58
2:B:226:ILE:HB	2:B:253:LEU:HD12	1.86	0.57
2:I:152:THR:HG22	2:I:154:MET:H	1.69	0.57
2:D:71:GLN:NE2	2:D:199:ASN:OD1	2.37	0.57
3:F:9:TYR:HB3	3:F:165:ILE:HD13	1.84	0.57
1:J:275:CYS:SG	1:J:278:SER:OG	2.60	0.57
3:F:141:ARG:HG3	3:F:172:TYR:CE1	2.38	0.57
1:J:35:ASN:ND2	1:J:395:GLY:O	2.37	0.57
2:B:323:ASP:OD2	2:B:381:LYS:NZ	2.37	0.57
1:C:356:GLY:HA2	1:C:380:GLU:HB2	1.86	0.57
2:I:91:GLY:HA3	2:I:152:THR:HB	1.85	0.57
1:A:136:ASP:O	1:A:140:THR:HG23	2.04	0.56
1:C:189:VAL:O	2:D:93:GLN:NE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:LYS:O	1:C:327:VAL:HG23	2.05	0.56
1:J:355:ILE:HG13	1:J:360:PRO:HG3	1.87	0.56
2:K:91:GLY:HA3	2:K:152:THR:HB	1.88	0.56
1:C:389:ARG:HA	1:C:392:LYS:HE3	1.86	0.56
2:D:96:VAL:HG21	2:D:115:SER:HB3	1.88	0.56
3:F:20:THR:O	3:F:24:VAL:HG23	2.06	0.56
2:I:379:LEU:HD21	2:I:443:ILE:HG21	1.88	0.56
1:J:417:LYS:NZ	14:J:604:HOH:O	2.39	0.56
1:A:133:LYS:O	1:A:137:GLU:HG3	2.06	0.56
2:B:71:GLN:NE2	2:B:190:VAL:O	2.26	0.56
1:C:357:GLY:HA3	7:C:502:ICS:S1A	2.45	0.56
2:K:90:HIS:ND1	2:K:116:ASP:OD1	2.35	0.56
2:D:200:MET:HE2	2:D:204:ILE:HG13	1.87	0.56
5:N:61:ARG:NH1	5:N:108:ASP:OD2	2.39	0.56
1:J:199:ASN:HD21	1:J:279:MET:HA	1.71	0.55
2:B:238:ARG:NE	2:B:258:GLU:OE1	2.31	0.55
2:I:19:ASP:OD1	2:I:20:TYR:N	2.39	0.55
3:L:195:GLU:O	3:L:198:ILE:HG22	2.06	0.55
1:C:226:ILE:HA	1:C:253:TRP:HB2	1.88	0.55
1:J:447:SER:OG	1:J:448:GLY:N	2.40	0.55
3:L:48:LEU:HD21	3:L:222:GLU:HG3	1.88	0.55
2:B:38:ASP:OD1	2:B:39:LYS:N	2.40	0.55
2:K:206:ARG:HG3	2:K:210:LEU:HD22	1.89	0.55
2:D:71:GLN:HG2	2:D:186:THR:HB	1.89	0.54
1:J:272:LEU:HD22	1:J:312:ILE:HD12	1.88	0.54
2:I:103:PHE:HB3	2:I:111:VAL:HG21	1.89	0.54
1:H:35:ASN:ND2	1:H:395:GLY:O	2.33	0.54
3:M:234:LYS:NZ	14:M:404:HOH:O	2.34	0.54
2:D:351:LEU:O	2:D:355:MET:HG3	2.06	0.54
1:H:357:GLY:HA3	7:H:502:ICS:S1A	2.48	0.54
1:H:385:ASP:HB2	1:H:389:ARG:HH12	1.73	0.54
2:K:178:GLU:OE2	2:K:178:GLU:N	2.37	0.54
3:M:16:LYS:N	10:M:301:ADP:O1B	2.39	0.54
3:M:246:ARG:NH2	14:M:408:HOH:O	2.40	0.54
3:L:266:GLU:OE2	3:M:47:ARG:NH2	2.40	0.53
2:D:172:GLU:OE2	2:D:172:GLU:N	2.42	0.53
3:E:224:ARG:HB3	3:E:226:MET:HG2	1.88	0.53
3:L:20:THR:O	3:L:24:VAL:HG22	2.08	0.53
3:M:9:TYR:HB3	3:M:165:ILE:HD13	1.89	0.53
2:K:129:GLN:NE2	2:K:133:ASP:OD1	2.40	0.53
2:B:103:PHE:HB3	2:B:111:VAL:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:TYR:OH	1:C:317:ASP:OD2	2.27	0.53
3:L:57:THR:HB	3:L:90:GLY:H	1.74	0.53
5:N:71:GLU:HG3	5:N:100:LEU:HD12	1.89	0.53
2:B:143:LYS:NZ	14:B:704:HOH:O	2.40	0.53
3:E:50:LEU:HD11	3:E:78:LYS:HB3	1.90	0.53
2:B:151:THR:HG23	2:B:162:LEU:HD11	1.91	0.53
2:B:96:VAL:HG21	2:B:115:SER:HB3	1.91	0.53
2:B:202:GLU:OE2	2:B:206:ARG:NH2	2.42	0.53
1:C:378:GLY:HA3	1:C:401:TYR:CD1	2.44	0.53
2:D:93:GLN:OE1	2:D:117:SER:OG	2.19	0.53
2:D:215:ASP:OD1	2:D:215:ASP:N	2.41	0.53
3:E:219:GLN:O	3:E:222:GLU:HG3	2.09	0.53
3:E:224:ARG:HE	3:F:285:LYS:HB2	1.74	0.53
1:A:355:ILE:HG22	1:A:356:GLY:H	1.75	0.52
1:J:155:PRO:HB3	2:K:157:VAL:HG21	1.91	0.52
1:A:93:ARG:HG3	1:A:113:ASN:HB2	1.91	0.52
2:B:279:GLU:OE1	2:B:279:GLU:N	2.42	0.52
3:E:269:LEU:HD22	3:E:274:ILE:HB	1.91	0.52
2:I:116:ASP:OD1	2:I:116:ASP:N	2.35	0.52
2:K:86:MET:HE2	2:K:87:PRO:HD2	1.92	0.52
3:M:192:ARG:NH1	14:M:410:HOH:O	2.42	0.52
1:A:22:GLU:OE2	1:A:25:ARG:NH2	2.43	0.52
1:J:100:TYR:HH	1:J:104:THR:HG1	1.57	0.52
1:A:252:GLN:NE2	1:A:255:GLY:O	2.42	0.52
2:D:135:LEU:HD13	2:D:175:ILE:HD13	1.91	0.52
3:L:46:THR:HG21	3:L:86:CYS:HB3	1.91	0.52
1:A:234:ASP:HB3	1:A:451:HIS:ND1	2.25	0.51
2:B:277:THR:HB	2:B:280:GLU:HG3	1.92	0.51
1:C:222:ASP:HB3	1:C:268:VAL:HA	1.91	0.51
3:E:264:GLU:HA	3:E:267:GLU:HG3	1.93	0.51
1:H:81:ILE:HD12	1:H:134:LEU:HD21	1.92	0.51
2:I:70:CYS:HB2	2:I:188:SER:HB3	1.92	0.51
3:M:39:CYS:HB3	3:M:103:VAL:HG22	1.92	0.51
3:E:237:GLN:NE2	3:E:240:GLU:OE1	2.43	0.51
1:J:209:LYS:HB3	1:J:263:GLU:OE2	2.10	0.51
2:I:119:THR:HG23	2:I:121:ASP:H	1.76	0.51
1:J:306:ILE:HG23	1:J:328:ILE:HD13	1.92	0.51
3:M:11:LYS:O	3:M:14:ILE:HG12	2.10	0.51
1:C:354:TYR:CZ	1:C:404:VAL:HG12	2.46	0.51
2:I:381:LYS:NZ	2:I:385:GLU:OE2	2.44	0.51
2:K:170:LYS:HG2	2:K:177:ASP:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:15:GLY:HA2	10:L:301:ADP:H5'1	1.92	0.51
3:E:67:THR:HG23	3:E:69:GLU:H	1.76	0.51
1:J:62:CYS:HB3	2:K:94:GLY:HA3	1.92	0.51
2:K:224:ILE:HD11	2:K:336:SER:HB2	1.92	0.51
2:K:445:ASN:ND2	14:K:710:HOH:O	2.44	0.51
1:C:430:ILE:HG13	2:D:110:PRO:HB3	1.93	0.51
3:E:140:ILE:HG23	3:E:178:VAL:HG11	1.93	0.51
4:G:76:LYS:HG3	4:G:81:LEU:HD23	1.93	0.51
1:J:300:PHE:CD2	1:J:362:HIS:HB3	2.46	0.51
2:K:247:MET:HB2	2:K:341:PRO:HD3	1.93	0.51
2:D:324:TRP:HH2	2:D:377:MET:HG2	1.75	0.51
1:H:5:SER:HB2	1:H:8:GLU:OE1	2.11	0.51
1:J:302:PRO:O	1:J:306:ILE:HG12	2.11	0.51
2:K:384:LEU:HD11	2:K:410:LEU:HD23	1.92	0.51
3:L:185:CYS:HB2	3:L:197:ILE:HG21	1.93	0.51
3:M:245:ALA:O	3:M:249:VAL:HG23	2.11	0.51
1:C:49:ASN:OD1	1:C:383:HIS:NE2	2.44	0.50
2:D:90:HIS:HB3	2:D:151:THR:HG22	1.93	0.50
2:I:105:ARG:NH1	14:I:710:HOH:O	2.39	0.50
3:L:192:ARG:HD2	3:L:195:GLU:OE1	2.11	0.50
1:A:74:PRO:HG3	1:A:98:ASN:HD22	1.76	0.50
1:A:158:LEU:HD13	2:B:158:ILE:HD13	1.94	0.50
2:B:213:MET:HE1	2:B:216:LYS:HG3	1.92	0.50
1:H:301:GLY:O	1:H:305:THR:OG1	2.24	0.50
1:H:364:ILE:HG12	1:H:374:VAL:HG21	1.93	0.50
3:M:242:ARG:O	3:M:246:ARG:HD2	2.11	0.50
2:I:397:ASN:OD1	2:I:397:ASN:N	2.41	0.50
1:J:234:ASP:HB3	1:J:451:HIS:ND1	2.26	0.50
1:C:57:MET:H	2:D:114:VAL:HG23	1.77	0.50
1:H:139:GLU:HG3	1:H:174:LEU:HD13	1.93	0.50
1:C:350:ARG:NH1	14:C:609:HOH:O	2.45	0.50
1:C:373:GLU:N	1:C:373:GLU:OE1	2.45	0.50
2:K:152:THR:HG22	2:K:154:MET:H	1.77	0.50
1:A:35:ASN:ND2	1:A:395:GLY:O	2.37	0.49
1:C:427:GLU:HB3	1:C:431:PHE:CE2	2.47	0.49
2:K:83:GLU:HG2	2:K:84:LYS:HG3	1.93	0.49
3:M:185:CYS:SG	3:M:197:ILE:HG13	2.52	0.49
1:H:354:TYR:CZ	1:H:404:VAL:HG12	2.47	0.49
1:H:429:PHE:O	1:H:433:LYS:HG2	2.11	0.49
1:H:8:GLU:HA	1:H:11:SER:OG	2.12	0.49
2:I:246:GLU:OE2	2:I:343:SER:OG	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:165:ILE:O	3:L:169:ILE:HG12	2.12	0.49
3:L:261:THR:HG23	3:L:264:GLU:H	1.77	0.49
3:M:238:ALA:HB1	3:M:242:ARG:HH21	1.78	0.49
2:B:231:GLU:CD	2:B:236:ASN:HD22	2.16	0.49
3:F:2:ALA:N	14:F:409:HOH:O	2.44	0.49
3:M:80:GLY:O	3:M:84:VAL:HG12	2.13	0.49
1:C:6:ARG:HH22	1:C:36:ASP:HB2	1.77	0.49
1:C:351:VAL:HG12	1:C:420:LEU:HB3	1.95	0.49
4:G:59:GLY:HA3	5:N:13:HIS:HB3	1.94	0.49
3:M:187:SER:HB2	3:M:211:PHE:CE1	2.47	0.49
1:C:97:ARG:NH1	1:C:443:SER:O	2.45	0.49
3:E:150:ILE:HB	3:E:183:LEU:HD23	1.94	0.49
1:H:334:GLU:O	1:H:338:VAL:HG23	2.13	0.49
3:L:140:ILE:HG23	3:L:178:VAL:HG11	1.94	0.49
1:J:259:ILE:O	1:J:263:GLU:HG2	2.13	0.49
2:K:70:CYS:HB2	2:K:188:SER:HB2	1.95	0.49
3:M:9:TYR:CZ	3:M:127:VAL:HG21	2.48	0.49
1:A:359:ARG:HB2	7:A:502:ICS:S3A	2.53	0.49
2:D:326:ASP:OD1	2:D:487:TYR:OH	2.27	0.49
3:E:71:LEU:HD21	3:E:76:VAL:HG13	1.95	0.49
3:E:210:HIS:HB3	3:E:244:LEU:HD12	1.95	0.49
1:J:6:ARG:HG3	1:J:34:VAL:HG11	1.94	0.49
3:L:187:SER:HB2	3:L:211:PHE:CE2	2.48	0.49
1:A:59:ILE:HG23	1:A:426:LYS:HE2	1.95	0.48
3:F:243:ALA:O	3:F:246:ARG:HG2	2.13	0.48
2:B:326:ASP:OD1	2:B:487:TYR:OH	2.29	0.48
3:E:117:GLU:HG2	3:E:118:ASP:HB3	1.94	0.48
3:E:215:ASP:OD1	3:E:216:ASN:N	2.46	0.48
1:J:12:LEU:HD13	1:J:415:ARG:HG3	1.95	0.48
2:D:44:PHE:O	2:D:47:THR:OG1	2.30	0.48
2:I:231:GLU:CD	2:I:236:ASN:HD22	2.17	0.48
2:B:322:LEU:HD11	2:B:352:VAL:HG22	1.95	0.48
3:E:191:ASP:OD2	3:E:191:ASP:N	2.42	0.48
3:L:14:ILE:HD11	3:L:153:SER:HB3	1.95	0.48
3:L:214:ARG:NH2	14:L:413:HOH:O	2.46	0.48
5:N:52:VAL:HG12	5:N:115:PHE:HB3	1.95	0.48
1:A:427:GLU:N	1:A:427:GLU:OE2	2.46	0.48
2:B:86:MET:HG2	2:B:138:CYS:SG	2.54	0.48
3:E:260:ILE:HG23	3:E:264:GLU:HG2	1.96	0.48
3:M:210:HIS:CE1	3:M:240:GLU:HG3	2.48	0.48
1:C:145:ASN:O	1:C:176:LYS:NZ	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:195:GLU:HG2	3:L:272:PHE:CE2	2.48	0.48
2:D:116:ASP:OD1	2:D:116:ASP:N	2.42	0.48
3:L:242:ARG:O	3:L:246:ARG:HG2	2.13	0.48
3:M:146:GLN:OE1	3:M:146:GLN:HA	2.13	0.48
2:B:379:LEU:HD21	2:B:443:ILE:HG21	1.94	0.48
3:F:47:ARG:NH2	14:F:407:HOH:O	2.39	0.48
1:H:60:ARG:HG3	1:H:380:GLU:HB2	1.95	0.48
1:J:210:ARG:HH11	1:J:263:GLU:HB2	1.79	0.48
1:J:346:LEU:HD21	1:J:464:ASP:HA	1.96	0.48
2:K:487:TYR:O	2:K:491:MET:HG3	2.13	0.48
3:L:5:GLN:HB3	3:L:145:ALA:HA	1.95	0.48
3:M:139:PRO:HA	3:M:144:LYS:HB2	1.96	0.48
3:E:16:LYS:HD2	3:E:126:ASP:OD1	2.14	0.48
3:E:245:ALA:O	3:E:249:VAL:HG23	2.14	0.48
2:I:59:ARG:NH2	2:I:426:ASP:OD2	2.47	0.48
2:I:59:ARG:NE	2:I:62:LEU:O	2.43	0.48
1:J:423:SER:HB3	1:J:438:PHE:HZ	1.79	0.48
1:A:134:LEU:O	1:A:138:VAL:HG23	2.14	0.48
1:A:224:ALA:HB2	1:A:268:VAL:HG21	1.96	0.48
1:A:341:LYS:HD3	2:B:5:VAL:HG22	1.95	0.48
2:B:463:GLU:OE2	2:B:504:ARG:NH1	2.30	0.48
3:E:215:ASP:HB2	3:E:237:GLN:OE1	2.14	0.48
1:H:338:VAL:HG11	1:H:457:ALA:HA	1.96	0.48
2:I:108:ARG:NH2	2:K:523:ARG:OXT	2.46	0.48
2:I:153:CYS:O	2:I:157:VAL:HG23	2.14	0.48
1:C:332:LYS:HA	1:C:335:TRP:NE1	2.29	0.47
3:F:260:ILE:HD11	3:F:265:LEU:HG	1.96	0.47
5:N:50:CYS:HB2	5:N:101:ALA:HB3	1.96	0.47
1:A:276:TYR:O	1:A:280:ASN:HB3	2.14	0.47
3:E:53:LYS:NZ	3:F:263:ASP:OD1	2.43	0.47
1:H:207:LEU:HD22	1:H:282:ILE:HD11	1.95	0.47
3:L:180:LEU:HG	3:L:206:THR:HG21	1.95	0.47
2:I:6:ASP:OD1	2:I:6:ASP:N	2.43	0.47
2:I:299:GLU:O	2:I:303:LYS:HG2	2.14	0.47
2:K:167:ASN:O	2:K:171:LYS:HG2	2.14	0.47
1:A:332:LYS:HA	1:A:335:TRP:NE1	2.28	0.47
2:B:340:ILE:HG21	1:C:479:TRP:CE2	2.49	0.47
2:D:28:ARG:HA	2:D:32:GLU:HB2	1.96	0.47
3:F:226:MET:HE3	3:F:230:GLU:HG2	1.96	0.47
1:H:12:LEU:HD13	1:H:415:ARG:HG2	1.95	0.47
1:H:323:LYS:O	1:H:327:VAL:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:326:ASP:OD1	2:K:487:TYR:OH	2.27	0.47
3:L:133:CYS:HB2	12:L:303:SF4:S2	2.55	0.47
2:D:56:ASN:ND2	2:D:59:ARG:HH21	2.12	0.47
2:I:324:TRP:HH2	2:I:377:MET:HG2	1.79	0.47
3:E:268:LEU:O	3:E:271:GLU:HG2	2.14	0.47
3:F:279:ASP:OD1	3:F:281:SER:OG	2.25	0.47
1:J:158:LEU:HD11	2:K:154:MET:HG3	1.97	0.47
1:J:223:VAL:HG12	1:J:270:LEU:HB3	1.97	0.47
2:K:119:THR:HG22	2:K:120:GLU:N	2.30	0.47
1:H:161:ASP:O	1:H:182:ARG:NH2	2.37	0.47
2:K:86:MET:HG2	2:K:138:CYS:SG	2.54	0.47
2:D:199:ASN:ND2	2:D:300:LYS:HE3	2.30	0.47
3:F:73:LEU:HD11	3:F:77:LEU:HD22	1.97	0.47
2:K:109:GLU:HG3	2:K:261:LEU:O	2.14	0.47
3:M:22:ASN:OD1	3:M:227:THR:OG1	2.26	0.47
3:M:45:SER:HB2	3:M:126:ASP:OD2	2.15	0.47
1:C:170:LYS:HD2	1:C:170:LYS:HA	1.59	0.47
3:E:170:VAL:HG23	3:E:257:PRO:HG2	1.97	0.47
1:H:10:GLU:OE1	1:H:14:GLN:NE2	2.48	0.47
2:K:105:ARG:NH1	14:K:708:HOH:O	2.37	0.47
3:M:81:TYR:OH	3:M:230:GLU:HB3	2.15	0.47
1:C:394:MET:SD	1:C:395:GLY:N	2.88	0.46
3:E:167:LYS:HG2	3:E:259:PRO:HB3	1.97	0.46
3:F:101:ARG:O	3:F:105:THR:HG23	2.15	0.46
2:K:6:ASP:OD2	2:K:6:ASP:N	2.33	0.46
3:L:227:THR:HG22	3:L:230:GLU:HG3	1.97	0.46
1:A:189:VAL:O	2:B:93:GLN:NE2	2.48	0.46
2:I:39:LYS:O	2:I:43:VAL:HG23	2.15	0.46
2:B:384:LEU:HD11	2:B:410:LEU:HD23	1.98	0.46
3:E:140:ILE:HG12	3:E:148:ILE:HD11	1.97	0.46
3:F:219:GLN:O	3:F:222:GLU:HG2	2.15	0.46
3:M:187:SER:HB3	3:M:213:PRO:HA	1.97	0.46
3:M:270:MET:HG3	3:M:275:MET:HG2	1.96	0.46
1:H:10:GLU:O	1:H:14:GLN:NE2	2.49	0.46
1:H:162:ASP:OD1	5:N:20:VAL:HG12	2.15	0.46
1:J:106:VAL:HG11	2:K:40:ILE:HG23	1.97	0.46
1:J:298:ASN:HD21	1:J:362:HIS:HA	1.79	0.46
3:M:264:GLU:HA	3:M:267:GLU:HG3	1.97	0.46
1:C:234:ASP:HB3	1:C:451:HIS:ND1	2.31	0.46
1:C:405:THR:OG1	1:C:408:GLU:HG3	2.16	0.46
3:E:17:SER:O	3:E:21:GLN:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:49:ILE:HD13	3:L:84:VAL:HG21	1.98	0.46
1:A:161:ASP:O	1:A:182:ARG:NH2	2.47	0.46
1:C:270:LEU:HD11	1:C:295:MET:HG2	1.97	0.46
1:A:355:ILE:HB	1:A:360:PRO:HD3	1.98	0.46
3:E:276:GLU:HB3	3:F:219:GLN:HB3	1.98	0.46
1:H:225:ILE:HD11	1:H:242:LEU:HD12	1.98	0.46
1:H:230:ASN:HA	1:H:235:ALA:H	1.80	0.46
2:K:199:ASN:OD1	2:K:300:LYS:HE2	2.16	0.46
1:A:378:GLY:HA3	1:A:401:TYR:O	2.16	0.46
2:D:315:LYS:HA	2:D:315:LYS:HD2	1.66	0.46
1:H:359:ARG:HB2	7:H:502:ICS:S3A	2.55	0.46
1:J:7:GLU:OE1	1:J:7:GLU:N	2.47	0.46
1:J:417:LYS:HE2	1:J:417:LYS:HB2	1.80	0.46
3:L:214:ARG:HG3	10:L:301:ADP:C2	2.50	0.46
3:M:263:ASP:OD1	3:M:264:GLU:N	2.49	0.46
1:C:223:VAL:HG11	1:C:247:LEU:HD13	1.97	0.46
1:C:413:VAL:HG21	1:C:431:PHE:CE1	2.50	0.46
2:D:177:ASP:OD2	2:D:177:ASP:N	2.44	0.46
2:D:226:ILE:HD13	2:D:291:VAL:HB	1.97	0.46
1:J:396:ASP:OD2	1:J:397:SER:N	2.49	0.46
1:A:459:PHE:O	1:A:463:MET:HG2	2.16	0.46
1:C:432:GLN:HG2	1:C:472:TRP:HH2	1.81	0.46
3:F:44:ASP:OD1	3:F:44:ASP:N	2.49	0.46
3:F:166:SER:O	3:F:170:VAL:HG12	2.16	0.46
1:J:415:ARG:NH1	1:J:415:ARG:HB3	2.31	0.46
2:B:59:ARG:HD3	2:B:62:LEU:HD23	1.97	0.45
1:H:214:THR:O	1:H:214:THR:OG1	2.34	0.45
1:H:433:LYS:HE3	2:K:353:ASP:OD2	2.16	0.45
2:K:119:THR:HG22	2:K:120:GLU:H	1.80	0.45
1:A:346:LEU:HD21	1:A:464:ASP:HA	1.98	0.45
1:A:430:ILE:HG13	2:B:110:PRO:HB3	1.98	0.45
2:I:299:GLU:OE1	2:I:401:ARG:NH2	2.50	0.45
1:C:51:LYS:HB3	1:C:51:LYS:HE3	1.73	0.45
1:H:209:LYS:HB3	1:H:263:GLU:HG2	1.96	0.45
2:I:96:VAL:HG21	2:I:115:SER:HB2	1.98	0.45
1:A:149:SER:OG	1:A:151:GLN:NE2	2.48	0.45
1:C:387:TYR:OH	1:C:402:ASP:HB2	2.17	0.45
2:D:56:ASN:ND2	2:D:428:TRP:HD1	2.14	0.45
3:E:263:ASP:OD2	3:E:264:GLU:N	2.49	0.45
3:F:210:HIS:HB3	3:F:244:LEU:HD12	1.97	0.45
3:M:53:LYS:HD3	3:M:53:LYS:HA	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ILE:HG21	1:C:78:MET:HG3	1.98	0.45
2:D:350:ARG:NH1	14:D:707:HOH:O	2.41	0.45
1:H:103:THR:OG1	2:K:513:GLN:NE2	2.50	0.45
2:K:401:ARG:HG3	2:K:401:ARG:HH11	1.81	0.45
2:D:475:ASP:OD1	2:D:475:ASP:N	2.39	0.45
1:A:26:LYS:HE3	1:A:26:LYS:HB3	1.59	0.45
3:E:147:GLU:OE2	3:E:149:TYR:OH	2.31	0.45
1:H:53:GLN:HB2	1:H:56:LEU:HD12	1.98	0.45
1:J:324:CYS:O	1:J:328:ILE:HG13	2.16	0.45
5:N:69:ASP:OD2	5:N:72:ARG:NH2	2.36	0.45
1:A:145:ASN:OD1	1:A:176:LYS:NZ	2.50	0.45
1:A:185:GLY:HA3	8:A:503:CLF:S2A	2.57	0.45
2:B:394:LEU:HD13	2:B:430:LEU:HB2	1.98	0.45
2:I:151:THR:HG23	2:I:162:LEU:HD11	1.99	0.45
1:A:359:ARG:NH1	7:A:502:ICS:S4B	2.91	0.45
1:H:184:GLU:OE1	1:H:187:ARG:NE	2.34	0.45
1:J:423:SER:HB3	1:J:438:PHE:CZ	2.52	0.45
3:L:6:CYS:HA	3:L:147:GLU:O	2.16	0.45
1:C:324:CYS:O	1:C:328:ILE:HD12	2.18	0.44
2:D:21:LYS:HE2	2:D:21:LYS:HB3	1.60	0.44
1:H:20:TYR:O	1:H:25:ARG:NH2	2.50	0.44
2:D:88:TYR:O	2:D:150:SER:N	2.44	0.44
3:F:21:GLN:HG2	3:F:49:ILE:HG13	1.98	0.44
1:H:258:SER:OG	1:H:261:GLU:HG3	2.17	0.44
2:I:289:ASN:ND2	2:I:312:GLU:O	2.44	0.44
2:B:202:GLU:HG3	2:B:300:LYS:HG2	2.00	0.44
1:H:176:LYS:NZ	14:H:605:HOH:O	2.44	0.44
2:I:266:ASP:OD2	2:I:270:ARG:NH2	2.41	0.44
1:A:350:ARG:NH1	14:A:601:HOH:O	2.50	0.44
1:H:253:TRP:HA	1:H:254:SER:HA	1.66	0.44
1:H:265:THR:HG22	1:H:286:MET:HE3	1.99	0.44
2:I:221:ASN:O	2:I:222:LYS:HG2	2.17	0.44
3:L:167:LYS:HG2	3:L:259:PRO:HB3	1.99	0.44
2:B:18:GLN:NE2	14:B:707:HOH:O	2.50	0.44
3:L:24:VAL:HB	3:L:34:VAL:HG11	1.99	0.44
2:B:45:GLN:O	2:B:49:THR:HG23	2.18	0.44
3:E:58:ILE:HG12	3:E:76:VAL:HG11	2.00	0.44
1:H:359:ARG:HD2	1:H:444:TRP:CH2	2.50	0.44
2:K:44:PHE:O	2:K:47:THR:OG1	2.31	0.44
3:M:24:VAL:HG22	3:M:34:VAL:HG21	2.00	0.44
1:C:59:ILE:HG21	1:C:354:TYR:HE2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:80:LEU:HD12	2:D:80:LEU:HA	1.87	0.44
2:K:376:VAL:O	2:K:380:VAL:HG23	2.17	0.44
1:A:81:ILE:HD12	1:A:134:LEU:HD21	1.99	0.44
3:E:14:ILE:O	3:E:186:ASN:ND2	2.46	0.44
3:M:34:VAL:HG12	3:M:122:PHE:HB2	2.00	0.44
1:A:191:GLN:NE2	6:A:501:HCA:O1	2.47	0.44
3:F:24:VAL:HG21	3:F:36:ILE:HD11	1.99	0.44
2:I:354:MET:SD	2:I:491:MET:HG2	2.57	0.44
2:I:458:LYS:HG2	2:I:462:PHE:CD2	2.53	0.44
3:L:245:ALA:O	3:L:249:VAL:HG12	2.18	0.44
3:M:109:PHE:O	3:M:113:GLU:HG2	2.17	0.44
4:G:49:SER:HA	4:G:120:GLY:H	1.82	0.43
2:K:322:LEU:HD13	2:K:351:LEU:HD23	2.00	0.43
3:L:96:VAL:HG22	3:M:171:LYS:HE2	2.00	0.43
1:A:253:TRP:HA	1:A:254:SER:HA	1.64	0.43
2:D:74:GLY:HA3	2:D:193:HIS:O	2.18	0.43
3:F:148:ILE:HG21	3:F:169:ILE:HD11	2.00	0.43
3:F:183:LEU:HD13	3:F:206:THR:HG21	1.99	0.43
1:H:179:VAL:HG13	1:H:205:TRP:HB2	1.99	0.43
2:I:28:ARG:NH1	2:I:29:ASP:OD2	2.51	0.43
2:I:512:MET:HG3	2:I:516:ASP:OD1	2.18	0.43
2:K:223:LYS:O	2:K:288:LEU:HD12	2.18	0.43
3:M:166:SER:O	3:M:170:VAL:HG13	2.17	0.43
3:M:214:ARG:HG3	10:M:301:ADP:C2	2.53	0.43
1:A:378:GLY:HA3	1:A:401:TYR:CD1	2.53	0.43
2:D:70:CYS:HB2	2:D:188:SER:HB2	2.00	0.43
3:E:163:ASN:O	3:E:167:LYS:HG3	2.18	0.43
2:B:266:ASP:OD2	2:B:270:ARG:NH2	2.43	0.43
3:E:195:GLU:HG3	3:E:272:PHE:CE2	2.54	0.43
2:K:59:ARG:HD3	2:K:62:LEU:HD23	2.00	0.43
3:L:152:CYS:SG	3:L:183:LEU:HD22	2.58	0.43
3:L:261:THR:HG22	3:L:264:GLU:HB2	2.01	0.43
3:M:170:VAL:HG11	3:M:259:PRO:HD3	2.00	0.43
1:C:462:ASP:HA	1:C:465:MET:HG2	2.00	0.43
3:E:141:ARG:HG3	3:E:172:TYR:CE1	2.53	0.43
1:H:306:ILE:HG23	1:H:328:ILE:HD13	2.00	0.43
1:H:357:GLY:O	1:H:379:TYR:HD2	2.00	0.43
2:K:50:LYS:HB2	2:K:50:LYS:HE2	1.75	0.43
2:K:219:GLY:HA2	2:K:288:LEU:HG	2.00	0.43
1:C:89:GLY:O	1:C:113:ASN:ND2	2.52	0.43
1:C:428:LYS:HB2	1:C:440:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:13:HIS:HB3	5:N:59:GLY:HA3	2.01	0.43
4:G:51:LEU:HD21	4:G:80:LYS:HG3	2.00	0.43
1:H:77:ASP:OD2	1:H:258:SER:HB2	2.18	0.43
3:M:24:VAL:HG21	3:M:36:ILE:HG13	2.00	0.43
2:B:28:ARG:HG3	2:B:34:LYS:HD2	2.01	0.43
1:C:165:SER:O	1:C:169:VAL:HG12	2.17	0.43
3:E:39:CYS:HB2	3:E:127:VAL:HG12	2.01	0.43
2:I:341:PRO:HD2	2:I:344:LEU:HD12	2.00	0.43
1:J:332:LYS:HA	1:J:335:TRP:CD1	2.54	0.43
2:K:320:MET:HE3	2:K:378:GLY:HA3	2.01	0.43
2:B:230:PHE:H	2:B:297:HIS:CE1	2.36	0.43
3:F:22:ASN:ND2	14:F:406:HOH:O	2.39	0.43
3:L:42:LYS:HB3	3:L:42:LYS:HE2	1.74	0.43
3:M:35:MET:HG3	3:M:85:LYS:HB2	2.00	0.43
2:B:47:THR:HA	2:B:52:TYR:CG	2.54	0.43
1:J:355:ILE:HD12	1:J:359:ARG:HB3	2.00	0.43
1:J:430:ILE:HG13	2:K:110:PRO:HB3	2.00	0.43
2:K:518:ASN:O	2:K:523:ARG:NH2	2.52	0.43
3:L:141:ARG:HG2	3:L:172:TYR:CZ	2.54	0.43
2:B:397:ASN:OD1	2:B:397:ASN:N	2.44	0.43
1:C:222:ASP:O	1:C:269:LYS:N	2.45	0.43
1:C:464:ASP:OD1	1:C:468:ASN:ND2	2.46	0.43
3:E:61:MET:HE2	3:E:61:MET:HB2	1.93	0.43
3:E:77:LEU:HD13	3:E:87:VAL:HG22	1.99	0.43
3:F:56:ASN:HB3	3:F:61:MET:SD	2.58	0.43
2:I:231:GLU:HB3	2:I:237:PHE:CZ	2.54	0.43
3:L:142:GLU:HB3	3:L:144:LYS:HD3	2.01	0.43
1:A:225:ILE:HD11	1:A:242:LEU:HD12	2.01	0.42
1:C:165:SER:HA	1:C:168:LYS:HG2	2.00	0.42
1:C:359:ARG:NH1	1:C:441:MET:O	2.52	0.42
2:D:119:THR:OG1	2:D:121:ASP:OD1	2.26	0.42
3:E:30:MET:H	3:E:30:MET:HG2	1.59	0.42
3:E:214:ARG:HG3	10:E:301:ADP:C2	2.54	0.42
2:I:214:ASP:OD1	2:I:215:ASP:N	2.52	0.42
2:I:215:ASP:N	2:I:215:ASP:OD2	2.51	0.42
1:J:332:LYS:HA	1:J:335:TRP:NE1	2.34	0.42
3:L:260:ILE:HD11	3:L:265:LEU:HD23	2.01	0.42
2:B:70:CYS:HB2	2:B:188:SER:HB2	2.01	0.42
1:C:247:LEU:HD23	1:C:247:LEU:HA	1.89	0.42
1:C:361:ARG:HB3	1:C:379:TYR:OH	2.19	0.42
3:F:267:GLU:OE2	3:F:267:GLU:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:464:ASP:OD1	1:H:468:ASN:ND2	2.51	0.42
1:J:241:LEU:HD23	1:J:241:LEU:HA	1.79	0.42
3:L:7:ALA:HB3	3:L:148:ILE:HG12	2.01	0.42
2:B:458:LYS:HG2	2:B:462:PHE:CD2	2.54	0.42
2:D:151:THR:HG23	2:D:162:LEU:HD11	2.01	0.42
4:G:51:LEU:HD11	4:G:98:TYR:HB3	2.02	0.42
2:I:83:GLU:HG2	2:I:84:LYS:HG3	2.01	0.42
2:K:71:GLN:OE1	2:K:199:ASN:ND2	2.51	0.42
1:C:20:TYR:HB2	1:C:25:ARG:HG2	2.01	0.42
1:C:245:MET:HG3	1:C:324:CYS:HB2	2.01	0.42
1:C:332:LYS:HE3	1:C:332:LYS:HB3	1.71	0.42
3:E:195:GLU:HA	3:E:198:ILE:HB	2.01	0.42
1:J:213:ASP:OD1	1:J:214:THR:N	2.53	0.42
1:J:229:TYR:HA	1:J:255:GLY:H	1.85	0.42
1:J:271:ASN:HD21	1:J:286:MET:CE	2.33	0.42
1:J:473:LYS:HB2	1:J:473:LYS:HE2	1.74	0.42
3:M:44:ASP:N	3:M:44:ASP:OD1	2.52	0.42
1:A:304:LYS:HD3	1:A:304:LYS:HA	1.92	0.42
2:B:7:LYS:HB3	2:B:7:LYS:HE3	1.60	0.42
1:C:120:GLU:O	1:C:124:VAL:HG22	2.20	0.42
2:D:153:CYS:O	2:D:157:VAL:HG23	2.19	0.42
1:C:17:LEU:HB3	1:C:25:ARG:HD2	2.01	0.42
1:H:97:ARG:O	1:H:231:ILE:HA	2.19	0.42
1:J:332:LYS:NZ	1:J:336:GLU:HG3	2.35	0.42
3:L:132:VAL:HG12	3:L:137:ALA:HB2	2.02	0.42
2:B:53:GLN:HG3	2:B:432:SER:HB3	2.02	0.42
2:B:88:TYR:O	2:B:149:VAL:HA	2.19	0.42
1:C:10:GLU:O	1:C:14:GLN:NE2	2.50	0.42
1:C:343:ARG:NH1	1:C:369:ASP:O	2.53	0.42
3:E:134:GLY:HA2	4:G:122:ALA:HB3	2.01	0.42
3:F:101:ARG:HG3	3:F:102:GLY:N	2.34	0.42
1:H:158:LEU:HD13	2:I:158:ILE:HG23	2.02	0.42
2:I:43:VAL:O	2:I:47:THR:HG23	2.19	0.42
3:L:39:CYS:HB2	3:L:127:VAL:HA	2.02	0.42
3:L:77:LEU:C	3:L:78:LYS:HD2	2.40	0.42
2:I:156:GLU:HG3	2:I:187:PRO:HA	2.02	0.42
2:K:88:TYR:O	2:K:150:SER:N	2.50	0.42
1:C:168:LYS:HG3	1:C:169:VAL:N	2.35	0.42
1:C:313:ALA:O	1:C:321:GLN:NE2	2.45	0.42
2:D:163:ASN:OD1	2:D:164:ALA:N	2.53	0.42
1:H:332:LYS:HA	1:H:335:TRP:NE1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:417:LYS:HE2	2:I:417:LYS:HB2	1.89	0.42
1:J:65:ALA:O	1:J:70:VAL:HG23	2.20	0.42
3:L:150:ILE:HB	3:L:183:LEU:HD23	2.01	0.42
1:A:205:TRP:O	1:A:209:LYS:NZ	2.41	0.42
1:C:198:ALA:O	1:C:202:VAL:HG12	2.20	0.42
2:D:253:LEU:HD23	2:D:253:LEU:HA	1.90	0.42
4:G:110:ASP:OD1	4:G:110:ASP:N	2.52	0.42
1:J:47:ILE:HD13	1:J:47:ILE:HA	1.94	0.42
3:L:9:TYR:HB3	3:L:165:ILE:HD13	2.01	0.42
2:B:120:GLU:O	2:B:124:VAL:HG23	2.19	0.41
1:C:17:LEU:HD11	1:C:32:LEU:HD12	2.02	0.41
2:D:504:ARG:HD2	2:D:504:ARG:HA	1.79	0.41
1:H:61:GLY:O	2:I:93:GLN:NE2	2.51	0.41
1:J:409:PHE:O	1:J:413:VAL:HG13	2.20	0.41
3:L:53:LYS:HG2	3:L:225:ARG:NH2	2.35	0.41
1:A:423:SER:O	1:A:440:GLU:HA	2.20	0.41
1:C:175:SER:O	1:C:175:SER:OG	2.37	0.41
2:I:72:PRO:O	2:I:76:VAL:HG23	2.20	0.41
2:I:243:MET:HG2	2:I:344:LEU:HD21	2.02	0.41
3:L:77:LEU:HD23	3:L:77:LEU:HA	1.78	0.41
5:N:27:LYS:HD2	5:N:113:VAL:HG21	2.02	0.41
1:A:23:LYS:HE2	1:A:23:LYS:HB3	1.88	0.41
1:A:90:GLN:HG3	2:B:68:LYS:O	2.20	0.41
1:C:282:ILE:HD12	1:C:282:ILE:HA	1.86	0.41
2:K:499:ASN:ND2	14:K:707:HOH:O	2.35	0.41
3:L:34:VAL:HG23	3:L:122:PHE:CB	2.51	0.41
3:L:151:VAL:HG22	3:L:184:ILE:HB	2.02	0.41
3:M:71:LEU:HD11	3:M:76:VAL:HG13	2.02	0.41
3:M:119:ASP:N	3:M:119:ASP:OD1	2.54	0.41
2:D:266:ASP:CG	2:D:270:ARG:HH12	2.22	0.41
3:F:71:LEU:HD23	3:F:71:LEU:HA	1.90	0.41
3:F:243:ALA:HA	3:F:246:ARG:HE	1.85	0.41
1:J:96:ARG:NH1	7:J:502:ICS:S5A	2.93	0.41
1:J:186:PHE:HB3	2:K:154:MET:SD	2.59	0.41
1:J:367:TYR:HD1	1:J:372:MET:HE3	1.84	0.41
2:K:435:PHE:CE2	2:K:458:LYS:HD3	2.55	0.41
3:M:218:VAL:HG21	10:M:301:ADP:C2	2.56	0.41
3:M:239:ASP:HA	3:M:242:ARG:HB2	2.02	0.41
1:C:186:PHE:HB3	2:D:154:MET:SD	2.61	0.41
1:C:332:LYS:HA	1:C:335:TRP:CD1	2.55	0.41
3:E:42:LYS:HB3	3:E:44:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:52:SER:OG	3:F:53:LYS:N	2.52	0.41
2:I:516:ASP:C	2:I:516:ASP:OD2	2.58	0.41
3:L:195:GLU:HA	3:L:198:ILE:HG22	2.03	0.41
3:L:195:GLU:N	3:L:195:GLU:OE2	2.53	0.41
1:A:124:VAL:HG12	1:A:125:PHE:HD2	1.86	0.41
3:F:178:VAL:O	3:F:179:ARG:NH1	2.50	0.41
2:K:362:LEU:HD13	2:K:386:LEU:HD13	2.01	0.41
1:A:131:LEU:O	1:A:135:ILE:HG13	2.21	0.41
1:A:152:SER:OG	1:A:182:ARG:HA	2.19	0.41
1:A:237:SER:O	1:A:240:ILE:HG22	2.21	0.41
1:C:131:LEU:O	1:C:135:ILE:HG13	2.21	0.41
2:B:368:ALA:O	2:B:442:MET:HA	2.20	0.41
1:C:66:GLY:O	1:C:70:VAL:HB	2.21	0.41
2:D:156:GLU:HG3	2:D:187:PRO:HA	2.03	0.41
1:J:240:ILE:HD11	2:K:19:ASP:HB2	2.02	0.41
2:K:453:ARG:NH2	14:K:712:HOH:O	2.45	0.41
2:B:153:CYS:HB3	2:B:188:SER:OG	2.20	0.41
2:D:50:LYS:O	2:D:54:GLU:HG2	2.20	0.41
3:E:49:ILE:HG21	3:E:84:VAL:HG11	2.03	0.41
3:E:151:VAL:HG22	3:E:184:ILE:HB	2.01	0.41
4:G:15:LYS:HB3	4:G:15:LYS:HE3	1.75	0.41
1:H:317:ASP:OD1	1:H:319:SER:OG	2.35	0.41
1:J:350:ARG:NH2	1:J:416:ILE:O	2.54	0.41
3:L:87:VAL:HG21	3:L:110:LEU:HD11	2.03	0.41
3:M:83:GLY:O	14:M:401:HOH:O	2.21	0.41
3:M:98:CYS:HB3	5:N:118:GLU:OE2	2.21	0.41
3:M:237:GLN:HA	3:M:237:GLN:OE1	2.21	0.41
1:A:276:TYR:H	1:A:358:LEU:HD13	1.86	0.41
1:A:439:ARG:HA	1:A:439:ARG:HD2	1.83	0.41
2:B:53:GLN:OE1	2:B:436:THR:OG1	2.17	0.41
1:C:203:ARG:HB2	1:C:282:ILE:HD11	2.02	0.41
4:G:5:TYR:CD1	5:N:57:LEU:HB3	2.56	0.41
3:L:21:GLN:OE1	3:L:49:ILE:HB	2.20	0.41
3:M:180:LEU:HD23	3:M:257:PRO:HB3	2.02	0.41
3:M:214:ARG:HG3	10:M:301:ADP:H2	1.86	0.41
5:N:116:THR:OG1	5:N:118:GLU:HG3	2.20	0.41
3:E:199:ALA:HA	3:E:202:ASN:OD1	2.21	0.40
2:I:474:PHE:HB3	2:K:522:VAL:HA	2.03	0.40
1:C:355:ILE:HB	1:C:360:PRO:HD3	2.03	0.40
1:H:209:LYS:HE2	1:H:209:LYS:HB2	1.90	0.40
1:H:423:SER:O	1:H:440:GLU:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:210:HIS:NE2	3:M:240:GLU:HG3	2.37	0.40
2:D:194:VAL:HB	2:D:297:HIS:CG	2.55	0.40
2:K:236:ASN:HD21	2:K:484:THR:HB	1.87	0.40
2:K:452:GLN:O	2:K:455:THR:OG1	2.32	0.40
3:M:103:VAL:O	3:M:107:ILE:HG13	2.21	0.40
3:M:155:GLU:HG3	3:M:156:MET:N	2.36	0.40
1:A:68:LYS:HG3	1:A:151:GLN:HG3	2.04	0.40
1:C:428:LYS:NZ	1:C:445:ASP:OD2	2.55	0.40
2:D:441:PHE:CE2	2:D:465:PRO:HG2	2.57	0.40
3:E:24:VAL:HG21	3:E:36:ILE:HG12	2.03	0.40
3:F:107:ILE:HG23	3:F:116:TYR:HE2	1.86	0.40
1:J:318:GLU:OE2	1:J:318:GLU:HA	2.21	0.40
5:N:27:LYS:HE3	5:N:27:LYS:HB3	1.74	0.40
2:B:471:PHE:HA	2:B:472:PRO:HA	1.94	0.40
1:C:87:GLY:HA3	2:D:70:CYS:SG	2.61	0.40
2:I:86:MET:HG2	2:I:138:CYS:SG	2.61	0.40
2:I:471:PHE:HA	2:I:472:PRO:HA	1.94	0.40
1:J:253:TRP:CD1	1:J:253:TRP:N	2.90	0.40
2:K:294:GLN:HA	2:K:374:ASP:OD1	2.21	0.40
3:M:247:LYS:HB2	3:M:247:LYS:HE2	1.75	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	A	476/492 (97%)	459 (96%)	17 (4%)	0	100	100
1	C	476/492 (97%)	465 (98%)	11 (2%)	0	100	100
1	H	476/492 (97%)	464 (98%)	12 (2%)	0	100	100
1	J	476/492 (97%)	464 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	520/523 (99%)	507 (98%)	13 (2%)	0	100	100
2	D	520/523 (99%)	509 (98%)	11 (2%)	0	100	100
2	I	520/523 (99%)	509 (98%)	11 (2%)	0	100	100
2	K	520/523 (99%)	508 (98%)	12 (2%)	0	100	100
3	E	272/290 (94%)	261 (96%)	11 (4%)	0	100	100
3	F	281/290 (97%)	274 (98%)	7 (2%)	0	100	100
3	L	270/290 (93%)	263 (97%)	7 (3%)	0	100	100
3	M	278/290 (96%)	269 (97%)	9 (3%)	0	100	100
4	G	119/122 (98%)	117 (98%)	2 (2%)	0	100	100
5	N	119/122 (98%)	118 (99%)	1 (1%)	0	100	100
All	All	5323/5464 (97%)	5187 (97%)	136 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2   Protein sidechains   ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	407/415 (98%)	392 (96%)	15 (4%)	29	54
1	C	408/415 (98%)	378 (93%)	30 (7%)	11	24
1	H	407/415 (98%)	393 (97%)	14 (3%)	32	57
1	J	408/415 (98%)	384 (94%)	24 (6%)	16	33
2	B	454/455 (100%)	436 (96%)	18 (4%)	27	51
2	D	454/455 (100%)	438 (96%)	16 (4%)	31	56
2	I	454/455 (100%)	442 (97%)	12 (3%)	41	67
2	K	454/455 (100%)	437 (96%)	17 (4%)	29	54
3	E	221/234 (94%)	206 (93%)	15 (7%)	13	27
3	F	229/234 (98%)	213 (93%)	16 (7%)	12	26
3	L	219/234 (94%)	207 (94%)	12 (6%)	18	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	226/234 (97%)	207 (92%)	19 (8%)	9	19
4	G	102/103 (99%)	97 (95%)	5 (5%)	21	42
5	N	102/103 (99%)	97 (95%)	5 (5%)	21	42
All	All	4545/4622 (98%)	4327 (95%)	218 (5%)	24	43

All (218) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	44	LYS
1	A	45	CYS
1	A	120	GLU
1	A	121	LYS
1	A	139	GLU
1	A	213	ASP
1	A	252	GLN
1	A	359	ARG
1	A	362	HIS
1	A	397	SER
1	A	401	TYR
1	A	445	ASP
1	A	467	LEU
1	A	480	GLU
2	B	2	SER
2	B	6	ASP
2	B	7	LYS
2	B	102	TYR
2	B	143	LYS
2	B	177	ASP
2	B	211	LYS
2	B	252	SER
2	B	279	GLU
2	B	281	MET
2	B	315	LYS
2	B	420	THR
2	B	426	ASP
2	B	442	MET
2	B	453	ARG
2	B	491	MET
2	B	506	ASP
2	B	512	MET

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Mol	Chain	Res	Type
1	C	4	MET
1	C	5	SER
1	C	8	GLU
1	C	18	GLU
1	C	45	CYS
1	C	49	ASN
1	C	51	LYS
1	C	57	MET
1	C	209	LYS
1	C	237	SER
1	C	277	ARG
1	C	281	TYR
1	C	288	GLU
1	C	350	ARG
1	C	352	MET
1	C	355	ILE
1	C	358	LEU
1	C	359	ARG
1	C	362	HIS
1	C	368	GLU
1	C	388	ASP
1	C	392	LYS
1	C	393	GLU
1	C	401	TYR
1	C	409	PHE
1	C	415	ARG
1	C	439	ARG
1	C	444	TRP
1	C	445	ASP
1	C	454	ASP
2	D	92	SER
2	D	101	SER
2	D	102	TYR
2	D	114	VAL
2	D	116	ASP
2	D	179	PHE
2	D	188	SER
2	D	189	PHE
2	D	206	ARG
2	D	214	ASP
2	D	222	LYS
2	D	238	ARG

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Mol	Chain	Res	Type
2	D	253	LEU
2	D	258	GLU
2	D	394	LEU
2	D	460	LYS
3	E	16	LYS
3	E	30	MET
3	E	61	MET
3	E	138	MET
3	E	156	MET
3	E	157	MET
3	E	185	CYS
3	E	202	ASN
3	E	214	ARG
3	E	222	GLU
3	E	250	ASP
3	E	258	ASN
3	E	262	MET
3	E	267	GLU
3	E	270	MET
3	F	33	LYS
3	F	52	SER
3	F	61	MET
3	F	74	GLU
3	F	81	TYR
3	F	101	ARG
3	F	117	GLU
3	F	119	ASP
3	F	138	MET
3	F	225	ARG
3	F	226	MET
3	F	239	ASP
3	F	246	ARG
3	F	252	LYS
3	F	268	LEU
3	F	272	PHE
4	G	11	MET
4	G	23	LYS
4	G	28	LEU
4	G	87	GLU
4	G	110	ASP
1	H	22	GLU
1	H	51	LYS

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Mol	Chain	Res	Type
1	H	68	LYS
1	H	116	SER
1	H	248	ARG
1	H	250	VAL
1	H	295	MET
1	H	324	CYS
1	H	336	GLU
1	H	355	ILE
1	H	358	LEU
1	H	401	TYR
1	H	445	ASP
1	H	465	MET
2	I	7	LYS
2	I	102	TYR
2	I	202	GLU
2	I	220	SER
2	I	258	GLU
2	I	276	THR
2	I	334	GLU
2	I	343	SER
2	I	369	LEU
2	I	420	THR
2	I	432	SER
2	I	512	MET
1	J	4	MET
1	J	6	ARG
1	J	29	ASN
1	J	41	GLN
1	J	45	CYS
1	J	161	ASP
1	J	209	LYS
1	J	218	SER
1	J	277	ARG
1	J	355	ILE
1	J	359	ARG
1	J	362	HIS
1	J	377	THR
1	J	401	TYR
1	J	409	PHE
1	J	410	GLU
1	J	414	LYS
1	J	420	LEU

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Mol	Chain	Res	Type
1	J	439	ARG
1	J	441	MET
1	J	445	ASP
1	J	463	MET
1	J	465	MET
1	J	473	LYS
2	K	6	ASP
2	K	19	ASP
2	K	23	MET
2	K	102	TYR
2	K	128	GLN
2	K	160	ASP
2	K	245	SER
2	K	256	ASP
2	K	258	GLU
2	K	288	LEU
2	K	315	LYS
2	K	320	MET
2	K	369	LEU
2	K	394	LEU
2	K	417	LYS
2	K	426	ASP
2	K	435	PHE
3	L	11	LYS
3	L	30	MET
3	L	33	LYS
3	L	46	THR
3	L	72	GLU
3	L	81	TYR
3	L	142	GLU
3	L	153	SER
3	L	204	LEU
3	L	207	GLN
3	L	226	MET
3	L	267	GLU
3	M	3	MET
3	M	45	SER
3	M	59	MET
3	M	81	TYR
3	M	84	VAL
3	M	89	SER
3	M	155	GLU

Continued from previous page...

Mol	Chain	Res	Type
3	M	188	ARG
3	M	194	ASP
3	M	207	GLN
3	M	208	MET
3	M	210	HIS
3	M	211	PHE
3	M	215	ASP
3	M	220	ARG
3	M	236	LYS
3	M	262	MET
3	M	267	GLU
3	M	280	GLU
5	N	23	LYS
5	N	27	LYS
5	N	28	LYS
5	N	83	LYS
5	N	103	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	113	ASN
1	C	145	ASN
1	C	199	ASN
1	C	362	HIS
1	H	271	ASN
2	I	128	GLN
1	J	199	ASN
1	J	271	ASN
2	K	104	ASN

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   ⓘ

Of 28 ligands modelled in this entry, 8 are monoatomic - leaving 20 for Mogul analysis.

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	$\#\|Z\| > 2$
10	ADP	M	301	11	24,29,29	0.89	0	29,45,45	1.21	2 (6%)
8	CLF	D	602	2,1	0,24,24	-	-	-		
7	ICS	C	502	1	6,30,30	1.72	1 (16%)	-		
13	FES	G	201	4	0,4,4	-	-	-		
8	CLF	K	602	2,1	0,24,24	-	-	-		
8	CLF	A	503	2,1	0,24,24	-	-	-		
6	HCA	C	501	-	13,13,13	1.28	1 (7%)	15,18,18	1.55	3 (20%)
6	HCA	J	501	-	13,13,13	1.15	1 (7%)	15,18,18	1.23	2 (13%)
12	SF4	L	303	3	0,12,12	-	-	-		
10	ADP	L	301	11	24,29,29	0.94	1 (4%)	29,45,45	1.21	2 (6%)
10	ADP	E	301	11	24,29,29	0.90	0	29,45,45	1.20	2 (6%)
13	FES	N	201	5	0,4,4	-	-	-		
8	CLF	H	503	2,1	0,24,24	-	-	-		
6	HCA	A	501	-	13,13,13	1.29	1 (7%)	15,18,18	1.61	3 (20%)
12	SF4	F	301	3	0,12,12	-	-	-		
6	HCA	H	501	-	13,13,13	1.16	1 (7%)	15,18,18	1.46	3 (20%)
7	ICS	H	502	1	6,30,30	1.83	1 (16%)	-		
10	ADP	F	302	11	24,29,29	0.91	0	29,45,45	1.23	3 (10%)
7	ICS	A	502	1	6,30,30	1.75	1 (16%)	-		
7	ICS	J	502	1	6,30,30	1.83	1 (16%)	-		

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
10	ADP	L	301	11	-	5/12/32/32	0/3/3/3
10	ADP	E	301	11	-	7/12/32/32	0/3/3/3
13	FES	N	201	5	-	-	0/1/1/1
10	ADP	M	301	11	-	5/12/32/32	0/3/3/3
8	CLF	H	503	2,1	-	-	0/12/10/10
8	CLF	K	602	2,1	-	-	0/12/10/10
12	SF4	F	301	3	-	-	0/6/5/5
6	HCA	A	501	-	-	1/17/17/17	-
10	ADP	F	302	11	-	7/12/32/32	0/3/3/3
8	CLF	D	602	2,1	-	-	0/12/10/10
13	FES	G	201	4	-	-	0/1/1/1
8	CLF	A	503	2,1	-	-	0/12/10/10
12	SF4	L	303	3	-	-	0/6/5/5
6	HCA	C	501	-	-	0/17/17/17	-
6	HCA	J	501	-	-	1/17/17/17	-
6	HCA	H	501	-	-	8/17/17/17	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	502	ICS	S2B-FE6	-3.68	2.16	2.24
7	H	502	ICS	S2B-FE6	-3.54	2.16	2.24
7	A	502	ICS	S2B-FE6	-3.28	2.17	2.24
7	C	502	ICS	S2B-FE6	-3.27	2.17	2.24
6	J	501	HCA	C3-C7	2.30	1.55	1.53
6	H	501	HCA	C3-C7	2.30	1.55	1.53
10	L	301	ADP	PA-O3A	2.14	1.61	1.59
6	C	501	HCA	C3-C7	2.13	1.55	1.53
6	A	501	HCA	C3-C7	2.07	1.55	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	501	HCA	O5-C7-C3	-3.76	114.80	122.09
6	C	501	HCA	O5-C7-C3	-3.74	114.84	122.09
10	E	301	ADP	N3-C2-N1	-3.63	123.74	128.67
10	F	302	ADP	N3-C2-N1	-3.62	123.75	128.67
10	M	301	ADP	N3-C2-N1	-3.57	123.83	128.67
10	L	301	ADP	N3-C2-N1	-3.45	124.00	128.67
6	H	501	HCA	O7-C3-C4	-3.35	103.53	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	501	HCA	O6-C7-C3	2.80	118.51	113.14
6	C	501	HCA	O6-C7-C3	2.71	118.33	113.14
10	M	301	ADP	C4-C5-N7	-2.63	106.56	109.34
10	E	301	ADP	C4-C5-N7	-2.62	106.57	109.34
10	F	302	ADP	C4-C5-N7	-2.60	106.58	109.34
10	L	301	ADP	C4-C5-N7	-2.53	106.67	109.34
6	H	501	HCA	O6-C7-C3	2.20	117.36	113.14
6	H	501	HCA	O5-C7-C3	-2.19	117.84	122.09
6	A	501	HCA	O1-C1-C2	-2.13	116.92	122.95
6	C	501	HCA	O1-C1-C2	-2.12	116.94	122.95
10	F	302	ADP	O4'-C1'-N9	2.08	111.50	108.75
6	J	501	HCA	O5-C7-C3	-2.01	118.20	122.09
6	J	501	HCA	O6-C7-C3	2.00	116.98	113.14

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	501	HCA	C2-C3-C4-C5
6	H	501	HCA	C2-C3-C4-C5
6	H	501	HCA	C7-C3-C4-C5
6	H	501	HCA	O7-C3-C4-C5
10	E	301	ADP	C5'-O5'-PA-O1A
10	E	301	ADP	C5'-O5'-PA-O2A
10	E	301	ADP	C5'-O5'-PA-O3A
10	F	302	ADP	C5'-O5'-PA-O2A
10	L	301	ADP	PB-O3A-PA-O5'
10	L	301	ADP	C5'-O5'-PA-O2A
10	M	301	ADP	C5'-O5'-PA-O2A
10	M	301	ADP	C5'-O5'-PA-O3A
10	M	301	ADP	O4'-C4'-C5'-O5'
10	F	302	ADP	O4'-C4'-C5'-O5'
10	M	301	ADP	C3'-C4'-C5'-O5'
10	E	301	ADP	O4'-C4'-C5'-O5'
6	H	501	HCA	C3-C4-C5-C6
6	J	501	HCA	C3-C4-C5-C6
10	F	302	ADP	C3'-C4'-C5'-O5'
10	E	301	ADP	C3'-C4'-C5'-O5'
10	L	301	ADP	O4'-C4'-C5'-O5'
10	F	302	ADP	PA-O3A-PB-O2B
10	F	302	ADP	C5'-O5'-PA-O1A
10	F	302	ADP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
10	L	301	ADP	C5'-O5'-PA-O1A
10	L	301	ADP	C5'-O5'-PA-O3A
10	M	301	ADP	C5'-O5'-PA-O1A
6	H	501	HCA	C1-C2-C3-C7
10	E	301	ADP	PB-O3A-PA-O2A
6	H	501	HCA	C4-C3-C7-O6
6	H	501	HCA	C4-C5-C6-O3
10	F	302	ADP	PA-O3A-PB-O3B
6	H	501	HCA	C4-C5-C6-O4
10	E	301	ADP	PB-O3A-PA-O1A

There are no ring outliers.

11 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	M	301	ADP	4	0
7	C	502	ICS	1	0
8	A	503	CLF	1	0
12	L	303	SF4	1	0
10	L	301	ADP	2	0
10	E	301	ADP	1	0
6	A	501	HCA	1	0
7	H	502	ICS	2	0
10	F	302	ADP	1	0
7	A	502	ICS	3	0
7	J	502	ICS	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 ADP M 301

Bond lengths

Bond angles

Torsions

Rings

Ligand CLF D 602

Bond lengths

Bond angles

Torsions

Rings

Ligand ICS C 502

Bond lengths

Bond angles

Torsions

Rings

Ligand FES G 201

Bond lengths

Bond angles

Torsions

Rings

Ligand CLF K 602

Bond lengths

Bond angles

Torsions

Rings

Ligand CLF A 503

Bond lengths

Bond angles

Torsions

Rings

Ligand HCA C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand HCA J 501

Bond lengths

Bond angles

Torsions

Rings

Ligand SF4 L 303

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP L 301

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP E 301

Bond lengths

Bond angles

Torsions

Rings

Ligand FES N 201

Bond lengths

Bond angles

Torsions

Rings

Ligand CLF H 503

Bond lengths

Bond angles

Torsions

Rings

Ligand HCA A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand SF4 F 301

Bond lengths

Bond angles

Torsions

Rings

Ligand HCA H 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ICS H 502

Bond lengths
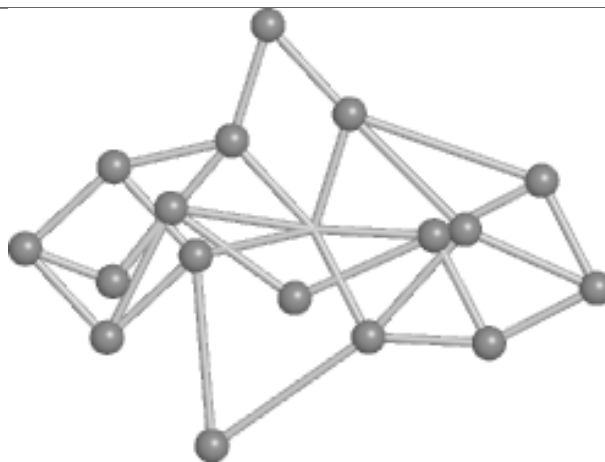
Bond angles
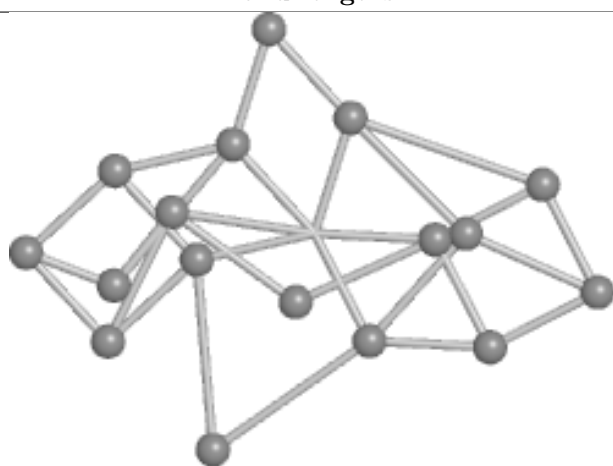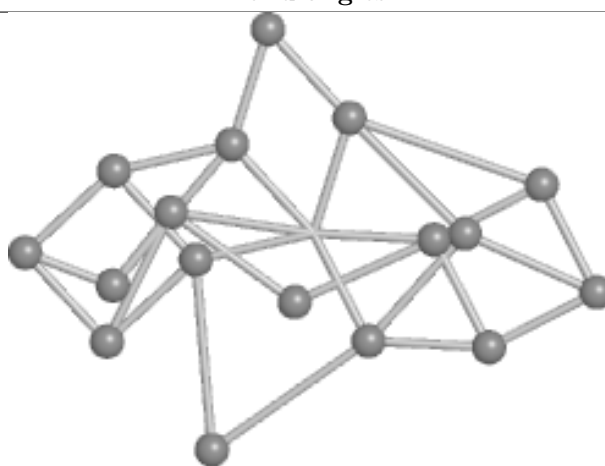
Torsions

Rings

Ligand ADP F 302

Bond lengths

Bond angles

Torsions

Rings

Ligand ICS A 502

Bond lengths

Bond angles

Torsions

Rings

Ligand ICS J 502
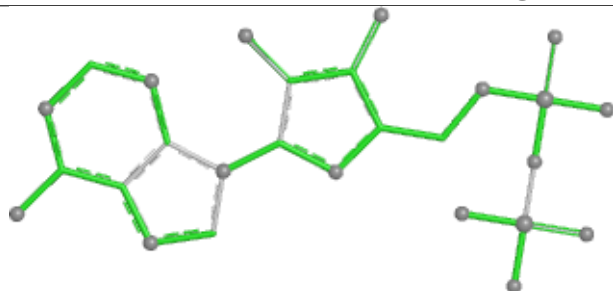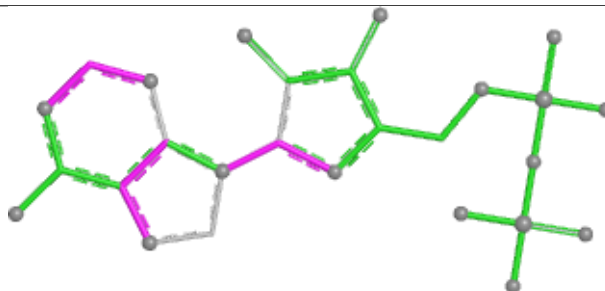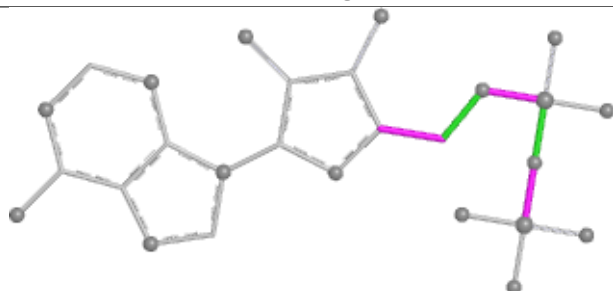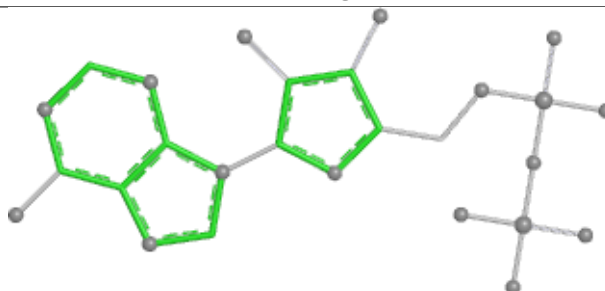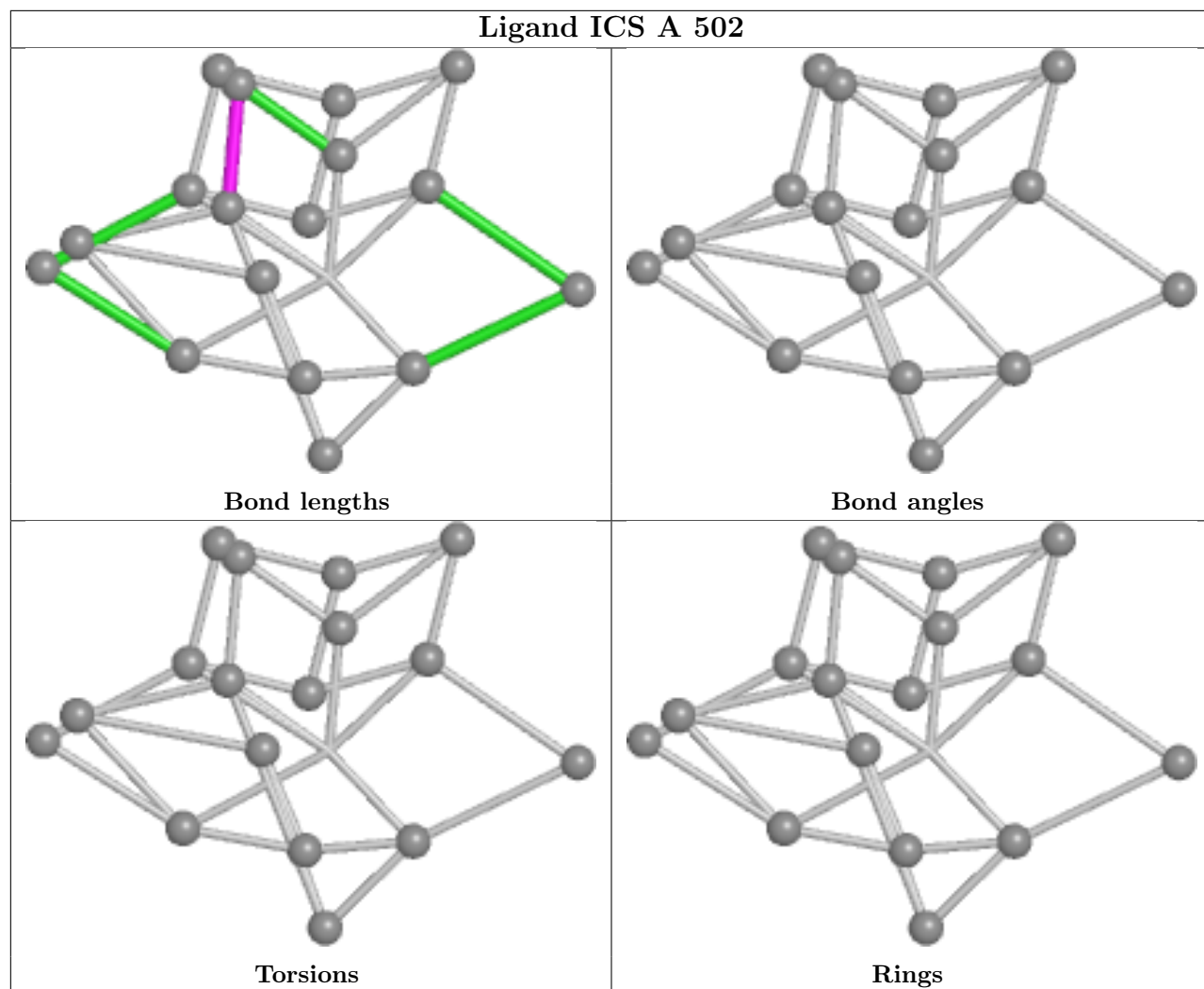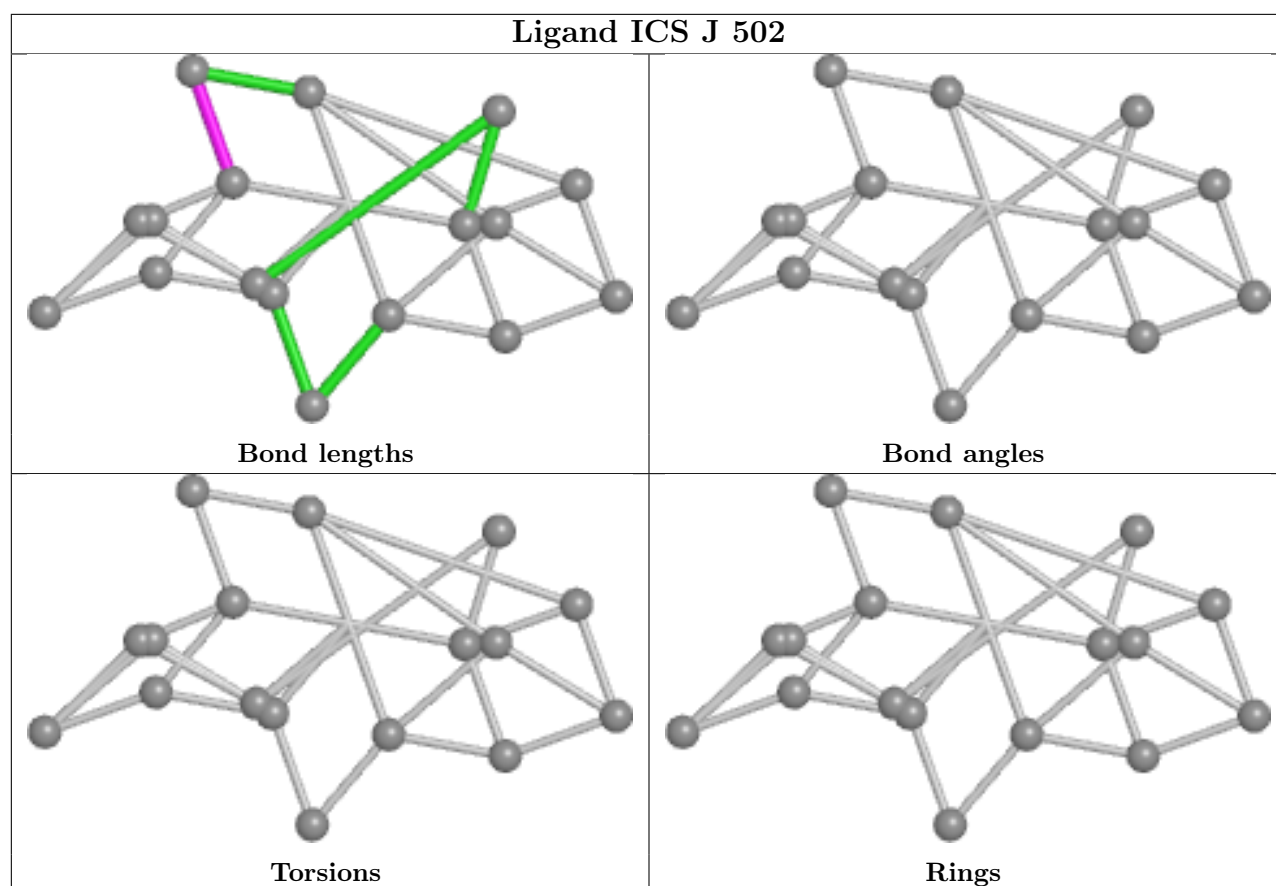
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-45925. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ
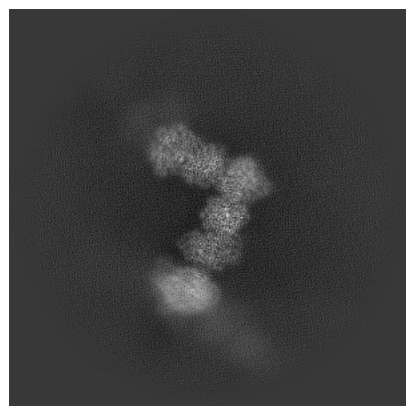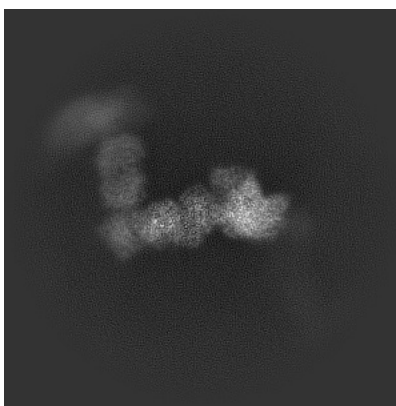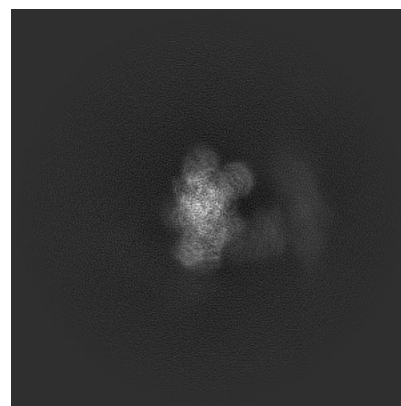
6.1.1 Primary map

X   Y   Z

6.1.2 Raw map

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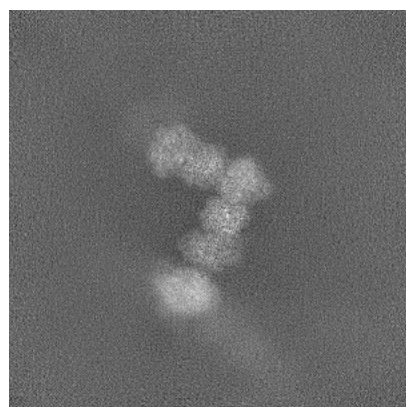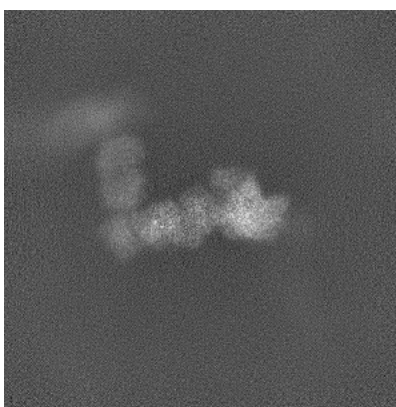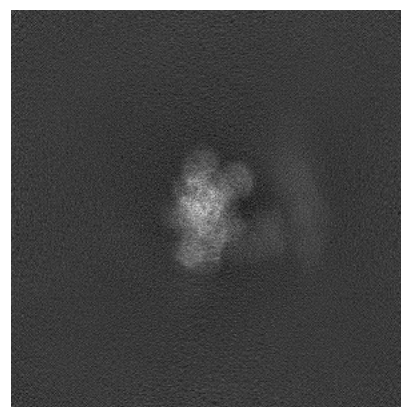
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
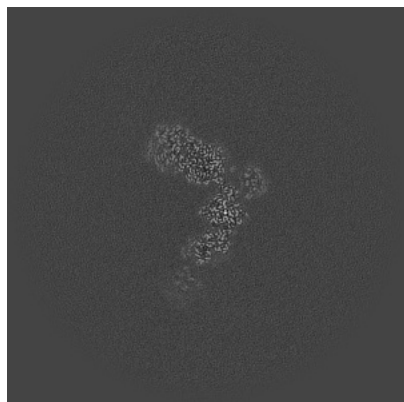
6.2.1 Primary map

X Index: 256
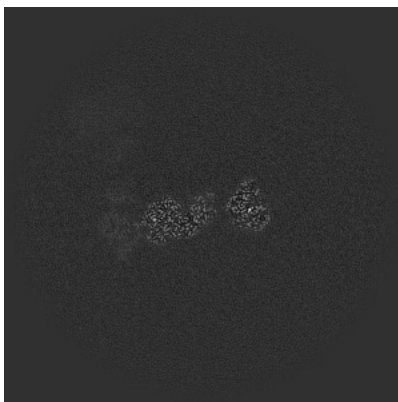
Y Index: 256
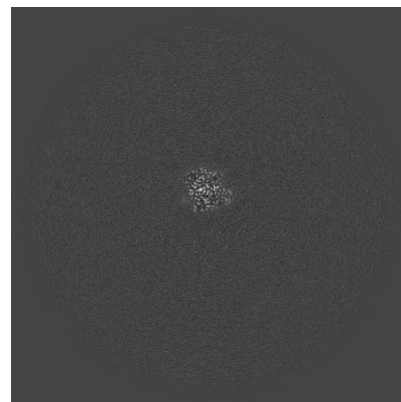
Z Index: 256

6.2.2 Raw map
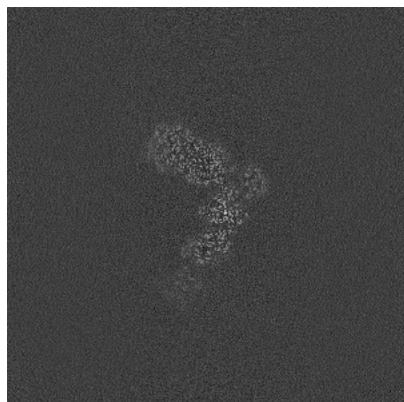
X Index: 256
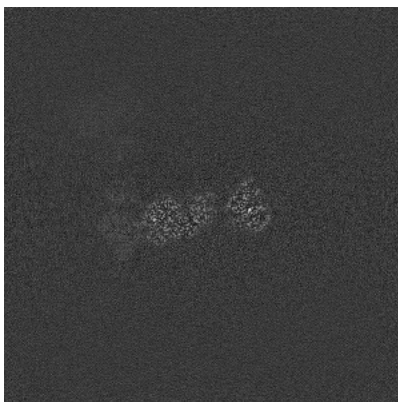
Y Index: 256
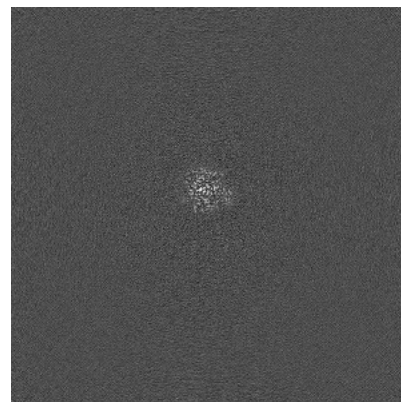
Z Index: 256

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

6.3 Largest variance slices (i)

6.3.1 Primary map
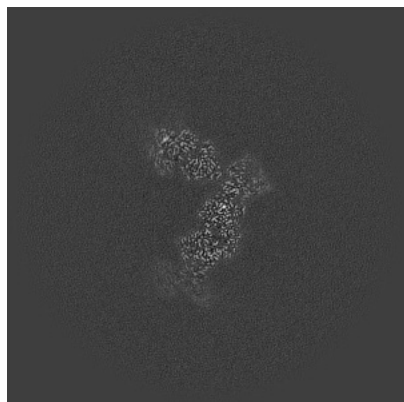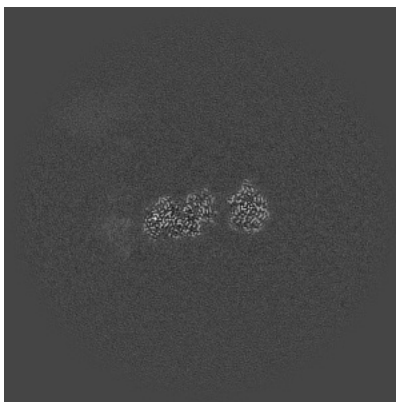
| X Index: 242 | Y Index: 261 | Z Index: 313 |
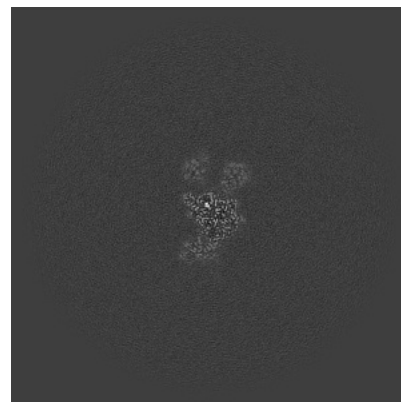
6.3.2 Raw map
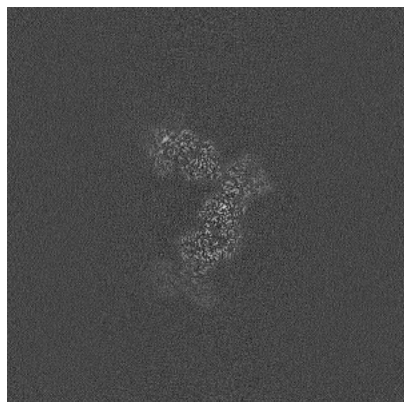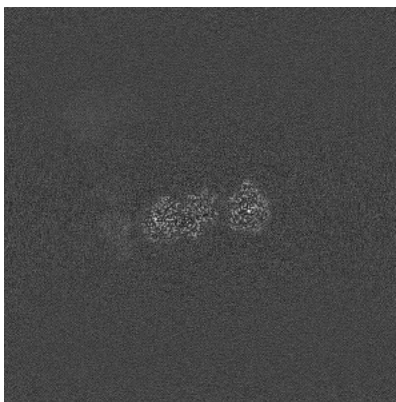
| X Index: 242 | Y Index: 260 | Z Index: 0 |
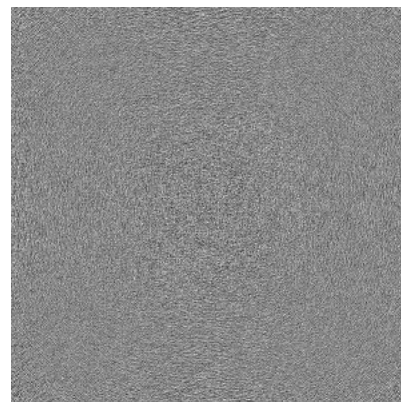
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map
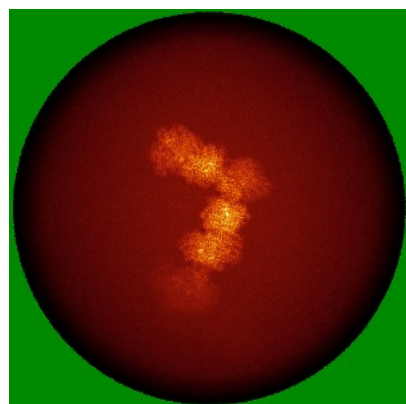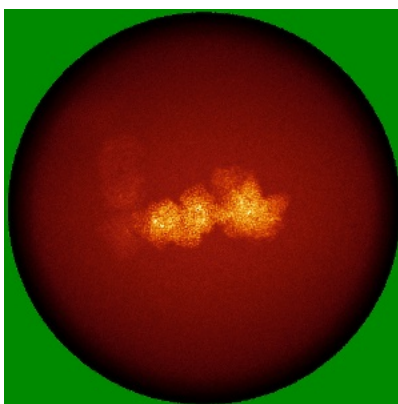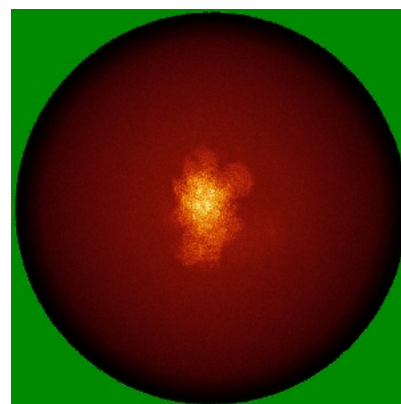
X   Y   Z

6.4.2 Raw map

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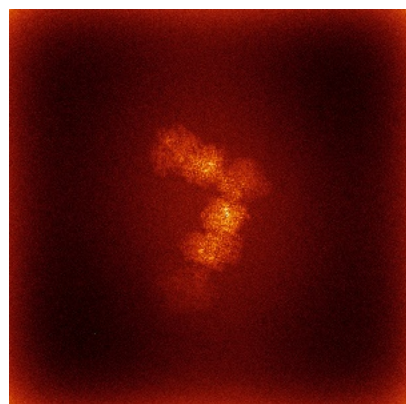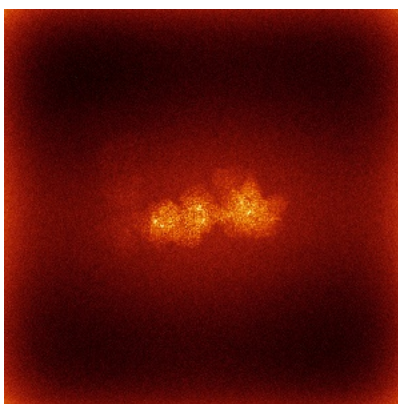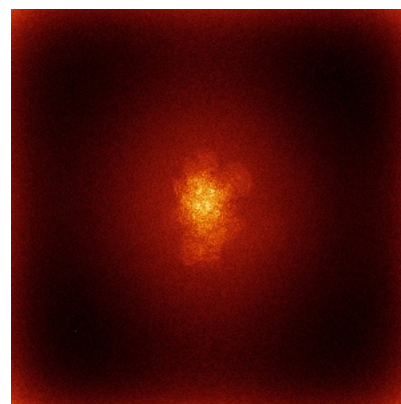
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X   Y   Z
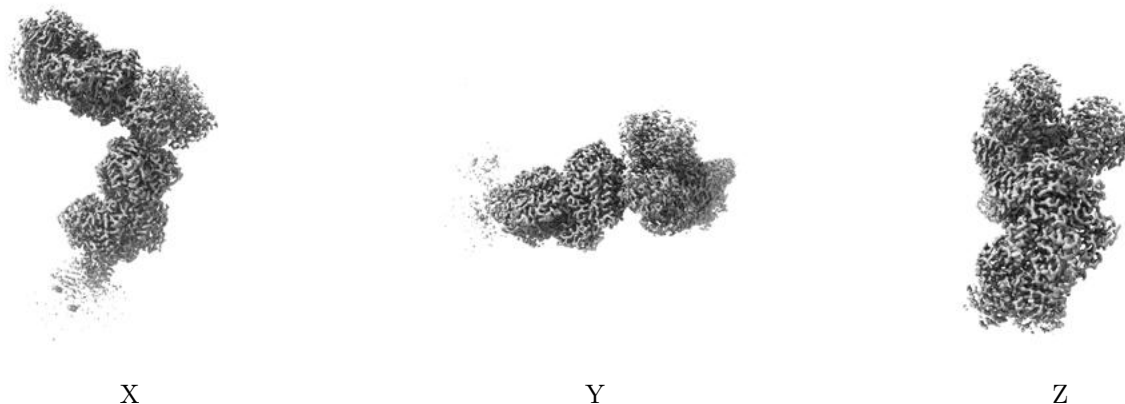
The images above show the 3D surface view of the map at the recommended contour level 0.221. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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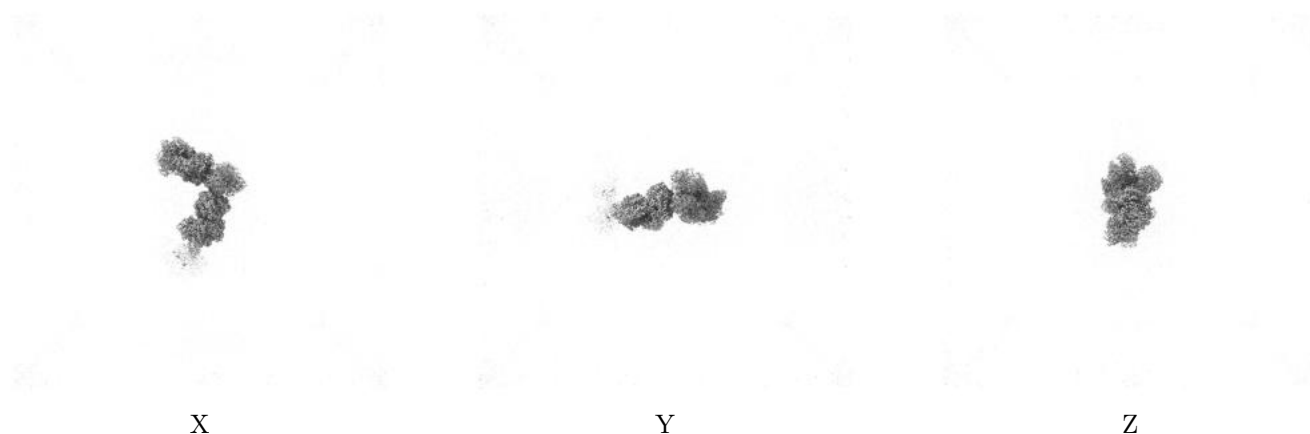
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6   Mask visualisation ⓘ

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_45925_msk_1.map ⓘ

X   Y   Z
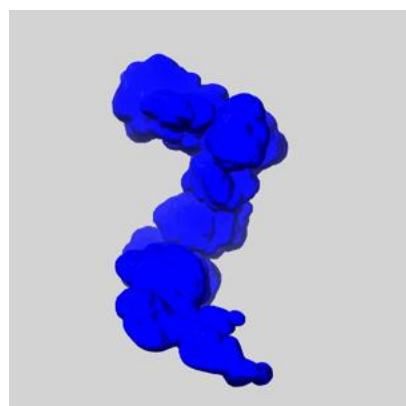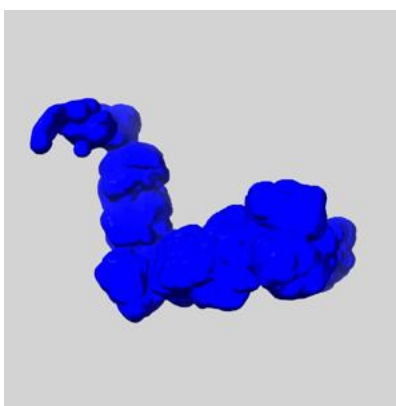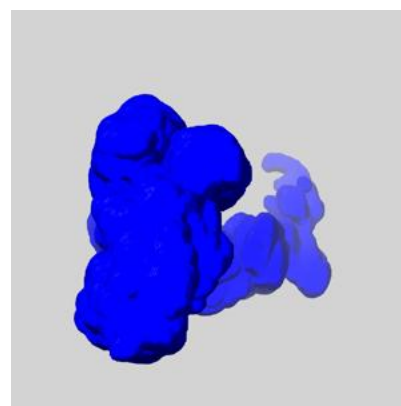
7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
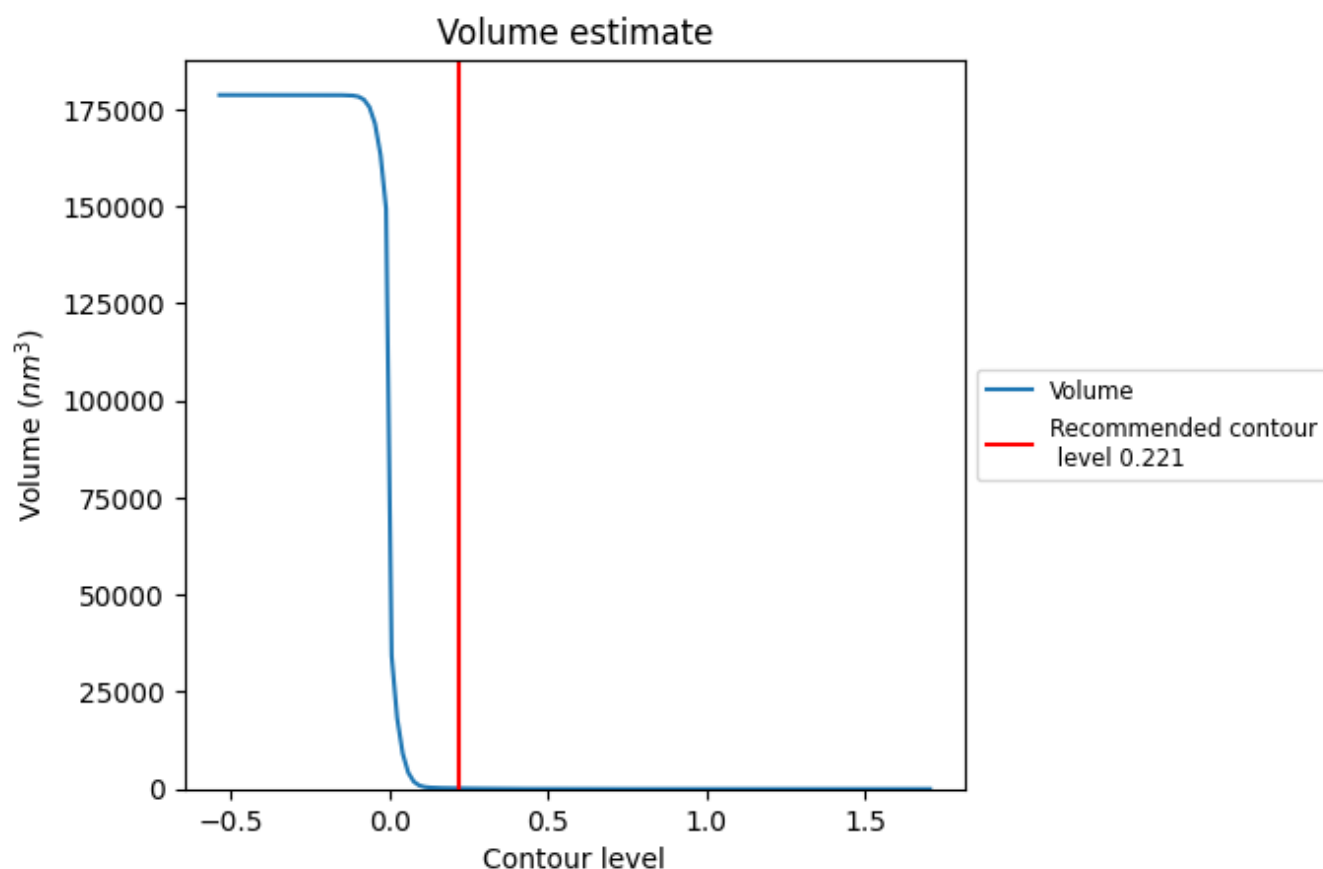
The volume at the recommended contour level is 152 nm^3; this corresponds to an approximate mass of 137 kDa.

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 ⓘ
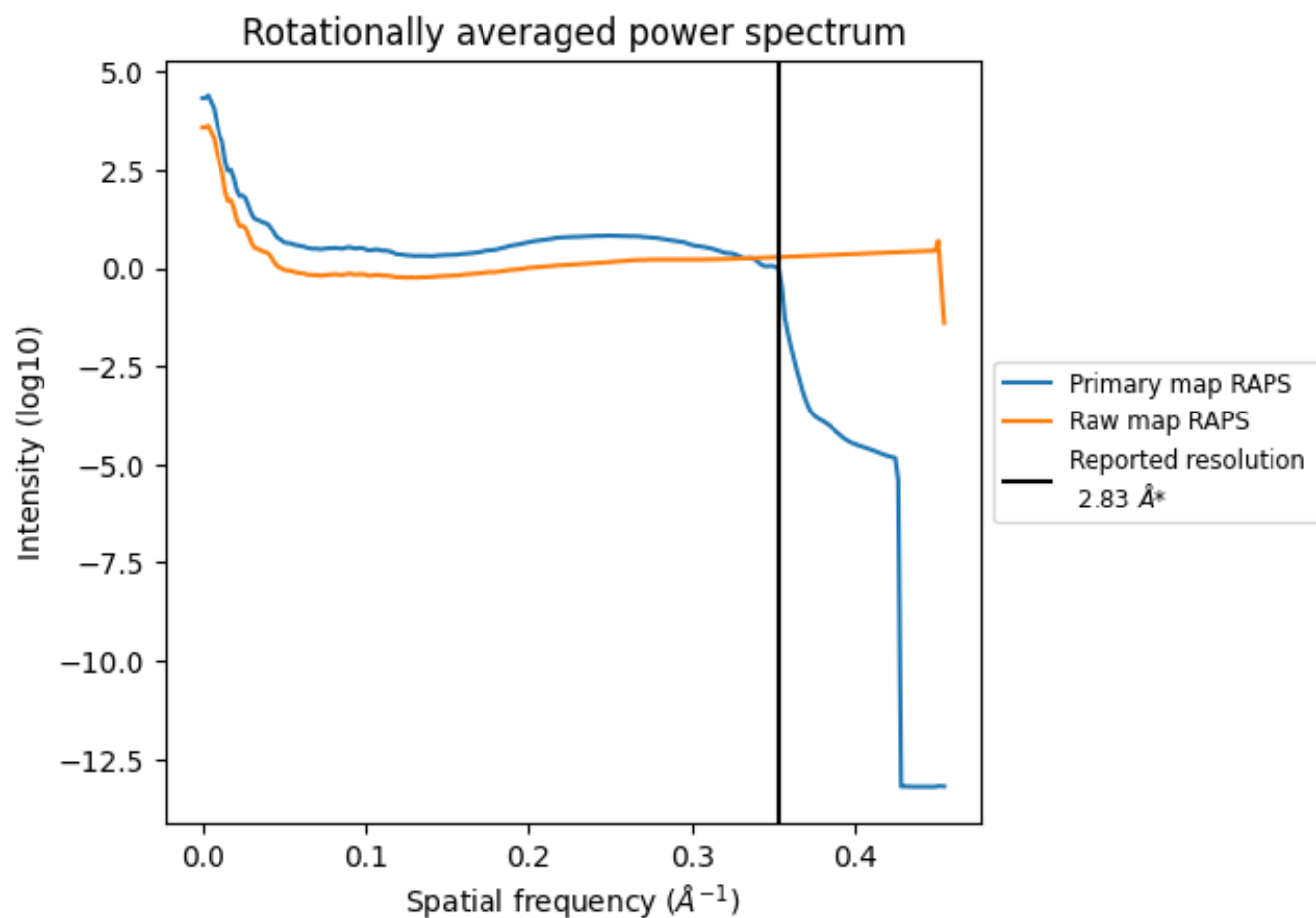
*Reported resolution corresponds to spatial frequency of 0.353 Å^{-1}

8 Fourier-Shell correlation ⓘ

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 ⓘ
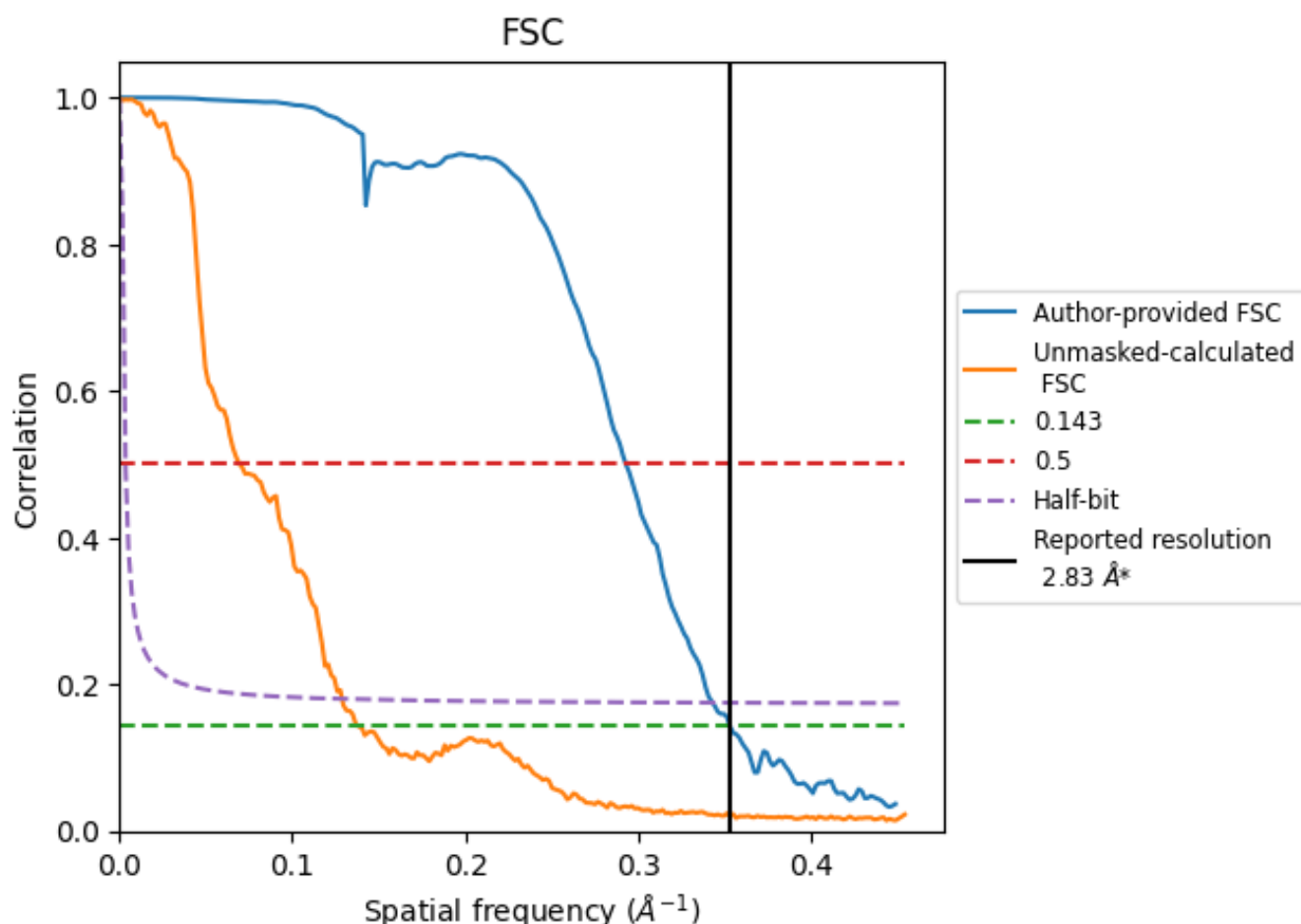
*Reported resolution corresponds to spatial frequency of 0.353 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.83	3.41	2.91
Unmasked-calculated*	7.25	14.37	7.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.25 differs from the reported value 2.83 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-45925 and PDB model 9CU1. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay ⓘ

| X | Y | Z |
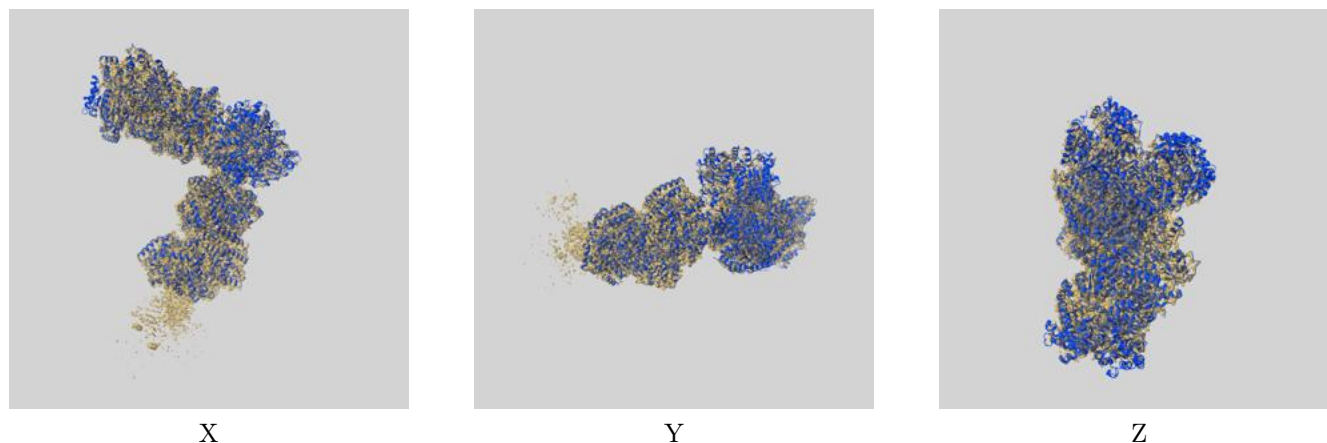
The images above show the 3D surface view of the map at the recommended contour level 0.221 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model　ⓘ

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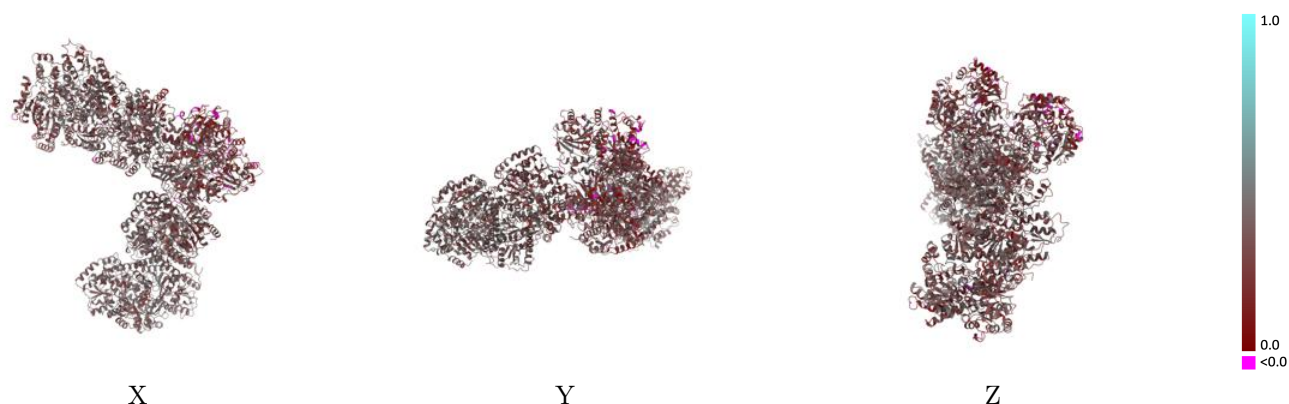
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X　　　　　　　　　　　Y　　　　　　　　　　　Z
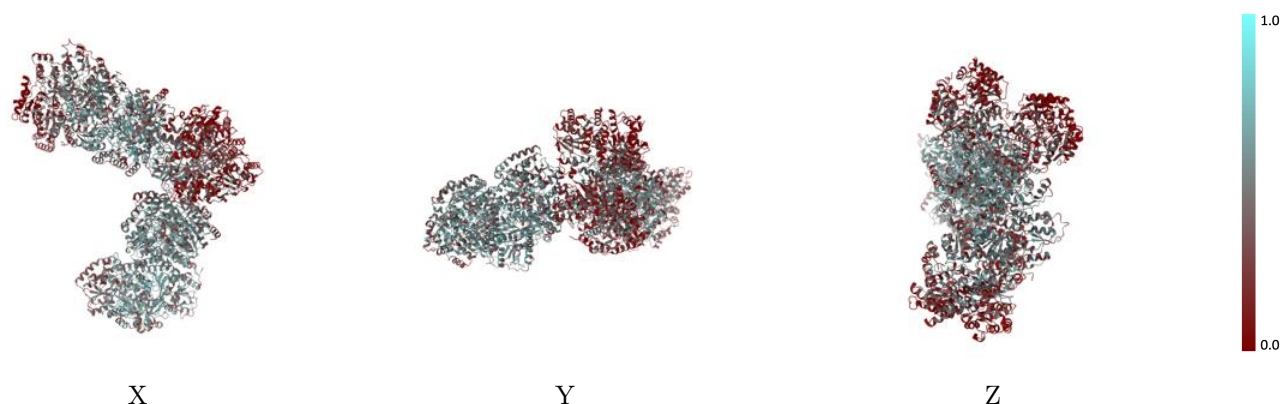
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.221).

9.4　Atom inclusion ⓘ
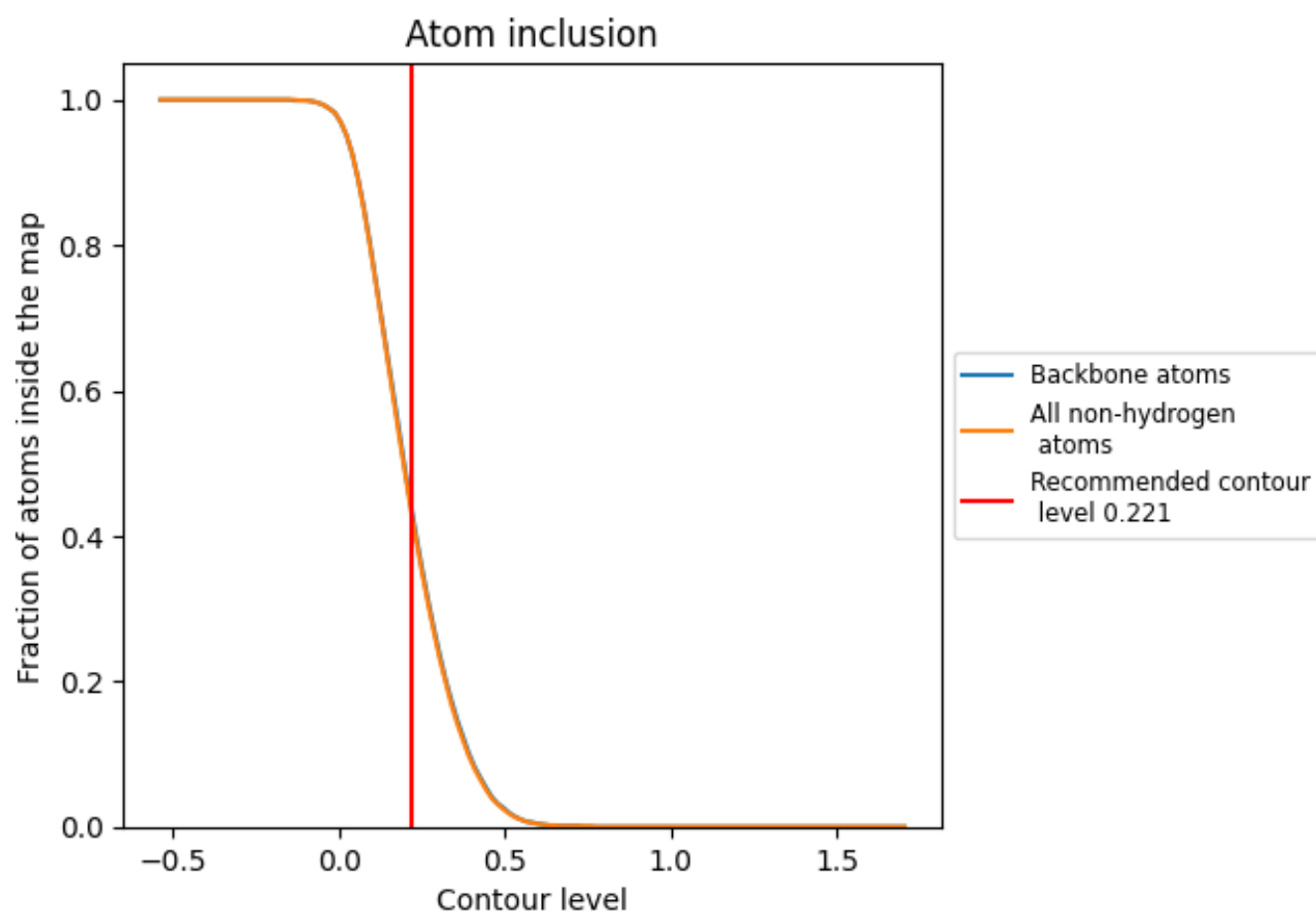
Atom inclusion

At the recommended contour level, 43% of all backbone atoms, 43% 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 (0.221) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4260	0.3330
A	0.5110	0.3420
B	0.4940	0.3450
C	0.2410	0.3160
D	0.4080	0.3320
E	0.1470	0.2150
F	0.2160	0.3020
G	0.5330	0.3600
H	0.5440	0.3440
I	0.5760	0.3670
J	0.5050	0.3680
K	0.5630	0.3800
L	0.2220	0.2530
M	0.2690	0.2980
N	0.5330	0.3500

1.0

0.0
<0.0