Full wwPDB EM Validation Report (i)

Nov 7, 2022 – 12:06 AM EST

PDB ID	:	6NZZ
EMDB ID	:	EMD-0563
Title	:	LRRC8A-DCPIB in MSP1E3D1 nanodisc expanded state
Authors	:	Kern, D.M.; Hite, R.K.; Brohawn, S.G.
Deposited on	:	2019-02-14
Resolution	:	3.32 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:

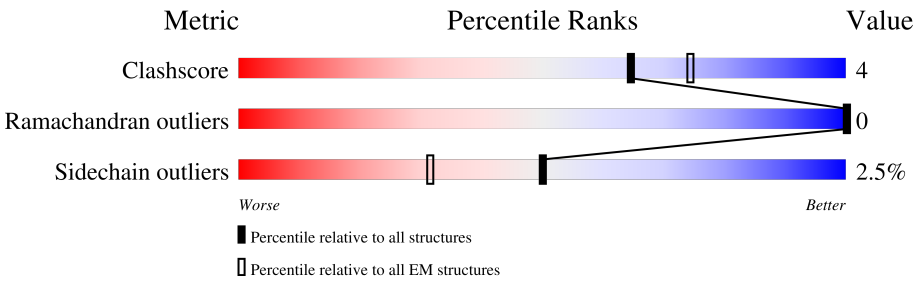
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.32 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	820	16% 33% • 63%
1	B	820	16% 33% • 63%
1	C	820	16% 33% • 63%
1	D	820	16% 33% • 63%
1	E	820	16% 33% • 63%
1	F	820	16% 33% • 63%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 31327 atoms, of which 15669 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 Volume-regulated anion channel subunit LRRC8A.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	306	5123	1697	2555	411	443	17	0	0
1	B	306	5123	1697	2555	411	443	17	0	0
1	C	306	5123	1697	2555	411	443	17	0	0
1	D	306	5123	1697	2555	411	443	17	0	0
1	E	306	5123	1697	2555	411	443	17	0	0
1	F	306	5123	1697	2555	411	443	17	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	811	SER	-	expression tag	UNP Q80WG5
A	812	ASN	-	expression tag	UNP Q80WG5
A	813	SER	-	expression tag	UNP Q80WG5
A	814	LEU	-	expression tag	UNP Q80WG5
A	815	GLU	-	expression tag	UNP Q80WG5
A	816	VAL	-	expression tag	UNP Q80WG5
A	817	LEU	-	expression tag	UNP Q80WG5
A	818	PHE	-	expression tag	UNP Q80WG5
A	819	GLN	-	expression tag	UNP Q80WG5
A	820	GLY	-	expression tag	UNP Q80WG5
B	811	SER	-	expression tag	UNP Q80WG5
B	812	ASN	-	expression tag	UNP Q80WG5
B	813	SER	-	expression tag	UNP Q80WG5
B	814	LEU	-	expression tag	UNP Q80WG5
B	815	GLU	-	expression tag	UNP Q80WG5
B	816	VAL	-	expression tag	UNP Q80WG5
B	817	LEU	-	expression tag	UNP Q80WG5
B	818	PHE	-	expression tag	UNP Q80WG5

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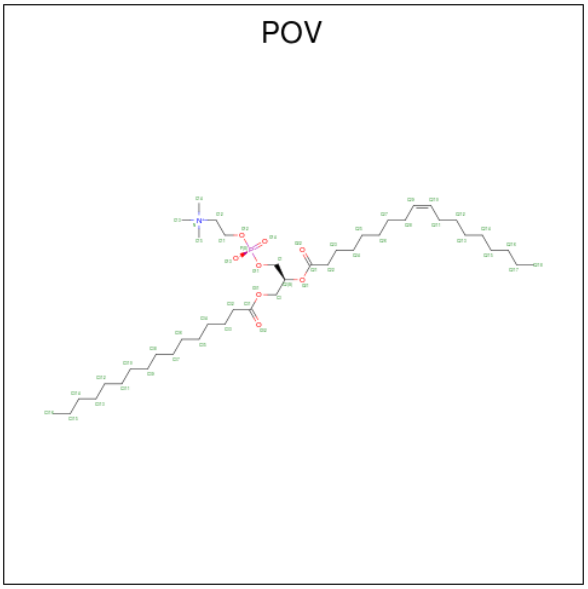
Chain	Residue	Modelled	Actual	Comment	Reference
B	819	GLN	-	expression tag	UNP Q80WG5
B	820	GLY	-	expression tag	UNP Q80WG5
C	811	SER	-	expression tag	UNP Q80WG5
C	812	ASN	-	expression tag	UNP Q80WG5
C	813	SER	-	expression tag	UNP Q80WG5
C	814	LEU	-	expression tag	UNP Q80WG5
C	815	GLU	-	expression tag	UNP Q80WG5
C	816	VAL	-	expression tag	UNP Q80WG5
C	817	LEU	-	expression tag	UNP Q80WG5
C	818	PHE	-	expression tag	UNP Q80WG5
C	819	GLN	-	expression tag	UNP Q80WG5
C	820	GLY	-	expression tag	UNP Q80WG5
D	811	SER	-	expression tag	UNP Q80WG5
D	812	ASN	-	expression tag	UNP Q80WG5
D	813	SER	-	expression tag	UNP Q80WG5
D	814	LEU	-	expression tag	UNP Q80WG5
D	815	GLU	-	expression tag	UNP Q80WG5
D	816	VAL	-	expression tag	UNP Q80WG5
D	817	LEU	-	expression tag	UNP Q80WG5
D	818	PHE	-	expression tag	UNP Q80WG5
D	819	GLN	-	expression tag	UNP Q80WG5
D	820	GLY	-	expression tag	UNP Q80WG5
E	811	SER	-	expression tag	UNP Q80WG5
E	812	ASN	-	expression tag	UNP Q80WG5
E	813	SER	-	expression tag	UNP Q80WG5
E	814	LEU	-	expression tag	UNP Q80WG5
E	815	GLU	-	expression tag	UNP Q80WG5
E	816	VAL	-	expression tag	UNP Q80WG5
E	817	LEU	-	expression tag	UNP Q80WG5
E	818	PHE	-	expression tag	UNP Q80WG5
E	819	GLN	-	expression tag	UNP Q80WG5
E	820	GLY	-	expression tag	UNP Q80WG5
F	811	SER	-	expression tag	UNP Q80WG5
F	812	ASN	-	expression tag	UNP Q80WG5
F	813	SER	-	expression tag	UNP Q80WG5
F	814	LEU	-	expression tag	UNP Q80WG5
F	815	GLU	-	expression tag	UNP Q80WG5
F	816	VAL	-	expression tag	UNP Q80WG5
F	817	LEU	-	expression tag	UNP Q80WG5
F	818	PHE	-	expression tag	UNP Q80WG5
F	819	GLN	-	expression tag	UNP Q80WG5
F	820	GLY	-	expression tag	UNP Q80WG5

- Molecule 2 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: $C_{42}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
2	A	1	89	31	52	6	0
			Total	C	H	O	
2	A	1	89	31	52	6	0
			Total	C	H	O	
2	A	1	89	31	52	6	0
			Total	C	H	O	
2	B	1	89	31	52	6	0
			Total	C	H	O	
2	B	1	89	31	52	6	0
			Total	C	H	O	
2	B	1	89	31	52	6	0
			Total	C	H	O	
2	C	1	89	31	52	6	0
			Total	C	H	O	
2	C	1	89	31	52	6	0
			Total	C	H	O	
2	C	1	89	31	52	6	0
			Total	C	H	O	
2	D	1	89	31	52	6	0
			Total	C	H	O	
2	D	1	89	31	52	6	0
			Total	C	H	O	
2	D	1	89	31	52	6	0

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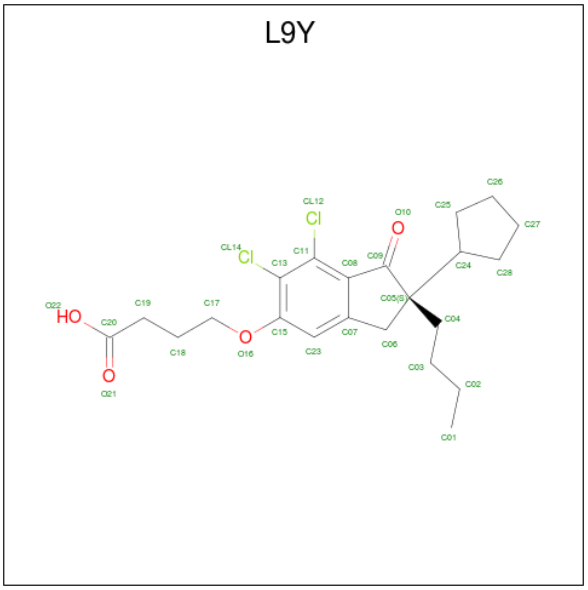
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
2	E	1	89	31	52	6	0
2	E	1	89	31	52	6	0
2	E	1	89	31	52	6	0
2	F	1	89	31	52	6	0
2	F	1	89	31	52	6	0
2	F	1	89	31	52	6	0

- Molecule 3 is 4-{[(2S)-2-butyl-6,7-dichloro-2-cyclopentyl-1-oxo-2,3-dihydro-1H-inden-5-yl]oxy}butanoic acid (three-letter code: L9Y) (formula: $C_{22}H_{28}Cl_2O_4$).



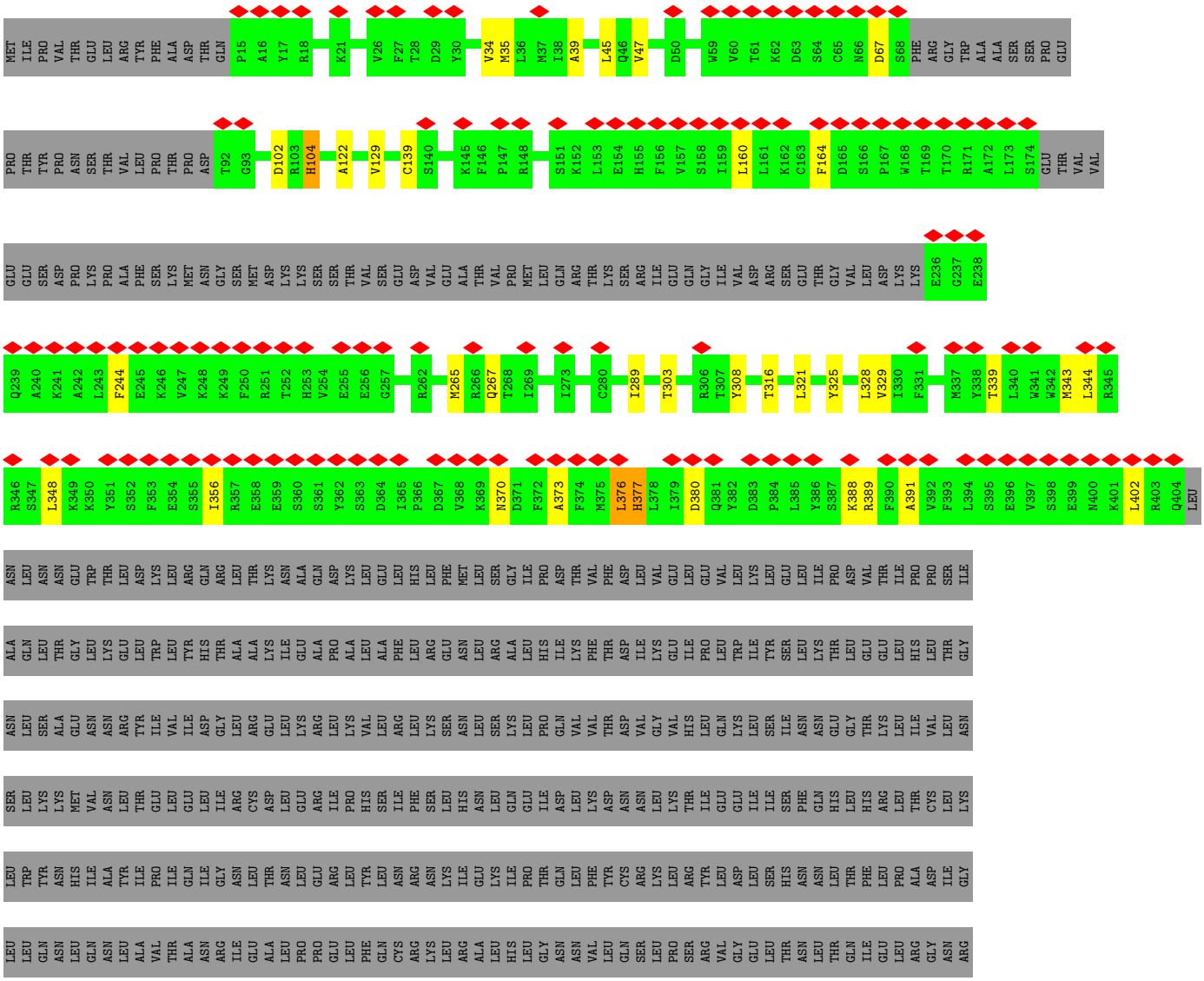
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	H	O	
3	F	1	55	22	2	27	4	0

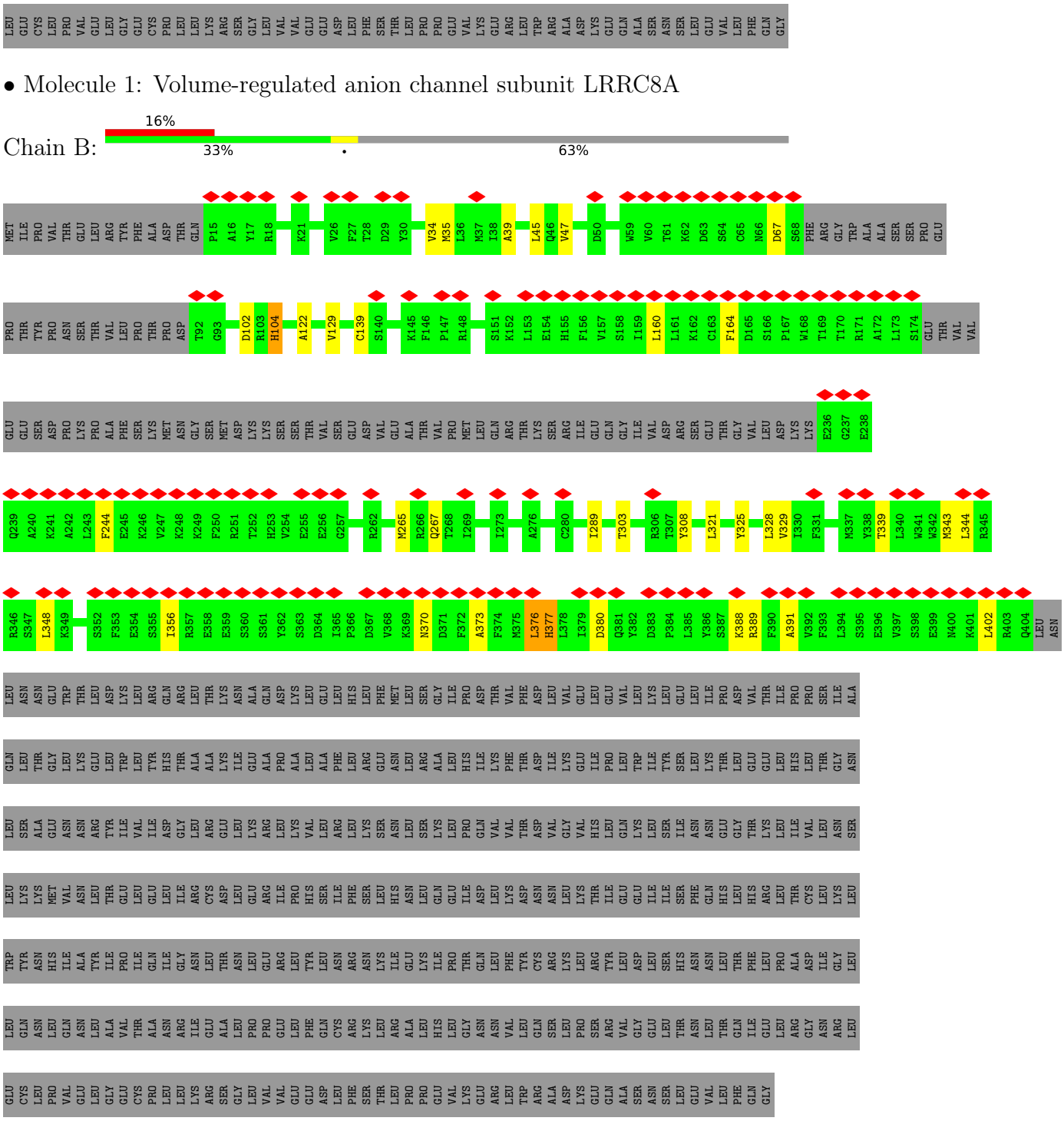
3 Residue-property plots (i)

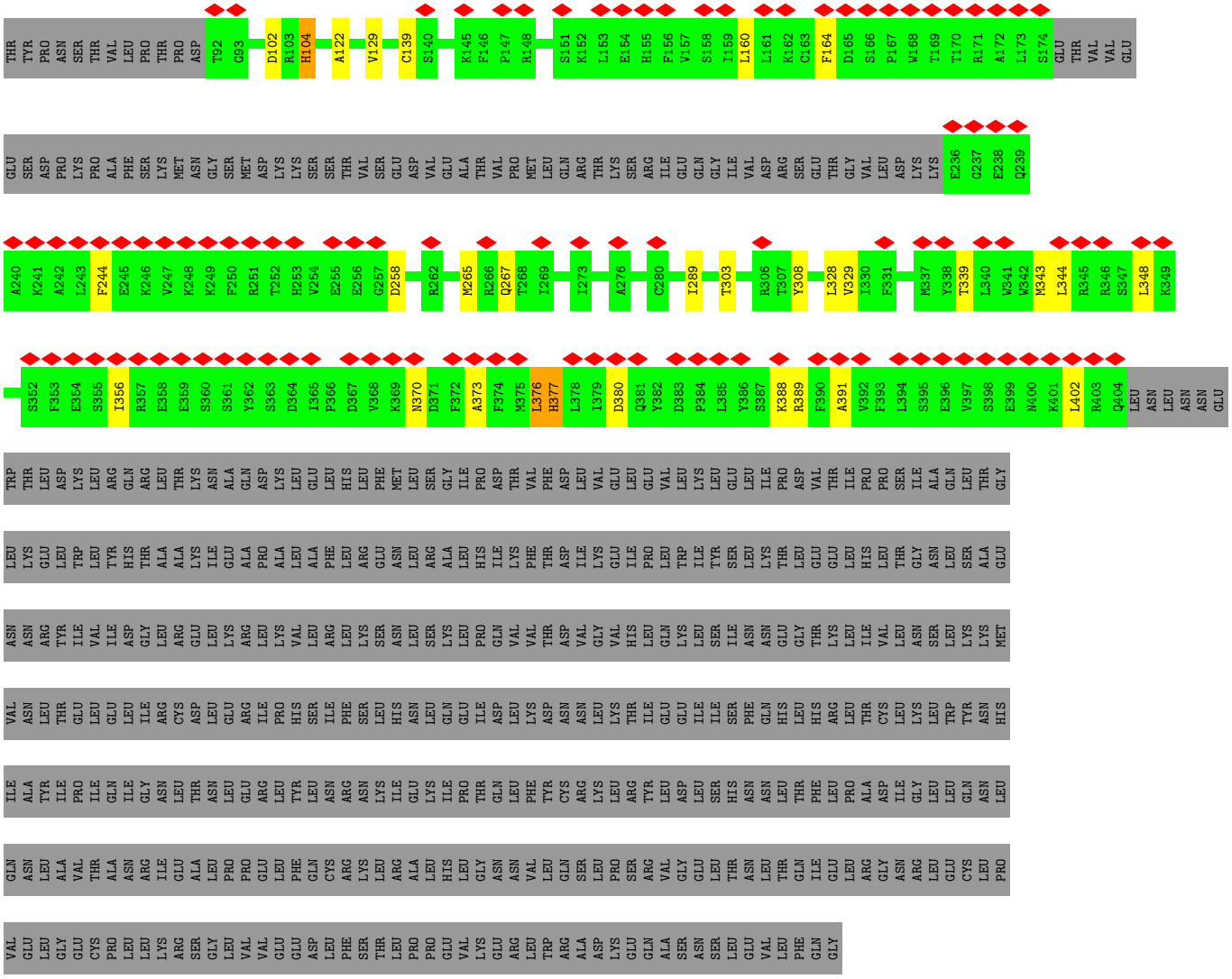
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Volume-regulated anion channel subunit LRRC8A

Chain A:

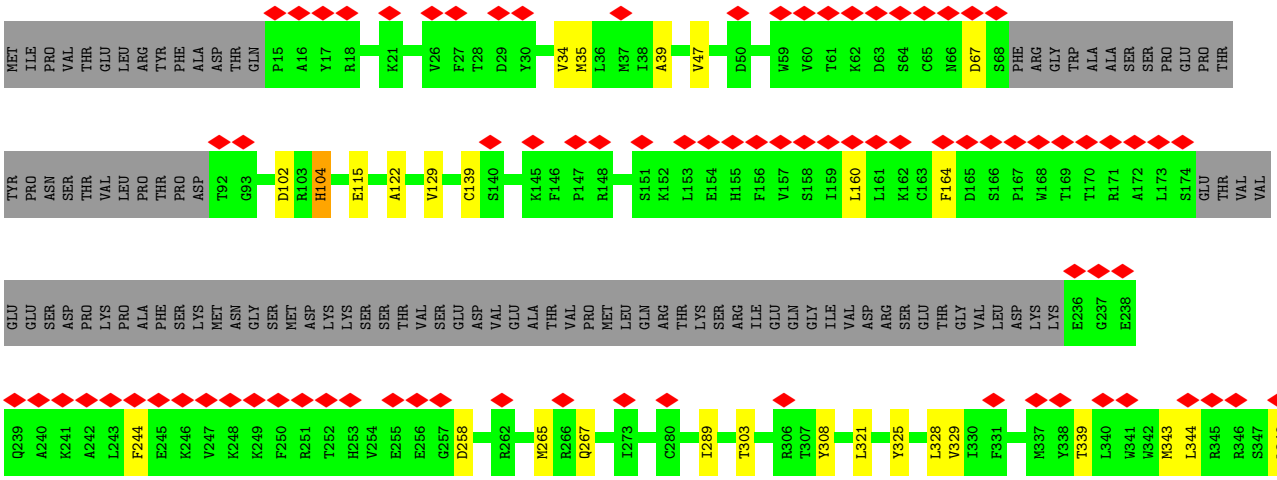


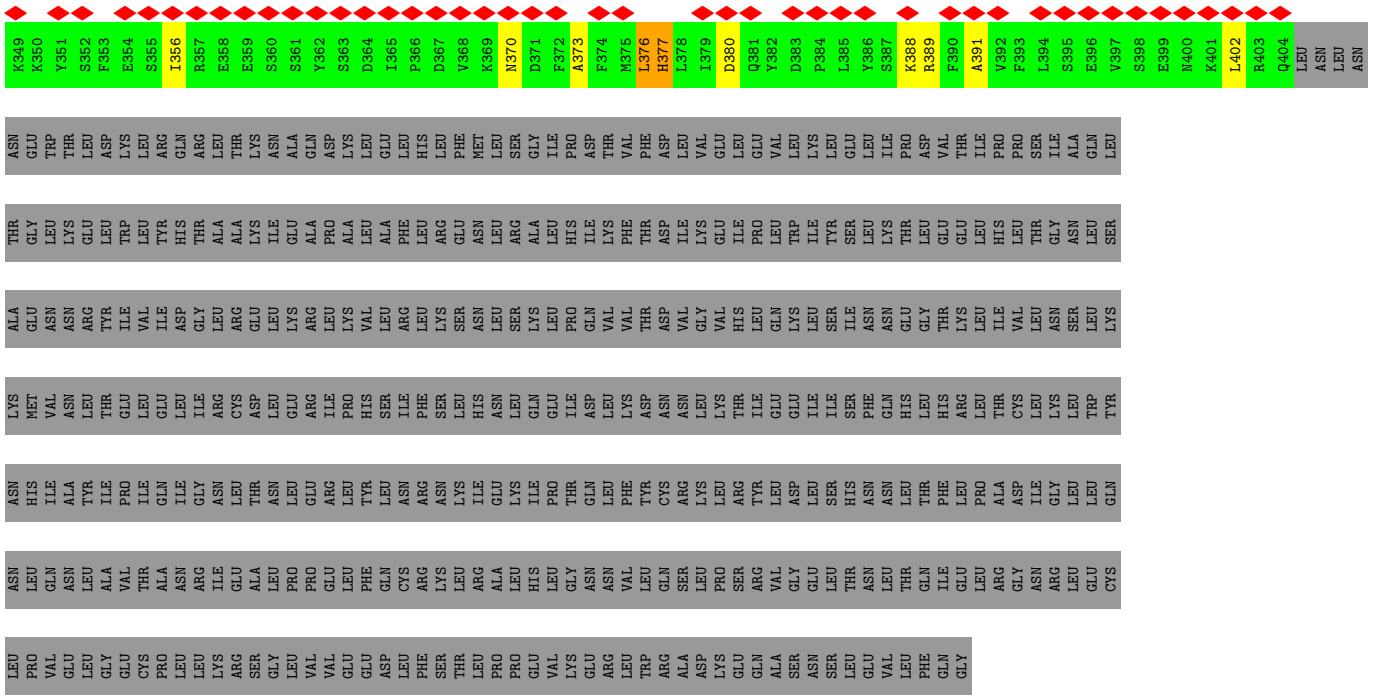

• Molecule 1: Volume-regulated anion channel subunit LRRC8A
Chain B:
16%
33%
63%
• Molecule 1: Volume-regulated anion channel subunit LRRC8A
Chain C:
16%
33%
63%



- Molecule 1: Volume-regulated anion channel subunit LRRC8A

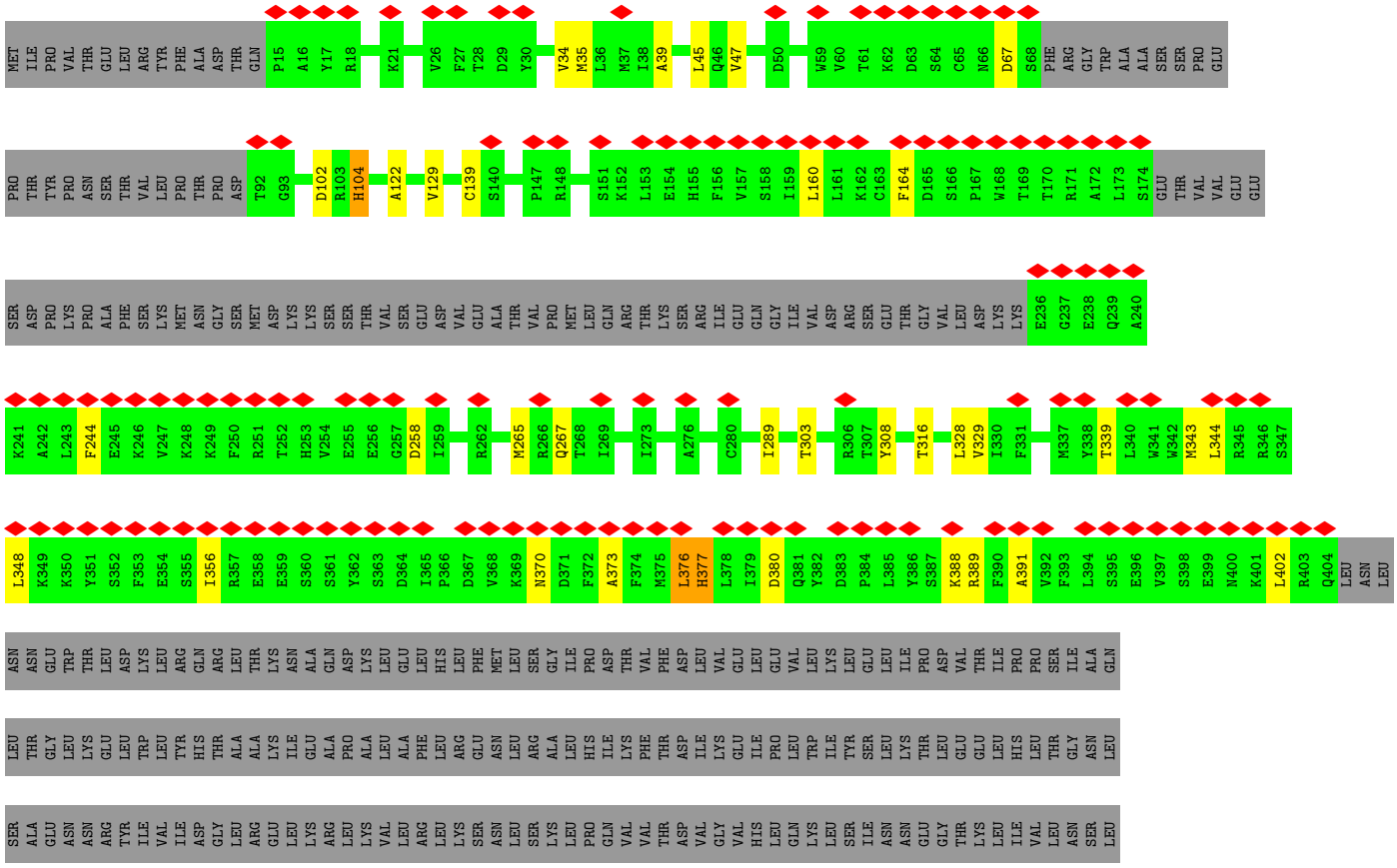
Chain D:

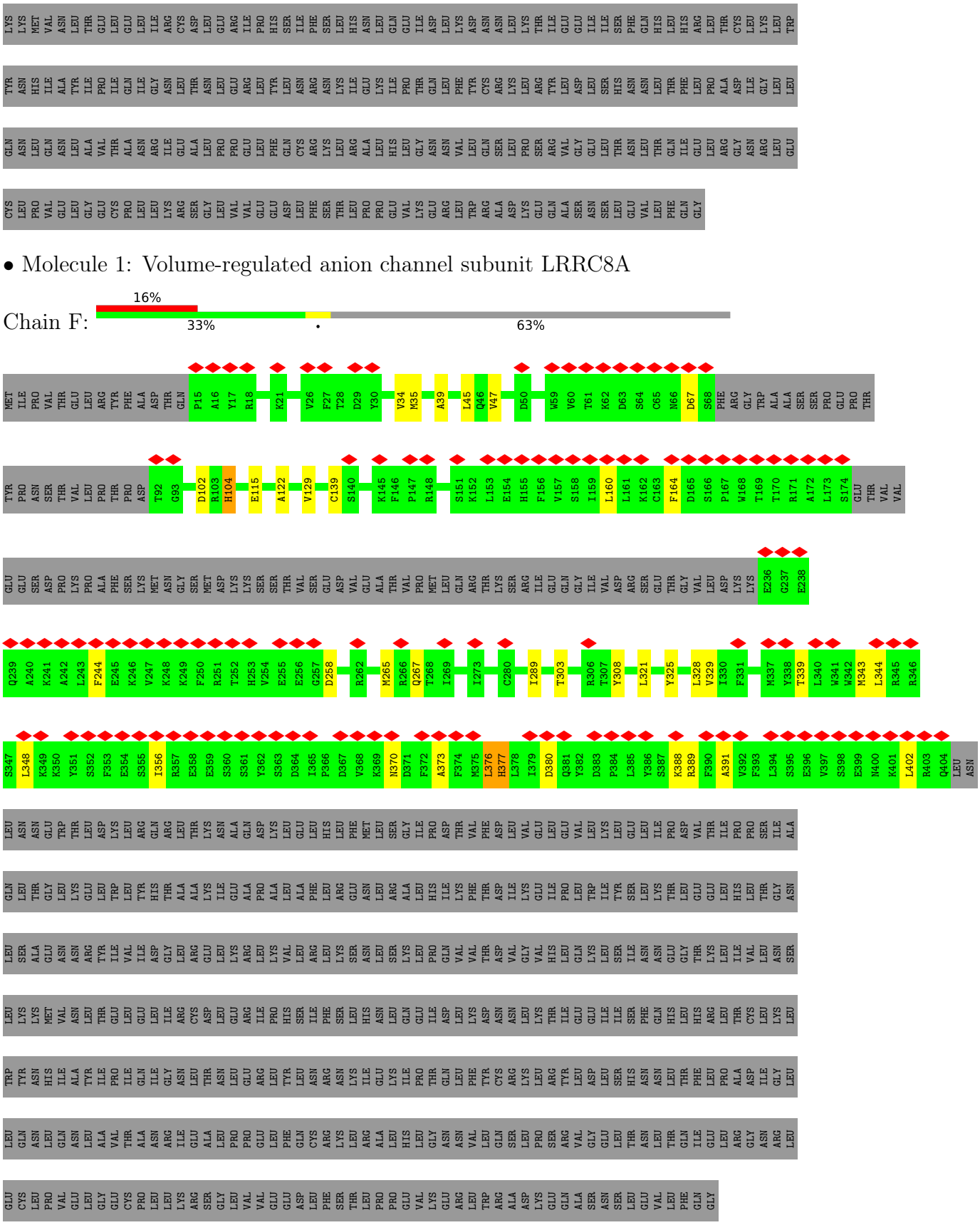




- Molecule 1: Volume-regulated anion channel subunit LRRC8A

Chain E:




LYS LYS MET VAL ASN LEU THR GLU LEU GLU LEU ILE ARG CYS ASP LEU GLU ARG ILE PRO HIS SER ILE PHE SER LEU HIS ASN LEU GLN GLU ILE ASP LEU LYS ASP ASN ASN LEU LYS THR ILE GLU GLU ILE ILE SER PHE GLN HIS LEU HIS ARG LEU THR CYS LEU LYS LEU TRP
TYR ASN HIS ILE ALA TYR ILE PRO ILE GLN ILE GLY ASN LEU THR ASN LEU GLU ARG LEU TYR LEU ASN ARG ASN LYS ILE GLU LYS ILE PRO THR GLN LEU PHE TYR CYS ARG LYS LEU ASP LEU SER HIS ASN ASN LEU THR PHE LEU PRO ALA ASP ILE GLY LEU LEU
GLN ASN LEU GLN ASN LEU ALA VAL THR ALA ALA ASN ARG ILE GLU ALA LEU PRO PRO GLU LEU PHE GLN CYS ARG LYS LEU ARG ALA LEU HIS LEU GLY ASN ASN VAL LEU GLN SER LEU PRO SER ARG VAL GLY GLU LEU THR ASN LEU THR GLN ILE GLU LEU ARG GLY ASN ARG LEU GLU
CYS LEU PRO VAL GLU LEU GLY GLU CYS PRO LEU LEU LYS ARG SER GLY LEU VAL VAL GLU GLU ASP LEU PHE SER THR LEU PRO PRO GLU VAL LYS GLU ARG LEU TRP ARG ALA ASP LYS GLU GLN ALA SER ASN SER LEU GLU VAL LEU PHE GLN GLY
• Molecule 1: Volume-regulated anion channel subunit LRRC8A
Chain F:
16%
33%
63%
MET ILE PRO VAL THR GLU LEU ARG TYR PHE ALA ASP THR GLN P15 A16 Y17 R18 K21 V26 F27 T28 D29 Y30 V34 M35 A39 L45 Q46 V47 D50 W59 V60 T61 K62 D63 S64 C65 N66 D67 S68 PHE ARG GLY TRP ALA ALA SER SER PRO GLU PRO THR
TYR PRO ASN SER THR VAL LEU PRO THR PRO ASP T92 G93 D102 R103 H104 E115 A122 V129 C139 S140 K145 F146 P147 R148 S151 K152 L153 E154 H155 F156 V157 S158 I159 L160 L161 K162 C163 F164 D165 S166 P167 W168 T169 T170 R171 A172 L173 S174 GLU THR VAL VAL
GLU GLU SER ASP PRO LYS PRO ALA PHE SER LYS MET ASN GLY SER MET ASP LYS LYS SER SER THR VAL SER GLU ASP VAL GLU ALA THR VAL PRO MET LEU GLN ARG THR LYS SER ARG ILE GLU GLN GLY ILE VAL ASP ARG SER GLU THR GLY VAL LEU ASP LYS LYS E236 G237 E238
Q239 A240 K241 A242 L243 F244 E245 K246 V247 K248 K249 F250 R251 T252 H253 V254 E255 E256 G257 D258 R262 M265 R266 Q267 T268 I269 I273 C280 I289 T303 R306 T307 Y308 L321 Y325 L328 V329 I330 F331 M337 Y338 T339 L340 W341 W342 M343 L344 R345 R346
S347 L348 K349 K350 Y351 S352 F353 E354 S355 I356 R357 E358 E359 S360 S361 Y362 S363 D364 I365 P366 D367 V368 K369 N370 D371 F372 A373 F374 M375 L376 H377 L378 I379 D380 Q381 Y382 D383 P384 L385 Y386 S387 K388 R389 F390 A391 V392 F393 L394 S395 E396 V397 S398 E399 M400 K401 L402 R403 Q404 LEU ASN
LEU ASN ASN GLU TRP THR LEU ASP LYS LEU ARG GLN ARG LEU THR LYS ASN ALA GLN ASP LYS LEU GLU LEU HIS LEU PHE MET LEU SER GLY ILE PRO ASP THR VAL PHE ASP LEU VAL GLU LEU GLU VAL LEU LYS LEU GLU LEU ILE PRO ASP VAL THR ILE PRO PRO SER ILE ALA
GLN LEU THR GLY LEU LYS GLU LEU TRP LEU TYR HIS THR ALA ALA LYS ILE GLU ALA PRO ALA LEU ALA PHE LEU ARG GLU ASN LEU ARG ALA LEU HIS ILE LYS PHE THR ASP ILE LYS GLU ILE PRO LEU TRP ILE TYR SER LEU LYS THR LEU GLU GLU LEU HIS LEU THR GLY ASN
LEU SER ALA GLU ASN ASN ARG TYR ILE VAL ILE ASP GLY LEU ARG GLU LEU LYS ARG LEU LYS VAL LEU ARG LEU LYS SER ASN LEU SER LYS LEU PRO GLN VAL VAL THR ASP VAL GLY VAL HIS LEU GLN LYS LEU SER ILE ASN ASN GLU GLY THR LYS LEU ILE VAL LEU ASN SER
LEU LYS LYS MET VAL ASN LEU THR GLU LEU GLU LEU ILE ARG CYS ASP LEU GLU ARG ILE PRO HIS SER ILE PHE SER LEU HIS ASN LEU GLN GLU ILE ASP LEU LYS ASP ASN ASN LEU LYS THR ILE GLU GLU ILE ILE SER PHE GLN HIS LEU HIS ARG LEU THR CYS LEU LYS LEU
TRP TYR ASN HIS ILE ALA TYR ILE PRO ILE GLN ILE GLY ASN LEU THR ASN LEU GLU ARG LEU TYR LEU ASN ARG ASN LYS ILE GLU LYS ILE PRO THR GLN LEU PHE TYR CYS ARG LYS LEU ARG TYR LEU ASP LEU SER HIS ASN ASN LEU THR PHE LEU PRO ALA ASP ILE GLY LEU
LEU GLN ASN LEU GLN ASN LEU ALA VAL THR ALA ALA ASN ARG ILE GLU ALA LEU PRO PRO GLU LEU PHE GLN CYS ARG LYS LEU ARG ALA LEU HIS LEU GLY ASN ASN VAL LEU GLN SER LEU PRO SER ARG VAL GLY GLU LEU THR ASN LEU THR GLN ILE GLU LEU ARG GLY ASN ARG LEU
GLU CYS LEU PRO VAL GLU LEU GLY GLU CYS PRO LEU LEU LYS ARG SER GLY LEU VAL VAL GLU GLU ASP LEU PHE SER THR LEU PRO PRO GLU VAL LYS GLU ARG LEU TRP ARG ALA ASP LYS GLU GLN ALA SER ASN SER LEU GLU VAL LEU PHE GLN GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	35435	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 ($e^-/Å^2$)	60.8	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	64.370	Depositor
Minimum map value	-35.093	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	10.0	Depositor
Map size (Å)	396.032, 396.032, 396.032	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.088, 1.088, 1.088	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: POV, L9Y

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	0.31	0/2643	0.52	0/3580
1	B	0.31	0/2643	0.52	0/3580
1	C	0.31	0/2643	0.52	0/3580
1	D	0.31	0/2643	0.52	0/3580
1	E	0.31	0/2643	0.53	0/3580
1	F	0.31	0/2643	0.53	0/3580
All	All	0.31	0/15858	0.52	0/21480

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	A	2568	2555	2555	24	0
1	B	2568	2555	2555	22	0
1	C	2568	2555	2555	22	0
1	D	2568	2555	2555	23	0
1	E	2568	2555	2555	22	0
1	F	2568	2555	2555	25	0
2	A	37	52	50	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	37	52	50	0	0
2	C	37	52	50	0	0
2	D	37	52	50	0	0
2	E	37	52	50	0	0
2	F	37	52	50	0	0
3	F	28	27	0	0	0
All	All	15658	15669	15630	130	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 4.

All (130) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:VAL:HG13	1:F:328:LEU:HD21	1.75	0.69
1:A:34:VAL:HG13	1:A:328:LEU:HD21	1.75	0.69
1:B:34:VAL:HG13	1:B:328:LEU:HD21	1.75	0.69
1:E:34:VAL:HG13	1:E:328:LEU:HD21	1.75	0.69
1:D:34:VAL:HG13	1:D:328:LEU:HD21	1.75	0.69
1:C:34:VAL:HG13	1:C:328:LEU:HD21	1.75	0.68
1:A:122:ALA:HB2	1:A:289:ILE:HG22	1.76	0.68
1:F:122:ALA:HB2	1:F:289:ILE:HG22	1.76	0.67
1:B:122:ALA:HB2	1:B:289:ILE:HG22	1.76	0.67
1:E:122:ALA:HB2	1:E:289:ILE:HG22	1.76	0.67
1:C:122:ALA:HB2	1:C:289:ILE:HG22	1.76	0.66
1:D:122:ALA:HB2	1:D:289:ILE:HG22	1.76	0.66
1:A:45:LEU:HD12	1:F:47:VAL:HG21	1.78	0.66
1:D:303:THR:HG1	1:D:308:TYR:HH	1.46	0.64
1:E:303:THR:HG1	1:E:308:TYR:HH	1.47	0.63
1:C:303:THR:HG1	1:C:308:TYR:HH	1.47	0.63
1:D:139:CYS:O	1:D:267:GLN:NE2	2.33	0.62
1:A:139:CYS:O	1:A:267:GLN:NE2	2.33	0.62
1:F:139:CYS:O	1:F:267:GLN:NE2	2.33	0.62
1:C:139:CYS:O	1:C:267:GLN:NE2	2.33	0.62
1:E:139:CYS:O	1:E:267:GLN:NE2	2.33	0.62
1:B:139:CYS:O	1:B:267:GLN:NE2	2.33	0.61
1:B:303:THR:OG1	1:B:308:TYR:OH	2.21	0.59
1:A:39:ALA:HB2	1:A:129:VAL:HG23	1.85	0.58
1:F:39:ALA:HB2	1:F:129:VAL:HG23	1.85	0.58
1:E:39:ALA:HB2	1:E:129:VAL:HG23	1.85	0.58
1:F:303:THR:OG1	1:F:308:TYR:OH	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ALA:HB2	1:D:129:VAL:HG23	1.85	0.58
1:B:39:ALA:HB2	1:B:129:VAL:HG23	1.85	0.58
1:C:39:ALA:HB2	1:C:129:VAL:HG23	1.85	0.57
1:F:160:LEU:HD21	1:F:376:LEU:CD2	2.34	0.57
1:D:160:LEU:HD21	1:D:376:LEU:CD2	2.34	0.57
1:E:160:LEU:HD21	1:E:376:LEU:CD2	2.34	0.57
1:C:160:LEU:HD21	1:C:376:LEU:CD2	2.34	0.57
1:B:160:LEU:HD21	1:B:376:LEU:CD2	2.34	0.56
1:A:160:LEU:HD21	1:A:376:LEU:CD2	2.34	0.56
1:E:47:VAL:HG21	1:F:45:LEU:HD12	1.87	0.56
1:F:164:PHE:O	1:F:389:ARG:NH2	2.39	0.56
1:B:339:THR:O	1:B:343:MET:N	2.39	0.56
1:C:164:PHE:O	1:C:389:ARG:NH2	2.39	0.56
1:C:339:THR:O	1:C:343:MET:N	2.39	0.55
1:F:339:THR:O	1:F:343:MET:N	2.39	0.55
1:D:339:THR:O	1:D:343:MET:N	2.39	0.55
1:E:164:PHE:O	1:E:389:ARG:NH2	2.39	0.55
1:A:339:THR:O	1:A:343:MET:N	2.39	0.55
1:E:339:THR:O	1:E:343:MET:N	2.39	0.54
1:C:356:ILE:HD12	1:C:388:LYS:HG2	1.90	0.54
1:B:373:ALA:O	1:B:377:HIS:N	2.41	0.54
1:D:356:ILE:HD12	1:D:388:LYS:HG2	1.90	0.54
1:D:373:ALA:O	1:D:377:HIS:N	2.41	0.54
1:B:356:ILE:HD12	1:B:388:LYS:HG2	1.90	0.53
1:E:373:ALA:O	1:E:377:HIS:N	2.41	0.53
1:F:373:ALA:O	1:F:377:HIS:N	2.41	0.53
1:C:373:ALA:O	1:C:377:HIS:N	2.41	0.53
1:E:356:ILE:HD12	1:E:388:LYS:HG2	1.90	0.53
1:A:164:PHE:O	1:A:389:ARG:NH2	2.39	0.53
1:D:164:PHE:O	1:D:389:ARG:NH2	2.39	0.53
1:B:164:PHE:O	1:B:389:ARG:NH2	2.39	0.53
1:A:373:ALA:O	1:A:377:HIS:N	2.41	0.53
1:B:47:VAL:HG21	1:C:45:LEU:HD12	1.91	0.53
1:A:356:ILE:HD12	1:A:388:LYS:HG2	1.90	0.52
1:D:244:PHE:CE2	1:D:402:LEU:HD22	2.44	0.52
1:E:244:PHE:CE2	1:E:402:LEU:HD22	2.44	0.52
1:F:356:ILE:HD12	1:F:388:LYS:HG2	1.90	0.52
1:B:244:PHE:CE2	1:B:402:LEU:HD22	2.44	0.52
1:C:244:PHE:CE2	1:C:402:LEU:HD22	2.44	0.52
1:A:47:VAL:HG21	1:B:45:LEU:HD12	1.91	0.52
1:F:244:PHE:CE2	1:F:402:LEU:HD22	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:PHE:CE2	1:A:402:LEU:HD22	2.44	0.51
1:E:370:ASN:N	1:E:370:ASN:OD1	2.45	0.50
1:D:47:VAL:HG21	1:E:45:LEU:HD12	1.94	0.50
1:F:370:ASN:OD1	1:F:370:ASN:N	2.44	0.50
1:D:370:ASN:N	1:D:370:ASN:OD1	2.45	0.50
1:B:370:ASN:N	1:B:370:ASN:OD1	2.44	0.49
1:C:370:ASN:N	1:C:370:ASN:OD1	2.44	0.49
1:A:370:ASN:N	1:A:370:ASN:OD1	2.44	0.49
1:D:356:ILE:HD13	1:D:391:ALA:CB	2.45	0.47
1:E:356:ILE:HD13	1:E:391:ALA:CB	2.44	0.47
1:A:45:LEU:HD12	1:F:47:VAL:CG2	2.43	0.47
1:A:316:THR:OG1	1:F:115:GLU:OE2	2.27	0.47
1:C:356:ILE:HD13	1:C:391:ALA:CB	2.45	0.47
1:F:356:ILE:HD13	1:F:391:ALA:CB	2.45	0.47
1:A:356:ILE:HD13	1:A:391:ALA:CB	2.45	0.46
1:D:115:GLU:OE2	1:E:316:THR:OG1	2.31	0.46
1:A:303:THR:OG1	1:A:308:TYR:OH	2.21	0.46
1:B:356:ILE:HD13	1:B:391:ALA:CB	2.45	0.46
1:E:356:ILE:HD12	1:E:388:LYS:CG	2.46	0.45
1:F:356:ILE:HD12	1:F:388:LYS:CG	2.46	0.45
1:D:356:ILE:HD12	1:D:388:LYS:CG	2.46	0.45
1:C:356:ILE:HD12	1:C:388:LYS:CG	2.46	0.45
1:B:356:ILE:HD12	1:B:388:LYS:CG	2.46	0.45
1:F:258:ASP:OD1	1:F:258:ASP:N	2.50	0.45
1:A:356:ILE:HD12	1:A:388:LYS:CG	2.46	0.44
1:C:303:THR:OG1	1:C:308:TYR:OH	2.21	0.44
1:E:258:ASP:OD1	1:E:258:ASP:N	2.50	0.44
1:C:102:ASP:OD1	1:C:104:HIS:N	2.51	0.43
1:D:102:ASP:OD1	1:D:104:HIS:N	2.51	0.43
1:A:39:ALA:CB	1:A:129:VAL:HG23	2.50	0.42
1:B:244:PHE:CD2	1:B:402:LEU:HD22	2.54	0.42
1:E:102:ASP:OD1	1:E:104:HIS:N	2.51	0.42
1:A:321:LEU:O	1:A:325:TYR:N	2.51	0.42
1:B:102:ASP:OD1	1:B:104:HIS:N	2.51	0.42
1:D:39:ALA:CB	1:D:129:VAL:HG23	2.50	0.42
1:C:244:PHE:CD2	1:C:402:LEU:HD22	2.54	0.42
1:C:265:MET:CE	1:C:344:LEU:HD21	2.50	0.42
1:D:321:LEU:O	1:D:325:TYR:N	2.51	0.42
1:A:265:MET:CE	1:A:344:LEU:HD21	2.50	0.42
1:F:244:PHE:CD2	1:F:402:LEU:HD22	2.54	0.42
1:F:265:MET:CE	1:F:344:LEU:HD21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:PHE:CD2	1:A:402:LEU:HD22	2.54	0.42
1:B:265:MET:CE	1:B:344:LEU:HD21	2.50	0.42
1:E:244:PHE:CD2	1:E:402:LEU:HD22	2.55	0.42
1:B:39:ALA:CB	1:B:129:VAL:HG23	2.50	0.41
1:F:39:ALA:CB	1:F:129:VAL:HG23	2.50	0.41
1:C:258:ASP:OD1	1:C:258:ASP:N	2.50	0.41
1:F:321:LEU:O	1:F:325:TYR:N	2.51	0.41
1:F:102:ASP:OD1	1:F:104:HIS:N	2.51	0.41
1:A:102:ASP:OD1	1:A:104:HIS:N	2.51	0.41
1:B:321:LEU:O	1:B:325:TYR:N	2.51	0.41
1:D:244:PHE:CD2	1:D:402:LEU:HD22	2.55	0.41
1:D:258:ASP:OD1	1:D:258:ASP:N	2.50	0.41
1:D:265:MET:CE	1:D:344:LEU:HD21	2.50	0.41
1:D:35:MET:HG3	1:D:328:LEU:HD23	2.03	0.41
1:E:35:MET:HG3	1:E:328:LEU:HD23	2.03	0.41
1:E:265:MET:CE	1:E:344:LEU:HD21	2.50	0.41
1:F:35:MET:HG3	1:F:328:LEU:HD23	2.03	0.41
1:C:39:ALA:CB	1:C:129:VAL:HG23	2.50	0.41
1:C:35:MET:HG3	1:C:328:LEU:HD23	2.03	0.40
1:A:35:MET:HG3	1:A:328:LEU:HD23	2.03	0.40
1:B:35:MET:HG3	1:B:328:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	300/820 (37%)	284 (95%)	16 (5%)	0	100	100
1	B	300/820 (37%)	284 (95%)	16 (5%)	0	100	100
1	C	300/820 (37%)	284 (95%)	16 (5%)	0	100	100
1	D	300/820 (37%)	284 (95%)	16 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	300/820 (37%)	284 (95%)	16 (5%)	0	100	100
1	F	300/820 (37%)	284 (95%)	16 (5%)	0	100	100
All	All	1800/4920 (37%)	1704 (95%)	96 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/758 (38%)	277 (98%)	7 (2%)	47	73
1	B	284/758 (38%)	277 (98%)	7 (2%)	47	73
1	C	284/758 (38%)	277 (98%)	7 (2%)	47	73
1	D	284/758 (38%)	277 (98%)	7 (2%)	47	73
1	E	284/758 (38%)	277 (98%)	7 (2%)	47	73
1	F	284/758 (38%)	277 (98%)	7 (2%)	47	73
All	All	1704/4548 (38%)	1662 (98%)	42 (2%)	50	73

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ASP
1	A	104	HIS
1	A	329	VAL
1	A	348	LEU
1	A	376	LEU
1	A	377	HIS
1	A	380	ASP
1	B	67	ASP
1	B	104	HIS
1	B	329	VAL
1	B	348	LEU
1	B	376	LEU

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Mol	Chain	Res	Type
1	B	377	HIS
1	B	380	ASP
1	C	67	ASP
1	C	104	HIS
1	C	329	VAL
1	C	348	LEU
1	C	376	LEU
1	C	377	HIS
1	C	380	ASP
1	D	67	ASP
1	D	104	HIS
1	D	329	VAL
1	D	348	LEU
1	D	376	LEU
1	D	377	HIS
1	D	380	ASP
1	E	67	ASP
1	E	104	HIS
1	E	329	VAL
1	E	348	LEU
1	E	376	LEU
1	E	377	HIS
1	E	380	ASP
1	F	67	ASP
1	F	104	HIS
1	F	329	VAL
1	F	348	LEU
1	F	376	LEU
1	F	377	HIS
1	F	380	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	GLN
1	B	267	GLN
1	C	267	GLN
1	D	267	GLN
1	E	267	GLN
1	F	267	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

19 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	$\#\|Z\| > 2$
2	POV	D	902	-	11,11,51	0.51	0	11,11,59	1.06	1 (9%)
2	POV	C	901	-	14,14,51	1.30	2 (14%)	14,14,59	1.48	3 (21%)
2	POV	F	902	-	11,11,51	0.51	0	11,11,59	1.06	1 (9%)
2	POV	E	903	-	9,9,51	0.53	0	9,9,59	1.07	1 (11%)
2	POV	D	901	-	14,14,51	1.30	2 (14%)	14,14,59	1.48	3 (21%)
2	POV	E	901	-	14,14,51	1.31	2 (14%)	14,14,59	1.49	3 (21%)
2	POV	B	902	-	11,11,51	0.51	0	11,11,59	1.06	1 (9%)
2	POV	A	901	-	14,14,51	1.31	2 (14%)	14,14,59	1.49	3 (21%)
2	POV	C	902	-	11,11,51	0.50	0	11,11,59	1.05	1 (9%)
2	POV	F	903	-	9,9,51	0.54	0	9,9,59	1.07	1 (11%)
2	POV	F	901	-	14,14,51	1.30	2 (14%)	14,14,59	1.49	3 (21%)
2	POV	B	903	-	9,9,51	0.54	0	9,9,59	1.07	1 (11%)
2	POV	A	902	-	11,11,51	0.51	0	11,11,59	1.05	1 (9%)
3	L9Y	F	904	-	29,30,30	1.95	9 (31%)	35,43,43	3.09	13 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	POV	B	901	-	14,14,51	1.31	2 (14%)	14,14,59	1.49	3 (21%)
2	POV	D	903	-	9,9,51	0.54	0	9,9,59	1.07	1 (11%)
2	POV	E	902	-	11,11,51	0.50	0	11,11,59	1.05	1 (9%)
2	POV	A	903	-	9,9,51	0.54	0	9,9,59	1.07	1 (11%)
2	POV	C	903	-	9,9,51	0.54	0	9,9,59	1.07	1 (11%)

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
2	POV	D	902	-	-	4/9/9/55	-
2	POV	C	901	-	-	2/12/12/55	-
2	POV	F	902	-	-	4/9/9/55	-
2	POV	E	903	-	-	3/7/7/55	-
2	POV	D	901	-	-	2/12/12/55	-
2	POV	E	901	-	-	2/12/12/55	-
2	POV	B	902	-	-	4/9/9/55	-
2	POV	A	901	-	-	2/12/12/55	-
2	POV	C	902	-	-	4/9/9/55	-
2	POV	F	903	-	-	3/7/7/55	-
2	POV	F	901	-	-	2/12/12/55	-
2	POV	B	903	-	-	3/7/7/55	-
2	POV	A	902	-	-	4/9/9/55	-
3	L9Y	F	904	-	-	13/18/40/40	0/3/3/3
2	POV	B	901	-	-	2/12/12/55	-
2	POV	D	903	-	-	3/7/7/55	-
2	POV	E	902	-	-	4/9/9/55	-
2	POV	A	903	-	-	3/7/7/55	-
2	POV	C	903	-	-	3/7/7/55	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	904	L9Y	C06-C07	4.95	1.57	1.51
2	E	901	POV	O32-C31	4.22	1.36	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	POV	O32-C31	4.21	1.36	1.22
2	A	901	POV	O32-C31	4.21	1.36	1.22
2	D	901	POV	O32-C31	4.20	1.36	1.22
2	C	901	POV	O32-C31	4.19	1.36	1.22
2	F	901	POV	O32-C31	4.19	1.36	1.22
3	F	904	L9Y	C18-C17	3.43	1.65	1.51
3	F	904	L9Y	C23-C15	3.01	1.44	1.38
3	F	904	L9Y	O16-C17	2.94	1.53	1.43
3	F	904	L9Y	O10-C09	2.87	1.26	1.21
3	F	904	L9Y	O16-C15	2.82	1.43	1.37
3	F	904	L9Y	C04-C05	2.77	1.59	1.54
2	F	901	POV	O31-C31	-2.42	1.22	1.30
2	A	901	POV	O31-C31	-2.42	1.22	1.30
3	F	904	L9Y	C19-C20	2.41	1.56	1.50
2	E	901	POV	O31-C31	-2.39	1.22	1.30
2	B	901	POV	O31-C31	-2.39	1.22	1.30
2	D	901	POV	O31-C31	-2.39	1.22	1.30
2	C	901	POV	O31-C31	-2.38	1.22	1.30
3	F	904	L9Y	C13-CL14	-2.04	1.68	1.72

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	904	L9Y	C06-C05-C09	-13.25	91.60	103.64
3	F	904	L9Y	C06-C07-C23	4.33	136.55	129.05
3	F	904	L9Y	C06-C07-C08	-4.23	104.69	110.94
3	F	904	L9Y	O16-C15-C13	4.23	122.83	115.78
3	F	904	L9Y	C23-C15-C13	-4.14	115.59	120.76
3	F	904	L9Y	C28-C24-C25	-3.85	100.11	104.39
2	E	901	POV	O31-C31-C32	3.36	124.84	114.03
2	A	901	POV	O31-C31-C32	3.35	124.80	114.03
2	F	901	POV	O31-C31-C32	3.35	124.79	114.03
2	B	901	POV	O31-C31-C32	3.35	124.78	114.03
2	D	901	POV	O31-C31-C32	3.34	124.76	114.03
2	C	901	POV	O31-C31-C32	3.33	124.74	114.03
3	F	904	L9Y	O10-C09-C08	-2.95	123.84	130.66
3	F	904	L9Y	C07-C08-C09	-2.80	105.89	108.97
2	B	901	POV	C33-C32-C31	-2.68	107.73	114.47
2	C	901	POV	C33-C32-C31	-2.67	107.74	114.47
2	E	901	POV	C33-C32-C31	-2.66	107.77	114.47
2	F	901	POV	C33-C32-C31	-2.66	107.78	114.47
2	A	901	POV	C33-C32-C31	-2.65	107.78	114.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	901	POV	C33-C32-C31	-2.65	107.79	114.47
3	F	904	L9Y	C26-C25-C24	2.63	109.10	105.00
3	F	904	L9Y	O16-C17-C18	2.58	117.91	108.33
3	F	904	L9Y	C19-C18-C17	2.58	117.26	112.35
2	F	902	POV	C33-C32-C31	-2.57	108.00	114.47
2	E	902	POV	C33-C32-C31	-2.57	108.00	114.47
2	D	902	POV	C33-C32-C31	-2.57	108.01	114.47
2	A	902	POV	C33-C32-C31	-2.55	108.03	114.47
2	C	902	POV	C33-C32-C31	-2.55	108.05	114.47
2	B	902	POV	C33-C32-C31	-2.55	108.05	114.47
2	A	903	POV	C23-C22-C21	-2.42	108.38	114.47
2	D	903	POV	C23-C22-C21	-2.42	108.38	114.47
2	F	903	POV	C23-C22-C21	-2.42	108.39	114.47
2	E	903	POV	C23-C22-C21	-2.41	108.39	114.47
2	C	903	POV	C23-C22-C21	-2.41	108.40	114.47
2	B	903	POV	C23-C22-C21	-2.40	108.43	114.47
2	E	901	POV	O32-C31-C32	-2.36	115.50	123.08
2	F	901	POV	O32-C31-C32	-2.36	115.50	123.08
2	A	901	POV	O32-C31-C32	-2.36	115.50	123.08
2	D	901	POV	O32-C31-C32	-2.35	115.53	123.08
2	B	901	POV	O32-C31-C32	-2.35	115.54	123.08
2	C	901	POV	O32-C31-C32	-2.33	115.59	123.08
3	F	904	L9Y	C27-C28-C24	2.05	108.19	105.00
3	F	904	L9Y	C11-C08-C07	-2.02	120.17	121.52

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	904	L9Y	C04-C05-C24-C25
3	F	904	L9Y	C04-C05-C24-C28
3	F	904	L9Y	C06-C05-C24-C25
3	F	904	L9Y	C06-C05-C24-C28
3	F	904	L9Y	C09-C05-C24-C25
3	F	904	L9Y	C09-C05-C24-C28
3	F	904	L9Y	C13-C15-O16-C17
2	A	903	POV	C21-C22-C23-C24
2	B	903	POV	C21-C22-C23-C24
2	C	903	POV	C21-C22-C23-C24
2	D	903	POV	C21-C22-C23-C24
2	E	903	POV	C21-C22-C23-C24
2	F	903	POV	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
3	F	904	L9Y	C02-C03-C04-C05
2	F	901	POV	C33-C34-C35-C36
2	B	901	POV	C33-C34-C35-C36
2	C	901	POV	C33-C34-C35-C36
2	E	901	POV	C33-C34-C35-C36
2	A	901	POV	C33-C34-C35-C36
2	D	901	POV	C33-C34-C35-C36
3	F	904	L9Y	C17-C18-C19-C20
3	F	904	L9Y	C03-C04-C05-C24
3	F	904	L9Y	C03-C04-C05-C09
2	B	902	POV	C36-C37-C38-C39
2	D	902	POV	C36-C37-C38-C39
2	E	902	POV	C36-C37-C38-C39
2	F	902	POV	C36-C37-C38-C39
2	A	902	POV	C36-C37-C38-C39
2	C	902	POV	C36-C37-C38-C39
3	F	904	L9Y	C23-C15-O16-C17
3	F	904	L9Y	C18-C17-O16-C15
2	A	902	POV	C34-C35-C36-C37
2	B	902	POV	C34-C35-C36-C37
2	C	902	POV	C34-C35-C36-C37
2	D	902	POV	C34-C35-C36-C37
2	F	902	POV	C34-C35-C36-C37
2	E	902	POV	C34-C35-C36-C37
2	A	903	POV	O21-C21-C22-C23
2	B	903	POV	O21-C21-C22-C23
2	C	903	POV	O21-C21-C22-C23
2	D	903	POV	O21-C21-C22-C23
2	E	903	POV	O21-C21-C22-C23
2	F	903	POV	O21-C21-C22-C23
2	B	903	POV	O22-C21-C22-C23
2	A	903	POV	O22-C21-C22-C23
2	C	903	POV	O22-C21-C22-C23
2	D	903	POV	O22-C21-C22-C23
2	E	903	POV	O22-C21-C22-C23
2	F	903	POV	O22-C21-C22-C23
2	A	902	POV	O32-C31-C32-C33
2	B	902	POV	O32-C31-C32-C33
2	E	902	POV	O32-C31-C32-C33
2	F	902	POV	O32-C31-C32-C33
2	C	902	POV	O32-C31-C32-C33
2	D	902	POV	O32-C31-C32-C33

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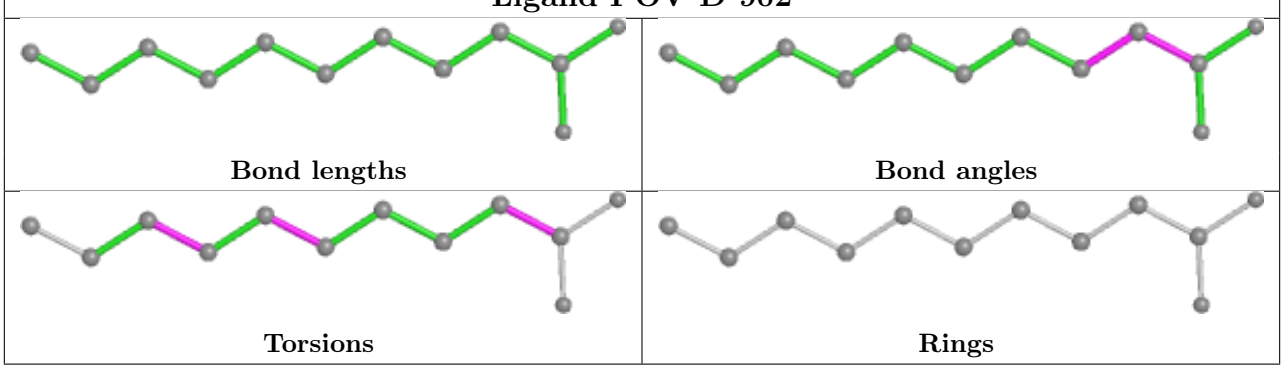
Mol	Chain	Res	Type	Atoms
2	A	902	POV	O31-C31-C32-C33
2	D	902	POV	O31-C31-C32-C33
2	E	902	POV	O31-C31-C32-C33
2	F	902	POV	O31-C31-C32-C33
2	B	902	POV	O31-C31-C32-C33
2	C	902	POV	O31-C31-C32-C33
2	E	901	POV	C32-C33-C34-C35
2	D	901	POV	C32-C33-C34-C35
2	F	901	POV	C32-C33-C34-C35
2	C	901	POV	C32-C33-C34-C35
2	A	901	POV	C32-C33-C34-C35
2	B	901	POV	C32-C33-C34-C35

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand POV D 902



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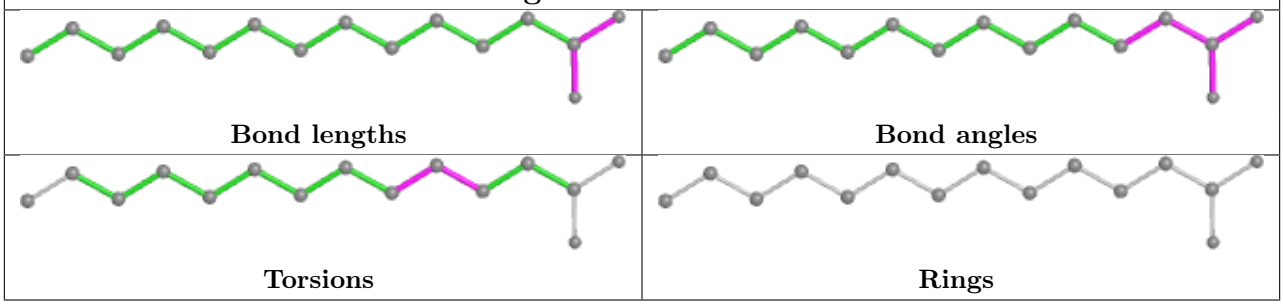
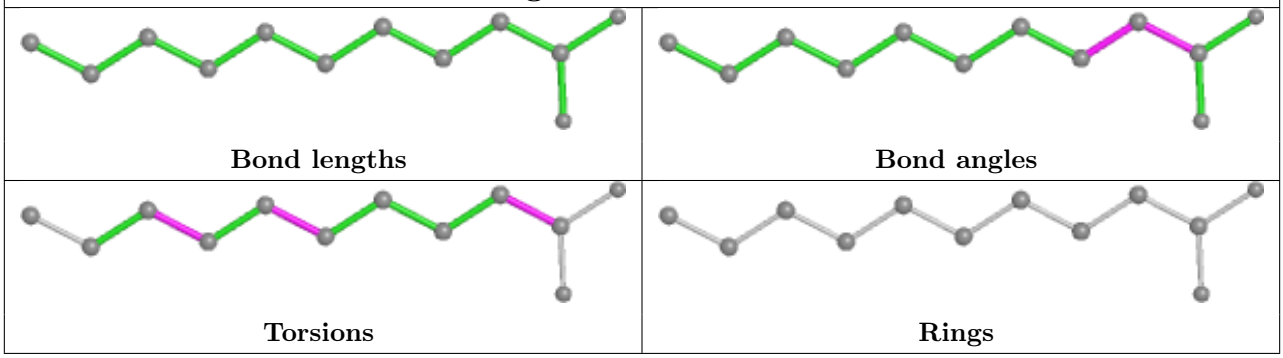


Ligand POV F 902



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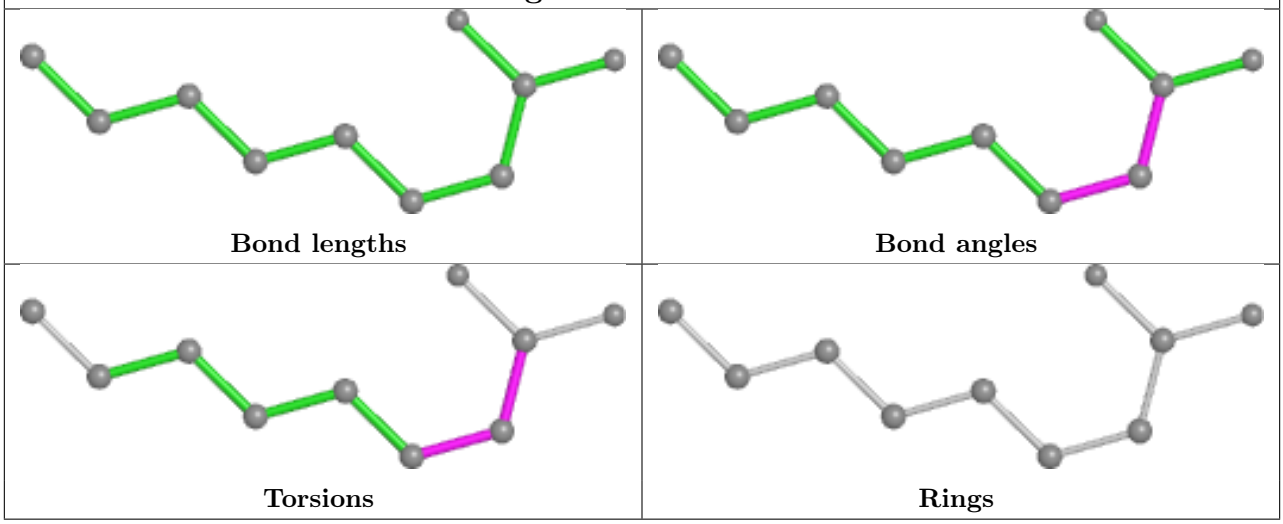

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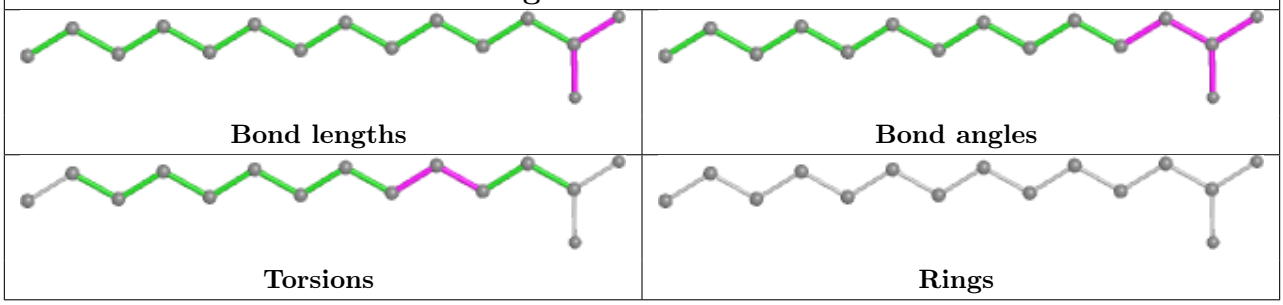

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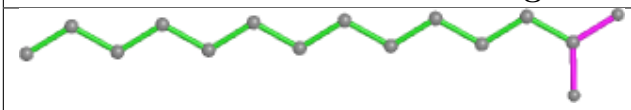
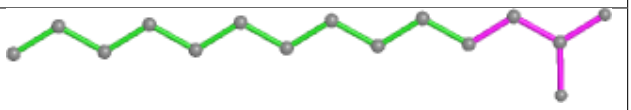
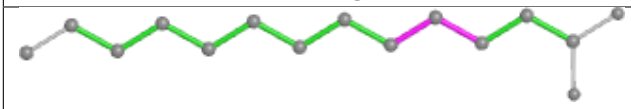
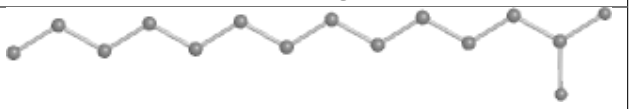
 Bond lengths	 Bond angles
 Torsions	 Rings

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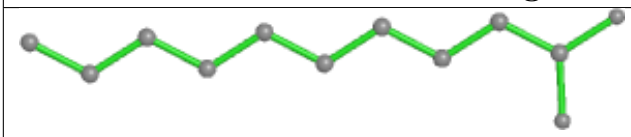
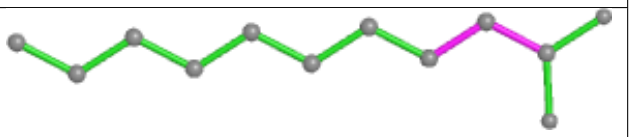
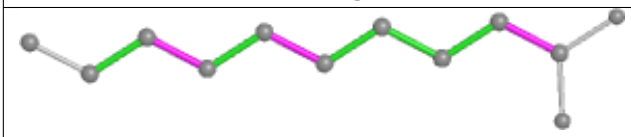
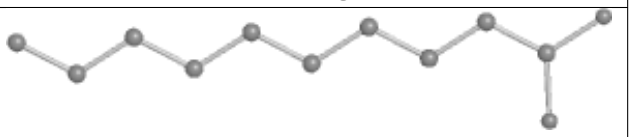
 Bond lengths	 Bond angles
 Torsions	 Rings

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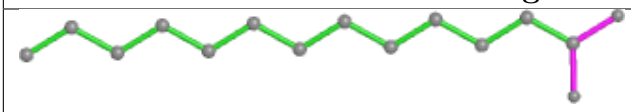
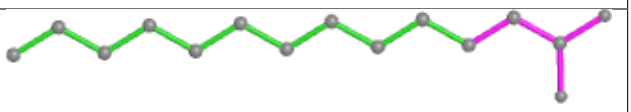
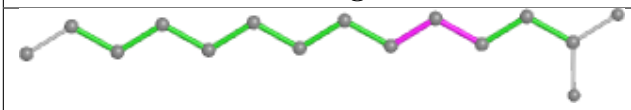
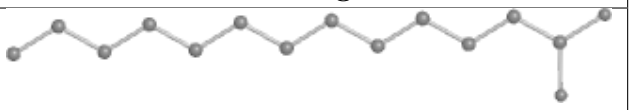
 Bond lengths	 Bond angles
 Torsions	 Rings

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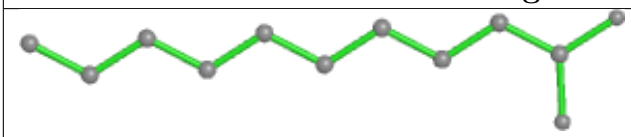
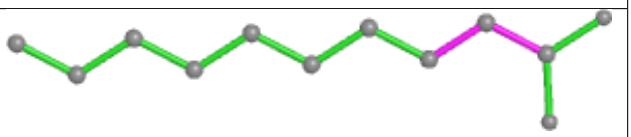
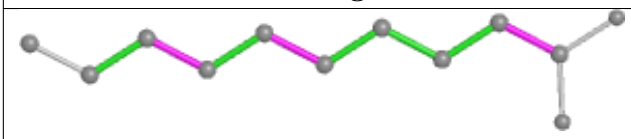
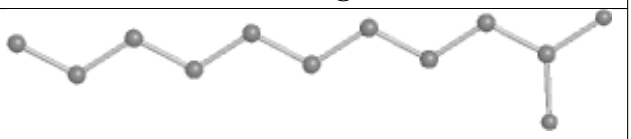
 Bond lengths	 Bond angles
 Torsions	 Rings

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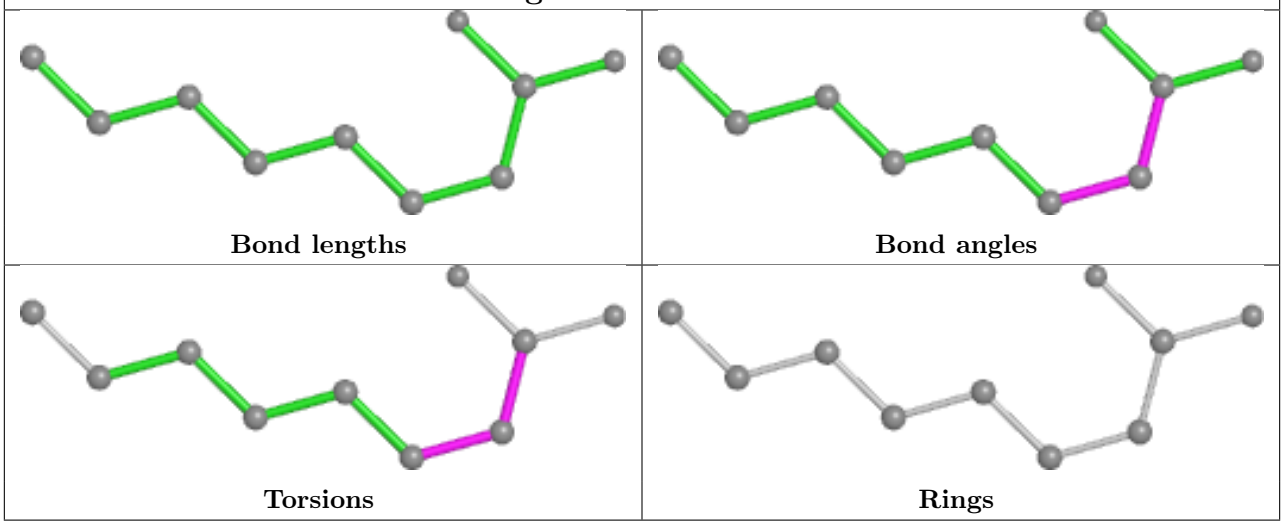

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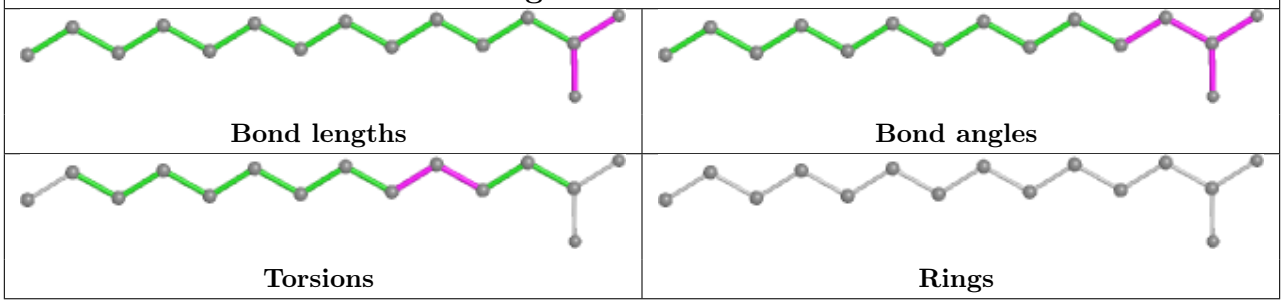

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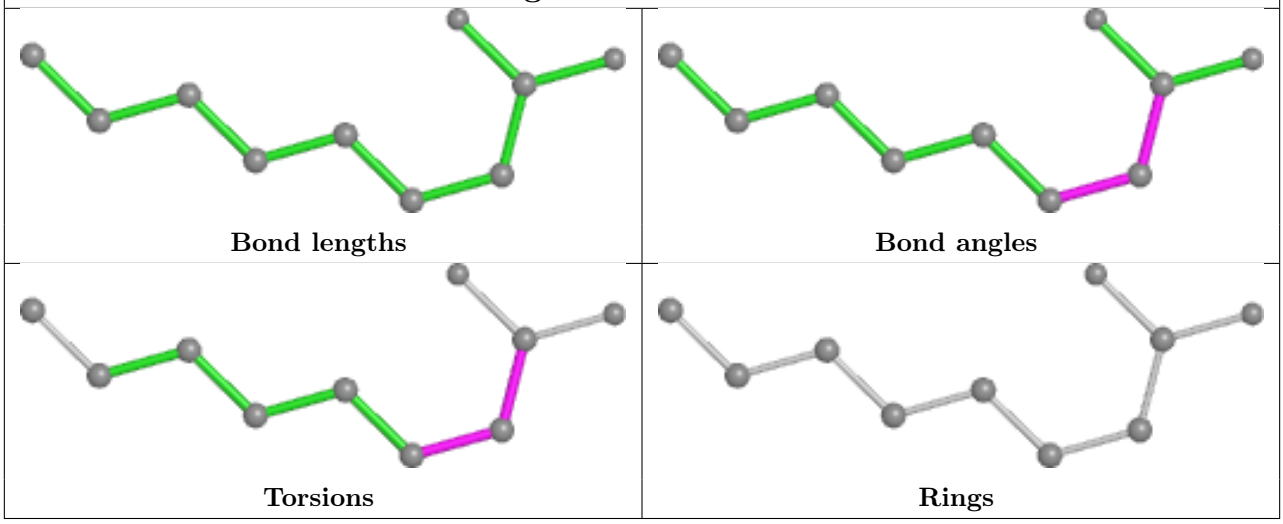

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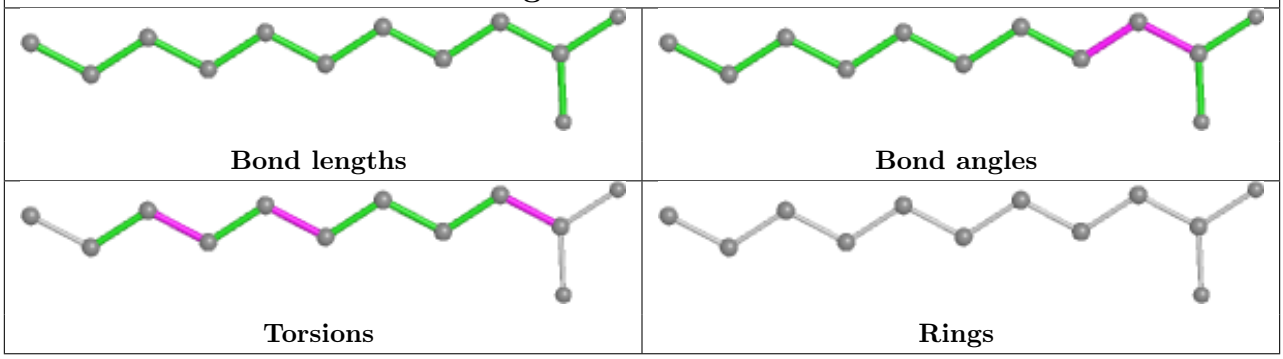
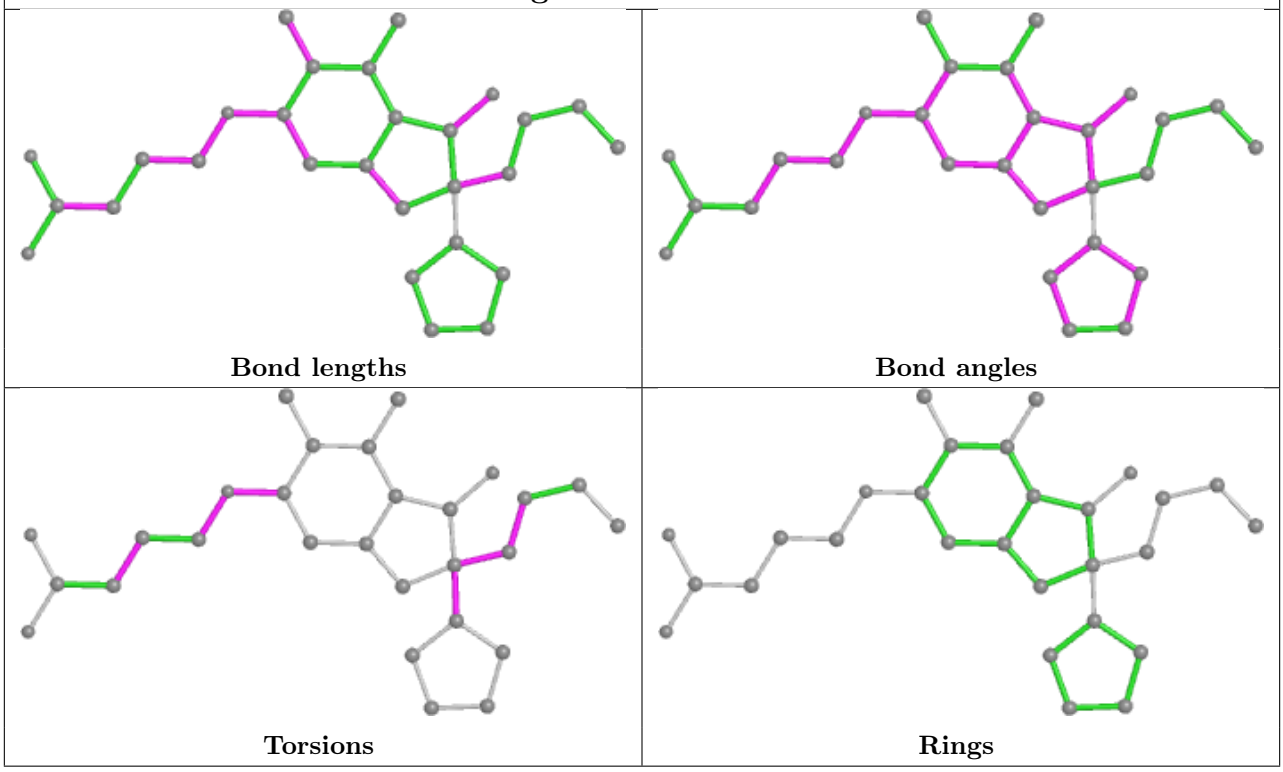


Ligand L9Y F 904



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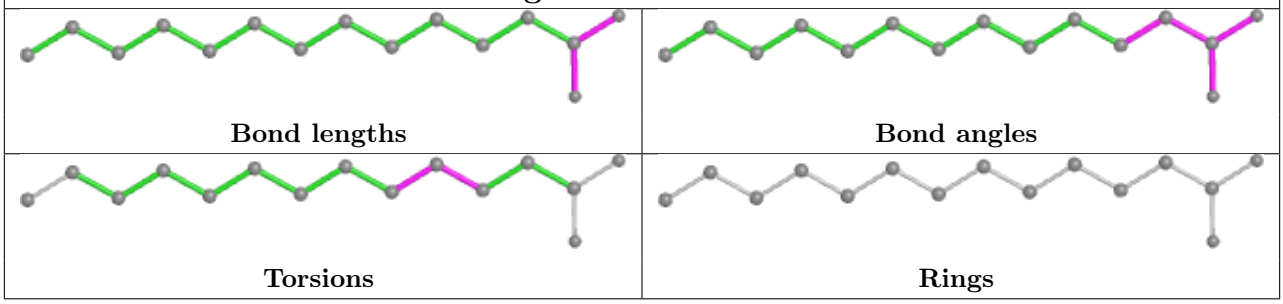

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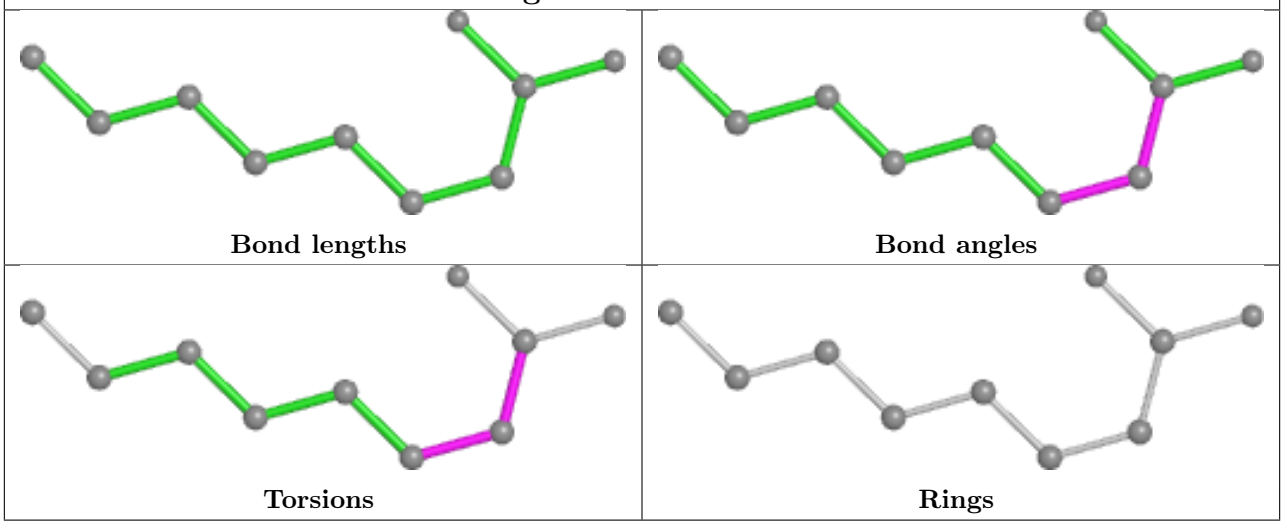

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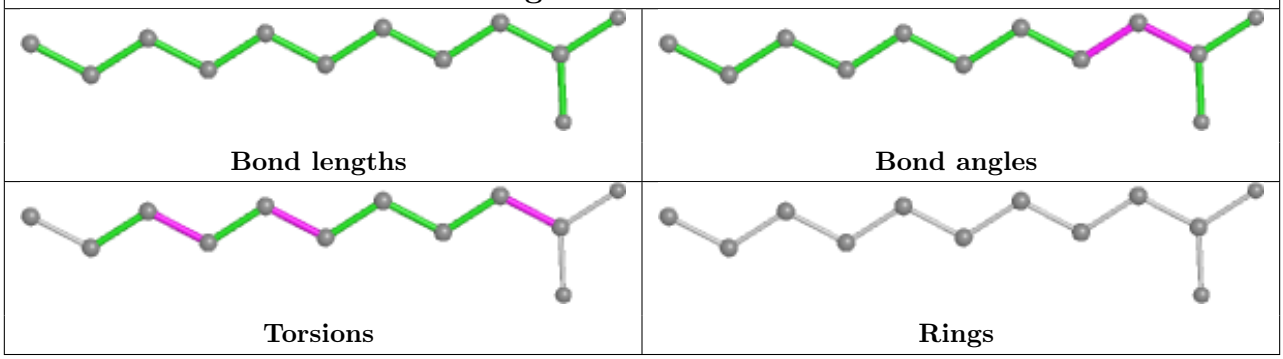

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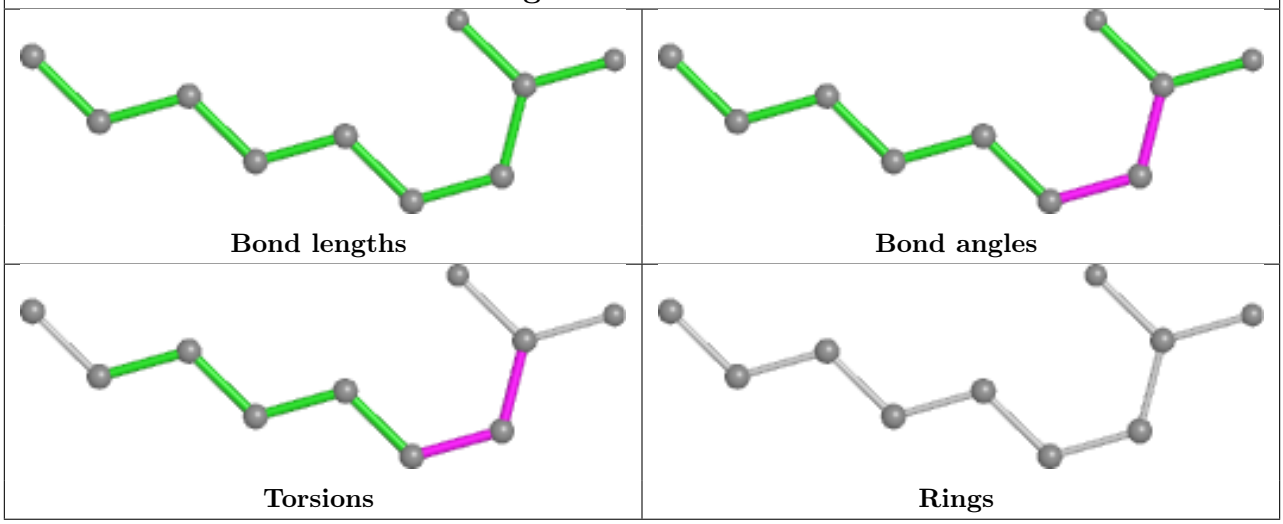

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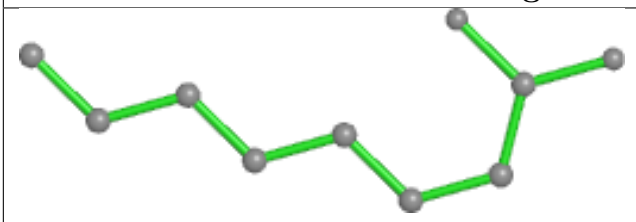
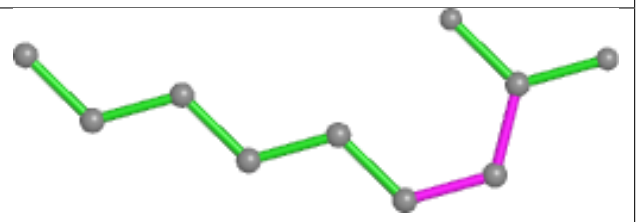
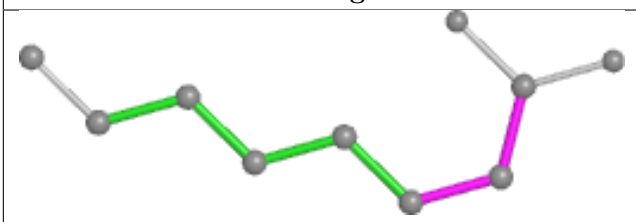
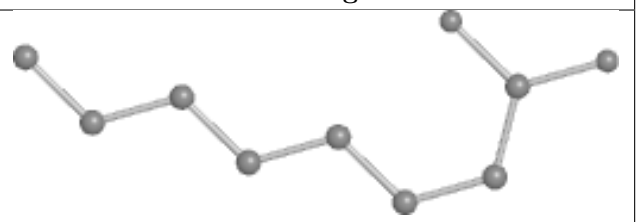
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

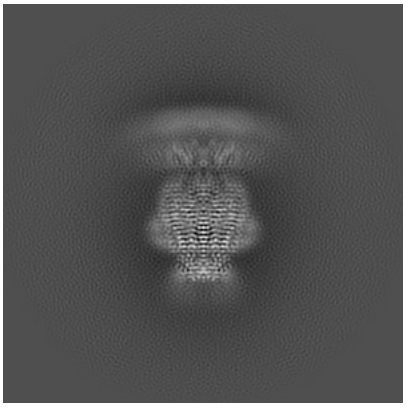
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0563. These allow visual inspection of the internal detail of the map and identification of artifacts.

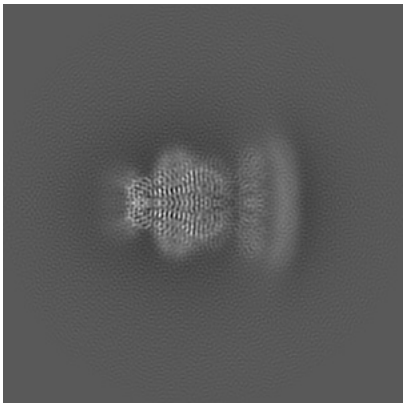
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

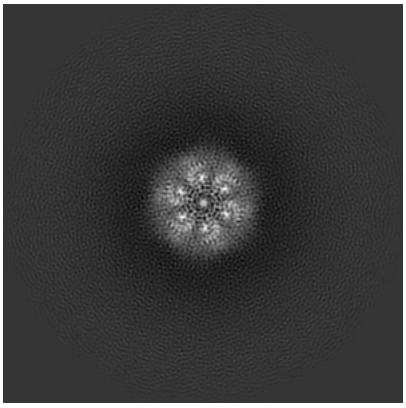
6.1.1 Primary map



X



Y

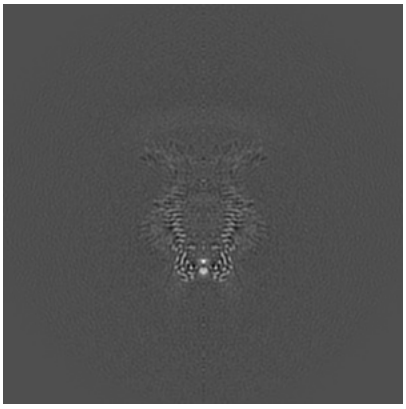


Z

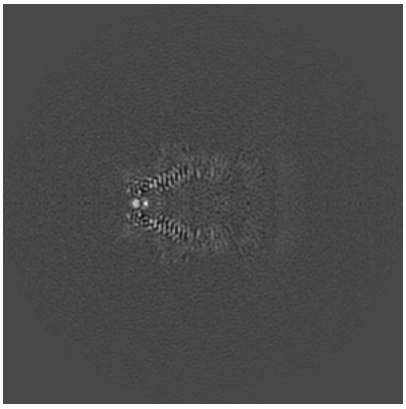
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

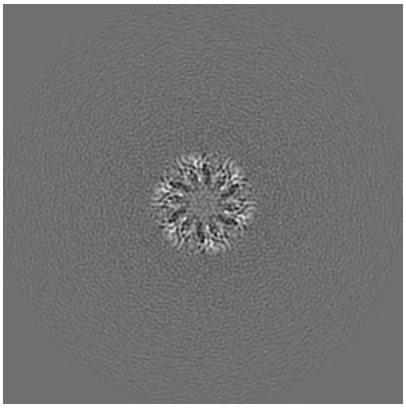
6.2.1 Primary map



X Index: 182



Y Index: 182

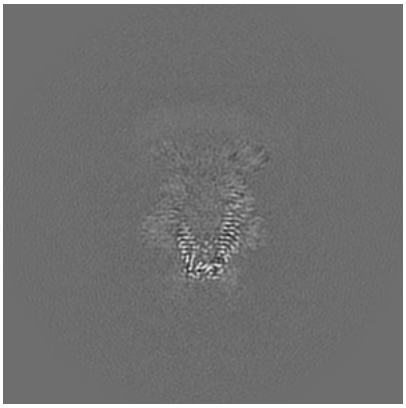


Z Index: 182

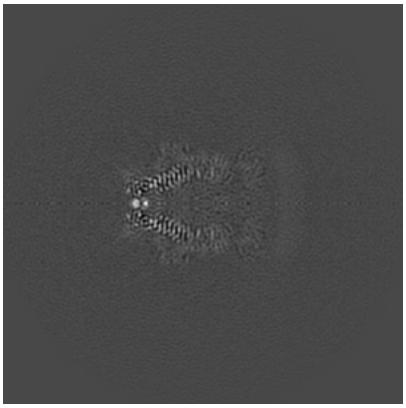
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

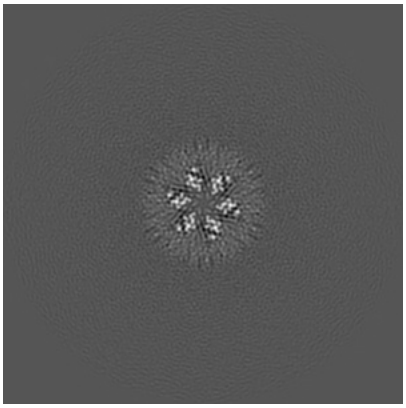
6.3.1 Primary map



X Index: 172



Y Index: 182



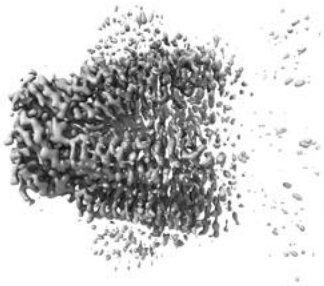
Z Index: 151

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

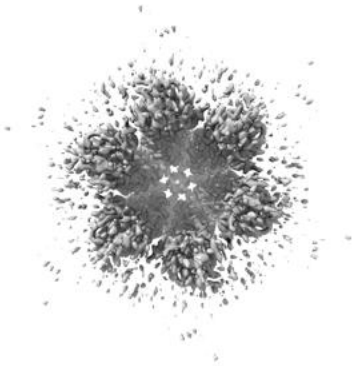
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 10.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

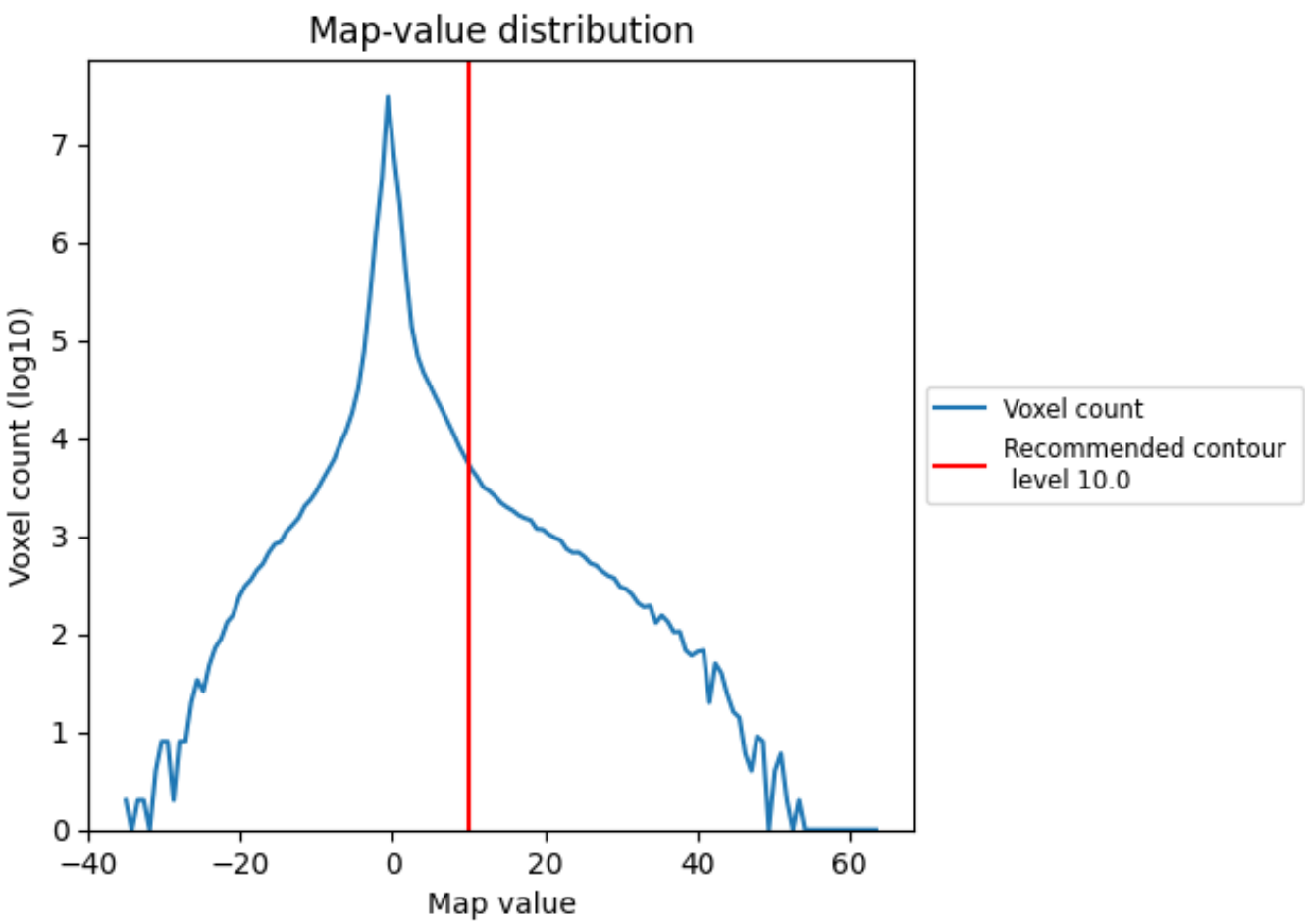
6.5 Mask visualisation (i)

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

7 Map analysis (i)

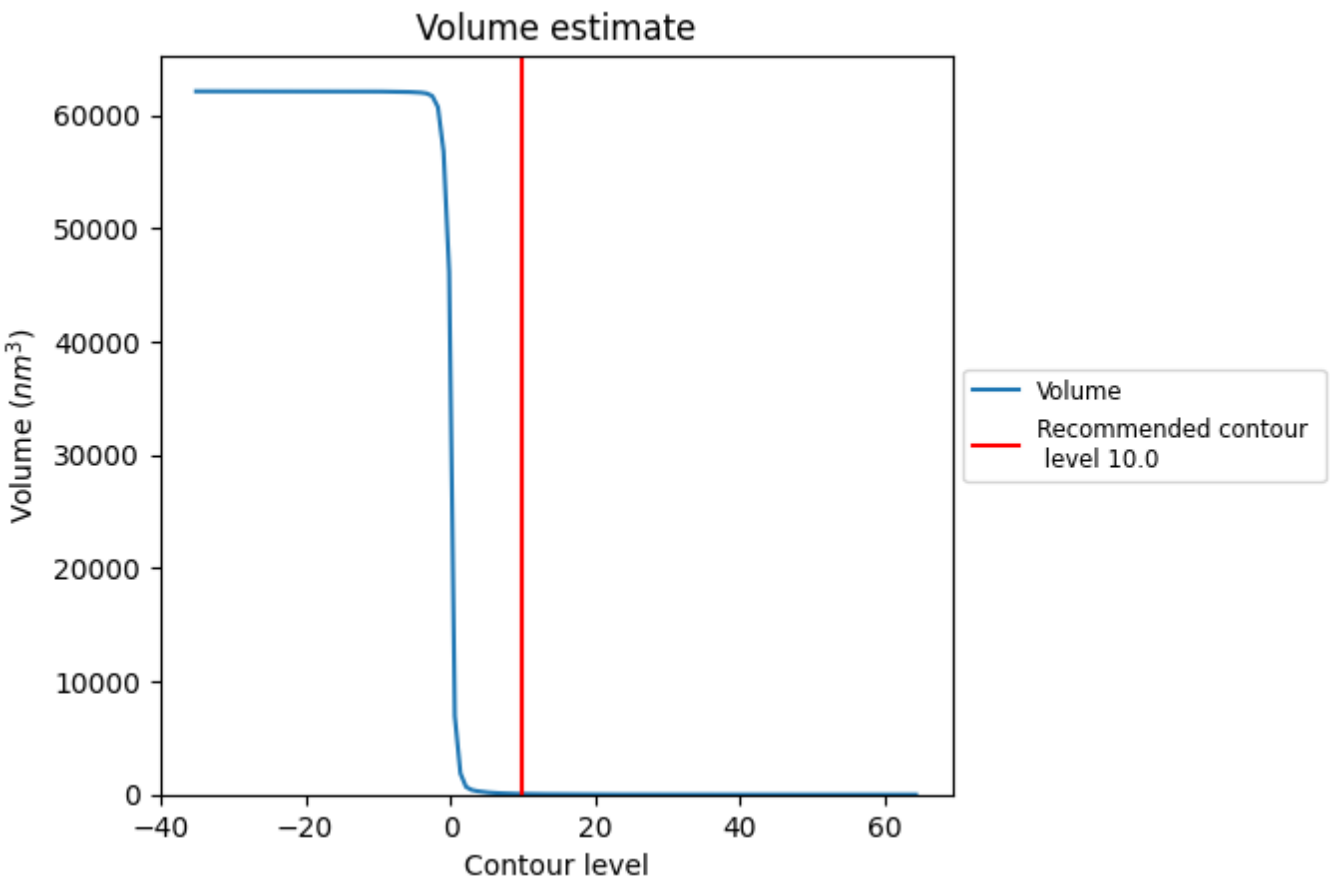
This section contains the results of statistical analysis of the map.

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.

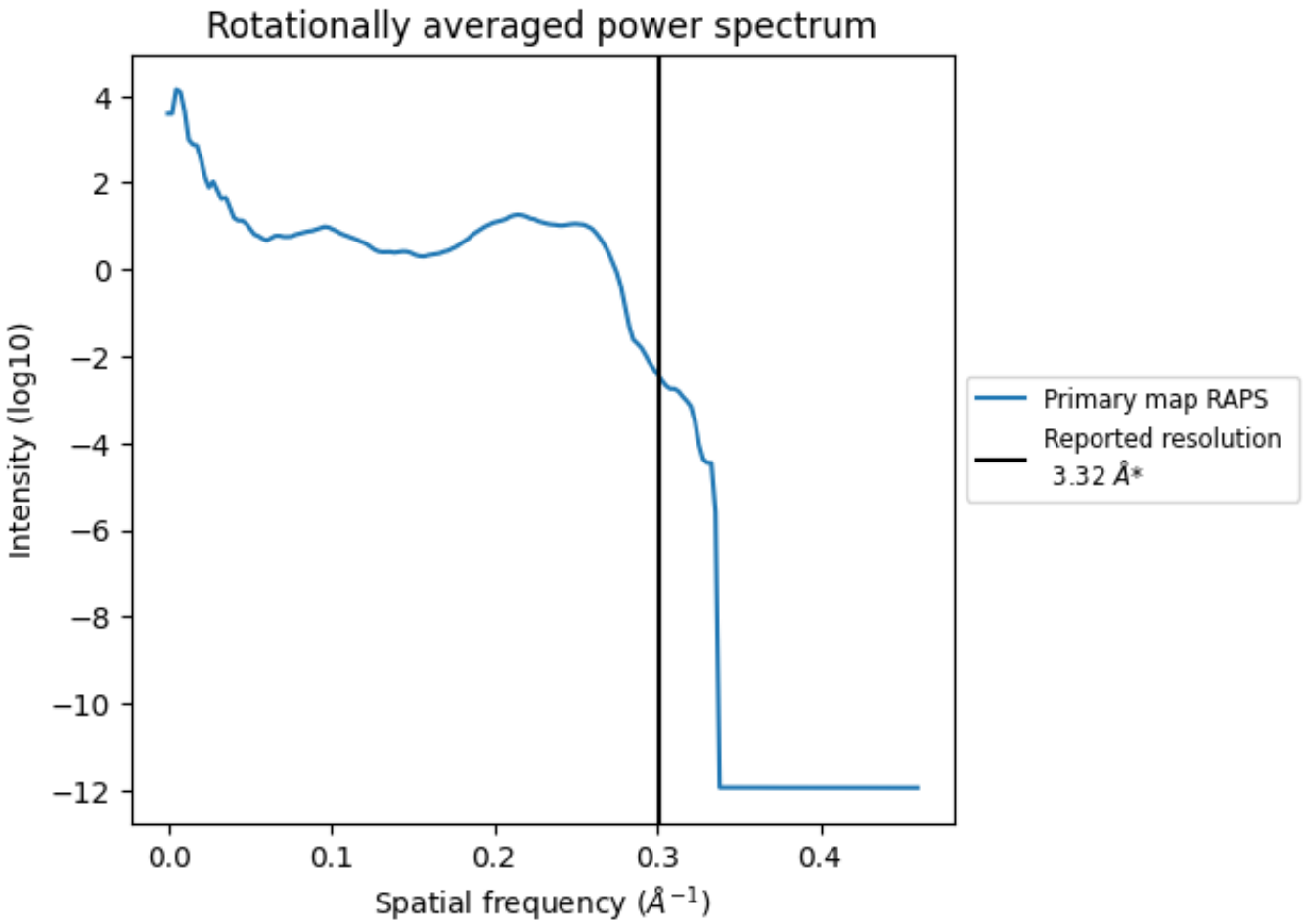
7.2 Volume estimate (i)



The volume at the recommended contour level is 56 nm^3; this corresponds to an approximate mass of 50 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 0.301 Å^{-1}

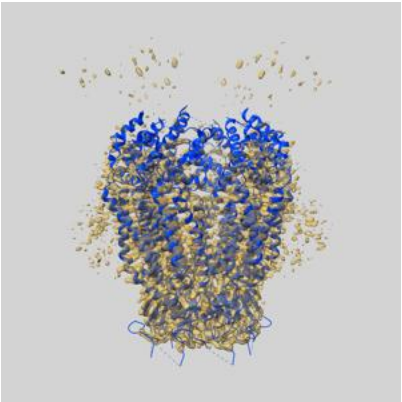
8 Fourier-Shell correlation (i)

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

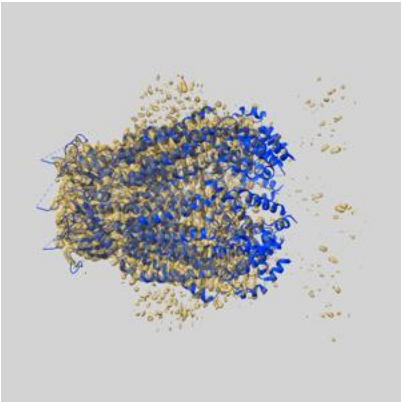
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0563 and PDB model 6NZZ. Per-residue inclusion information can be found in section 3 on page 7.

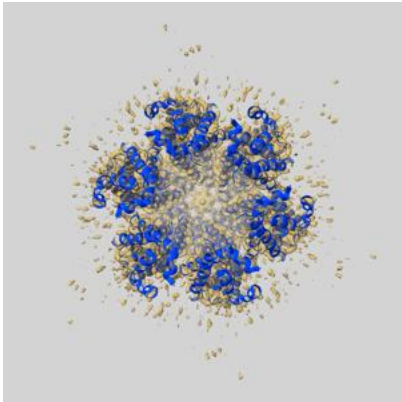
9.1 Map-model overlay (i)



X



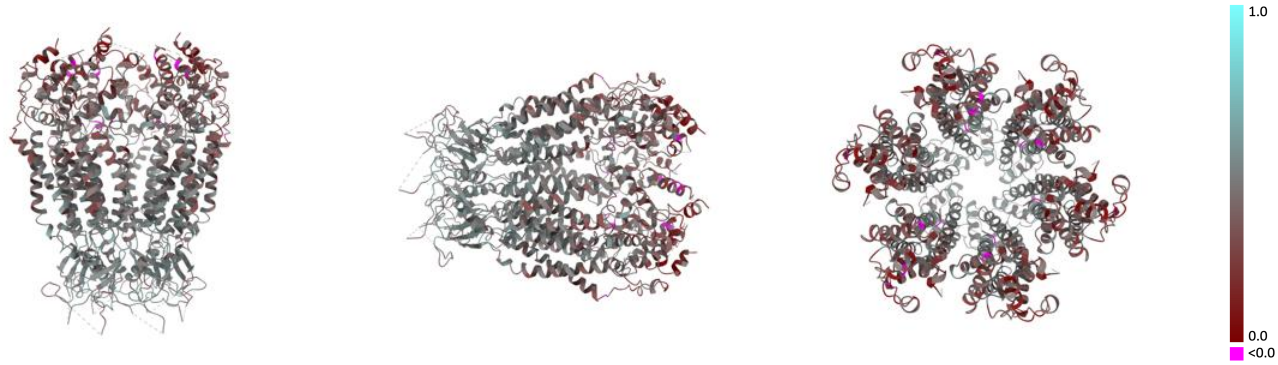
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 10.0 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.

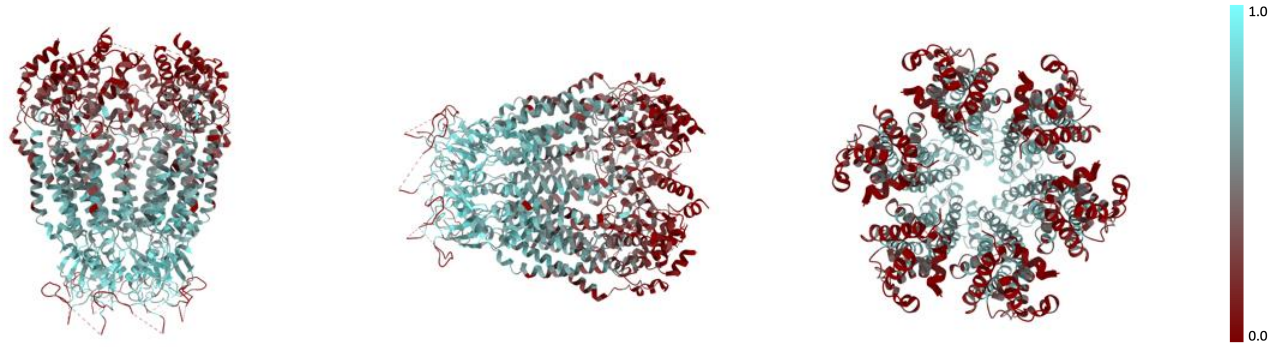
9.2 Q-score mapped to coordinate model (i)



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.

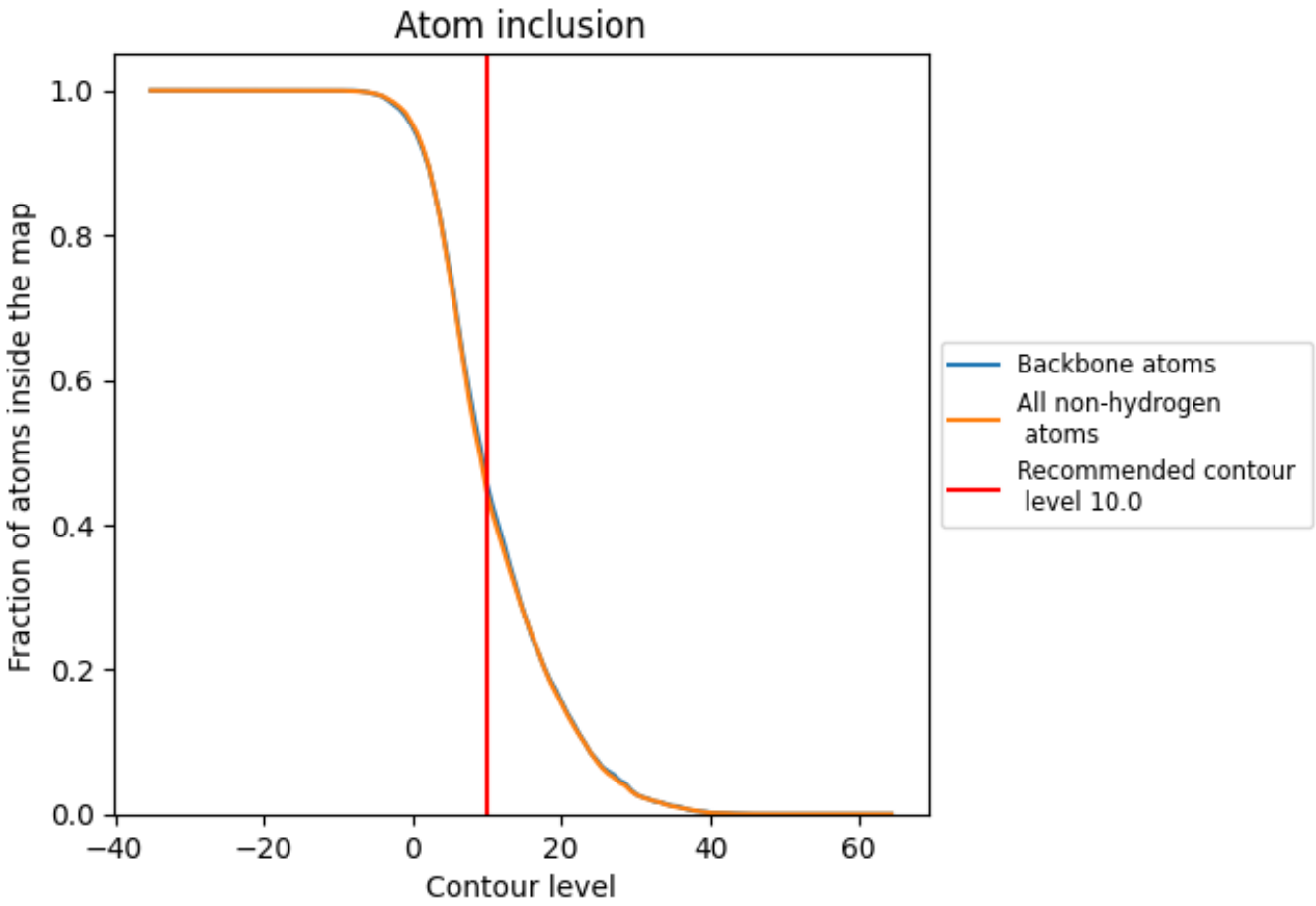
9.3 Atom inclusion mapped to coordinate model (i)



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 (10.0).

9.4 Atom inclusion (i)



At the recommended contour level, 46% of all backbone atoms, 45% 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 (10.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4457	0.4220
A	0.4621	0.4250
B	0.4617	0.4240
C	0.4558	0.4210
D	0.4652	0.4240
E	0.4538	0.4190
F	0.4672	0.4230