Full wwPDB EM Validation Report (i)

Nov 6, 2022 – 04:18 PM EST

PDB ID	:	6N7K
EMDB ID	:	EMD-0358
Title	:	Cryo-EM structure of tetrameric Ptch1 in complex with ShhNp (form II)
Authors	:	Yan, N.; Gong, X.; Qian, H.W.
Deposited on	:	2018-11-27
Resolution	:	6.50 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:

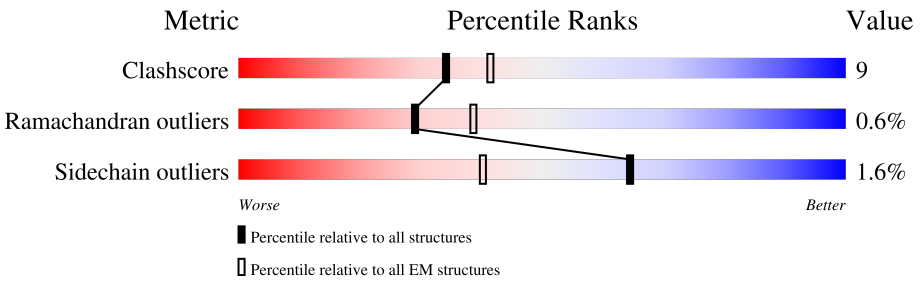
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 6.50 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	1349	35% 59% 14% • 27%
1	B	1349	37% 61% 11% • 27%
1	D	1349	62% 59% 13% • 27%
1	E	1349	55% 61% 12% • 27%
2	C	174	20% 71% 26% •
2	F	174	60% 71% 27% •
3	G	2	100% 100%
3	H	2	100% 50% 50%

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Mol	Chain	Length	Quality of chain
3	I	2	100% 100%
3	J	2	100% 50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CLR	A	1808	-	-	X	-
5	CLR	B	1508	-	-	X	-
5	CLR	D	1808	-	-	X	-
5	CLR	E	1508	-	-	X	-
8	PLM	C	205	-	-	X	-
8	PLM	F	205	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 34484 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 Protein patched homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	991	7807	5091	1282	1392	42	0	0
1	B	988	7708	5029	1267	1372	40	0	0
1	D	991	7807	5091	1282	1392	42	0	0
1	E	988	7708	5029	1267	1372	40	0	0

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q13635
A	-19	ALA	-	expression tag	UNP Q13635
A	-18	ASP	-	expression tag	UNP Q13635
A	-17	TYR	-	expression tag	UNP Q13635
A	-16	LYS	-	expression tag	UNP Q13635
A	-15	ASP	-	expression tag	UNP Q13635
A	-14	ASP	-	expression tag	UNP Q13635
A	-13	ASP	-	expression tag	UNP Q13635
A	-12	ASP	-	expression tag	UNP Q13635
A	-11	LYS	-	expression tag	UNP Q13635
A	-10	SER	-	expression tag	UNP Q13635
A	-9	GLY	-	expression tag	UNP Q13635
A	-8	PRO	-	expression tag	UNP Q13635
A	-7	ASP	-	expression tag	UNP Q13635
A	-6	GLU	-	expression tag	UNP Q13635
A	-5	VAL	-	expression tag	UNP Q13635
A	-4	ASP	-	expression tag	UNP Q13635
A	-3	ALA	-	expression tag	UNP Q13635
A	-2	SER	-	expression tag	UNP Q13635
A	-1	GLY	-	expression tag	UNP Q13635
A	0	ARG	-	expression tag	UNP Q13635
A	1306	LEU	-	expression tag	UNP Q13635

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1307	GLU	-	expression tag	UNP Q13635
A	1308	GLY	-	expression tag	UNP Q13635
A	1309	SER	-	expression tag	UNP Q13635
A	1310	ASP	-	expression tag	UNP Q13635
A	1311	GLU	-	expression tag	UNP Q13635
A	1312	VAL	-	expression tag	UNP Q13635
A	1313	ASP	-	expression tag	UNP Q13635
A	1314	ALA	-	expression tag	UNP Q13635
A	1315	VAL	-	expression tag	UNP Q13635
A	1316	GLU	-	expression tag	UNP Q13635
A	1317	GLY	-	expression tag	UNP Q13635
A	1318	SER	-	expression tag	UNP Q13635
A	1319	HIS	-	expression tag	UNP Q13635
A	1320	HIS	-	expression tag	UNP Q13635
A	1321	HIS	-	expression tag	UNP Q13635
A	1322	HIS	-	expression tag	UNP Q13635
A	1323	HIS	-	expression tag	UNP Q13635
A	1324	HIS	-	expression tag	UNP Q13635
A	1325	HIS	-	expression tag	UNP Q13635
A	1326	HIS	-	expression tag	UNP Q13635
A	1327	HIS	-	expression tag	UNP Q13635
A	1328	HIS	-	expression tag	UNP Q13635
B	-20	MET	-	initiating methionine	UNP Q13635
B	-19	ALA	-	expression tag	UNP Q13635
B	-18	ASP	-	expression tag	UNP Q13635
B	-17	TYR	-	expression tag	UNP Q13635
B	-16	LYS	-	expression tag	UNP Q13635
B	-15	ASP	-	expression tag	UNP Q13635
B	-14	ASP	-	expression tag	UNP Q13635
B	-13	ASP	-	expression tag	UNP Q13635
B	-12	ASP	-	expression tag	UNP Q13635
B	-11	LYS	-	expression tag	UNP Q13635
B	-10	SER	-	expression tag	UNP Q13635
B	-9	GLY	-	expression tag	UNP Q13635
B	-8	PRO	-	expression tag	UNP Q13635
B	-7	ASP	-	expression tag	UNP Q13635
B	-6	GLU	-	expression tag	UNP Q13635
B	-5	VAL	-	expression tag	UNP Q13635
B	-4	ASP	-	expression tag	UNP Q13635
B	-3	ALA	-	expression tag	UNP Q13635
B	-2	SER	-	expression tag	UNP Q13635
B	-1	GLY	-	expression tag	UNP Q13635

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ARG	-	expression tag	UNP Q13635
B	1306	LEU	-	expression tag	UNP Q13635
B	1307	GLU	-	expression tag	UNP Q13635
B	1308	GLY	-	expression tag	UNP Q13635
B	1309	SER	-	expression tag	UNP Q13635
B	1310	ASP	-	expression tag	UNP Q13635
B	1311	GLU	-	expression tag	UNP Q13635
B	1312	VAL	-	expression tag	UNP Q13635
B	1313	ASP	-	expression tag	UNP Q13635
B	1314	ALA	-	expression tag	UNP Q13635
B	1315	VAL	-	expression tag	UNP Q13635
B	1316	GLU	-	expression tag	UNP Q13635
B	1317	GLY	-	expression tag	UNP Q13635
B	1318	SER	-	expression tag	UNP Q13635
B	1319	HIS	-	expression tag	UNP Q13635
B	1320	HIS	-	expression tag	UNP Q13635
B	1321	HIS	-	expression tag	UNP Q13635
B	1322	HIS	-	expression tag	UNP Q13635
B	1323	HIS	-	expression tag	UNP Q13635
B	1324	HIS	-	expression tag	UNP Q13635
B	1325	HIS	-	expression tag	UNP Q13635
B	1326	HIS	-	expression tag	UNP Q13635
B	1327	HIS	-	expression tag	UNP Q13635
B	1328	HIS	-	expression tag	UNP Q13635
D	-20	MET	-	initiating methionine	UNP Q13635
D	-19	ALA	-	expression tag	UNP Q13635
D	-18	ASP	-	expression tag	UNP Q13635
D	-17	TYR	-	expression tag	UNP Q13635
D	-16	LYS	-	expression tag	UNP Q13635
D	-15	ASP	-	expression tag	UNP Q13635
D	-14	ASP	-	expression tag	UNP Q13635
D	-13	ASP	-	expression tag	UNP Q13635
D	-12	ASP	-	expression tag	UNP Q13635
D	-11	LYS	-	expression tag	UNP Q13635
D	-10	SER	-	expression tag	UNP Q13635
D	-9	GLY	-	expression tag	UNP Q13635
D	-8	PRO	-	expression tag	UNP Q13635
D	-7	ASP	-	expression tag	UNP Q13635
D	-6	GLU	-	expression tag	UNP Q13635
D	-5	VAL	-	expression tag	UNP Q13635
D	-4	ASP	-	expression tag	UNP Q13635
D	-3	ALA	-	expression tag	UNP Q13635

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	expression tag	UNP Q13635
D	-1	GLY	-	expression tag	UNP Q13635
D	0	ARG	-	expression tag	UNP Q13635
D	1306	LEU	-	expression tag	UNP Q13635
D	1307	GLU	-	expression tag	UNP Q13635
D	1308	GLY	-	expression tag	UNP Q13635
D	1309	SER	-	expression tag	UNP Q13635
D	1310	ASP	-	expression tag	UNP Q13635
D	1311	GLU	-	expression tag	UNP Q13635
D	1312	VAL	-	expression tag	UNP Q13635
D	1313	ASP	-	expression tag	UNP Q13635
D	1314	ALA	-	expression tag	UNP Q13635
D	1315	VAL	-	expression tag	UNP Q13635
D	1316	GLU	-	expression tag	UNP Q13635
D	1317	GLY	-	expression tag	UNP Q13635
D	1318	SER	-	expression tag	UNP Q13635
D	1319	HIS	-	expression tag	UNP Q13635
D	1320	HIS	-	expression tag	UNP Q13635
D	1321	HIS	-	expression tag	UNP Q13635
D	1322	HIS	-	expression tag	UNP Q13635
D	1323	HIS	-	expression tag	UNP Q13635
D	1324	HIS	-	expression tag	UNP Q13635
D	1325	HIS	-	expression tag	UNP Q13635
D	1326	HIS	-	expression tag	UNP Q13635
D	1327	HIS	-	expression tag	UNP Q13635
D	1328	HIS	-	expression tag	UNP Q13635
E	-20	MET	-	initiating methionine	UNP Q13635
E	-19	ALA	-	expression tag	UNP Q13635
E	-18	ASP	-	expression tag	UNP Q13635
E	-17	TYR	-	expression tag	UNP Q13635
E	-16	LYS	-	expression tag	UNP Q13635
E	-15	ASP	-	expression tag	UNP Q13635
E	-14	ASP	-	expression tag	UNP Q13635
E	-13	ASP	-	expression tag	UNP Q13635
E	-12	ASP	-	expression tag	UNP Q13635
E	-11	LYS	-	expression tag	UNP Q13635
E	-10	SER	-	expression tag	UNP Q13635
E	-9	GLY	-	expression tag	UNP Q13635
E	-8	PRO	-	expression tag	UNP Q13635
E	-7	ASP	-	expression tag	UNP Q13635
E	-6	GLU	-	expression tag	UNP Q13635
E	-5	VAL	-	expression tag	UNP Q13635

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	ASP	-	expression tag	UNP Q13635
E	-3	ALA	-	expression tag	UNP Q13635
E	-2	SER	-	expression tag	UNP Q13635
E	-1	GLY	-	expression tag	UNP Q13635
E	0	ARG	-	expression tag	UNP Q13635
E	1306	LEU	-	expression tag	UNP Q13635
E	1307	GLU	-	expression tag	UNP Q13635
E	1308	GLY	-	expression tag	UNP Q13635
E	1309	SER	-	expression tag	UNP Q13635
E	1310	ASP	-	expression tag	UNP Q13635
E	1311	GLU	-	expression tag	UNP Q13635
E	1312	VAL	-	expression tag	UNP Q13635
E	1313	ASP	-	expression tag	UNP Q13635
E	1314	ALA	-	expression tag	UNP Q13635
E	1315	VAL	-	expression tag	UNP Q13635
E	1316	GLU	-	expression tag	UNP Q13635
E	1317	GLY	-	expression tag	UNP Q13635
E	1318	SER	-	expression tag	UNP Q13635
E	1319	HIS	-	expression tag	UNP Q13635
E	1320	HIS	-	expression tag	UNP Q13635
E	1321	HIS	-	expression tag	UNP Q13635
E	1322	HIS	-	expression tag	UNP Q13635
E	1323	HIS	-	expression tag	UNP Q13635
E	1324	HIS	-	expression tag	UNP Q13635
E	1325	HIS	-	expression tag	UNP Q13635
E	1326	HIS	-	expression tag	UNP Q13635
E	1327	HIS	-	expression tag	UNP Q13635
E	1328	HIS	-	expression tag	UNP Q13635

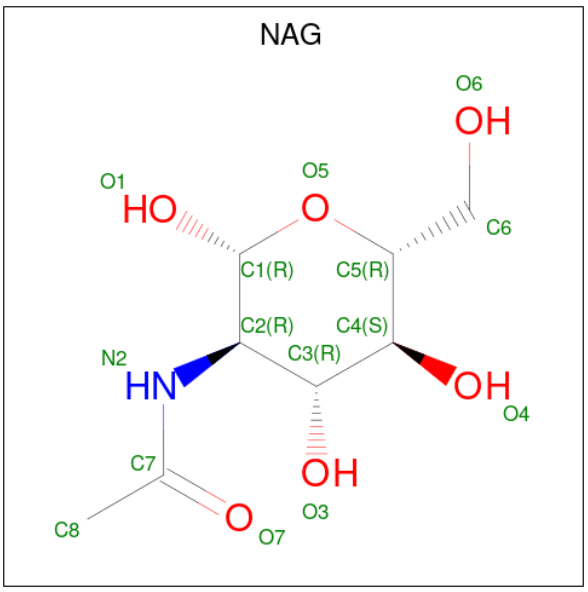
- Molecule 2 is a protein called Sonic hedgehog protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	174	1371	853	253	259	6	0	0
			Total	C	N	O	S		
2	F	174	1371	853	253	259	6	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	G	2	28	16	2	10	0	0
			Total	C	N	O		
3	H	2	28	16	2	10	0	0
			Total	C	N	O		
3	I	2	28	16	2	10	0	0
			Total	C	N	O		
3	J	2	28	16	2	10	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	70	40	5	25	0
			Total	C	N	O	
4	A	1	70	40	5	25	0
			Total	C	N	O	
4	A	1	70	40	5	25	0
			Total	C	N	O	
4	A	1	70	40	5	25	0
			Total	C	N	O	
4	A	1	70	40	5	25	0

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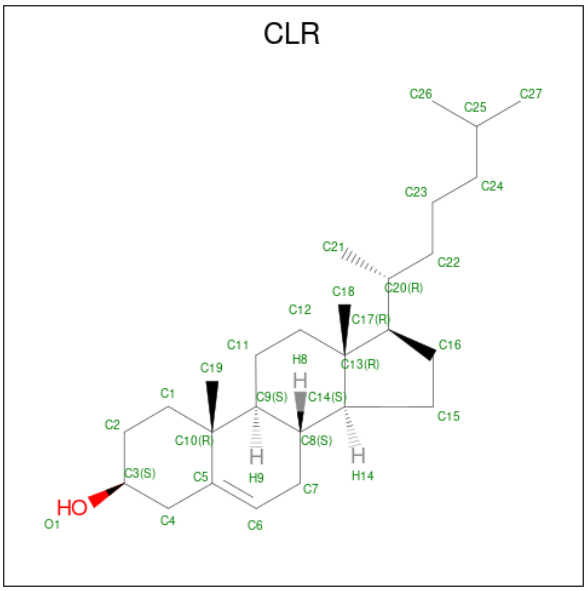
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	B	1	70	40	5	25	0
4	B	1	70	40	5	25	0
4	B	1	70	40	5	25	0
4	B	1	70	40	5	25	0
4	B	1	70	40	5	25	0
4	D	1	70	40	5	25	0
4	D	1	70	40	5	25	0
4	D	1	70	40	5	25	0
4	D	1	70	40	5	25	0
4	D	1	70	40	5	25	0
4	E	1	70	40	5	25	0
4	E	1	70	40	5	25	0
4	E	1	70	40	5	25	0
4	E	1	70	40	5	25	0
4	E	1	70	40	5	25	0

- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
5	A	1	84	81	3	0
			Total	C	O	
5	A	1	84	81	3	0
			Total	C	O	
5	A	1	84	81	3	0
			Total	C	O	
5	B	1	28	27	1	0
			Total	C	O	
5	C	1	28	27	1	0
			Total	C	O	
5	D	1	84	81	3	0
			Total	C	O	
5	D	1	84	81	3	0
			Total	C	O	
5	D	1	84	81	3	0
			Total	C	O	
5	E	1	28	27	1	0
			Total	C	O	
5	F	1	28	27	1	0

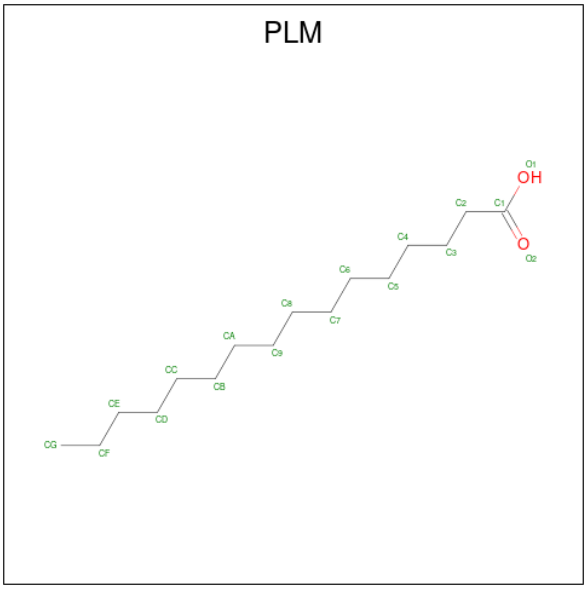
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
6	C	1	1	1	0
			Total	Zn	
6	F	1	1	1	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
7	C	2	2	2	0
			Total	Ca	
7	F	2	2	2	0

- Molecule 8 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



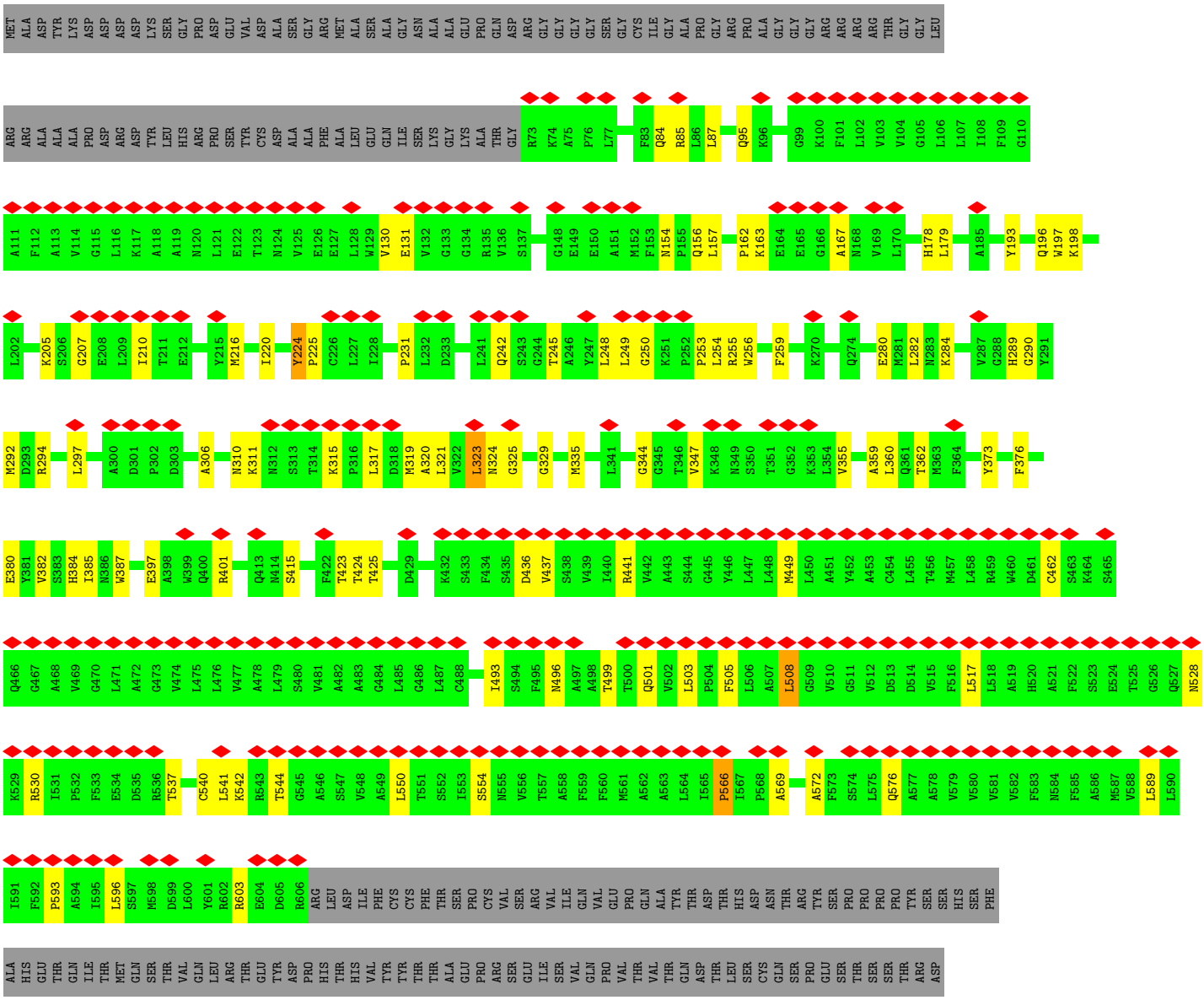
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
8	C	1	17	16	1	0
			Total	C	O	
8	F	1	17	16	1	0

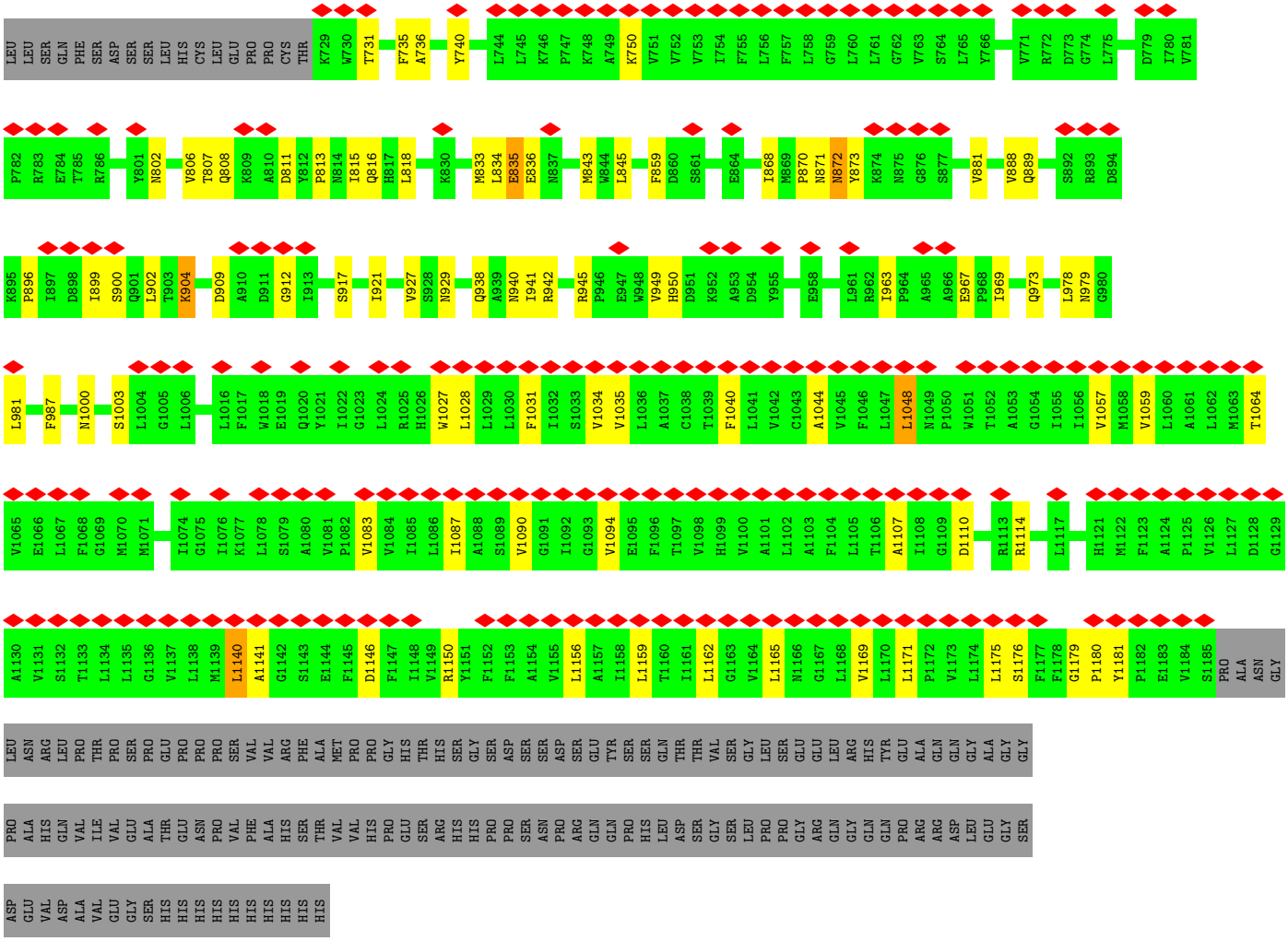
3 Residue-property plots (i)

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: Protein patched homolog 1

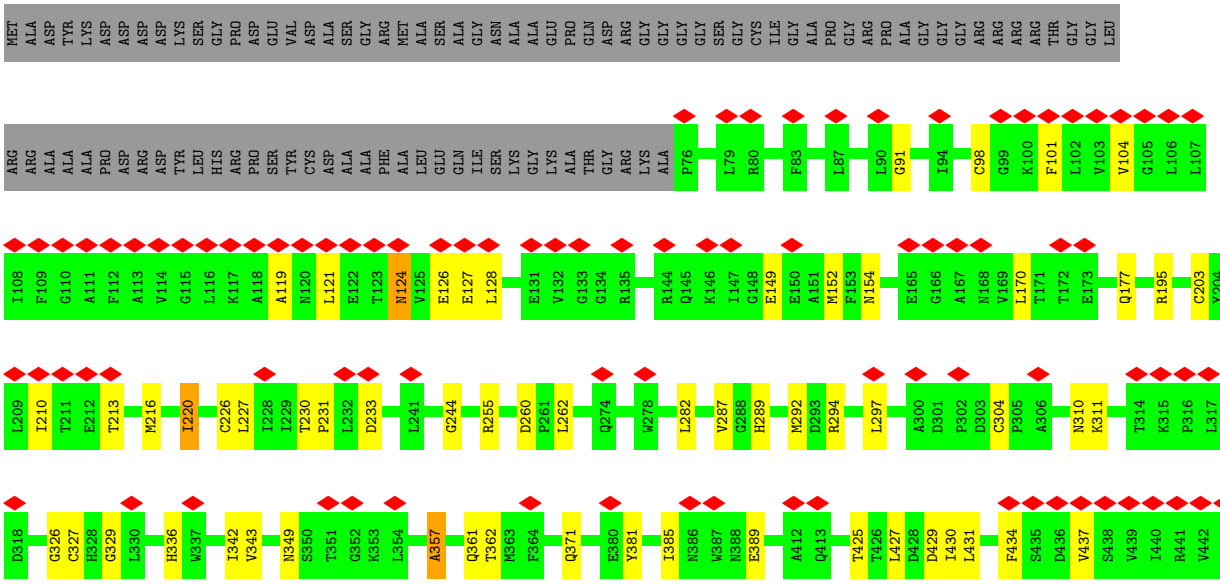
Chain A:

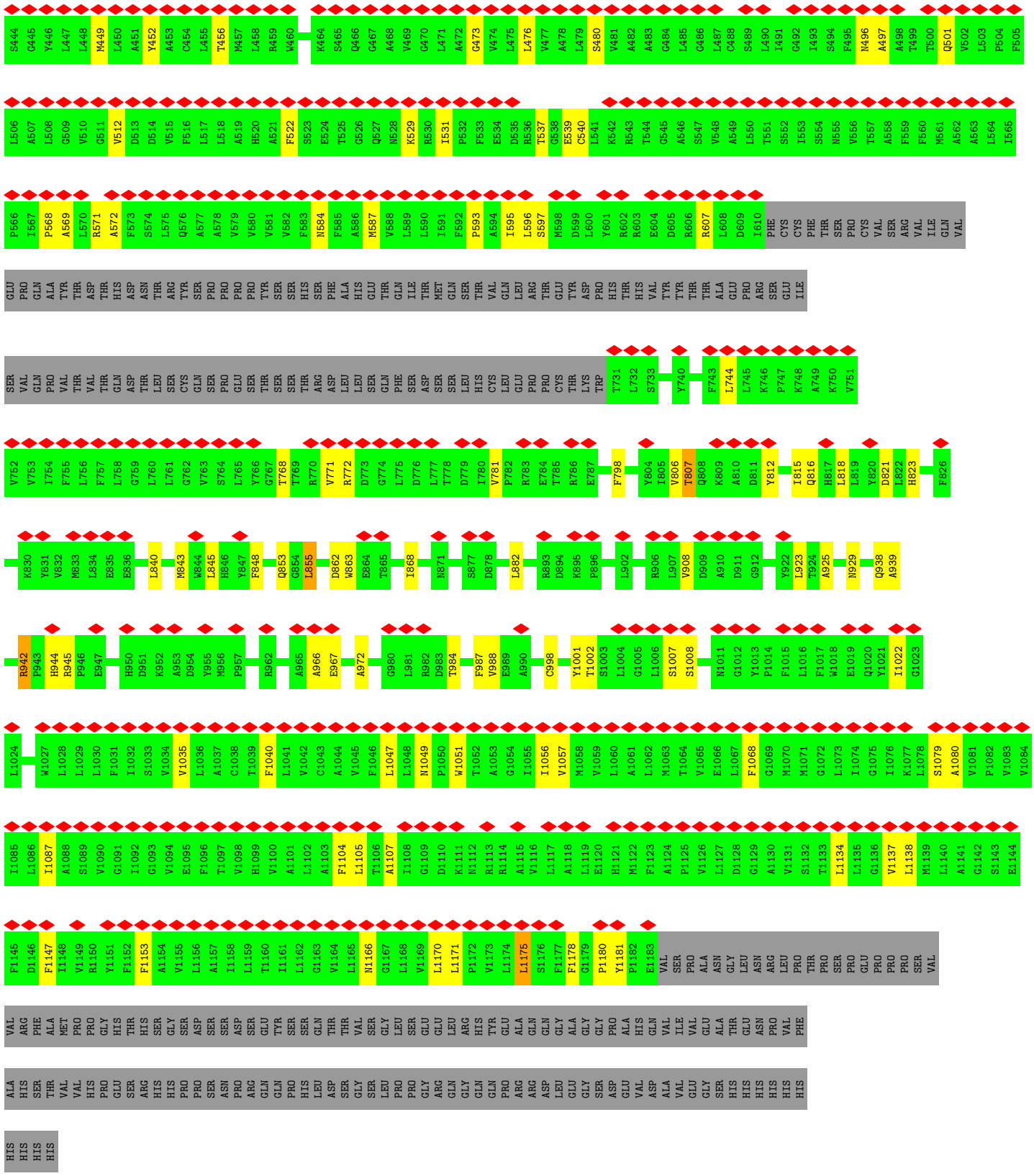




- Molecule 1: Protein patched homolog 1

Chain B:





- Molecule 1: Protein patched homolog 1

Chain D:

MET ALA ASP TYR LYS ASP ASP ASP LYS SER GLY PRO ASP GLU VAL ASP ALA SER GLY ARG MET ALA SER ALA GLY ASN ALA ALA GLU PRO GLN ASP ARG GLY GLY GLY GLY SER GLY CYS ILE GLY ALA PRO GLY ARG PRO ALA GLY GLY GLY ARG ARG ARG ARG THR GLY GLY LEU

ARG ARG ALA ALA ALA PRO ASP ARG ASP TYR LEU HIS ARG PRO SER TYR CYS ASP ALA ALA PHE ALA LEU GLU GLN ILE SER LYS GLY LYS ALA THR GLY R73 K74 A75 P76 L77 W78 L79 R80 F83 Q84 R85 L86 L87 C92 Y93 I94 Q95 K96 N97 C98 G99 K100 F101 L102 V103

V104 G105 L106 L107 I108 F109 G110 A111 F112 A113 V114 G115 L116 K117 A118 A119 N120 L121 E122 T123 N124 V125 E126 E127 L128 W129 V130 E131 V132 G133 G134 R135 V136 S137 R138 E139 L140 N141 Y142 I147 G148 E149 E150 A151 M152 F153 N154 P155 Q156 L157 M158 I159 Q160 T161 P162 K163 E164 E165 G166

A167 N168 V169 L170 T171 T172 E173 A174 L175 L176 Q177 H178 L179 D180 S181 A182 L183 Q184 A185 S186 R187 M192 Y193 Q196 W197 K198 L199 E200 H201 L202 C203 Y204 K205 S206 G207 E208 L209 I210 T211 E212 T213 G214 Y215 M216 D217 I220 E221 Y224 P225 C226 L227 I228 I229 T230 P231 L232

D233 C234 F235 W236 E237 G238 A239 K240 L241 Q242 S243 G244 T245 A246 Y247 L248 L249 G250 K251 P252 P253 L254 R255 W256 T257 N258 F259 L262 E263 F264 L265 E266 E267 L268 K269 K270 I271 N272 Y273 Q274 V275 D276 S277 W278 E279 E280 M281 L282 N283 K284 A285 E286 V287 G288 H289 G290 Y291 M292 D293

R294 P295 C296 L297 N298 P299 A300 D301 P302 D303 C304 P305 A306 T307 A308 P309 N310 K311 N312 S313 T314 K315 P316 L317 D318 M319 A320 L321 V322 L323 N324 G325 G326 G329 K333 Y334 M335 H336 W337 Q338 E339 E340 L341 I342 V343 G344 G345 T346 V347 K348 N349 S350 T351 G352 K353 L354 V355 S356

A357 H358 A359 L360 Q361 T362 M363 F364 Q365 L366 M367 T368 Q371 M372 Y373 E374 H375 F376 K377 G378 Y379 E380 Y381 V382 S383 H384 I385 N386 W387 D390 I395 L396 E397 A398 W399 Q400 R401 T402 Y403 V404 E405 V406 V407 H408 Q409 S410 V411 A412 Q413 N414 S415 T416 L420 S421 F422 T423

T424 T425 T426 L427 D428 D429 I430 L431 K432 S433 F434 S435 D436 V437 S438 V439 I440 R441 V442 A443 S444 G445 Y446 L447 L448 M449 L450 A451 Y452 A453 C454 L455 T456 M457 L458 R459 W460 D461 C462 S463 K464 S465 Q466 G467 A468 V469 G470 L471 A472 G473 V474 L475 L476 V477 A478 L479 S480 V481 A482 A483

G484 L485 G486 L487 C488 S489 L490 I491 G492 I493 S494 F495 N496 A497 A498 T499 T500 Q501 V502 L503 P504 F505 L506 A507 L508 G509 V510 G511 V512 D513 D514 V515 F516 L517 L518 A519 H520 A521 F522 S523 E524 T525 G526 Q527 N528 K529 R530 I531 P532 F533 E534 D535 R536 T537 G538 E539 C540 L541 K542 R543

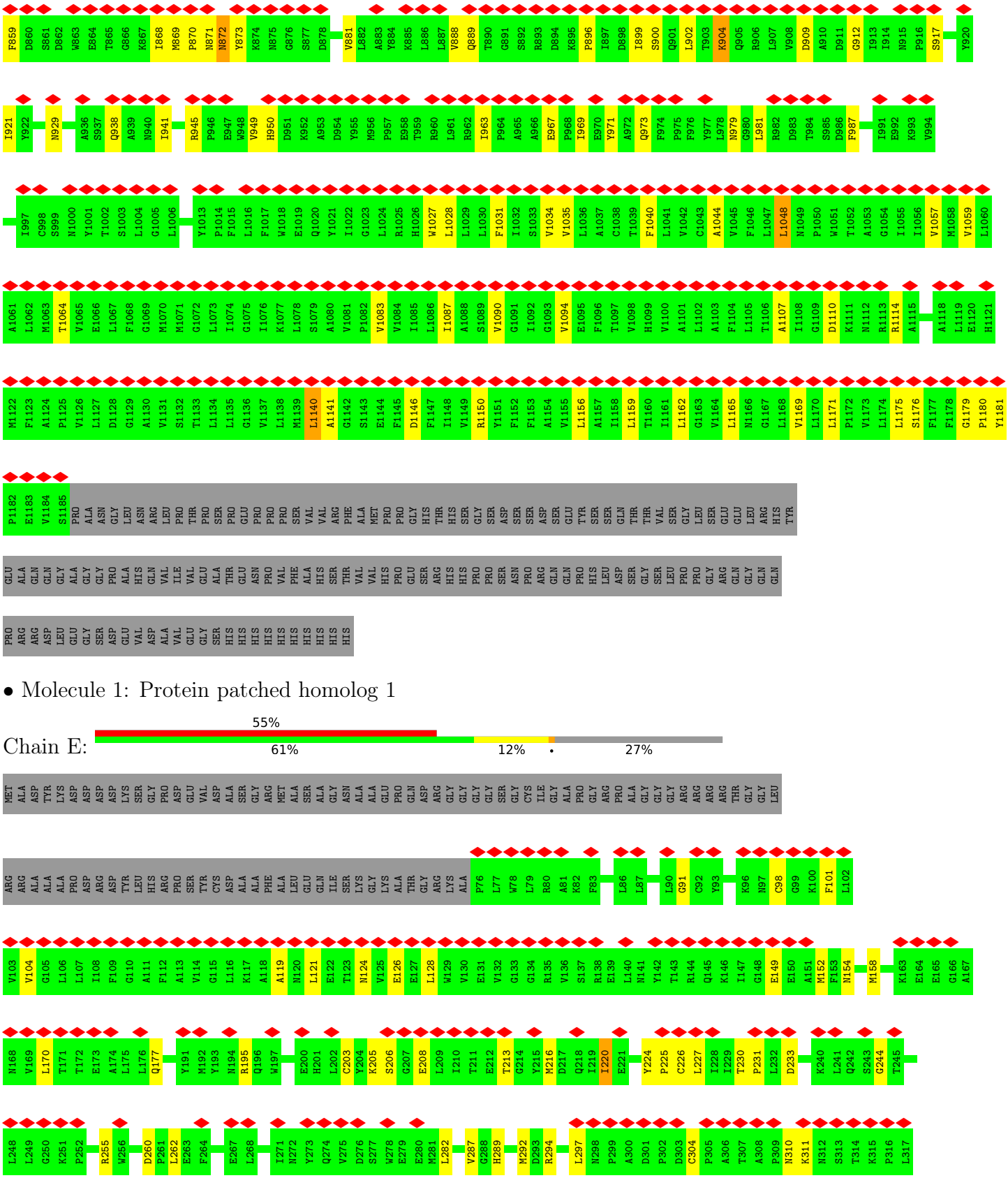
T544 G545 A546 S547 V548 A549 L550 T551 S552 I553 S554 N555 V556 T557 A558 F559 F560 M561 A562 A563 L564 I565 P566 I567 P568 A569 L570 R571 A572 F573 S574 L575 Q576 A577 A578 V579 V580 V581 V582 F583 N584 F585 A586 M587 V588 L589 L590 I591 F592 P593 A594 I595 L596 S597 M598 D599 L600 Y601 R602 R603

E604 D605 R606 ARG LEU ASP ILE PHE CYS CYS PHE THR SER PRO CYS VAL SER ARG VAL ILE GLN VAL GLU PRO GLN ALA TYR THR ASP THR HIS ASP ASN THR ARG TYR SER PRO PRO PRO PRO TYR SER SER HIS SER PHE ALA HIS GLU THR GLN ILE THR MET GLN SER THR VAL GLN

LEU ARG THR GLU TYR ASP PRO HIS THR HIS VAL TYR TYR THR THR ALA GLU PRO ARG SER GLU ILE SER VAL GLN PRO VAL THR VAL THR GLN ASP THR LEU SER CYS GLN SER PRO GLU SER THR SER SER THR ARG ASP LEU LEU SER GLN PHE SER ASP SER SER LEU HIS CYS LEU

GLU PRO PRO CYS THR K729 W730 T731 L732 S733 S734 F735 A736 E737 K738 H739 Y740 A741 P742 F743 L744 L745 K746 P747 K748 A749 K750 V751 V752 V753 I754 F755 L756 F757 L758 G759 L760 L761 G762 V763 S764 L765 V766 G767 T768 T769 R770 V771 R772 D773 G774 L775 D776 L777 T778 D779 I780 V781 P782 R783

E784 T785 R786 E787 Y788 D789 F790 I791 A792 A793 K796 Y797 F798 S799 F800 Y801 N802 I805 V806 T807 Q808 K809 A810 D811 Y812 P813 N814 I815 Q816 H817 L818 R824 S827 N828 V829 K830 Y831 V832 M833 L834 E835 E836 N837 K838 Q839 L840 P841 K842 M843 W844 L845 W851 D857 A858



- Molecule 1: Protein patched homolog 1

Chain E:

D318 M319 A320 L323 G326 C327 H328 G329 L330 H336 W337 Q338 E339 E340 L341 I342 V343 V347 K348 N349 S350 T351 G352 K353 L354 V355 S356 A357 L360 Q361 T362 M363 F364 Q365 L366 Q371 E374 H375 F376 K377 G378 Y379 E380 Y381 V382 S383 H384 I385 N386 W387 N388 E389 D390

W399 Q400 R401 H408 Q409 S410 V411 A412 Q413 N414 S415 L420 S421 F422 T423 T424 T425 T426 L427 D428 D429 I430 L431 K432 S433 F434 S435 D436 V437 S438 V439 I440 R441 V442 A443 S444 G445 Y446 L447 L448 M449 L450 A451 Y452 A453 C454 L455 T456 M457 L458 R459 C462 S463 K464 S465 Q466

G467 A468 V469 G470 L471 A472 G473 V474 L475 L476 V477 A478 L479 S480 V481 A482 A483 G484 L485 G486 L487 C488 S489 L490 I491 G492 I493 S494 F495 N496 A497 A498 T499 T500 Q501 V502 L503 P504 F505 L506 A507 L508 G509 V510 G511 V512 D513 D514 V515 F516 L517 L518 A519 H520 A521 F522 S523 E524 T525 G526

Q527 N528 K529 R530 I531 P532 F533 E534 D535 R536 T537 G538 E539 C540 L541 K542 R543 T544 G545 A546 S547 V548 A549 L550 T551 S552 I553 S554 N555 V556 T557 A558 F559 F560 M561 A562 A563 L564 I565 P566 I567 P568 A569 L570 R571 A572 F573 S574 L575 Q576 A577 A578 V579 V580 V581 V582 F583 N584 F585 A586

M587 V588 L589 L590 I591 F592 P593 A594 I595 L596 S597 M598 D599 L600 Y601 R602 R603 E604 D605 R606 R607 L608 D609 I610 PHE CYS CYS PHE THR SER PRO CYS VAL SER ARG VAL ILE GLN VAL GLU PRO GLN ALA TYR THR ASP THR HIS ASP ASN THR ARG TYR SER PRO PRO PRO PRO TYR SER

SER HIS SER PHE ALA HIS GLU THR GLN ILE THR MET GLN SER THR VAL GLN LEU ARG THR GLU TYR ASP PRO HIS THR HIS VAL TYR TYR THR THR ALA GLU PRO ARG SER GLU ILE SER VAL GLN PRO VAL THR VAL THR GLN ASP THR LEU SER CYS GLN LEU SER PRO GLU SER THR SER

SER THR ARG ASP LEU LEU SER GLN PHE SER ASP SER SER LEU HIS CYS LEU GLU PRO PRO CYS THR LYS ASP TRP T731 L732 S733 S734 F735 Y740 F743 L744 L745 K746 P747 K748 A749 K750 V751 V752 V753 I754 F755 L756 F757 L758 G759 L760 L761 G762 V763 S764 L765 Y766 G767 T768 T769 R770

V771 R772 D773 G774 L775 D776 L777 T778 D779 I780 V781 P782 R783 E784 T785 R786 E787 Y788 D789 F790 I791 F795 K796 Y797 F798 N802 M803 Y804 I805 V806 T807 Q808 K809 A810 D811 Y812 P813 N814 I815 Q816 H817 L818 L819 Y820 D821 L822 H823 R824 S825 F826 S827 N828 V829 K830 Y831 V832 M833 L834

E835 E836 N837 L840 P841 K842 M843 W844 L845 H846 Y847 F848 R849 D850 W851 L852 Q853 G854 L855 Q856 D857 A858 F859 D860 S861 D862 W863 E864 T865 G866 K867 I868 M869 P870 N871 N872 Y873 K874 N875 G876 S877 D878 D879 G880 V881 L882 A883 Y884 K885 L886 L887 V888 Q889 T890 G891 S892 R893 D894 K895

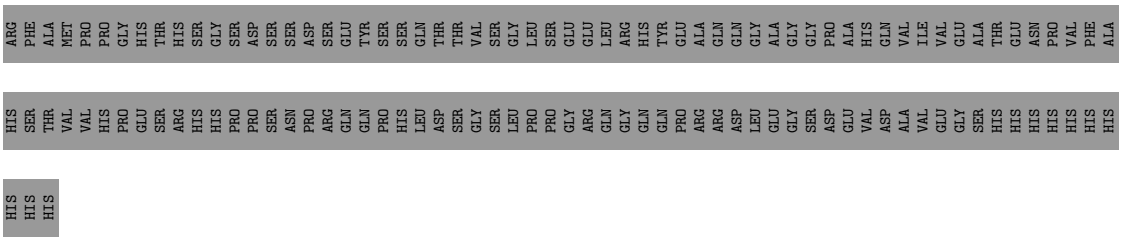
P896 I897 D898 I899 S900 Q901 L902 T903 K904 Q905 R906 L907 V908 D909 A910 D911 G912 I913 I914 N915 P916 S917 A918 F919 Y920 I921 Y922 L923 T924 A925 N929 V932 A935 A936 S937 Q938 A939 R942 P943 H944 R945 P946 E947 W948 V949 H950 D951 K952 A953 D954 Y955 M956 P957 E958 T959 R960

L961 R962 I963 P964 A965 A966 E967 P968 I969 E970 Y971 A972 Q973 F974 P975 N979 G980 L981 R982 D983 T984 S985 D986 F987 V988 E989 A990 V994 R995 T996 I997 C998 Y1001 T1002 S1003 L1004 G1005 L1006 S1007 S1008 Y1009 P1010 N1011 G1012 Y1013 P1014 F1015 L1016 F1017 W1018 E1019 Q1020 Y1021 I1022 G1023 L1024 R1025

H1026 W1027 L1028 L1029 L1030 F1031 I1032 S1033 V1034 V1035 L1036 A1037 C1038 T1039 F1040 L1041 V1042 C1043 A1044 V1045 F1046 L1047 L1048 N1049 P1050 W1051 T1052 A1053 G1054 I1055 I1056 V1057 M1058 V1059 L1060 A1061 L1062 M1063 T1064 V1065 E1066 L1067 F1068 G1069 M1070 M1071 G1072 L1073 I1074 G1075 I1076 K1077 L1078 S1079 A1080 V1081 P1082 V1083 V1084 I1085

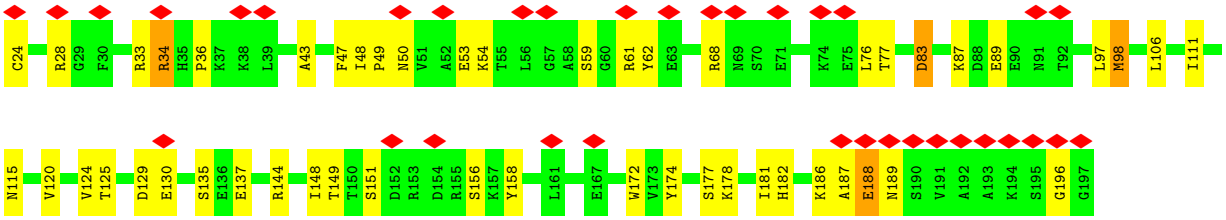
L1086 I1087 A1088 S1089 V1090 G1091 I1092 G1093 V1094 E1095 F1096 T1097 V1098 H1099 V1100 A1101 L1102 A1103 F1104 L1105 T1106 A1107 I1108 G1109 D1110 K1111 N1112 R1113 R1114 A1115 V1116 L1117 A1118 L1119 E1120 H1121 M1122 F1123 A1124 P1125 V1126 L1127 D1128 G1129 A1130 V1131 S1132 T1133 L1134 L1135 G1136 V1137 L1138 M1139 L1140 A1141 G1142 S1143 E1144 F1145

D1146 F1147 I1148 V1149 R1150 Y1151 F1152 F1153 A1154 V1155 L1156 A1157 I1158 L1159 T1160 I1161 L1162 G1163 V1164 L1165 N1166 G1167 L1168 V1169 L1170 L1171 P1172 V1173 L1174 L1175 S1176 F1177 F1178 G1179 P1180 Y1181 P1182 E1183 VAL SER PRO ALA ASN GLY LEU ASN ARG LEU PRO THR PRO SER PRO GLU PRO PRO PRO SER VAL VAL



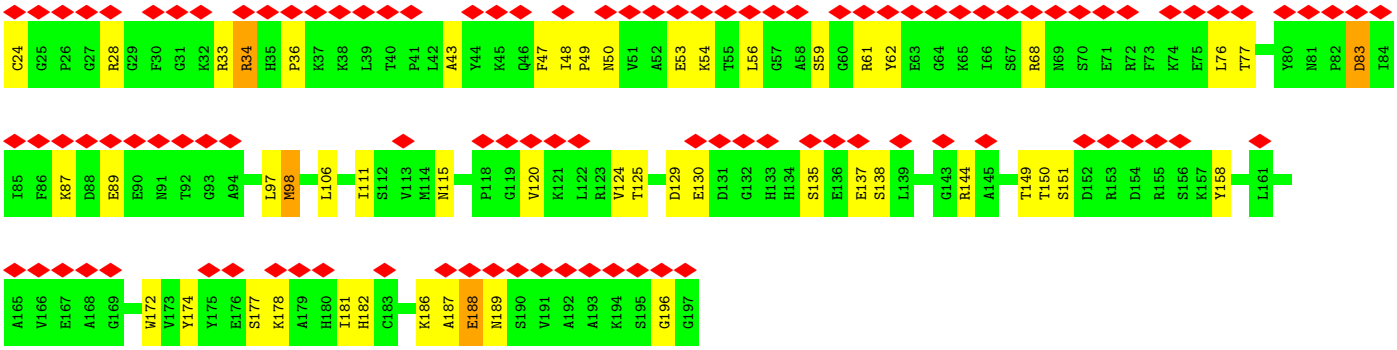
• Molecule 2: Sonic hedgehog protein

Chain C:



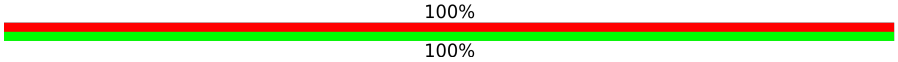
• Molecule 2: Sonic hedgehog protein

Chain F:



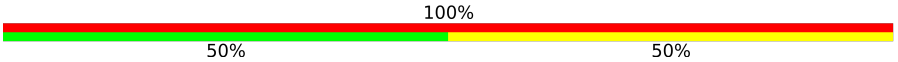
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

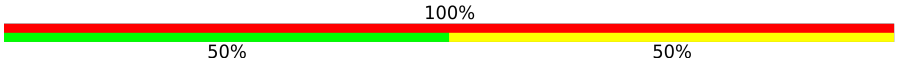
Chain H:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25510	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.077	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	311.91998, 311.91998, 311.91998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.114, 1.114, 1.114	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: ZN, PLM, NAG, CA, CLR

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	0.45	0/8000	0.71	6/10883 (0.1%)
1	B	0.48	0/7897	0.70	5/10749 (0.0%)
1	D	0.45	0/8000	0.71	6/10883 (0.1%)
1	E	0.48	0/7897	0.70	5/10749 (0.0%)
2	C	0.56	1/1401 (0.1%)	0.76	3/1886 (0.2%)
2	F	0.56	1/1401 (0.1%)	0.76	4/1886 (0.2%)
All	All	0.47	2/34596 (0.0%)	0.71	29/47036 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	6
1	D	0	7
1	E	0	6
2	C	0	1
2	F	0	1
All	All	0	28

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	98	MET	C-N	8.19	1.52	1.34
2	F	98	MET	C-N	8.16	1.52	1.34

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	83	ASP	O-C-N	-7.34	110.96	122.70
2	C	83	ASP	O-C-N	-7.33	110.97	122.70
1	B	297	LEU	CA-CB-CG	7.03	131.48	115.30
1	E	297	LEU	CA-CB-CG	6.99	131.39	115.30
1	A	323	LEU	CA-CB-CG	6.33	129.86	115.30
1	D	323	LEU	CA-CB-CG	6.32	129.82	115.30
1	E	262	LEU	CA-CB-CG	6.29	129.76	115.30
1	B	262	LEU	CA-CB-CG	6.28	129.74	115.30
1	D	508	LEU	CA-CB-CG	6.22	129.62	115.30
1	A	508	LEU	CA-CB-CG	6.20	129.55	115.30
2	C	83	ASP	C-N-CA	5.92	136.50	121.70
2	F	83	ASP	C-N-CA	5.91	136.48	121.70
1	D	1140	LEU	CA-CB-CG	5.55	128.06	115.30
1	A	1140	LEU	CA-CB-CG	5.55	128.06	115.30
1	E	855	LEU	CA-CB-CG	5.53	128.02	115.30
1	E	744	LEU	CA-CB-CG	5.52	127.99	115.30
1	B	855	LEU	CA-CB-CG	5.51	127.98	115.30
1	B	744	LEU	CA-CB-CG	5.50	127.96	115.30
2	C	196	GLY	N-CA-C	5.50	126.84	113.10
1	D	179	LEU	CA-CB-CG	5.49	127.91	115.30
1	A	179	LEU	CA-CB-CG	5.47	127.89	115.30
1	D	589	LEU	CA-CB-CG	5.47	127.88	115.30
2	F	196	GLY	N-CA-C	5.47	126.77	113.10
1	A	589	LEU	CA-CB-CG	5.47	127.88	115.30
1	B	1175	LEU	CB-CG-CD2	-5.25	102.08	111.00
1	E	1175	LEU	CB-CG-CD2	-5.23	102.11	111.00
1	A	517	LEU	CA-CB-CG	5.17	127.18	115.30
1	D	517	LEU	CA-CB-CG	5.16	127.16	115.30
2	F	138	SER	C-N-CA	-5.01	109.17	121.70

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	VAL	Peptide
1	A	224	TYR	Peptide
1	A	317	LEU	Peptide
1	A	835	GLU	Peptide
1	A	836	GLU	Peptide
1	A	870	PRO	Peptide
1	A	912	GLY	Peptide
1	B	1107	ALA	Peptide
1	B	327	CYS	Peptide

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Mol	Chain	Res	Type	Group
1	B	357	ALA	Peptide
1	B	385	ILE	Peptide
1	B	938	GLN	Peptide
1	B	942	ARG	Peptide
2	C	83	ASP	Mainchain
1	D	130	VAL	Peptide
1	D	224	TYR	Peptide
1	D	317	LEU	Peptide
1	D	835	GLU	Peptide
1	D	836	GLU	Peptide
1	D	870	PRO	Peptide
1	D	912	GLY	Peptide
1	E	1107	ALA	Peptide
1	E	327	CYS	Peptide
1	E	357	ALA	Peptide
1	E	385	ILE	Peptide
1	E	938	GLN	Peptide
1	E	942	ARG	Peptide
2	F	83	ASP	Mainchain

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	7807	0	7828	111	0
1	B	7708	0	7664	120	0
1	D	7807	0	7828	110	0
1	E	7708	0	7664	123	0
2	C	1371	0	1329	37	0
2	F	1371	0	1329	35	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
4	A	70	0	65	0	0
4	B	70	0	65	1	0
4	D	70	0	65	1	0
4	E	70	0	65	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	84	0	138	35	0
5	B	28	0	46	30	0
5	C	28	0	45	19	0
5	D	84	0	138	35	0
5	E	28	0	46	33	0
5	F	28	0	45	19	0
6	C	1	0	0	0	0
6	F	1	0	0	0	0
7	C	2	0	0	0	0
7	F	2	0	0	0	0
8	C	17	0	31	16	0
8	F	17	0	31	16	0
All	All	34484	0	34522	615	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 9.

All (615) 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:B:1147:PHE:HE2	8:C:205:PLM:CG	1.16	1.54
1:A:220:ILE:CD1	5:A:1808:CLR:C6	1.84	1.53
1:E:1147:PHE:HE2	8:F:205:PLM:CG	1.16	1.53
1:D:220:ILE:CD1	5:D:1808:CLR:C6	1.84	1.52
1:B:1147:PHE:CE2	8:C:205:PLM:CG	1.93	1.50
1:E:1147:PHE:CE2	8:F:205:PLM:CG	1.93	1.48
1:D:220:ILE:CD1	5:D:1808:CLR:H6	0.96	1.43
1:A:220:ILE:CD1	5:A:1808:CLR:H6	0.96	1.41
1:E:216:MET:SD	5:F:201:CLR:H41	1.65	1.35
1:B:216:MET:SD	5:C:201:CLR:H41	1.65	1.34
1:A:220:ILE:HD13	5:A:1808:CLR:C6	1.53	1.29
1:B:1147:PHE:CZ	8:C:205:PLM:HG2	1.73	1.24
1:D:220:ILE:HD13	5:D:1808:CLR:C6	1.53	1.23
1:E:1147:PHE:CZ	8:F:205:PLM:HG2	1.73	1.20
1:E:216:MET:SD	5:F:201:CLR:C4	2.29	1.19
1:B:216:MET:SD	5:C:201:CLR:C4	2.29	1.18
1:B:1147:PHE:HE2	8:C:205:PLM:HG1	0.99	1.15
1:E:121:LEU:HD12	5:E:1508:CLR:H192	1.16	1.14
1:E:1147:PHE:CE2	8:F:205:PLM:HG2	1.71	1.10
1:E:1147:PHE:HE2	8:F:205:PLM:HG1	0.99	1.08
1:B:121:LEU:HD12	5:B:1508:CLR:H192	1.16	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ILE:HD11	5:A:1808:CLR:H6	1.09	1.07
1:B:1147:PHE:CE2	8:C:205:PLM:HG2	1.71	1.07
1:E:437:VAL:HG11	5:E:1508:CLR:H121	1.09	1.06
1:B:437:VAL:HG11	5:B:1508:CLR:H121	1.09	1.05
5:D:1808:CLR:H162	5:D:1808:CLR:H231	1.39	1.04
1:D:220:ILE:HD11	5:D:1808:CLR:H6	1.09	1.04
5:A:1808:CLR:H162	5:A:1808:CLR:H231	1.39	1.03
8:F:205:PLM:HC2	8:F:205:PLM:H81	1.39	1.03
1:E:121:LEU:HD12	5:E:1508:CLR:C19	1.89	1.02
8:C:205:PLM:H81	8:C:205:PLM:HC2	1.39	1.02
1:B:121:LEU:HD12	5:B:1508:CLR:C19	1.89	1.01
1:E:152:MET:SD	2:F:28:ARG:NH1	2.33	1.01
1:B:152:MET:SD	2:C:28:ARG:NH1	2.33	1.01
1:A:220:ILE:HD11	5:A:1808:CLR:C6	1.66	1.00
1:E:437:VAL:HG11	5:E:1508:CLR:C12	1.94	0.97
1:B:437:VAL:HG11	5:B:1508:CLR:C12	1.94	0.96
1:D:220:ILE:HD11	5:D:1808:CLR:C6	1.66	0.96
1:B:1147:PHE:CE2	8:C:205:PLM:HG1	1.82	0.95
1:E:1147:PHE:HE2	8:F:205:PLM:HG3	1.33	0.94
2:F:187:ALA:O	2:F:189:ASN:N	2.01	0.93
2:F:76:LEU:HD23	2:F:97:LEU:HB3	1.50	0.92
2:C:187:ALA:O	2:C:189:ASN:N	2.01	0.92
1:B:1147:PHE:CE2	8:C:205:PLM:HG3	2.02	0.92
1:E:216:MET:SD	5:F:201:CLR:H6	2.10	0.92
5:B:1508:CLR:H273	5:B:1508:CLR:H221	1.50	0.91
2:C:76:LEU:HD23	2:C:97:LEU:HB3	1.50	0.91
1:E:437:VAL:CG1	5:E:1508:CLR:H121	2.01	0.91
1:B:216:MET:SD	5:C:201:CLR:H6	2.10	0.91
1:E:1147:PHE:CE2	8:F:205:PLM:HG1	1.82	0.90
5:E:1508:CLR:H211	5:E:1508:CLR:H242	1.54	0.90
5:E:1508:CLR:H221	5:E:1508:CLR:H273	1.50	0.90
1:B:437:VAL:CG1	5:B:1508:CLR:H121	2.01	0.89
5:B:1508:CLR:H242	5:B:1508:CLR:H211	1.54	0.88
1:B:119:ALA:HB1	5:B:1508:CLR:H72	1.55	0.88
1:E:119:ALA:HB1	5:E:1508:CLR:H72	1.55	0.87
1:E:1147:PHE:CE2	8:F:205:PLM:HG3	2.02	0.87
1:B:1147:PHE:HE2	8:C:205:PLM:HG3	1.32	0.84
5:A:1808:CLR:H221	5:A:1808:CLR:H181	1.59	0.83
1:E:282:LEU:HD21	5:F:201:CLR:C21	2.09	0.83
5:E:1508:CLR:H213	5:E:1508:CLR:C27	2.09	0.83
5:B:1508:CLR:H213	5:B:1508:CLR:C27	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1808:CLR:H181	5:D:1808:CLR:H221	1.59	0.82
8:C:205:PLM:HC2	8:C:205:PLM:C8	2.03	0.81
1:A:249:LEU:HD12	2:C:135:SER:HB2	1.63	0.81
1:B:282:LEU:HD21	5:C:201:CLR:C21	2.09	0.81
1:A:1171:LEU:O	1:A:1175:LEU:HB2	1.80	0.81
1:D:1171:LEU:O	1:D:1175:LEU:HB2	1.81	0.81
1:B:1147:PHE:HZ	8:C:205:PLM:HG2	1.45	0.81
5:E:1508:CLR:H221	5:E:1508:CLR:H262	1.64	0.80
5:A:1808:CLR:H162	5:A:1808:CLR:C23	2.02	0.80
5:A:1808:CLR:C25	5:A:1808:CLR:H213	2.12	0.80
1:D:249:LEU:HD12	2:F:135:SER:HB2	1.63	0.79
5:D:1808:CLR:H162	5:D:1808:CLR:C23	2.02	0.79
5:B:1508:CLR:H221	5:B:1508:CLR:H262	1.64	0.79
1:B:121:LEU:CD1	5:B:1508:CLR:H192	2.08	0.79
1:B:216:MET:SD	5:C:201:CLR:C6	2.70	0.79
1:E:149:GLU:OE1	2:F:28:ARG:NH1	2.16	0.79
1:E:216:MET:SD	5:F:201:CLR:C6	2.70	0.79
5:D:1808:CLR:C25	5:D:1808:CLR:H213	2.12	0.79
1:B:149:GLU:OE1	2:C:28:ARG:NH1	2.16	0.77
5:C:201:CLR:H183	5:C:201:CLR:H212	1.67	0.76
1:E:121:LEU:CD1	5:E:1508:CLR:H192	2.08	0.75
5:F:201:CLR:H183	5:F:201:CLR:H212	1.67	0.75
8:F:205:PLM:HC2	8:F:205:PLM:C8	2.03	0.74
5:A:1808:CLR:H213	5:A:1808:CLR:H25	1.70	0.74
1:B:220:ILE:HG13	5:C:201:CLR:H152	1.70	0.73
1:E:220:ILE:HG13	5:F:201:CLR:H152	1.70	0.73
5:A:1808:CLR:H231	5:A:1808:CLR:C16	2.18	0.73
5:D:1808:CLR:H213	5:D:1808:CLR:H25	1.70	0.73
5:E:1508:CLR:H262	5:E:1508:CLR:C22	2.17	0.72
1:A:1028:LEU:HD12	1:A:1083:VAL:HG22	1.72	0.72
1:D:1028:LEU:HD12	1:D:1083:VAL:HG22	1.72	0.72
1:A:220:ILE:CD1	5:A:1808:CLR:C7	2.67	0.72
1:A:220:ILE:HD12	5:A:1808:CLR:C6	2.15	0.71
5:B:1508:CLR:H262	5:B:1508:CLR:C22	2.17	0.71
5:B:1508:CLR:H273	5:B:1508:CLR:C22	2.20	0.71
1:A:220:ILE:HD13	5:A:1808:CLR:H6	0.71	0.71
1:D:220:ILE:HD13	5:D:1808:CLR:H6	0.71	0.71
5:B:1508:CLR:H273	5:B:1508:CLR:H213	1.72	0.70
5:E:1508:CLR:H273	5:E:1508:CLR:C22	2.20	0.70
1:D:220:ILE:CD1	5:D:1808:CLR:C7	2.67	0.70
5:D:1808:CLR:H231	5:D:1808:CLR:C16	2.18	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1808:CLR:H221	5:D:1808:CLR:C18	2.23	0.69
5:E:1508:CLR:H273	5:E:1508:CLR:H213	1.72	0.69
5:A:1808:CLR:H221	5:A:1808:CLR:C18	2.23	0.68
1:D:220:ILE:HD12	5:D:1808:CLR:C6	2.15	0.68
5:A:1808:CLR:H213	5:A:1808:CLR:H272	1.76	0.68
1:B:154:ASN:ND2	2:C:28:ARG:HG2	2.08	0.68
5:E:1508:CLR:H242	5:E:1508:CLR:C21	2.24	0.68
5:B:1508:CLR:H242	5:B:1508:CLR:C21	2.24	0.68
1:E:1147:PHE:HZ	8:F:205:PLM:HG2	1.45	0.68
1:D:335:MET:SD	5:D:1808:CLR:H211	2.34	0.68
1:E:216:MET:SD	5:F:201:CLR:C5	2.81	0.68
1:E:282:LEU:HD21	5:F:201:CLR:H212	1.75	0.67
1:A:335:MET:SD	5:A:1808:CLR:H211	2.34	0.67
1:E:434:PHE:HZ	8:F:205:PLM:HG3	1.60	0.67
1:E:154:ASN:ND2	2:F:28:ARG:HG2	2.08	0.67
1:B:434:PHE:HZ	8:C:205:PLM:HG3	1.60	0.67
1:B:216:MET:SD	5:C:201:CLR:C5	2.82	0.67
1:B:282:LEU:HD21	5:C:201:CLR:H212	1.75	0.67
5:D:1808:CLR:H213	5:D:1808:CLR:H272	1.76	0.67
5:D:1808:CLR:H213	5:D:1808:CLR:C27	2.26	0.66
1:B:154:ASN:HD22	2:C:28:ARG:HG2	1.60	0.65
5:E:1508:CLR:H213	5:E:1508:CLR:H272	1.77	0.65
1:B:496:ASN:HD21	1:B:572:ALA:HB3	1.61	0.65
5:A:1808:CLR:H213	5:A:1808:CLR:C27	2.26	0.65
1:D:248:LEU:HD23	1:D:250:GLY:H	1.62	0.65
2:C:144:ARG:HH21	2:C:186:LYS:HA	1.62	0.65
1:E:496:ASN:HD21	1:E:572:ALA:HB3	1.61	0.65
5:B:1508:CLR:H213	5:B:1508:CLR:H272	1.78	0.65
1:E:154:ASN:HD22	2:F:28:ARG:HG2	1.60	0.64
2:F:144:ARG:HH21	2:F:186:LYS:HA	1.62	0.64
1:A:248:LEU:HD23	1:A:250:GLY:H	1.62	0.64
1:B:121:LEU:CD1	5:B:1508:CLR:C19	2.73	0.63
1:B:988:VAL:HG13	1:B:1022:ILE:HG22	1.81	0.63
1:D:1114:ARG:HH22	1:D:1181:TYR:HA	1.64	0.63
1:D:736:ALA:O	1:D:740:TYR:HB2	1.99	0.63
1:A:736:ALA:O	1:A:740:TYR:HB2	1.99	0.62
1:E:945:ARG:NH1	1:E:967:GLU:O	2.32	0.62
1:D:873:TYR:HB2	1:D:881:VAL:HG22	1.82	0.62
1:D:282:LEU:HD21	5:D:1808:CLR:H192	1.82	0.62
1:B:945:ARG:NH1	1:B:967:GLU:O	2.32	0.62
1:E:988:VAL:HG13	1:E:1022:ILE:HG22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1114:ARG:HH22	1:A:1181:TYR:HA	1.64	0.61
1:B:128:LEU:HB2	1:B:569:ALA:HB2	1.82	0.61
1:D:210:ILE:HD11	1:D:949:VAL:HG21	1.83	0.61
1:B:119:ALA:CB	5:B:1508:CLR:H72	2.30	0.61
1:B:342:ILE:HD12	1:B:343:VAL:HG23	1.82	0.61
1:E:342:ILE:HD12	1:E:343:VAL:HG23	1.82	0.61
2:C:187:ALA:C	2:C:189:ASN:N	2.54	0.61
5:F:201:CLR:C16	5:F:201:CLR:H232	2.31	0.61
1:E:216:MET:HE2	1:E:216:MET:HA	1.83	0.61
1:E:121:LEU:CD1	5:E:1508:CLR:C19	2.73	0.60
5:C:201:CLR:C16	5:C:201:CLR:H232	2.31	0.60
1:A:210:ILE:HD11	1:A:949:VAL:HG21	1.82	0.60
1:A:290:GLY:O	1:A:294:ARG:NH1	2.34	0.60
1:E:128:LEU:HB2	1:E:569:ALA:HB2	1.82	0.60
1:A:873:TYR:HB2	1:A:881:VAL:HG22	1.82	0.60
1:E:434:PHE:CZ	8:F:205:PLM:HG3	2.37	0.60
1:B:434:PHE:CZ	8:C:205:PLM:HG3	2.37	0.60
1:D:290:GLY:O	1:D:294:ARG:NH1	2.33	0.60
1:A:282:LEU:HD21	5:A:1808:CLR:H192	1.82	0.59
1:E:1104:PHE:HE2	1:E:1180:PRO:HD2	1.67	0.59
2:F:187:ALA:C	2:F:189:ASN:N	2.54	0.59
1:B:216:MET:HE2	1:B:216:MET:HA	1.85	0.59
1:E:925:ALA:O	1:E:929:ASN:HB2	2.02	0.59
1:B:289:HIS:HB3	1:B:292:MET:HB2	1.85	0.59
5:F:201:CLR:H232	5:F:201:CLR:H161	1.85	0.59
1:B:1104:PHE:HE2	1:B:1180:PRO:HD2	1.67	0.59
1:B:862:ASP:HB3	1:B:868:ILE:HG12	1.86	0.58
1:B:925:ALA:O	1:B:929:ASN:HB2	2.03	0.58
1:D:205:LYS:HD2	1:D:224:TYR:HD2	1.68	0.58
1:E:289:HIS:HB3	1:E:292:MET:HB2	1.85	0.58
1:E:476:LEU:HD11	1:E:595:ILE:HD12	1.85	0.58
5:A:1808:CLR:H25	5:A:1808:CLR:C21	2.33	0.58
5:B:1508:CLR:H221	5:B:1508:CLR:C27	2.17	0.58
1:D:833:MET:HB2	1:D:979:ASN:HB2	1.86	0.58
1:E:119:ALA:CB	5:E:1508:CLR:H72	2.30	0.58
1:E:203:CYS:O	2:F:33:ARG:NH2	2.37	0.58
1:D:306:ALA:HA	1:D:311:LYS:HD3	1.86	0.58
5:E:1508:CLR:H221	5:E:1508:CLR:C27	2.17	0.58
1:B:476:LEU:HD11	1:B:595:ILE:HD12	1.85	0.58
1:B:203:CYS:O	2:C:33:ARG:NH2	2.37	0.58
5:D:1808:CLR:H25	5:D:1808:CLR:C21	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:201:CLR:H232	5:C:201:CLR:H161	1.85	0.57
1:E:1049:ASN:HD22	1:E:1105:LEU:HD21	1.69	0.57
1:A:306:ALA:HA	1:A:311:LYS:HD3	1.86	0.57
1:E:855:LEU:HD11	1:E:882:LEU:HD22	1.86	0.57
2:F:158:TYR:HB3	2:F:181:ILE:HD11	1.86	0.57
1:A:833:MET:HB2	1:A:979:ASN:HB2	1.86	0.57
1:E:862:ASP:HB3	1:E:868:ILE:HG12	1.86	0.57
1:A:1107:ALA:HB3	1:A:1114:ARG:HG3	1.87	0.57
1:D:566:PRO:HD2	1:D:1027:TRP:HH2	1.70	0.57
1:B:216:MET:SD	5:C:201:CLR:H42	2.39	0.57
1:A:449:MET:HG2	1:A:508:LEU:HD21	1.86	0.57
1:D:1107:ALA:HB3	1:D:1114:ARG:HG3	1.87	0.57
1:A:205:LYS:HD2	1:A:224:TYR:HD2	1.68	0.57
2:C:158:TYR:HB3	2:C:181:ILE:HD11	1.86	0.57
1:B:326:GLY:O	1:B:336:HIS:NE2	2.37	0.57
1:B:855:LEU:HD11	1:B:882:LEU:HD22	1.86	0.57
1:D:593:PRO:HA	1:D:596:LEU:HG	1.87	0.56
1:A:593:PRO:HA	1:A:596:LEU:HG	1.87	0.56
1:A:806:VAL:HG23	1:A:973:GLN:HB3	1.87	0.56
1:B:98:CYS:SG	1:B:597:SER:OG	2.61	0.56
1:D:449:MET:HG2	1:D:508:LEU:HD21	1.86	0.56
1:B:1049:ASN:HD22	1:B:1105:LEU:HD21	1.69	0.56
1:D:806:VAL:HG23	1:D:973:GLN:HB3	1.87	0.56
1:E:326:GLY:O	1:E:336:HIS:NE2	2.37	0.56
1:B:1051:TRP:HH2	1:B:1178:PHE:HB3	1.71	0.56
1:D:929:ASN:HD21	1:D:950:HIS:H	1.54	0.56
1:A:929:ASN:HD21	1:A:950:HIS:H	1.53	0.56
1:E:205:LYS:HA	1:E:226:CYS:HA	1.88	0.56
1:B:821:ASP:OD2	1:B:1001:TYR:OH	2.24	0.56
1:A:566:PRO:HD2	1:A:1027:TRP:HH2	1.70	0.56
5:B:1508:CLR:H221	5:B:1508:CLR:C26	2.26	0.55
2:C:120:VAL:HG13	2:C:151:SER:HB3	1.88	0.55
1:D:373:TYR:HA	1:D:387:TRP:HE1	1.72	0.55
1:E:1147:PHE:CZ	8:F:205:PLM:CG	2.50	0.55
1:D:294:ARG:NH2	1:D:329:GLY:O	2.40	0.55
1:D:220:ILE:HD12	5:D:1808:CLR:C7	2.37	0.55
1:E:821:ASP:OD2	1:E:1001:TYR:OH	2.24	0.55
2:F:120:VAL:HG13	2:F:151:SER:HB3	1.88	0.55
1:E:216:MET:SD	5:F:201:CLR:H42	2.39	0.55
2:C:62:TYR:CE2	2:C:137:GLU:HG2	2.42	0.55
5:D:1808:CLR:C21	5:D:1808:CLR:C24	2.85	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:425:THR:O	1:E:429:ASP:N	2.38	0.55
1:E:1051:TRP:HH2	1:E:1178:PHE:HB3	1.71	0.55
1:A:294:ARG:NH2	1:A:329:GLY:O	2.40	0.54
1:B:205:LYS:HA	1:B:226:CYS:HA	1.88	0.54
1:B:101:PHE:HA	1:B:104:VAL:HG12	1.89	0.54
1:E:101:PHE:HA	1:E:104:VAL:HG12	1.89	0.54
1:E:529:LYS:NZ	1:E:531:ILE:O	2.41	0.54
1:A:436:ASP:O	1:A:501:GLN:NE2	2.39	0.54
5:A:1808:CLR:C25	5:A:1808:CLR:C21	2.85	0.54
5:E:1508:CLR:C21	5:E:1508:CLR:C24	2.85	0.54
1:A:373:TYR:HA	1:A:387:TRP:HE1	1.72	0.54
5:B:1508:CLR:H273	5:B:1508:CLR:C21	2.37	0.54
2:F:62:TYR:CE2	2:F:137:GLU:HG2	2.42	0.54
5:A:1808:CLR:C21	5:A:1808:CLR:C24	2.85	0.54
1:B:425:THR:O	1:B:429:ASP:N	2.38	0.54
5:E:1508:CLR:H221	5:E:1508:CLR:C26	2.26	0.54
1:D:436:ASP:O	1:D:501:GLN:NE2	2.39	0.54
5:C:201:CLR:C16	5:C:201:CLR:C23	2.85	0.54
1:D:813:PRO:O	1:D:816:GLN:NE2	2.41	0.54
1:A:220:ILE:HD12	5:A:1808:CLR:C7	2.37	0.53
1:B:213:THR:HG22	1:B:216:MET:HB2	1.91	0.53
1:A:84:GLN:HB3	1:A:542:LYS:HD2	1.90	0.53
1:A:868:ILE:HG22	1:A:872:ASN:HB2	1.90	0.53
1:B:195:ARG:O	1:B:381:TYR:OH	2.24	0.53
1:A:813:PRO:O	1:A:816:GLN:NE2	2.42	0.53
1:A:540:CYS:SG	1:A:541:LEU:N	2.82	0.53
2:C:53:GLU:OE2	2:C:54:LYS:NZ	2.32	0.53
1:D:84:GLN:HB3	1:D:542:LYS:HD2	1.90	0.53
1:D:131:GLU:HA	1:D:566:PRO:HB2	1.90	0.53
1:D:868:ILE:HG22	1:D:872:ASN:HB2	1.90	0.53
1:A:131:GLU:HA	1:A:566:PRO:HB2	1.90	0.53
1:B:529:LYS:NZ	1:B:531:ILE:O	2.41	0.53
1:E:195:ARG:O	1:E:381:TYR:OH	2.24	0.53
1:E:807:THR:HG23	1:E:972:ALA:HB3	1.91	0.53
5:F:201:CLR:C16	5:F:201:CLR:C23	2.85	0.53
1:B:807:THR:HG23	1:B:972:ALA:HB3	1.91	0.52
1:E:522:PHE:HD1	1:E:540:CYS:HB2	1.74	0.52
1:A:540:CYS:O	1:A:544:THR:N	2.39	0.52
1:D:945:ARG:NH2	1:D:967:GLU:O	2.43	0.52
5:E:1508:CLR:H273	5:E:1508:CLR:C21	2.37	0.52
1:E:1002:THR:HG22	1:E:1007:SER:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:PHE:HD1	1:B:540:CYS:HB2	1.74	0.52
1:A:156:GLN:HG3	1:A:423:THR:HB	1.92	0.52
2:C:68:ARG:HD2	2:C:130:GLU:OE1	2.09	0.52
5:F:201:CLR:C21	5:F:201:CLR:H183	2.34	0.52
1:A:528:ASN:ND2	1:A:530:ARG:O	2.43	0.52
5:B:1508:CLR:C27	5:B:1508:CLR:C21	2.86	0.52
1:D:335:MET:SD	5:D:1808:CLR:C21	2.98	0.52
1:E:213:THR:HG22	1:E:216:MET:HB2	1.90	0.52
5:E:1508:CLR:C27	5:E:1508:CLR:C21	2.85	0.52
1:A:462:CYS:O	1:A:603:ARG:NH1	2.41	0.52
1:A:1040:PHE:HB2	1:A:1057:VAL:HG21	1.92	0.52
1:D:540:CYS:SG	1:D:541:LEU:N	2.82	0.52
1:E:119:ALA:HB1	5:E:1508:CLR:C7	2.36	0.52
2:F:68:ARG:HD2	2:F:130:GLU:OE1	2.09	0.52
1:B:437:VAL:HG11	5:B:1508:CLR:H212	1.92	0.52
1:B:1002:THR:HG22	1:B:1007:SER:HA	1.91	0.52
5:B:1508:CLR:C21	5:B:1508:CLR:C24	2.85	0.52
1:D:528:ASN:ND2	1:D:530:ARG:O	2.43	0.52
1:B:998:CYS:SG	1:B:1008:SER:OG	2.67	0.51
1:E:449:MET:HE2	1:E:512:VAL:HG11	1.92	0.51
1:A:731:THR:O	1:A:735:PHE:CB	2.59	0.51
1:D:156:GLN:HG3	1:D:423:THR:HB	1.92	0.51
1:D:1040:PHE:HB2	1:D:1057:VAL:HG21	1.92	0.51
1:B:1040:PHE:HB2	1:B:1057:VAL:HG21	1.91	0.51
1:D:245:THR:H	1:D:255:ARG:HG3	1.75	0.51
1:E:1040:PHE:HB2	1:E:1057:VAL:HG21	1.91	0.51
1:A:245:THR:H	1:A:255:ARG:HG3	1.75	0.51
1:B:812:TYR:O	1:B:816:GLN:NE2	2.44	0.51
1:E:437:VAL:HG11	5:E:1508:CLR:H212	1.92	0.51
1:A:335:MET:SD	5:A:1808:CLR:C21	2.98	0.51
1:A:380:GLU:HB3	2:C:43:ALA:HB3	1.93	0.51
1:D:163:LYS:NZ	1:D:415:SER:O	2.41	0.51
1:E:812:TYR:O	1:E:816:GLN:NE2	2.44	0.51
1:D:731:THR:O	1:D:735:PHE:CB	2.59	0.51
1:A:945:ARG:NH2	1:A:967:GLU:O	2.43	0.51
1:A:162:PRO:HB3	1:A:167:ALA:HB3	1.93	0.51
1:A:750:LYS:NZ	1:A:1176:SER:OG	2.44	0.51
1:D:750:LYS:NZ	1:D:1176:SER:OG	2.44	0.51
1:D:811:ASP:H	1:D:815:ILE:HD12	1.76	0.51
1:B:942:ARG:HA	1:B:944:HIS:H	1.76	0.50
1:D:162:PRO:HB3	1:D:167:ALA:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:59:SER:O	2:F:144:ARG:NH2	2.45	0.50
1:E:998:CYS:SG	1:E:1008:SER:OG	2.67	0.50
1:A:225:PRO:O	1:A:242:GLN:NE2	2.34	0.50
1:A:815:ILE:HG23	1:A:818:LEU:HD12	1.94	0.50
1:E:942:ARG:HA	1:E:944:HIS:H	1.76	0.50
1:A:1165:LEU:O	1:A:1169:VAL:HB	2.12	0.50
1:B:119:ALA:HB1	5:B:1508:CLR:C7	2.36	0.50
5:D:1808:CLR:C25	5:D:1808:CLR:C21	2.85	0.50
1:A:921:ILE:HG23	1:A:963:ILE:HG21	1.94	0.50
1:D:921:ILE:HG23	1:D:963:ILE:HG21	1.93	0.50
1:A:499:THR:O	1:A:503:LEU:HB3	2.11	0.50
1:A:811:ASP:H	1:A:815:ILE:HD12	1.76	0.50
1:D:1165:LEU:O	1:D:1169:VAL:HB	2.12	0.50
1:D:462:CYS:O	1:D:603:ARG:NH1	2.41	0.50
1:D:540:CYS:O	1:D:544:THR:N	2.39	0.50
1:D:815:ILE:HG23	1:D:818:LEU:HD12	1.94	0.50
1:E:91:GLY:O	1:E:537:THR:OG1	2.30	0.50
1:E:430:ILE:HG12	1:E:781:VAL:HG12	1.94	0.50
1:A:154:ASN:O	1:A:156:GLN:NE2	2.39	0.50
1:D:207:GLY:O	1:D:224:TYR:OH	2.26	0.50
1:D:280:GLU:HG3	1:D:284:LYS:HE3	1.93	0.50
1:D:380:GLU:HB3	2:F:43:ALA:HB3	1.92	0.50
1:B:126:GLU:OE1	2:C:28:ARG:NH2	2.45	0.50
1:B:449:MET:HE2	1:B:512:VAL:HG11	1.93	0.50
1:D:95:GLN:NE2	1:D:537:THR:OG1	2.45	0.50
1:D:154:ASN:O	1:D:156:GLN:NE2	2.39	0.50
1:D:499:THR:O	1:D:503:LEU:HB3	2.11	0.49
5:D:1808:CLR:C18	5:D:1808:CLR:C22	2.87	0.49
1:D:245:THR:HG22	1:D:255:ARG:HD2	1.94	0.49
1:E:126:GLU:OE1	2:F:28:ARG:NH2	2.45	0.49
1:B:1147:PHE:CZ	8:C:205:PLM:CG	2.50	0.49
1:A:1059:VAL:HG21	1:A:1171:LEU:HD21	1.94	0.49
2:F:54:LYS:O	2:F:61:ARG:NH1	2.45	0.49
1:A:95:GLN:NE2	1:A:537:THR:OG1	2.45	0.49
1:A:245:THR:HG22	1:A:255:ARG:HD2	1.94	0.49
2:C:54:LYS:O	2:C:61:ARG:NH1	2.46	0.49
2:C:59:SER:O	2:C:144:ARG:NH2	2.45	0.49
2:C:77:THR:HG22	2:C:98:MET:O	2.12	0.49
5:E:1508:CLR:H121	5:E:1508:CLR:H212	1.95	0.49
1:B:984:THR:HA	1:B:987:PHE:HD2	1.78	0.49
1:D:1059:VAL:HG21	1:D:1171:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:GLU:HG3	2:F:34:ARG:HG2	1.94	0.49
1:E:984:THR:HA	1:E:987:PHE:HD2	1.78	0.49
1:B:91:GLY:O	1:B:537:THR:OG1	2.30	0.49
2:F:77:THR:HG22	2:F:98:MET:O	2.12	0.49
1:A:280:GLU:HG3	1:A:284:LYS:HE3	1.93	0.49
1:A:941:ILE:HG23	1:A:969:ILE:HG23	1.95	0.49
5:B:1508:CLR:H121	5:B:1508:CLR:H212	1.95	0.49
1:E:216:MET:HA	1:E:216:MET:CE	2.40	0.49
1:D:1044:ALA:O	1:D:1048:LEU:N	2.46	0.49
1:B:430:ILE:HG12	1:B:781:VAL:HG12	1.94	0.49
1:A:1035:VAL:HG21	1:A:1087:ILE:HG23	1.95	0.48
1:B:208:GLU:HG3	2:C:34:ARG:HG2	1.94	0.48
1:D:1035:VAL:HG21	1:D:1087:ILE:HG23	1.95	0.48
1:B:815:ILE:HG23	1:B:818:LEU:HD23	1.94	0.48
5:F:201:CLR:C27	5:F:201:CLR:H222	2.42	0.48
1:E:294:ARG:NH2	1:E:329:GLY:O	2.32	0.48
1:E:437:VAL:HG21	5:E:1508:CLR:C12	2.43	0.48
1:A:1146:ASP:O	1:A:1150:ARG:HB2	2.14	0.48
1:B:437:VAL:HG21	5:B:1508:CLR:C12	2.43	0.48
2:C:111:ILE:O	2:C:115:ASN:ND2	2.47	0.48
1:E:480:SER:HB3	1:E:587:MET:HG3	1.95	0.48
1:E:815:ILE:HG23	1:E:818:LEU:HD23	1.94	0.48
1:B:216:MET:HA	1:B:216:MET:CE	2.40	0.48
1:E:568:PRO:HA	1:E:571:ARG:HB3	1.95	0.48
1:A:1044:ALA:O	1:A:1048:LEU:N	2.46	0.48
1:B:480:SER:HB3	1:B:587:MET:HG3	1.95	0.48
1:E:1104:PHE:CG	1:E:1175:LEU:HD21	2.48	0.48
1:D:889:GLN:NE2	1:D:896:PRO:O	2.47	0.48
1:D:1146:ASP:O	1:D:1150:ARG:HB2	2.14	0.48
1:A:889:GLN:NE2	1:A:896:PRO:O	2.47	0.48
1:B:260:ASP:HB3	1:B:292:MET:HG3	1.96	0.48
1:B:1104:PHE:CG	1:B:1175:LEU:HD21	2.48	0.48
5:B:1508:CLR:C27	5:B:1508:CLR:C22	2.88	0.48
1:B:823:HIS:CE1	1:B:840:LEU:HB2	2.49	0.48
1:B:1171:LEU:O	1:B:1175:LEU:HB3	2.14	0.48
5:D:1810:CLR:H162	5:D:1810:CLR:H221	1.59	0.48
1:E:216:MET:HE2	1:E:216:MET:CA	2.44	0.48
2:F:53:GLU:HB3	2:F:172:TRP:CD2	2.49	0.48
2:F:111:ILE:O	2:F:115:ASN:ND2	2.47	0.47
1:E:1171:LEU:O	1:E:1175:LEU:HB3	2.14	0.47
2:F:87:LYS:HE2	2:F:89:GLU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ALA:HA	1:A:323:LEU:HG	1.96	0.47
1:D:193:TYR:H	1:D:197:TRP:HZ3	1.63	0.47
1:A:496:ASN:HD21	1:A:572:ALA:HB3	1.79	0.47
5:A:1808:CLR:C18	5:A:1808:CLR:C22	2.87	0.47
1:E:128:LEU:CD1	8:F:205:PLM:HB2	2.45	0.47
1:E:531:ILE:HG21	1:E:539:GLU:HG3	1.97	0.47
1:B:128:LEU:CD1	8:C:205:PLM:HB2	2.45	0.47
1:B:452:TYR:O	1:B:456:THR:OG1	2.29	0.47
1:D:941:ILE:HG23	1:D:969:ILE:HG23	1.95	0.47
1:B:1079:SER:OG	1:B:1080:ALA:N	2.48	0.47
1:D:320:ALA:HA	1:D:323:LEU:HG	1.96	0.47
1:D:505:PHE:HD2	1:D:1140:LEU:HD23	1.79	0.47
1:E:1166:ASN:HA	1:E:1170:LEU:HB3	1.97	0.47
1:A:889:GLN:HE22	1:A:896:PRO:HB2	1.79	0.47
1:B:497:ALA:O	1:B:501:GLN:NE2	2.48	0.47
1:B:568:PRO:HA	1:B:571:ARG:HB3	1.95	0.47
1:B:1166:ASN:HA	1:B:1170:LEU:HB3	1.97	0.47
1:D:347:VAL:HG13	1:D:355:VAL:HB	1.96	0.47
1:A:505:PHE:HD2	1:A:1140:LEU:HD23	1.79	0.47
1:B:170:LEU:HD23	1:B:357:ALA:HB2	1.97	0.47
1:B:853:GLN:HE21	1:B:908:VAL:HG11	1.80	0.47
2:C:87:LYS:HE2	2:C:89:GLU:HB3	1.96	0.47
1:D:889:GLN:HE22	1:D:896:PRO:HB2	1.79	0.47
1:E:823:HIS:CE1	1:E:840:LEU:HB2	2.49	0.47
1:E:1079:SER:OG	1:E:1080:ALA:N	2.48	0.47
5:E:1508:CLR:C27	5:E:1508:CLR:C22	2.88	0.47
1:A:207:GLY:O	1:A:224:TYR:OH	2.26	0.47
2:C:174:TYR:HB3	2:C:182:HIS:HB3	1.97	0.47
1:D:496:ASN:HD21	1:D:572:ALA:HB3	1.79	0.47
1:E:98:CYS:SG	1:E:597:SER:OG	2.61	0.47
1:A:297:LEU:H	1:A:310:ASN:HD22	1.63	0.46
1:D:1064:THR:HG21	1:D:1090:VAL:HG22	1.97	0.46
1:B:531:ILE:HG21	1:B:539:GLU:HG3	1.97	0.46
1:A:384:HIS:CD2	1:A:385:ILE:HG23	2.51	0.46
2:C:53:GLU:HB3	2:C:172:TRP:CD2	2.49	0.46
1:E:260:ASP:HB3	1:E:292:MET:HG3	1.96	0.46
1:A:163:LYS:NZ	1:A:415:SER:O	2.40	0.46
1:A:193:TYR:H	1:A:197:TRP:HZ3	1.63	0.46
1:A:1064:THR:HG21	1:A:1090:VAL:HG22	1.97	0.46
5:C:201:CLR:C27	5:C:201:CLR:H222	2.42	0.46
1:E:170:LEU:HD23	1:E:357:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:MET:HB3	1:D:216:MET:HE2	1.77	0.46
2:F:174:TYR:HB3	2:F:182:HIS:HB3	1.97	0.46
1:E:282:LEU:CD2	5:F:201:CLR:C21	2.89	0.46
1:D:297:LEU:H	1:D:310:ASN:HD22	1.63	0.46
1:E:244:GLY:HA3	1:E:255:ARG:HA	1.98	0.46
1:A:256:TRP:HH2	5:A:1808:CLR:H112	1.80	0.46
1:D:344:GLY:N	1:D:359:ALA:O	2.48	0.46
1:B:1137:VAL:HG12	1:B:1153:PHE:HD1	1.81	0.46
2:C:47:PHE:HB3	2:C:174:TYR:HD1	1.81	0.46
1:E:1137:VAL:HG12	1:E:1153:PHE:HD1	1.81	0.46
2:F:47:PHE:HB3	2:F:174:TYR:HD1	1.81	0.46
1:A:347:VAL:HG13	1:A:355:VAL:HB	1.96	0.45
5:C:201:CLR:H8	5:C:201:CLR:H182	1.62	0.45
1:E:1056:ILE:HD13	1:E:1056:ILE:HA	1.84	0.45
1:D:225:PRO:O	1:D:242:GLN:NE2	2.34	0.45
2:F:48:ILE:HG13	2:F:49:PRO:HD3	1.98	0.45
1:B:244:GLY:HA3	1:B:255:ARG:HA	1.98	0.45
1:D:256:TRP:HH2	5:D:1808:CLR:H112	1.80	0.45
1:E:497:ALA:O	1:E:501:GLN:NE2	2.48	0.45
1:A:493:ILE:HG22	1:A:576:GLN:HE21	1.81	0.45
1:E:452:TYR:O	1:E:456:THR:OG1	2.29	0.45
1:A:1110:ASP:N	1:A:1110:ASP:OD1	2.49	0.45
2:C:48:ILE:HG13	2:C:49:PRO:HD3	1.98	0.45
5:C:201:CLR:C21	5:C:201:CLR:H183	2.34	0.45
1:D:493:ILE:HG22	1:D:576:GLN:HE21	1.81	0.45
1:B:216:MET:HE2	1:B:216:MET:CA	2.46	0.45
1:D:384:HIS:CD2	1:D:385:ILE:HG23	2.51	0.45
5:D:1809:CLR:H193	5:D:1809:CLR:H111	1.84	0.45
5:D:1810:CLR:H183	5:D:1810:CLR:H20	1.83	0.45
1:B:768:THR:HG22	1:B:1068:PHE:HD2	1.83	0.45
1:D:909:ASP:OD1	1:D:909:ASP:N	2.50	0.45
1:E:216:MET:CE	1:E:216:MET:CA	2.95	0.45
1:D:1110:ASP:OD1	1:D:1110:ASP:N	2.49	0.44
1:A:259:PHE:CE2	5:A:1808:CLR:H21	2.53	0.44
1:A:437:VAL:HG11	5:A:1810:CLR:H151	1.99	0.44
1:D:196:GLN:OE1	1:D:198:LYS:NZ	2.50	0.44
1:D:437:VAL:HG11	5:D:1810:CLR:H151	1.99	0.44
1:A:1031:PHE:HA	1:A:1034:VAL:HG12	1.99	0.44
1:B:216:MET:CE	1:B:216:MET:CA	2.95	0.44
1:B:282:LEU:CD2	5:C:201:CLR:C21	2.89	0.44
1:D:259:PHE:CE2	5:D:1808:CLR:H21	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:853:GLN:HE21	1:E:908:VAL:HG11	1.80	0.44
1:A:344:GLY:N	1:A:359:ALA:O	2.48	0.44
1:A:909:ASP:N	1:A:909:ASP:OD1	2.50	0.44
1:D:938:GLN:O	1:D:973:GLN:NE2	2.51	0.44
1:E:768:THR:HG22	1:E:1068:PHE:HD2	1.83	0.44
2:F:106:LEU:HD21	2:F:124:VAL:HG21	1.99	0.44
1:A:196:GLN:OE1	1:A:198:LYS:NZ	2.50	0.44
1:A:938:GLN:O	1:A:973:GLN:NE2	2.51	0.44
1:B:427:LEU:HD22	2:C:24:CYS:SG	2.58	0.44
5:D:1808:CLR:H193	5:D:1808:CLR:H111	1.79	0.44
1:A:496:ASN:ND2	1:A:569:ALA:O	2.51	0.44
1:D:1031:PHE:HA	1:D:1034:VAL:HG12	2.00	0.44
1:B:437:VAL:CG1	5:B:1508:CLR:H212	2.48	0.44
5:A:1808:CLR:H8	5:A:1808:CLR:H182	1.68	0.43
1:D:1162:LEU:HD13	1:D:1165:LEU:HD21	2.00	0.43
5:B:1508:CLR:H273	5:B:1508:CLR:C20	2.48	0.43
1:D:441:ARG:NH2	1:D:1141:ALA:O	2.51	0.43
1:D:496:ASN:ND2	1:D:569:ALA:O	2.51	0.43
5:E:1508:CLR:H273	5:E:1508:CLR:C20	2.48	0.43
1:A:441:ARG:NH2	1:A:1141:ALA:O	2.51	0.43
1:A:900:SER:O	1:A:904:LYS:NZ	2.52	0.43
1:A:1162:LEU:HD13	1:A:1165:LEU:HD21	2.00	0.43
5:A:1808:CLR:C16	5:A:1808:CLR:H272	2.48	0.43
2:C:106:LEU:HD21	2:C:124:VAL:HG21	1.99	0.43
1:E:427:LEU:HD22	2:F:24:CYS:SG	2.58	0.43
1:E:230:THR:OG1	1:E:233:ASP:N	2.52	0.43
5:F:201:CLR:H182	5:F:201:CLR:H8	1.62	0.43
1:A:216:MET:HB3	1:A:216:MET:HE2	1.77	0.43
1:D:178:HIS:NE2	1:D:362:THR:OG1	2.48	0.43
1:D:872:ASN:ND2	4:D:1804:NAG:O7	2.51	0.43
5:D:1808:CLR:C16	5:D:1808:CLR:H272	2.48	0.43
1:A:981:LEU:HB3	1:A:987:PHE:CE1	2.54	0.43
1:D:319:MET:HB3	1:D:321:LEU:HG	2.00	0.43
1:D:900:SER:O	1:D:904:LYS:NZ	2.52	0.43
1:E:437:VAL:CG1	5:E:1508:CLR:H212	2.48	0.43
1:D:1156:LEU:HD13	1:D:1159:LEU:HD13	2.01	0.43
1:E:1130:ALA:O	1:E:1133:THR:OG1	2.31	0.43
5:F:201:CLR:H111	5:F:201:CLR:H193	1.72	0.43
5:A:1810:CLR:H221	5:A:1810:CLR:H162	1.58	0.43
1:B:294:ARG:NH2	1:B:329:GLY:O	2.32	0.43
1:D:981:LEU:HB3	1:D:987:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1179:GLY:HA2	1:D:1180:PRO:HD3	1.88	0.43
1:E:361:GLN:HB2	1:E:798:PHE:CE2	2.54	0.43
1:E:945:ARG:HA	1:E:945:ARG:HD3	1.85	0.43
1:E:1047:LEU:HD23	1:E:1105:LEU:HD22	2.00	0.43
1:A:1156:LEU:HD13	1:A:1159:LEU:HD13	2.01	0.43
5:A:1810:CLR:H183	5:A:1810:CLR:H20	1.83	0.43
1:B:848:PHE:HE1	1:B:923:LEU:HA	1.84	0.43
4:B:1501:NAG:N2	4:B:1501:NAG:O4	2.52	0.43
1:E:998:CYS:HG	1:E:1008:SER:HG	1.57	0.43
1:A:397:GLU:OE2	1:A:401:ARG:NH2	2.39	0.42
1:B:361:GLN:HB2	1:B:798:PHE:CE2	2.54	0.42
8:C:205:PLM:H91	8:C:205:PLM:H62	1.57	0.42
1:A:859:PHE:HZ	1:A:902:LEU:HD11	1.84	0.42
1:D:376:PHE:HB3	1:D:382:VAL:HG21	2.01	0.42
2:F:125:THR:CG2	2:F:149:THR:HG23	2.49	0.42
2:F:177:SER:OG	2:F:178:LYS:N	2.52	0.42
2:C:125:THR:CG2	2:C:149:THR:HG23	2.50	0.42
5:F:201:CLR:H222	5:F:201:CLR:H25	1.57	0.42
5:A:1808:CLR:H213	5:A:1808:CLR:C24	2.49	0.42
1:B:230:THR:OG1	1:B:233:ASP:N	2.52	0.42
1:A:376:PHE:HB3	1:A:382:VAL:HG21	2.01	0.42
5:A:1808:CLR:H231	5:A:1808:CLR:H272	1.59	0.42
1:B:771:VAL:O	1:B:772:ARG:NE	2.52	0.42
1:E:771:VAL:O	1:E:772:ARG:NE	2.52	0.42
1:B:945:ARG:HA	1:B:945:ARG:HD3	1.85	0.42
1:B:593:PRO:HA	1:B:596:LEU:HB2	2.02	0.42
1:B:945:ARG:HH11	1:B:966:ALA:HB1	1.85	0.42
1:D:554:SER:HB2	1:D:1094:VAL:HG21	2.02	0.42
2:F:68:ARG:CG	2:F:130:GLU:OE1	2.68	0.42
2:F:150:THR:HG1	2:F:158:TYR:HE1	1.64	0.42
1:A:319:MET:HB3	1:A:321:LEU:HG	2.01	0.42
1:A:1000:ASN:O	1:A:1003:SER:OG	2.28	0.42
1:B:206:SER:HB3	1:B:227:LEU:HD12	2.02	0.42
1:D:157:LEU:H	1:D:157:LEU:HG	1.67	0.42
1:E:473:GLY:HA2	1:E:476:LEU:HD12	2.01	0.42
4:E:1501:NAG:O4	4:E:1501:NAG:N2	2.52	0.42
1:A:554:SER:HB2	1:A:1094:VAL:HG21	2.02	0.42
2:C:68:ARG:CG	2:C:130:GLU:OE1	2.68	0.42
1:D:518:LEU:HA	1:D:544:THR:HG21	2.02	0.42
1:E:231:PRO:HG3	1:E:342:ILE:HD13	2.01	0.42
1:B:210:ILE:H	1:B:210:ILE:HG13	1.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:843:MET:H	1:B:843:MET:HG2	1.72	0.42
1:D:1146:ASP:O	1:D:1150:ARG:CB	2.68	0.42
1:E:437:VAL:HG11	5:E:1508:CLR:C11	2.50	0.42
2:F:76:LEU:HD23	2:F:97:LEU:CB	2.37	0.42
2:C:177:SER:OG	2:C:178:LYS:N	2.52	0.41
1:E:304:CYS:HB2	1:E:311:LYS:HD3	2.02	0.41
1:E:593:PRO:HA	1:E:596:LEU:HB2	2.01	0.41
1:E:1134:LEU:O	1:E:1138:LEU:HB2	2.20	0.41
1:A:1179:GLY:HA2	1:A:1180:PRO:HD3	1.89	0.41
1:B:1056:ILE:HD13	1:B:1056:ILE:HA	1.84	0.41
5:C:201:CLR:H222	5:C:201:CLR:H25	1.57	0.41
5:C:201:CLR:H222	5:C:201:CLR:H272	2.02	0.41
5:D:1809:CLR:H191	5:D:1809:CLR:H8	1.85	0.41
1:B:231:PRO:HG3	1:B:342:ILE:HD13	2.01	0.41
1:B:473:GLY:HA2	1:B:476:LEU:HD12	2.01	0.41
1:B:1134:LEU:O	1:B:1138:LEU:HB2	2.20	0.41
1:E:945:ARG:HH11	1:E:966:ALA:HB1	1.85	0.41
5:D:1808:CLR:H231	5:D:1808:CLR:H272	1.59	0.41
1:B:863:TRP:HA	1:B:868:ILE:HD11	2.03	0.41
1:B:1047:LEU:HD23	1:B:1105:LEU:HD22	2.00	0.41
1:A:1146:ASP:O	1:A:1150:ARG:CB	2.68	0.41
2:C:156:SER:O	2:C:156:SER:OG	2.37	0.41
5:E:1508:CLR:H211	5:E:1508:CLR:C24	2.29	0.41
2:F:56:LEU:HD13	2:F:56:LEU:HA	1.88	0.41
1:A:231:PRO:HG2	1:A:360:LEU:HD13	2.03	0.41
1:A:423:THR:O	1:A:425:THR:N	2.54	0.41
1:A:927:VAL:HG11	1:A:945:ARG:HB2	2.03	0.41
8:F:205:PLM:H91	8:F:205:PLM:H62	1.57	0.41
1:A:940:ASN:HD22	1:A:942:ARG:HH12	1.69	0.41
5:A:1809:CLR:H8	5:A:1809:CLR:H191	1.85	0.41
2:C:124:VAL:HG22	2:C:148:ILE:HG22	2.03	0.41
1:E:224:TYR:HA	1:E:225:PRO:HD3	1.89	0.41
1:E:848:PHE:HE1	1:E:923:LEU:HA	1.84	0.41
1:A:978:LEU:HD23	1:A:978:LEU:HA	1.86	0.41
1:B:124:ASN:HB3	1:B:127:GLU:OE1	2.22	0.41
1:D:807:THR:OG1	1:D:808:GLN:N	2.55	0.41
1:D:843:MET:HG2	1:D:845:LEU:H	1.85	0.41
1:E:206:SER:HB3	1:E:227:LEU:HD12	2.02	0.41
1:E:486:GLY:O	1:E:489:SER:OG	2.39	0.41
1:A:178:HIS:NE2	1:A:362:THR:OG1	2.48	0.40
1:A:807:THR:OG1	1:A:808:GLN:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:843:MET:HG2	1:A:845:LEU:H	1.85	0.40
1:D:859:PHE:HZ	1:D:902:LEU:HD11	1.84	0.40
1:B:149:GLU:CD	2:C:28:ARG:HH12	2.25	0.40
1:E:863:TRP:HA	1:E:868:ILE:HD11	2.03	0.40
1:A:289:HIS:CD2	1:A:292:MET:HB2	2.57	0.40
1:D:869:MET:SD	1:D:902:LEU:HG	2.62	0.40
1:A:888:VAL:HG13	1:A:899:ILE:HA	2.02	0.40
1:B:304:CYS:HB2	1:B:311:LYS:HD3	2.02	0.40
2:C:76:LEU:HD23	2:C:97:LEU:CB	2.37	0.40
1:D:147:ILE:HD11	1:D:971:TYR:CZ	2.56	0.40
1:D:570:LEU:HD23	1:D:570:LEU:HA	1.94	0.40
1:D:888:VAL:HG13	1:D:899:ILE:HA	2.02	0.40
1:E:231:PRO:HG2	1:E:360:LEU:HD23	2.03	0.40
1:B:371:GLN:NE2	2:C:33:ARG:H	2.19	0.40
1:B:1035:VAL:HG21	1:B:1087:ILE:HG23	2.04	0.40
1:D:827:SER:HB3	1:D:840:LEU:HD11	2.04	0.40
1:E:158:MET:HB3	1:E:362:THR:HG23	2.03	0.40
1:E:371:GLN:NE2	2:F:33:ARG:H	2.19	0.40
1:E:957:PRO:HA	1:E:960:ARG:HB3	2.03	0.40
5:E:1508:CLR:H8	5:E:1508:CLR:H182	1.79	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	987/1349 (73%)	857 (87%)	123 (12%)	7 (1%)	22	63
1	B	984/1349 (73%)	856 (87%)	125 (13%)	3 (0%)	41	76
1	D	987/1349 (73%)	858 (87%)	122 (12%)	7 (1%)	22	63
1	E	984/1349 (73%)	856 (87%)	125 (13%)	3 (0%)	41	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	172/174 (99%)	153 (89%)	17 (10%)	2 (1%)	13	50
2	F	172/174 (99%)	153 (89%)	17 (10%)	2 (1%)	13	50
All	All	4286/5744 (75%)	3733 (87%)	529 (12%)	24 (1%)	29	66

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	939	ALA
2	C	188	GLU
1	E	939	ALA
2	F	188	GLU
1	A	424	THR
1	B	389	GLU
1	D	424	THR
1	E	389	GLU
1	A	834	LEU
1	A	835	GLU
1	A	917	SER
1	D	834	LEU
1	D	835	GLU
1	D	917	SER
1	A	325	GLY
1	B	1181	TYR
1	D	325	GLY
1	E	1181	TYR
1	A	253	PRO
1	D	253	PRO
1	A	566	PRO
2	C	36	PRO
1	D	566	PRO
2	F	36	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	832/1147 (72%)	820 (99%)	12 (1%)	67	80
1	B	808/1147 (70%)	795 (98%)	13 (2%)	62	79
1	D	832/1147 (72%)	820 (99%)	12 (1%)	67	80
1	E	808/1147 (70%)	795 (98%)	13 (2%)	62	79
2	C	142/144 (99%)	138 (97%)	4 (3%)	43	65
2	F	142/144 (99%)	138 (97%)	4 (3%)	43	65
All	All	3564/4876 (73%)	3506 (98%)	58 (2%)	64	79

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	ARG
1	A	87	LEU
1	A	157	LEU
1	A	254	LEU
1	A	315	LYS
1	A	324	ASN
1	A	550	LEU
1	A	802	ASN
1	A	871	ASN
1	A	872	ASN
1	A	904	LYS
1	A	1048	LEU
1	B	124	ASN
1	B	177	GLN
1	B	220	ILE
1	B	287	VAL
1	B	310	ASN
1	B	349	ASN
1	B	362	THR
1	B	431	LEU
1	B	584	ASN
1	B	607	ARG
1	B	806	VAL
1	B	807	THR
1	B	845	LEU
2	C	34	ARG
2	C	50	ASN
2	C	129	ASP
2	C	188	GLU
1	D	85	ARG

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Mol	Chain	Res	Type
1	D	87	LEU
1	D	157	LEU
1	D	254	LEU
1	D	315	LYS
1	D	324	ASN
1	D	550	LEU
1	D	802	ASN
1	D	871	ASN
1	D	872	ASN
1	D	904	LYS
1	D	1048	LEU
1	E	124	ASN
1	E	177	GLN
1	E	220	ILE
1	E	287	VAL
1	E	310	ASN
1	E	349	ASN
1	E	362	THR
1	E	431	LEU
1	E	584	ASN
1	E	607	ARG
1	E	806	VAL
1	E	807	THR
1	E	845	LEU
2	F	34	ARG
2	F	50	ASN
2	F	129	ASP
2	F	188	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	310	ASN
1	A	324	ASN
1	A	496	ASN
1	A	576	GLN
1	A	871	ASN
1	A	889	GLN
1	A	929	ASN
1	B	124	ASN
1	B	154	ASN

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Mol	Chain	Res	Type
1	B	156	GLN
1	B	218	GLN
1	B	371	GLN
1	B	408	HIS
1	B	409	GLN
1	B	496	ASN
1	B	846	HIS
1	B	853	GLN
1	B	929	ASN
1	B	938	GLN
1	B	1049	ASN
1	B	1121	HIS
2	C	35	HIS
2	C	50	ASN
2	C	107	ASN
1	D	95	GLN
1	D	310	ASN
1	D	324	ASN
1	D	496	ASN
1	D	576	GLN
1	D	871	ASN
1	D	889	GLN
1	D	929	ASN
1	E	124	ASN
1	E	154	ASN
1	E	156	GLN
1	E	218	GLN
1	E	371	GLN
1	E	408	HIS
1	E	409	GLN
1	E	496	ASN
1	E	846	HIS
1	E	853	GLN
1	E	929	ASN
1	E	938	GLN
1	E	1049	ASN
1	E	1121	HIS
2	F	35	HIS
2	F	50	ASN
2	F	107	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

8 monosaccharides 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	$\#\|Z\| > 2$
3	NAG	G	1	3,1	14,14,15	0.24	0	17,19,21	0.57	0
3	NAG	G	2	3	14,14,15	0.26	0	17,19,21	0.53	0
3	NAG	H	1	3,1	14,14,15	0.43	0	17,19,21	0.66	0
3	NAG	H	2	3	14,14,15	0.27	0	17,19,21	0.69	1 (5%)
3	NAG	I	1	3,1	14,14,15	0.25	0	17,19,21	0.57	0
3	NAG	I	2	3	14,14,15	0.26	0	17,19,21	0.52	0
3	NAG	J	1	3,1	14,14,15	0.43	0	17,19,21	0.65	0
3	NAG	J	2	3	14,14,15	0.25	0	17,19,21	0.69	1 (5%)

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
3	NAG	G	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	2	NAG	C1-O5-C5	2.53	115.62	112.19
3	J	2	NAG	C1-O5-C5	2.52	115.60	112.19

There are no chirality outliers.

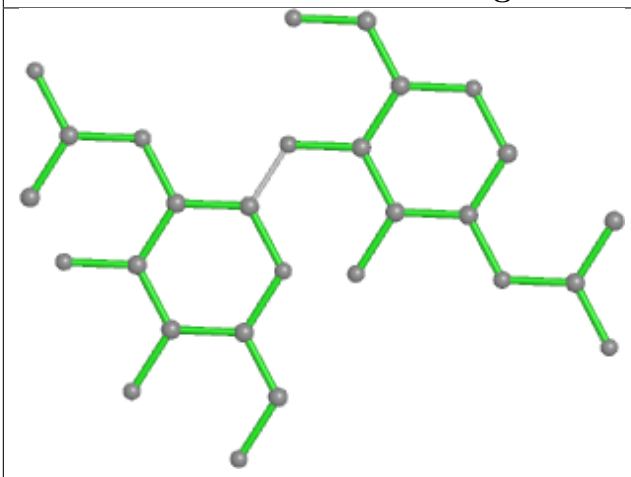
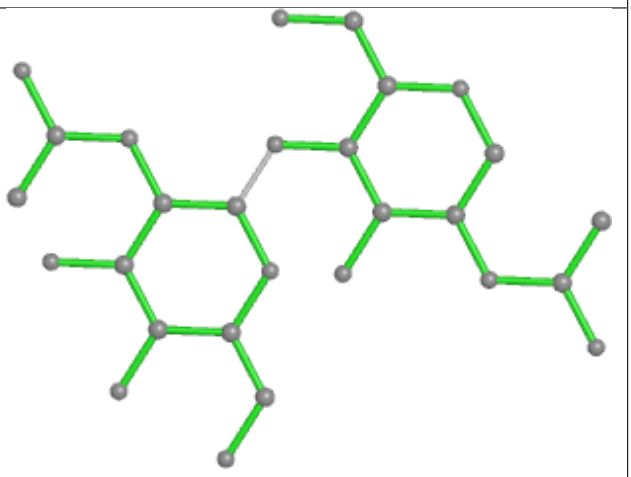
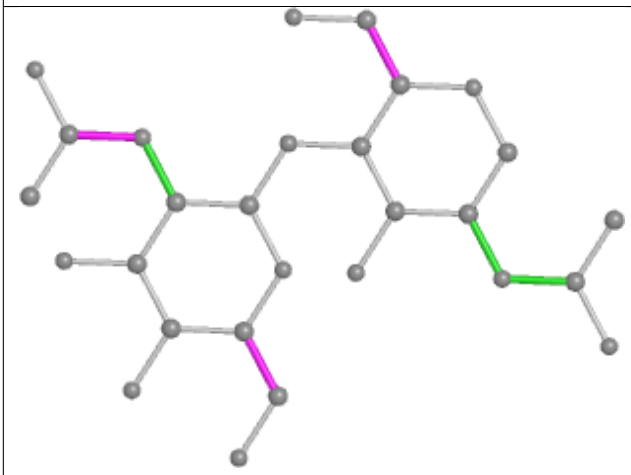
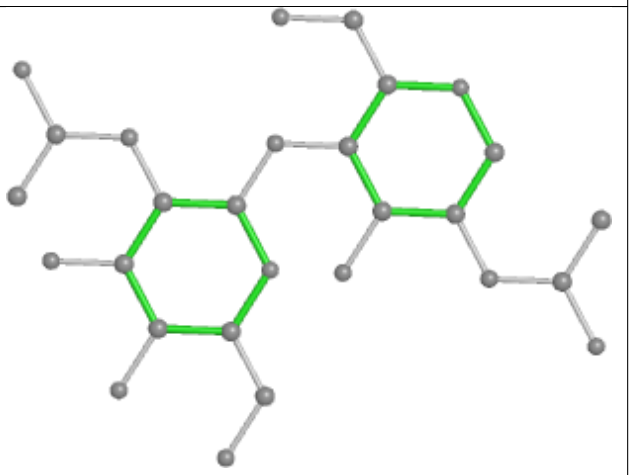
All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6

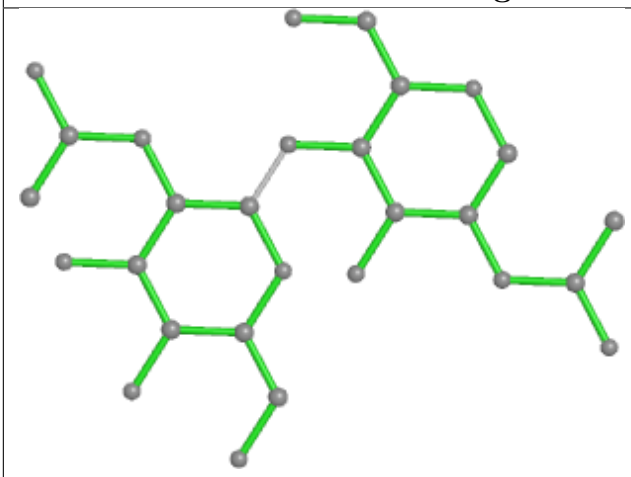
There are no ring outliers.

No monomer is involved in short contacts.

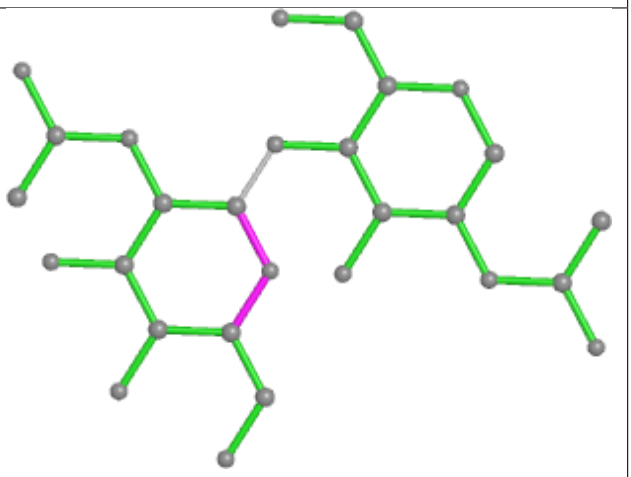
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain G	
 Bond lengths	 Bond angles
 Torsions	 Rings

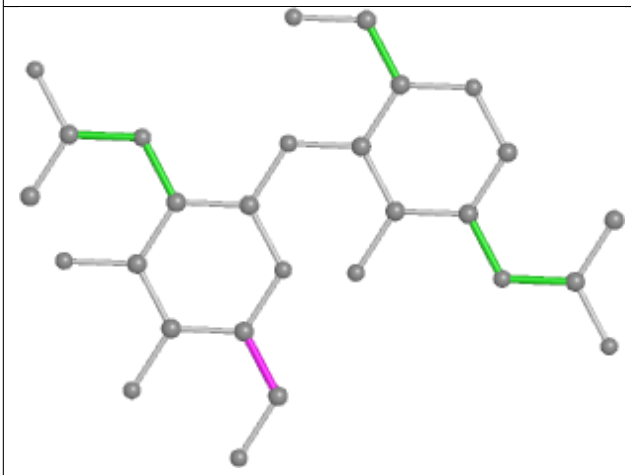
Oligosaccharide Chain H



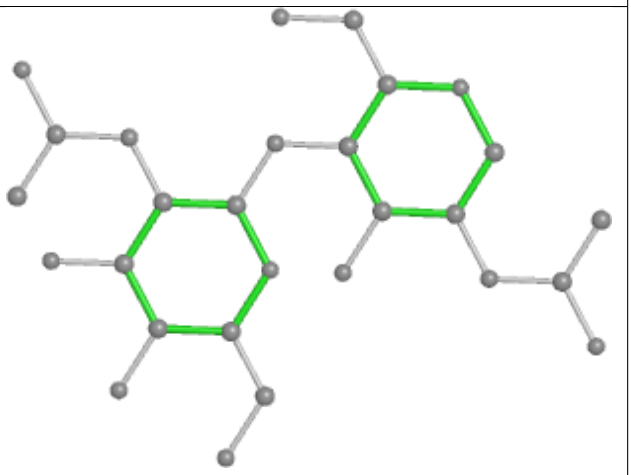
Bond lengths



Bond angles

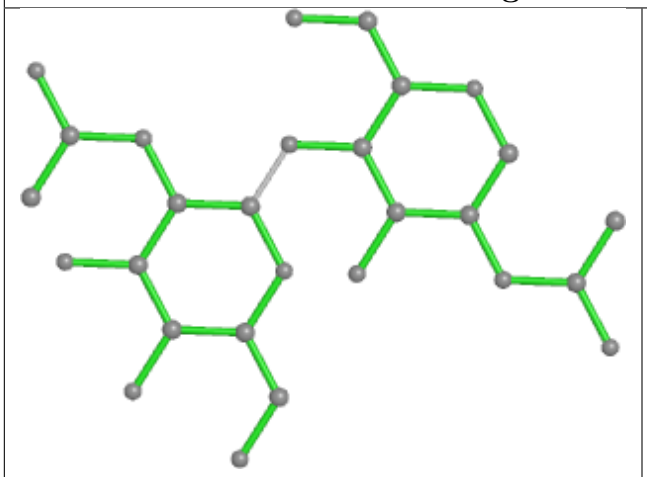


Torsions

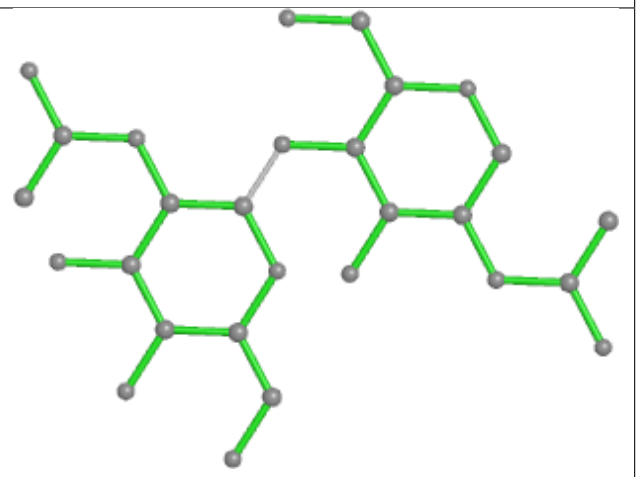


Rings

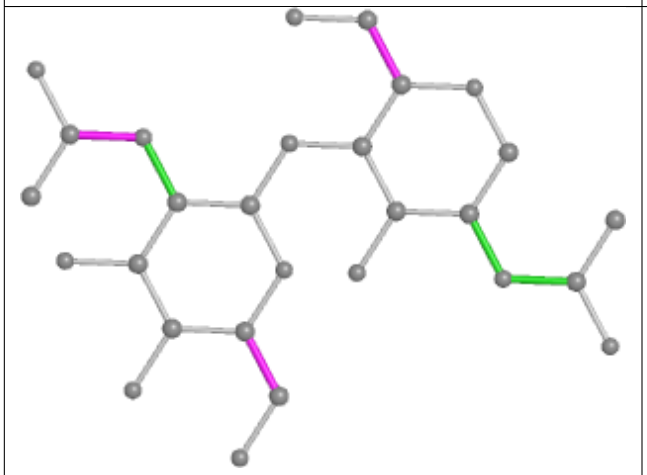
Oligosaccharide Chain I



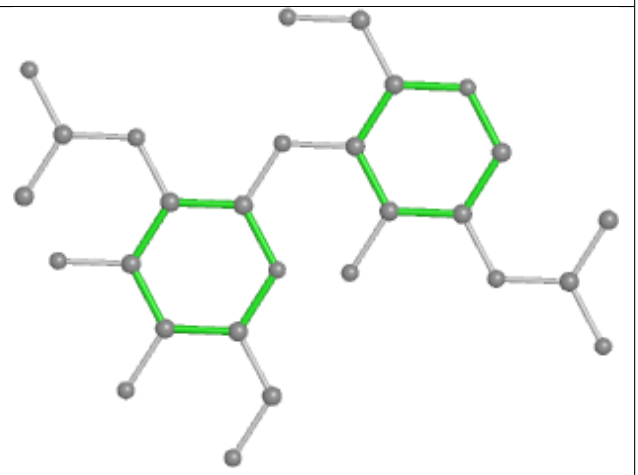
Bond lengths



Bond angles

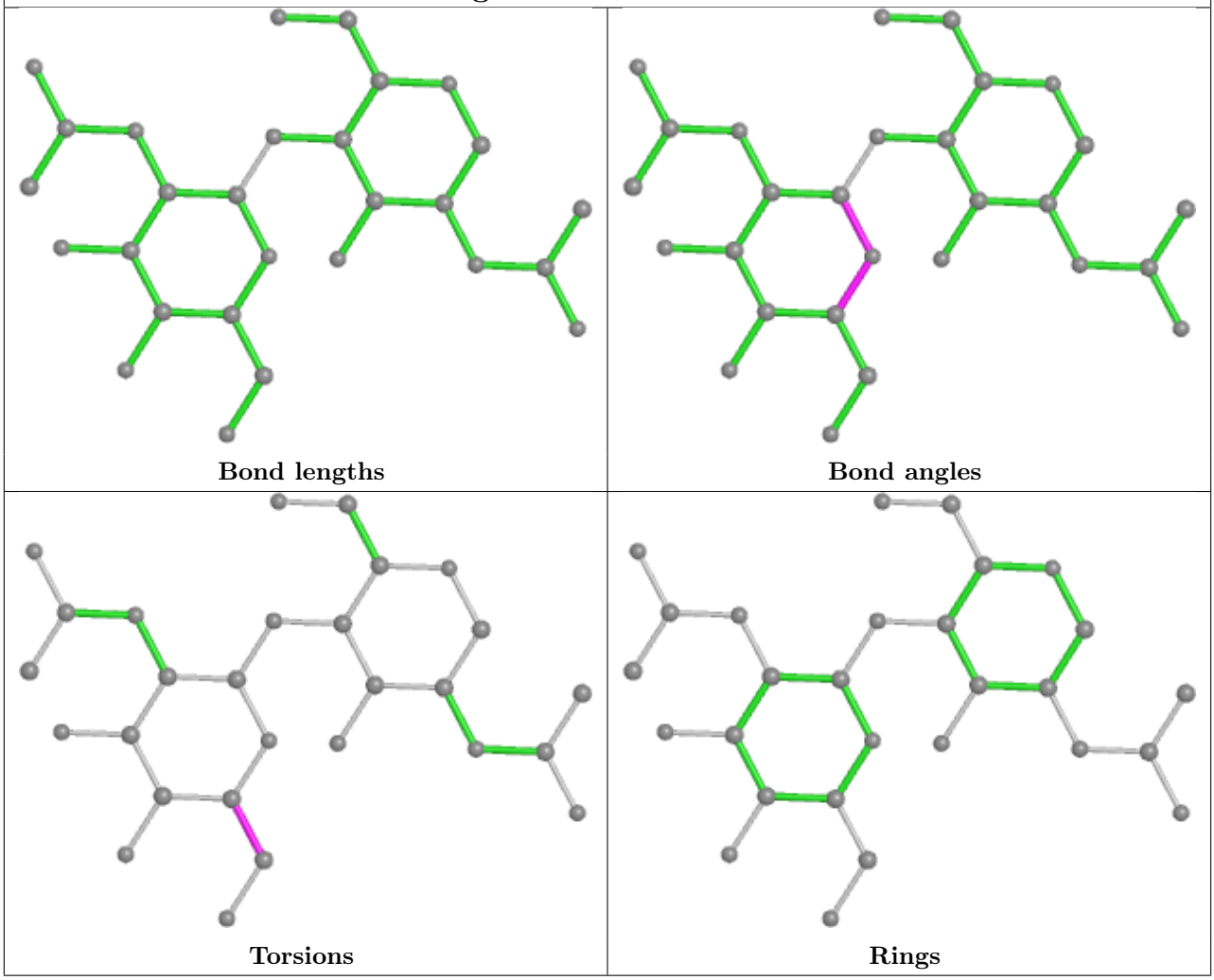


Torsions



Rings

Oligosaccharide Chain J



5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 6 are monoatomic - leaving 32 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	$\#\|Z\| > 2$
4	NAG	A	1807	1	14,14,15	0.39	0	17,19,21	0.39	0
4	NAG	A	1801	1	14,14,15	0.82	1 (7%)	17,19,21	2.25	3 (17%)
4	NAG	B	1501	1	14,14,15	0.70	1 (7%)	17,19,21	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	E	1505	1	14,14,15	0.25	0	17,19,21	0.47	0
4	NAG	D	1807	1	14,14,15	0.39	0	17,19,21	0.39	0
4	NAG	E	1501	1	14,14,15	0.70	1 (7%)	17,19,21	0.68	0
4	NAG	B	1504	1	14,14,15	0.74	1 (7%)	17,19,21	0.75	1 (5%)
4	NAG	A	1804	1	14,14,15	0.22	0	17,19,21	0.57	0
5	CLR	E	1508	-	31,31,31	0.87	2 (6%)	48,48,48	1.52	9 (18%)
4	NAG	E	1503	1	14,14,15	0.96	1 (7%)	17,19,21	1.34	3 (17%)
4	NAG	A	1802	1	14,14,15	0.23	0	17,19,21	0.55	0
8	PLM	C	205	2	16,16,17	0.35	0	15,15,17	0.74	0
4	NAG	B	1505	1	14,14,15	0.24	0	17,19,21	0.46	0
5	CLR	A	1809	-	31,31,31	0.70	0	48,48,48	1.51	9 (18%)
5	CLR	D	1810	-	31,31,31	0.66	0	48,48,48	1.24	5 (10%)
5	CLR	F	201	2	31,31,31	0.98	1 (3%)	48,48,48	1.91	8 (16%)
5	CLR	D	1809	-	31,31,31	0.70	0	48,48,48	1.51	9 (18%)
4	NAG	D	1803	1	14,14,15	0.81	1 (7%)	17,19,21	1.23	1 (5%)
8	PLM	F	205	2	16,16,17	0.34	0	15,15,17	0.74	0
5	CLR	B	1508	-	31,31,31	0.87	2 (6%)	48,48,48	1.53	9 (18%)
4	NAG	B	1502	1	14,14,15	0.52	0	17,19,21	0.38	0
4	NAG	E	1504	1	14,14,15	0.74	1 (7%)	17,19,21	0.75	1 (5%)
5	CLR	A	1808	-	31,31,31	1.00	2 (6%)	48,48,48	1.61	8 (16%)
4	NAG	D	1802	1	14,14,15	0.24	0	17,19,21	0.55	0
5	CLR	D	1808	-	31,31,31	1.00	2 (6%)	48,48,48	1.61	8 (16%)
5	CLR	C	201	2	31,31,31	0.99	1 (3%)	48,48,48	1.91	8 (16%)
4	NAG	D	1804	1	14,14,15	0.22	0	17,19,21	0.57	0
4	NAG	B	1503	1	14,14,15	0.93	1 (7%)	17,19,21	1.34	3 (17%)
5	CLR	A	1810	-	31,31,31	0.65	0	48,48,48	1.24	5 (10%)
4	NAG	E	1502	1	14,14,15	0.50	0	17,19,21	0.38	0
4	NAG	D	1801	1	14,14,15	0.82	1 (7%)	17,19,21	2.25	4 (23%)
4	NAG	A	1803	1	14,14,15	0.82	1 (7%)	17,19,21	1.22	1 (5%)

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
4	NAG	A	1807	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1801	1	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1501	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1505	1	-	4/6/23/26	0/1/1/1
4	NAG	D	1807	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1501	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1504	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1804	1	-	1/6/23/26	0/1/1/1
5	CLR	E	1508	-	-	4/10/68/68	0/4/4/4
4	NAG	E	1503	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1802	1	-	1/6/23/26	0/1/1/1
8	PLM	C	205	2	-	7/13/14/15	-
4	NAG	B	1505	1	-	4/6/23/26	0/1/1/1
5	CLR	A	1809	-	-	2/10/68/68	0/4/4/4
5	CLR	D	1810	-	-	6/10/68/68	0/4/4/4
5	CLR	F	201	2	-	3/10/68/68	0/4/4/4
5	CLR	D	1809	-	-	2/10/68/68	0/4/4/4
4	NAG	D	1803	1	-	3/6/23/26	0/1/1/1
8	PLM	F	205	2	-	7/13/14/15	-
5	CLR	B	1508	-	-	4/10/68/68	0/4/4/4
4	NAG	B	1502	1	-	0/6/23/26	0/1/1/1
4	NAG	E	1504	1	-	4/6/23/26	0/1/1/1
5	CLR	A	1808	-	-	9/10/68/68	0/4/4/4
4	NAG	D	1802	1	-	1/6/23/26	0/1/1/1
5	CLR	D	1808	-	-	9/10/68/68	0/4/4/4
5	CLR	C	201	2	-	3/10/68/68	0/4/4/4
4	NAG	D	1804	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1503	1	-	2/6/23/26	0/1/1/1
5	CLR	A	1810	-	-	6/10/68/68	0/4/4/4
4	NAG	E	1502	1	-	0/6/23/26	0/1/1/1
4	NAG	D	1801	1	-	5/6/23/26	0/1/1/1
4	NAG	A	1803	1	-	3/6/23/26	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1503	NAG	O5-C1	-2.75	1.39	1.43
4	A	1803	NAG	O5-C1	-2.73	1.39	1.43
4	D	1803	NAG	O5-C1	-2.71	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	201	CLR	C13-C14	-2.70	1.49	1.55
4	B	1503	NAG	O5-C1	-2.68	1.39	1.43
5	F	201	CLR	C13-C14	-2.67	1.49	1.55
5	A	1808	CLR	C13-C14	-2.52	1.50	1.55
5	D	1808	CLR	C13-C14	-2.50	1.50	1.55
4	D	1801	NAG	C1-C2	2.43	1.56	1.52
5	D	1808	CLR	C10-C9	-2.41	1.52	1.56
4	A	1801	NAG	C1-C2	2.40	1.55	1.52
5	A	1808	CLR	C10-C9	-2.36	1.52	1.56
4	B	1501	NAG	O5-C1	2.20	1.47	1.43
4	E	1501	NAG	O5-C1	2.19	1.47	1.43
5	E	1508	CLR	C10-C9	-2.17	1.52	1.56
4	B	1504	NAG	O5-C1	2.14	1.47	1.43
5	B	1508	CLR	C10-C9	-2.12	1.52	1.56
4	E	1504	NAG	O5-C1	2.09	1.47	1.43
5	E	1508	CLR	C13-C14	-2.04	1.51	1.55
5	B	1508	CLR	C13-C14	-2.03	1.51	1.55

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1801	NAG	C2-N2-C7	7.90	134.16	122.90
4	A	1801	NAG	C2-N2-C7	7.89	134.14	122.90
5	F	201	CLR	C13-C17-C20	-5.56	110.77	119.49
5	C	201	CLR	C13-C17-C20	-5.56	110.78	119.49
5	C	201	CLR	C13-C14-C8	-5.36	106.44	114.38
5	F	201	CLR	C13-C14-C8	-5.35	106.46	114.38
5	C	201	CLR	C8-C7-C6	-4.74	105.92	112.73
5	E	1508	CLR	C13-C17-C20	-4.72	112.09	119.49
5	F	201	CLR	C8-C7-C6	-4.70	105.98	112.73
5	B	1508	CLR	C13-C17-C20	-4.69	112.14	119.49
5	D	1808	CLR	C13-C14-C8	-4.50	107.72	114.38
5	A	1808	CLR	C13-C14-C8	-4.48	107.75	114.38
5	A	1809	CLR	C10-C9-C8	-4.40	106.14	112.73
5	D	1809	CLR	C10-C9-C8	-4.39	106.16	112.73
5	D	1808	CLR	C13-C17-C20	-4.37	112.64	119.49
5	A	1808	CLR	C13-C17-C20	-4.35	112.68	119.49
5	C	201	CLR	C3-C4-C5	-4.29	104.75	112.03
5	F	201	CLR	C3-C4-C5	-4.28	104.77	112.03
5	B	1508	CLR	C13-C14-C8	-3.86	108.66	114.38
5	E	1508	CLR	C13-C14-C8	-3.85	108.67	114.38
4	B	1503	NAG	C2-N2-C7	3.69	128.16	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1503	NAG	C2-N2-C7	3.69	128.15	122.90
5	F	201	CLR	C17-C13-C14	3.60	104.33	100.07
5	C	201	CLR	C17-C13-C14	3.56	104.30	100.07
4	A	1801	NAG	C1-C2-N2	3.48	116.44	110.49
4	D	1801	NAG	C1-C2-N2	3.46	116.40	110.49
4	D	1803	NAG	C2-N2-C7	3.27	127.56	122.90
4	A	1803	NAG	C2-N2-C7	3.25	127.54	122.90
5	A	1808	CLR	C17-C13-C14	3.05	103.68	100.07
5	D	1808	CLR	C17-C13-C14	2.98	103.60	100.07
5	B	1508	CLR	C7-C8-C9	2.96	113.30	109.71
5	E	1508	CLR	C7-C8-C9	2.93	113.27	109.71
5	D	1808	CLR	C11-C9-C10	-2.86	109.32	113.08
5	A	1808	CLR	C11-C9-C10	-2.85	109.33	113.08
5	A	1810	CLR	C13-C17-C20	-2.82	115.06	119.49
5	D	1809	CLR	C14-C8-C9	2.78	112.81	109.09
5	D	1809	CLR	C1-C10-C9	2.77	112.60	108.73
5	A	1809	CLR	C14-C8-C9	2.77	112.79	109.09
5	A	1809	CLR	C1-C10-C9	2.77	112.59	108.73
5	D	1810	CLR	C13-C17-C20	-2.76	115.16	119.49
5	B	1508	CLR	C14-C8-C9	-2.73	105.44	109.09
5	E	1508	CLR	C14-C8-C9	-2.69	105.48	109.09
5	D	1809	CLR	C21-C20-C17	2.66	117.00	112.92
5	D	1808	CLR	C1-C10-C9	2.66	112.44	108.73
5	A	1809	CLR	C21-C20-C17	2.65	116.98	112.92
5	A	1808	CLR	C1-C10-C9	2.65	112.43	108.73
5	B	1508	CLR	C17-C13-C14	2.60	103.16	100.07
5	E	1508	CLR	C4-C5-C10	2.60	119.88	116.42
5	B	1508	CLR	C4-C5-C10	2.60	119.87	116.42
5	E	1508	CLR	C17-C13-C14	2.59	103.14	100.07
5	D	1809	CLR	C19-C10-C9	-2.58	108.61	111.68
5	A	1809	CLR	C19-C10-C9	-2.57	108.61	111.68
5	A	1809	CLR	C1-C2-C3	2.55	113.73	110.47
5	D	1809	CLR	C1-C2-C3	2.53	113.72	110.47
5	E	1508	CLR	C11-C12-C13	-2.43	108.62	112.78
5	B	1508	CLR	C11-C12-C13	-2.42	108.63	112.78
4	E	1503	NAG	C4-C3-C2	2.42	114.56	111.02
5	D	1808	CLR	C7-C6-C5	-2.42	120.60	125.06
4	B	1503	NAG	C4-C3-C2	2.41	114.54	111.02
5	D	1810	CLR	C22-C20-C17	2.39	115.23	110.28
5	A	1808	CLR	C7-C6-C5	-2.39	120.66	125.06
5	A	1810	CLR	C8-C7-C6	-2.39	109.30	112.73
5	A	1810	CLR	C22-C20-C17	2.38	115.19	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	1810	CLR	C8-C7-C6	-2.35	109.35	112.73
5	A	1810	CLR	C14-C8-C9	2.33	112.21	109.09
5	D	1810	CLR	C14-C8-C9	2.33	112.20	109.09
5	D	1810	CLR	C10-C9-C8	-2.28	109.32	112.73
4	B	1504	NAG	C1-O5-C5	2.26	115.26	112.19
4	E	1504	NAG	C1-O5-C5	2.26	115.26	112.19
5	A	1810	CLR	C10-C9-C8	-2.25	109.37	112.73
5	E	1508	CLR	C7-C6-C5	-2.20	121.01	125.06
5	B	1508	CLR	C7-C6-C5	-2.18	121.04	125.06
5	C	201	CLR	C4-C5-C6	-2.16	117.49	120.61
5	D	1809	CLR	C4-C5-C10	2.15	119.28	116.42
5	A	1809	CLR	C4-C5-C10	2.14	119.27	116.42
4	E	1503	NAG	C1-C2-N2	2.14	114.14	110.49
4	B	1503	NAG	C1-C2-N2	2.12	114.11	110.49
4	A	1801	NAG	C8-C7-N2	2.11	119.67	116.10
5	F	201	CLR	C4-C5-C6	-2.11	117.57	120.61
5	A	1809	CLR	C7-C6-C5	-2.11	121.17	125.06
5	D	1809	CLR	C7-C6-C5	-2.10	121.18	125.06
4	D	1801	NAG	C8-C7-N2	2.10	119.66	116.10
5	A	1808	CLR	C10-C9-C8	-2.09	109.60	112.73
5	D	1808	CLR	C10-C9-C8	-2.09	109.60	112.73
5	C	201	CLR	C16-C17-C13	2.08	106.35	103.84
5	C	201	CLR	C11-C12-C13	-2.07	109.22	112.78
5	A	1808	CLR	C7-C8-C9	2.06	112.21	109.71
5	F	201	CLR	C11-C12-C13	-2.05	109.27	112.78
5	D	1808	CLR	C7-C8-C9	2.04	112.19	109.71
5	D	1809	CLR	C1-C10-C5	-2.03	105.04	108.75
5	F	201	CLR	C16-C17-C13	2.03	106.29	103.84
5	B	1508	CLR	C10-C5-C6	-2.03	119.80	122.90
5	A	1809	CLR	C1-C10-C5	-2.02	105.05	108.75
5	E	1508	CLR	C10-C5-C6	-2.01	119.83	122.90
4	D	1801	NAG	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

All (110) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	201	CLR	C17-C20-C22-C23
5	F	201	CLR	C17-C20-C22-C23
5	A	1810	CLR	C13-C17-C20-C21
5	D	1810	CLR	C13-C17-C20-C21
5	C	201	CLR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
5	F	201	CLR	C22-C23-C24-C25
5	A	1810	CLR	C16-C17-C20-C21
5	D	1810	CLR	C16-C17-C20-C21
5	A	1810	CLR	C13-C17-C20-C22
5	D	1810	CLR	C13-C17-C20-C22
4	A	1801	NAG	C4-C5-C6-O6
4	D	1801	NAG	C4-C5-C6-O6
5	A	1810	CLR	C16-C17-C20-C22
5	D	1810	CLR	C16-C17-C20-C22
4	B	1505	NAG	O5-C5-C6-O6
4	E	1505	NAG	O5-C5-C6-O6
4	A	1803	NAG	O5-C5-C6-O6
4	D	1803	NAG	O5-C5-C6-O6
4	B	1505	NAG	C4-C5-C6-O6
4	E	1505	NAG	C4-C5-C6-O6
4	E	1504	NAG	C4-C5-C6-O6
8	C	205	PLM	C6-C7-C8-C9
8	F	205	PLM	C6-C7-C8-C9
4	B	1504	NAG	C4-C5-C6-O6
4	A	1801	NAG	O5-C5-C6-O6
4	D	1801	NAG	O5-C5-C6-O6
5	A	1810	CLR	C17-C20-C22-C23
5	D	1810	CLR	C17-C20-C22-C23
4	A	1803	NAG	C4-C5-C6-O6
4	D	1803	NAG	C4-C5-C6-O6
4	A	1801	NAG	C8-C7-N2-C2
4	A	1801	NAG	O7-C7-N2-C2
4	B	1504	NAG	C8-C7-N2-C2
4	B	1504	NAG	O7-C7-N2-C2
4	B	1505	NAG	C8-C7-N2-C2
4	B	1505	NAG	O7-C7-N2-C2
4	D	1801	NAG	C8-C7-N2-C2
4	D	1801	NAG	O7-C7-N2-C2
4	E	1504	NAG	C8-C7-N2-C2
4	E	1504	NAG	O7-C7-N2-C2
4	E	1505	NAG	C8-C7-N2-C2
4	E	1505	NAG	O7-C7-N2-C2
5	A	1808	CLR	C22-C23-C24-C25
5	D	1808	CLR	C22-C23-C24-C25
5	A	1810	CLR	C21-C20-C22-C23
5	D	1810	CLR	C21-C20-C22-C23
5	A	1808	CLR	C13-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
5	D	1808	CLR	C13-C17-C20-C22
8	C	205	PLM	C9-CA-CB-CC
8	F	205	PLM	C9-CA-CB-CC
5	A	1808	CLR	C16-C17-C20-C21
5	D	1808	CLR	C16-C17-C20-C21
5	A	1808	CLR	C13-C17-C20-C21
5	D	1808	CLR	C13-C17-C20-C21
4	A	1807	NAG	O5-C5-C6-O6
4	D	1807	NAG	O5-C5-C6-O6
4	B	1504	NAG	O5-C5-C6-O6
4	E	1504	NAG	O5-C5-C6-O6
8	C	205	PLM	C2-C3-C4-C5
8	F	205	PLM	C2-C3-C4-C5
8	C	205	PLM	CA-CB-CC-CD
8	F	205	PLM	CA-CB-CC-CD
5	C	201	CLR	C21-C20-C22-C23
5	F	201	CLR	C21-C20-C22-C23
8	F	205	PLM	CD-CE-CF-CG
8	C	205	PLM	CD-CE-CF-CG
8	C	205	PLM	C3-C4-C5-C6
8	F	205	PLM	C3-C4-C5-C6
5	A	1808	CLR	C17-C20-C22-C23
5	D	1808	CLR	C17-C20-C22-C23
5	A	1808	CLR	C23-C24-C25-C26
5	D	1808	CLR	C23-C24-C25-C26
4	A	1802	NAG	O5-C5-C6-O6
4	D	1802	NAG	O5-C5-C6-O6
4	A	1804	NAG	O5-C5-C6-O6
4	D	1804	NAG	O5-C5-C6-O6
5	A	1808	CLR	C23-C24-C25-C27
5	D	1808	CLR	C23-C24-C25-C27
4	B	1501	NAG	C1-C2-N2-C7
4	E	1501	NAG	C1-C2-N2-C7
5	B	1508	CLR	C22-C23-C24-C25
5	E	1508	CLR	C22-C23-C24-C25
8	F	205	PLM	C8-C9-CA-CB
8	C	205	PLM	C8-C9-CA-CB
5	A	1808	CLR	C16-C17-C20-C22
5	D	1808	CLR	C16-C17-C20-C22
5	B	1508	CLR	C23-C24-C25-C26
5	E	1508	CLR	C23-C24-C25-C26
4	A	1801	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	A	1803	NAG	C3-C2-N2-C7
4	D	1801	NAG	C3-C2-N2-C7
4	D	1803	NAG	C3-C2-N2-C7
5	A	1809	CLR	C22-C23-C24-C25
5	D	1809	CLR	C22-C23-C24-C25
5	B	1508	CLR	C20-C22-C23-C24
5	E	1508	CLR	C20-C22-C23-C24
5	B	1508	CLR	C23-C24-C25-C27
5	E	1508	CLR	C23-C24-C25-C27
5	A	1808	CLR	C20-C22-C23-C24
5	D	1808	CLR	C20-C22-C23-C24
4	B	1501	NAG	O5-C5-C6-O6
4	E	1501	NAG	O5-C5-C6-O6
4	B	1503	NAG	C1-C2-N2-C7
4	E	1503	NAG	C1-C2-N2-C7
4	A	1807	NAG	C4-C5-C6-O6
4	D	1807	NAG	C4-C5-C6-O6
4	B	1503	NAG	C3-C2-N2-C7
4	E	1503	NAG	C3-C2-N2-C7
5	A	1809	CLR	C23-C24-C25-C27
5	D	1809	CLR	C23-C24-C25-C27

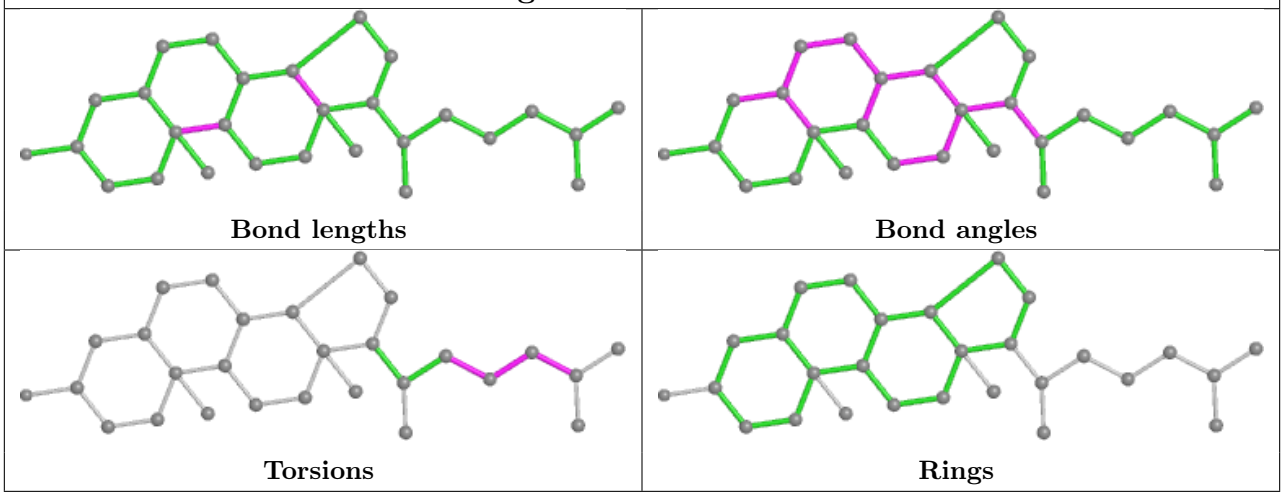
There are no ring outliers.

15 monomers are involved in 206 short contacts:

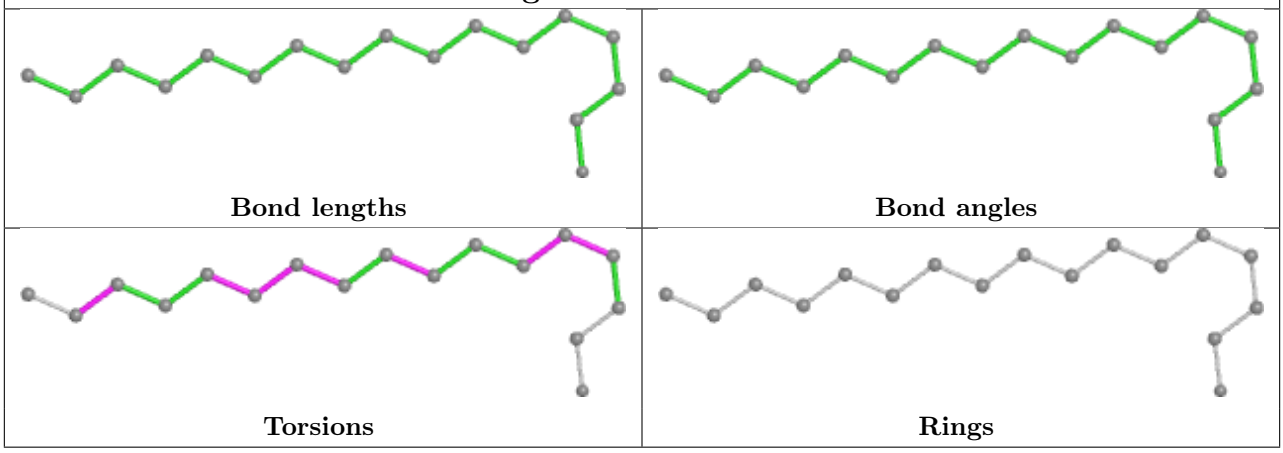
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1501	NAG	1	0
4	E	1501	NAG	1	0
5	E	1508	CLR	33	0
8	C	205	PLM	16	0
5	A	1809	CLR	1	0
5	D	1810	CLR	3	0
5	F	201	CLR	19	0
5	D	1809	CLR	2	0
8	F	205	PLM	16	0
5	B	1508	CLR	30	0
5	A	1808	CLR	31	0
5	D	1808	CLR	30	0
5	C	201	CLR	19	0
4	D	1804	NAG	1	0
5	A	1810	CLR	3	0

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.

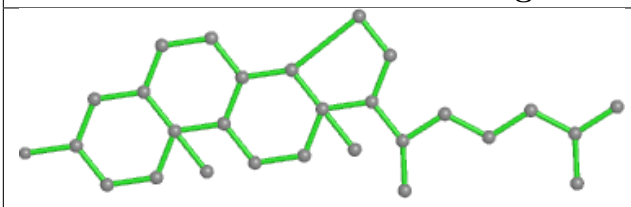
Ligand CLR E 1508



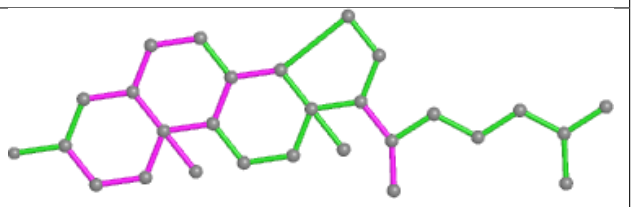
Ligand PLM C 205



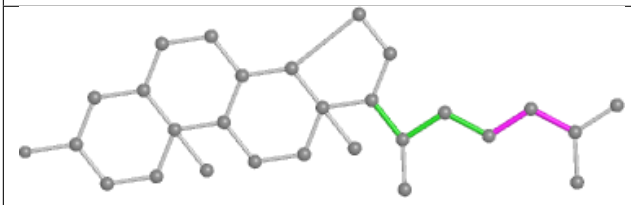
Ligand CLR A 1809



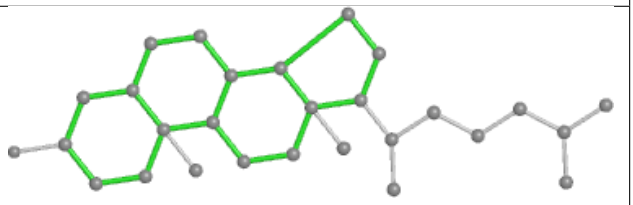
Bond lengths



Bond angles

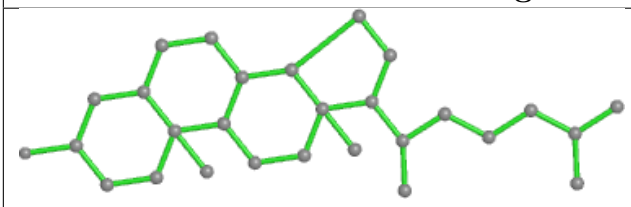


Torsions



Rings

Ligand CLR D 1810



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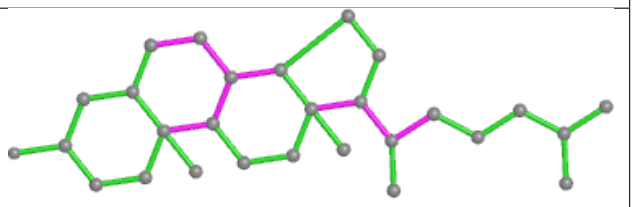

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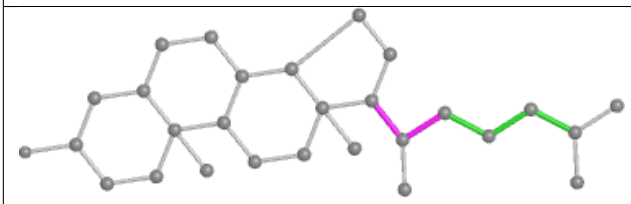

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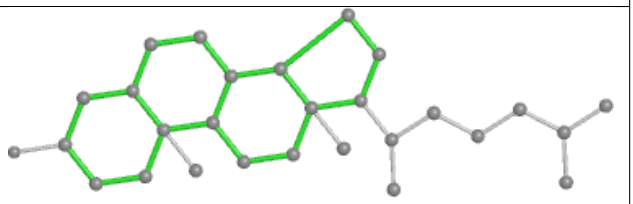
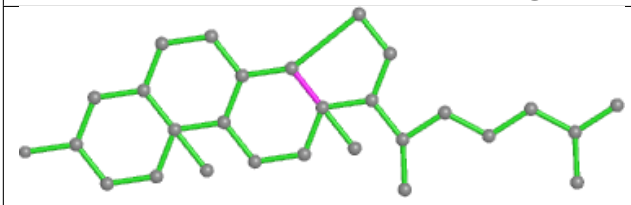
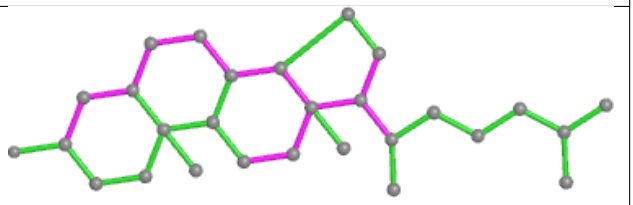


Rings

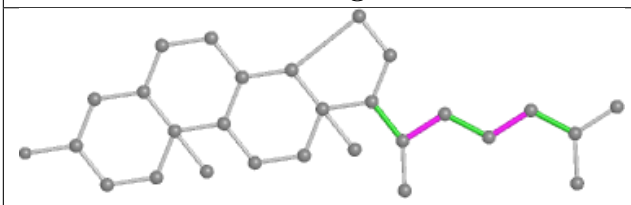
Ligand CLR F 201



Bond lengths



Bond angles



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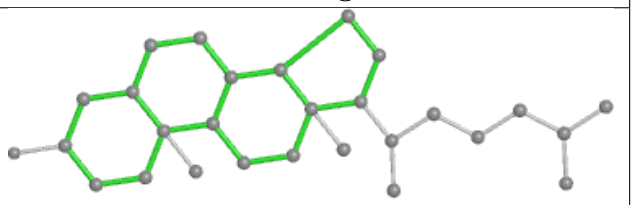
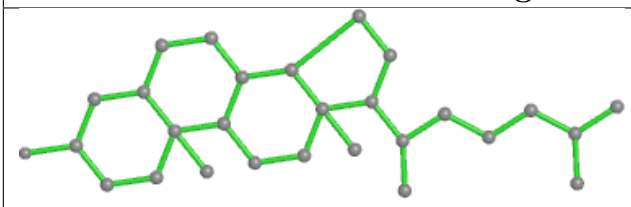


Rings

Ligand CLR D 1809



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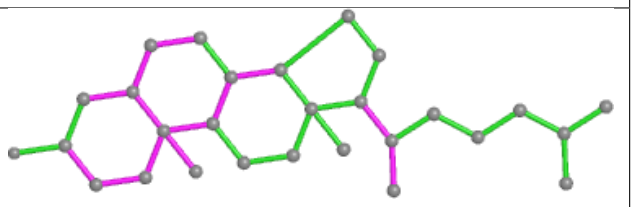
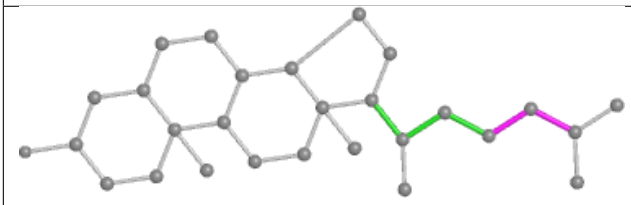


Bond angles



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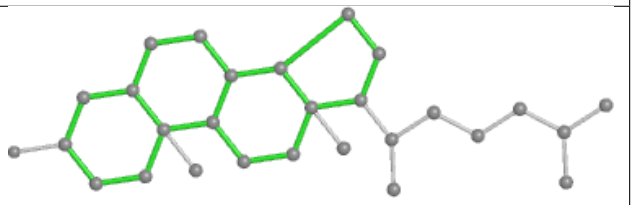
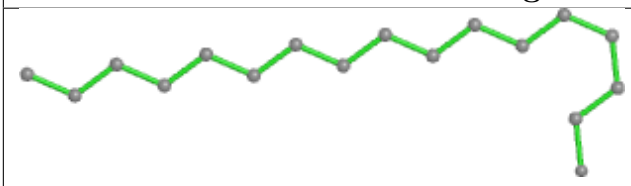


Rings

Ligand PLM F 205



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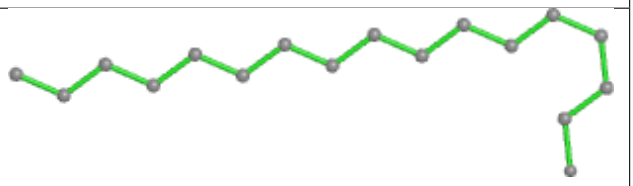
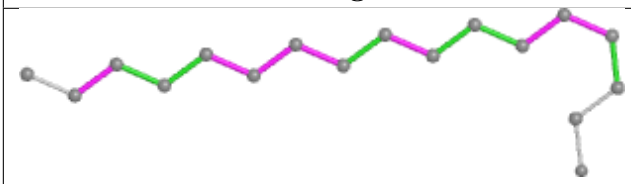


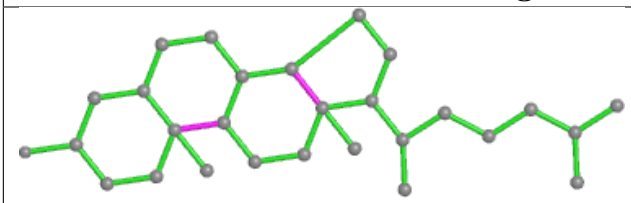
Bond angles



Torsions

Rings

Ligand CLR B 1508



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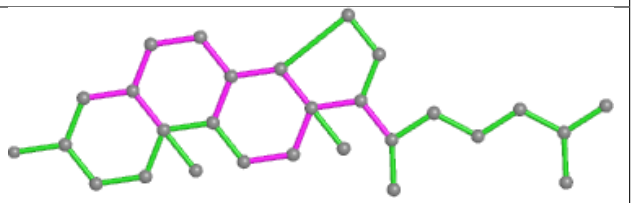

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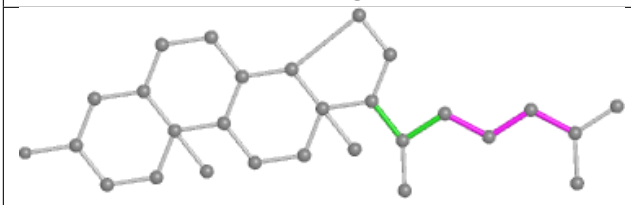

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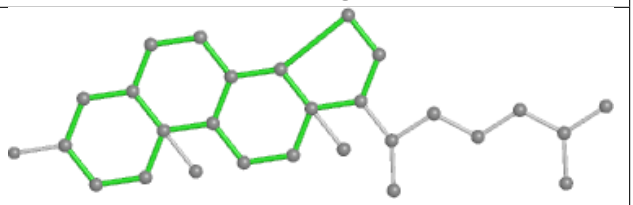
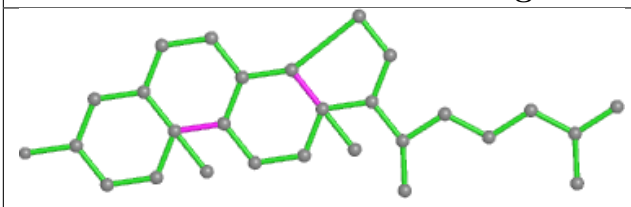


Rings

Ligand CLR A 1808



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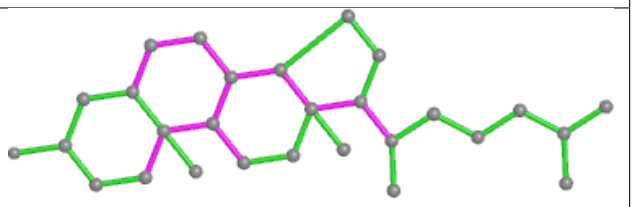
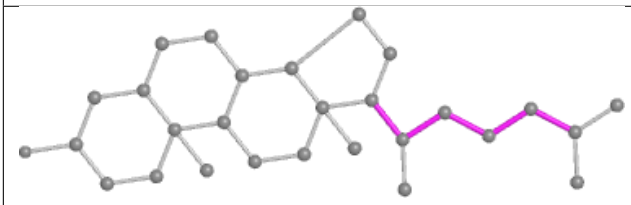


Bond angles



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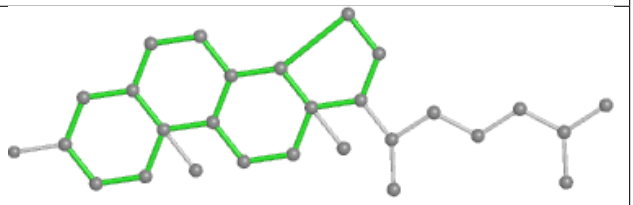
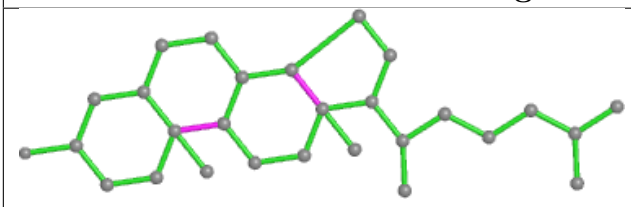
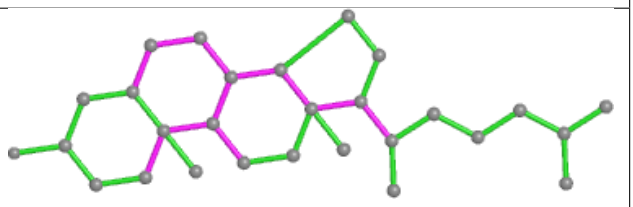


Rings

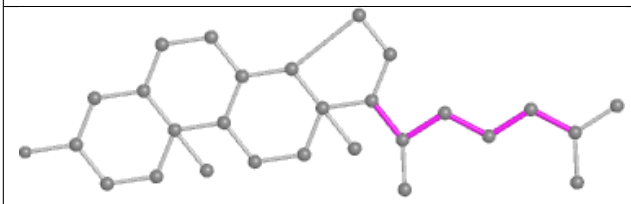
Ligand CLR D 1808



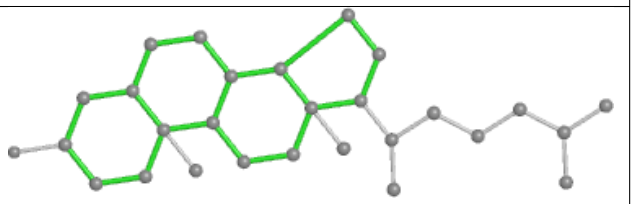
Bond lengths



Bond angles

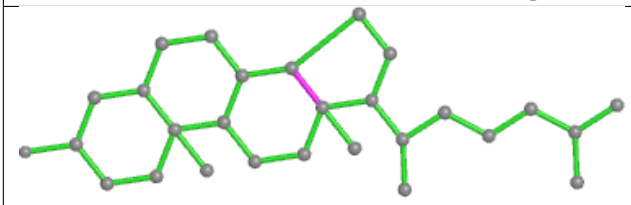


Torsions

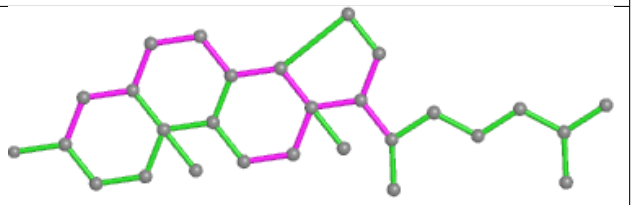


Rings

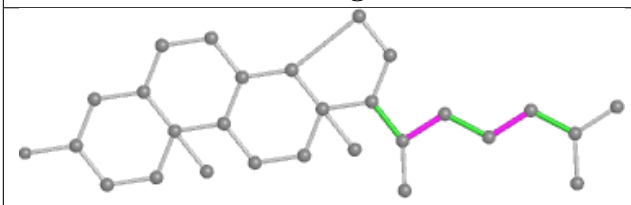
Ligand CLR C 201



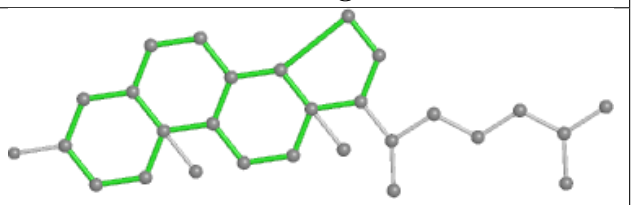
Bond lengths



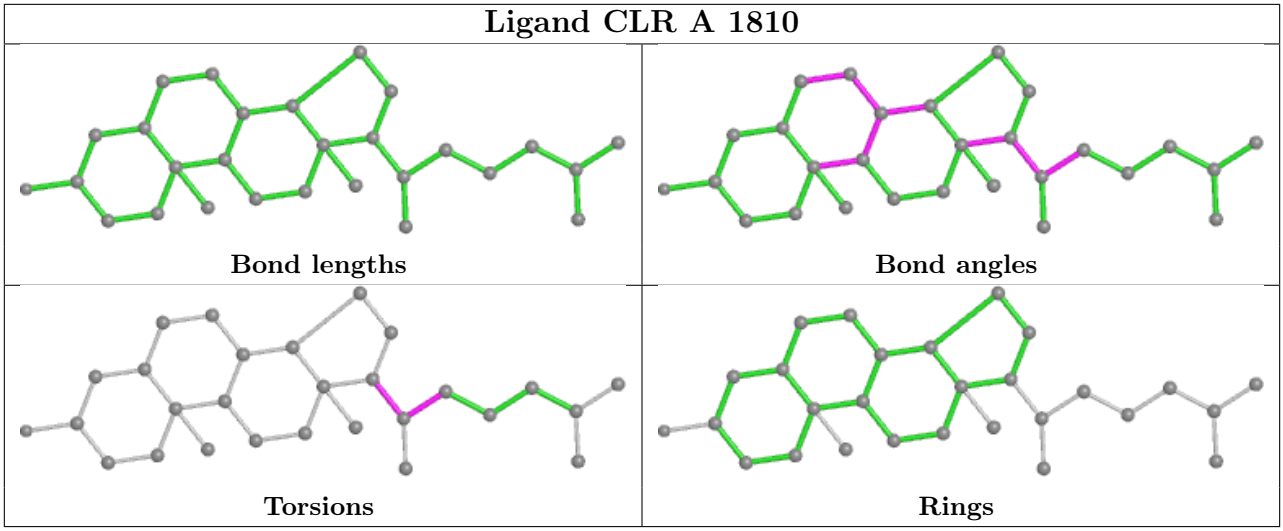
Bond angles



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.

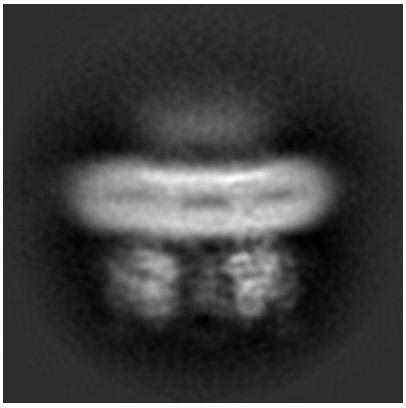
6 Map visualisation (i)

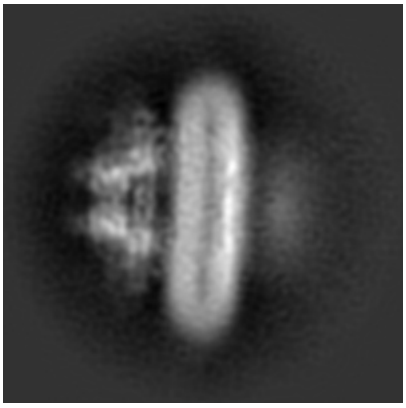
This section contains visualisations of the EMDB entry EMD-0358. These allow visual inspection of the internal detail of the map and identification of artifacts.

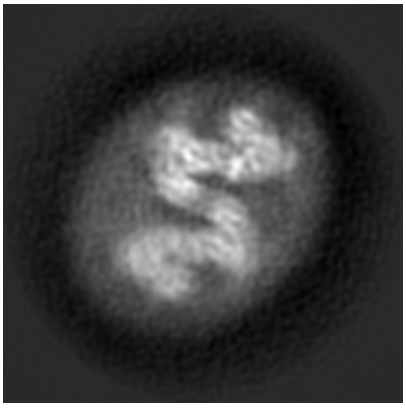
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

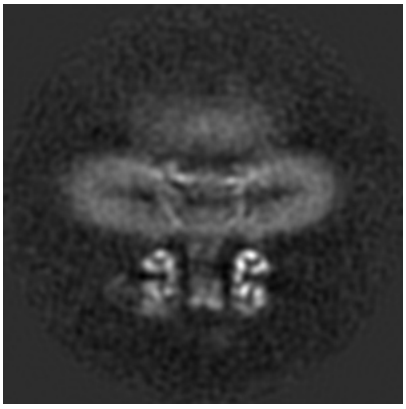

Y

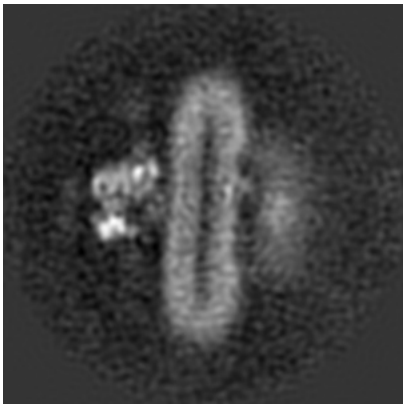

Z

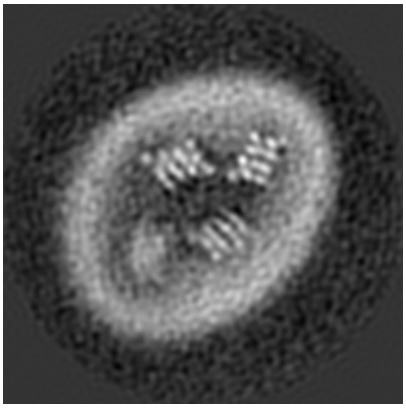
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 140

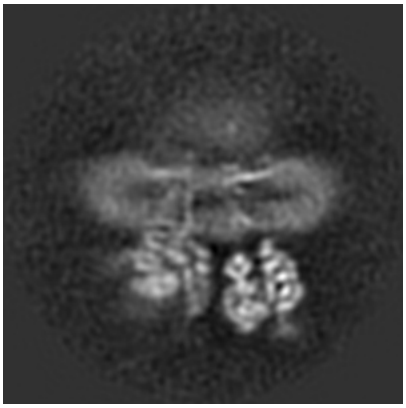

Y Index: 140


Z Index: 140

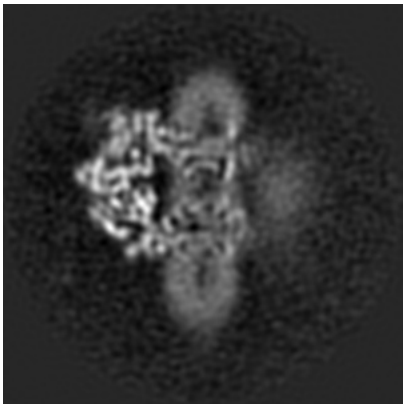
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

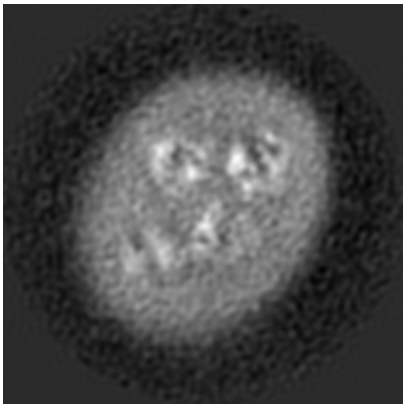
6.3.1 Primary map



X Index: 163



Y Index: 167

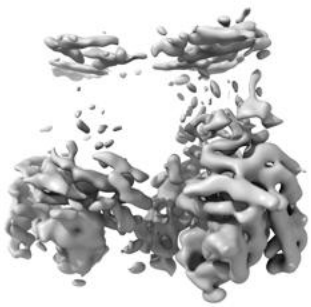


Z Index: 158

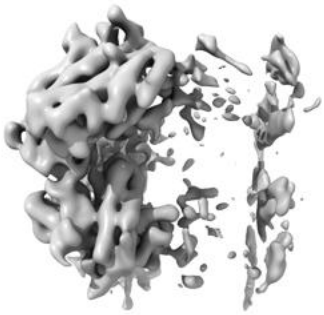
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

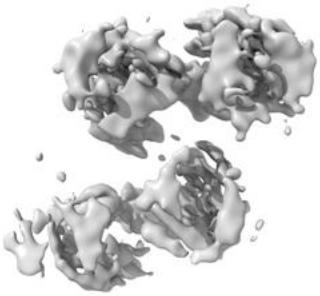
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

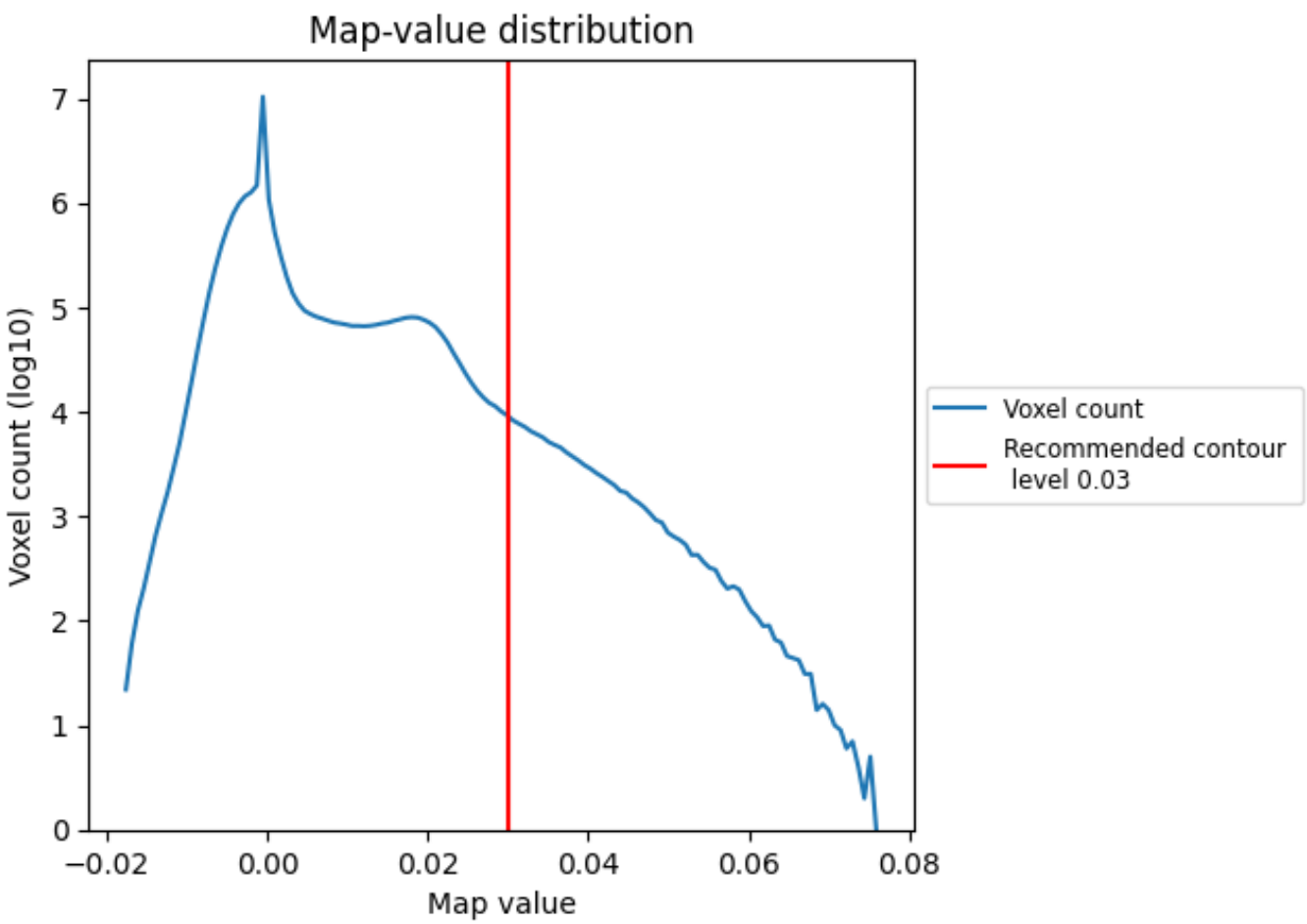
6.5 Mask visualisation (i)

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

7 Map analysis (i)

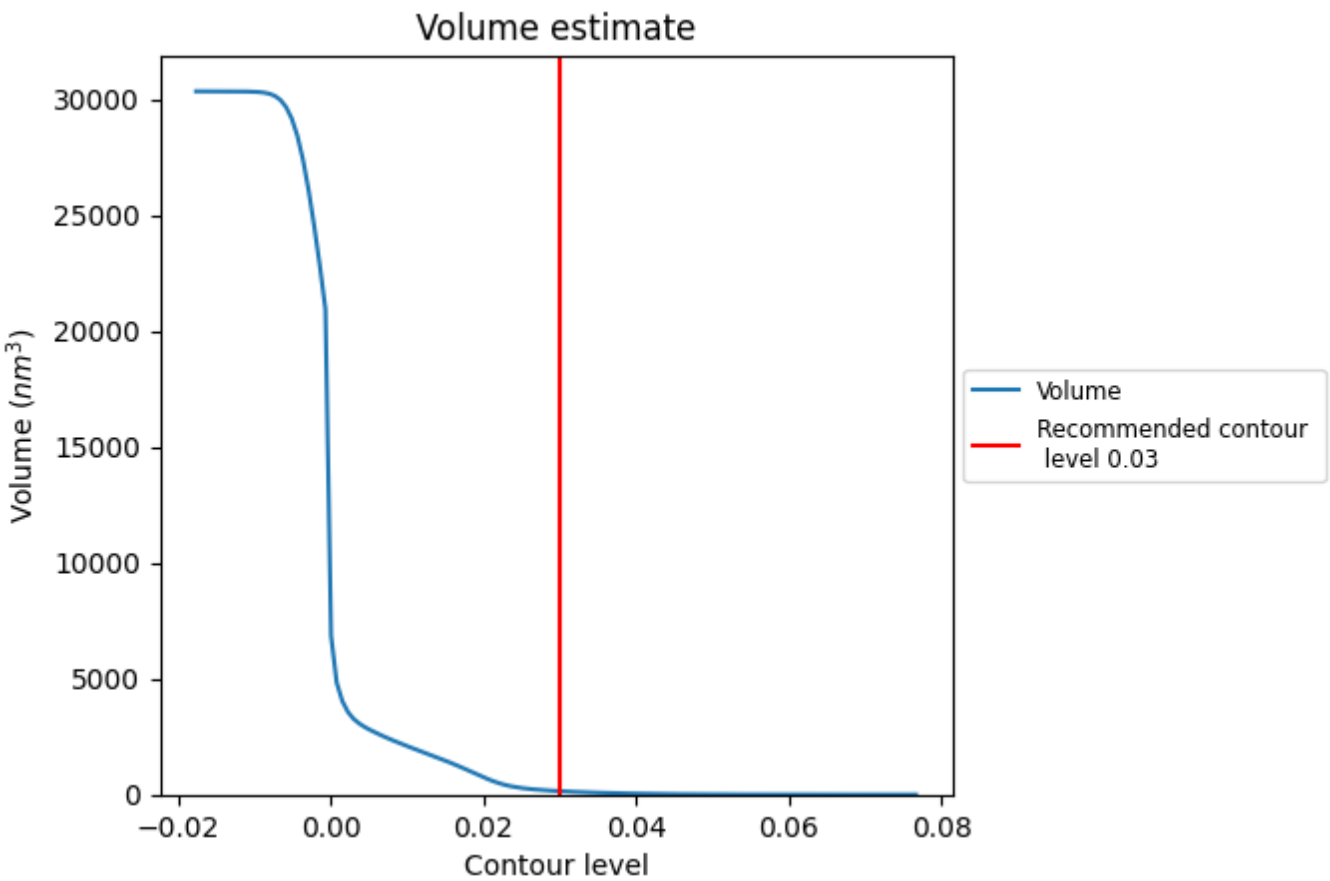
This section contains the results of statistical analysis of the map.

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.

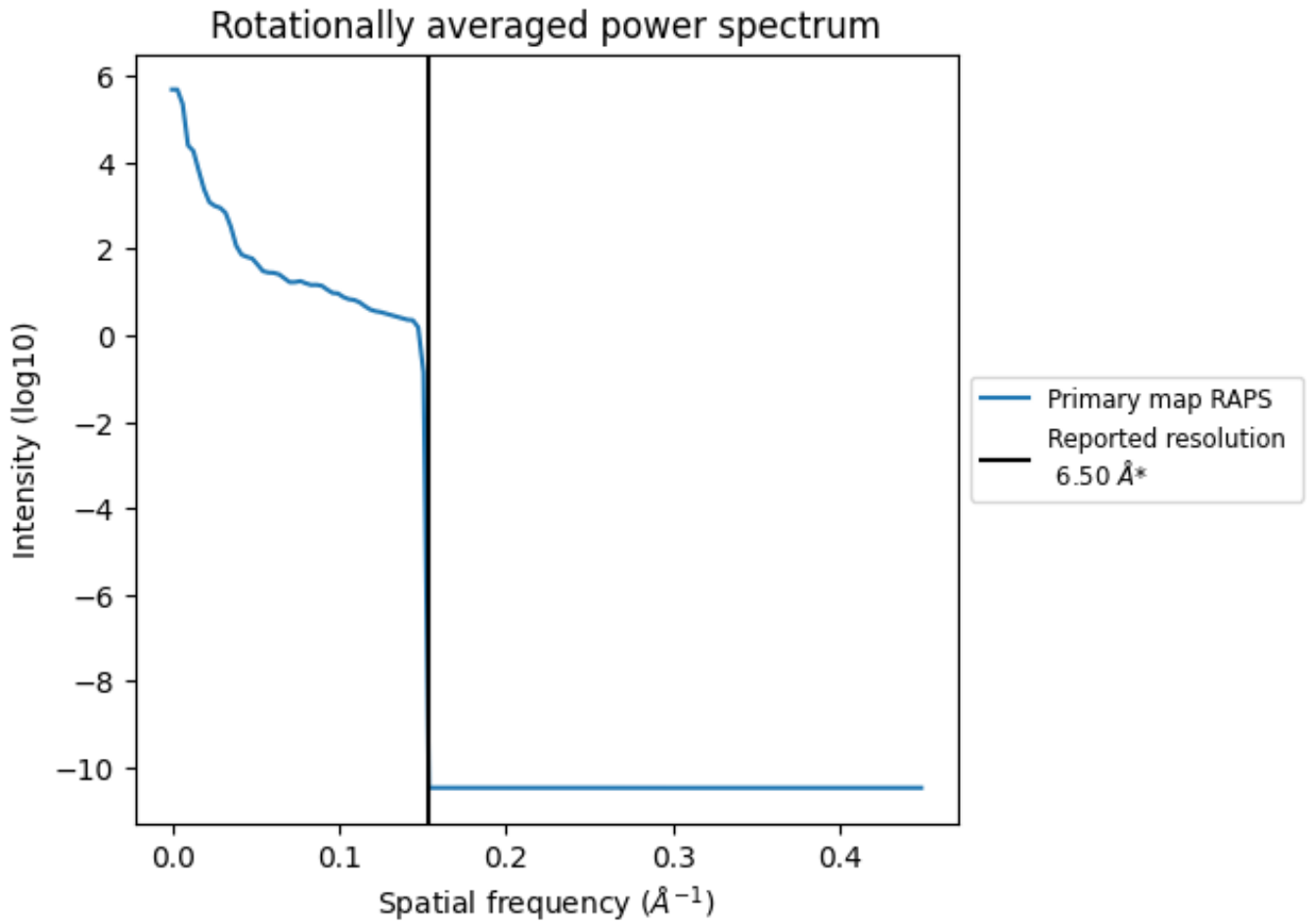
7.2 Volume estimate (i)



The volume at the recommended contour level is 148 nm^3; this corresponds to an approximate mass of 134 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 0.154 Å^{-1}

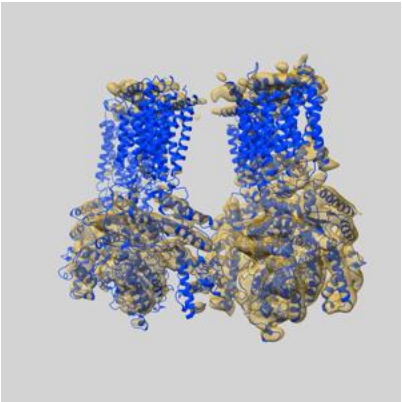
8 Fourier-Shell correlation (i)

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

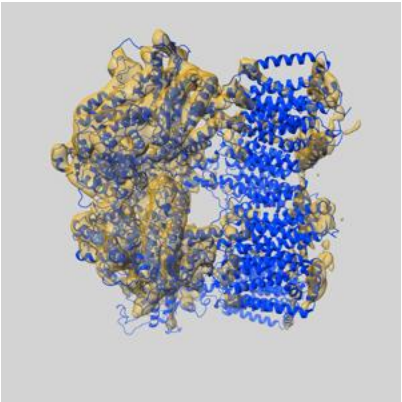
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0358 and PDB model 6N7K. Per-residue inclusion information can be found in section 3 on page 13.

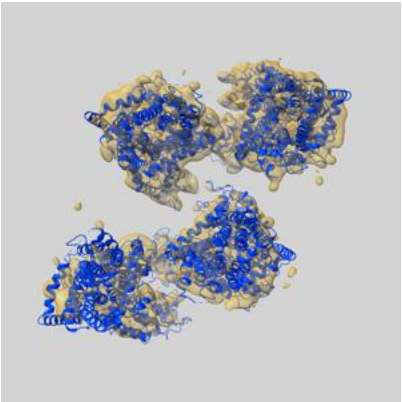
9.1 Map-model overlay (i)



X



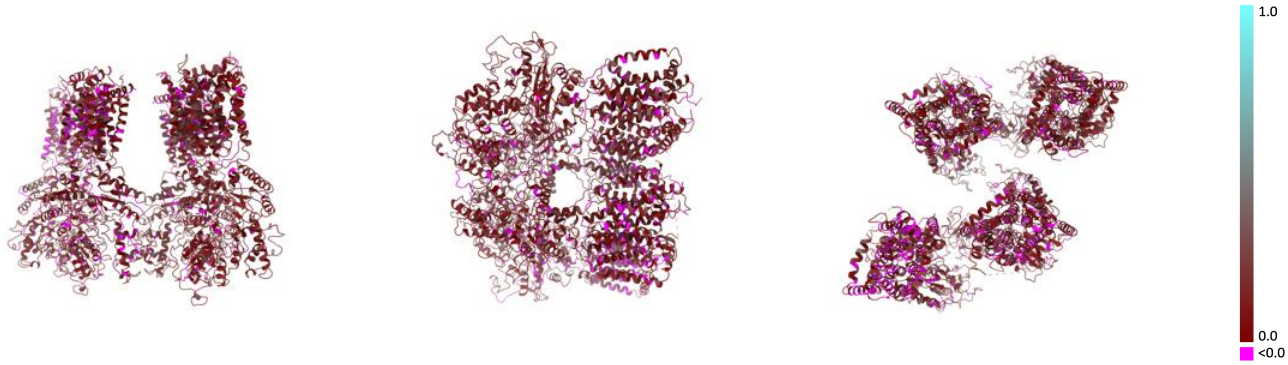
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

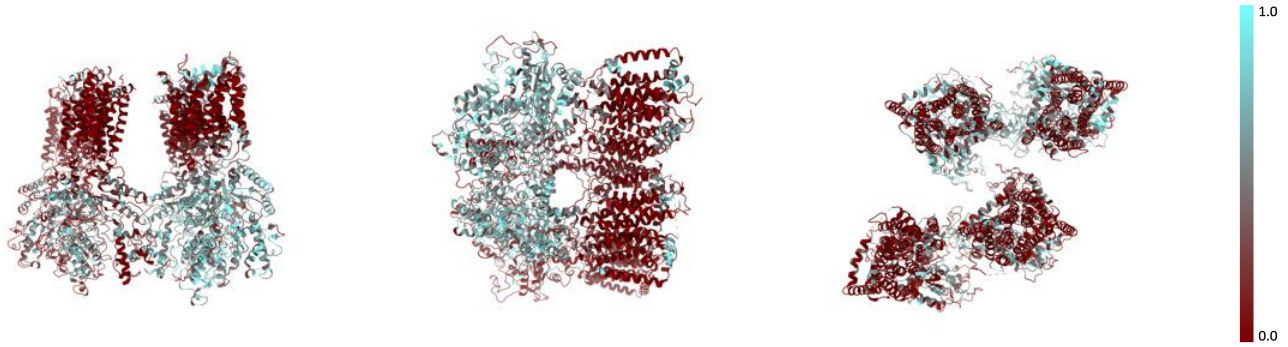
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

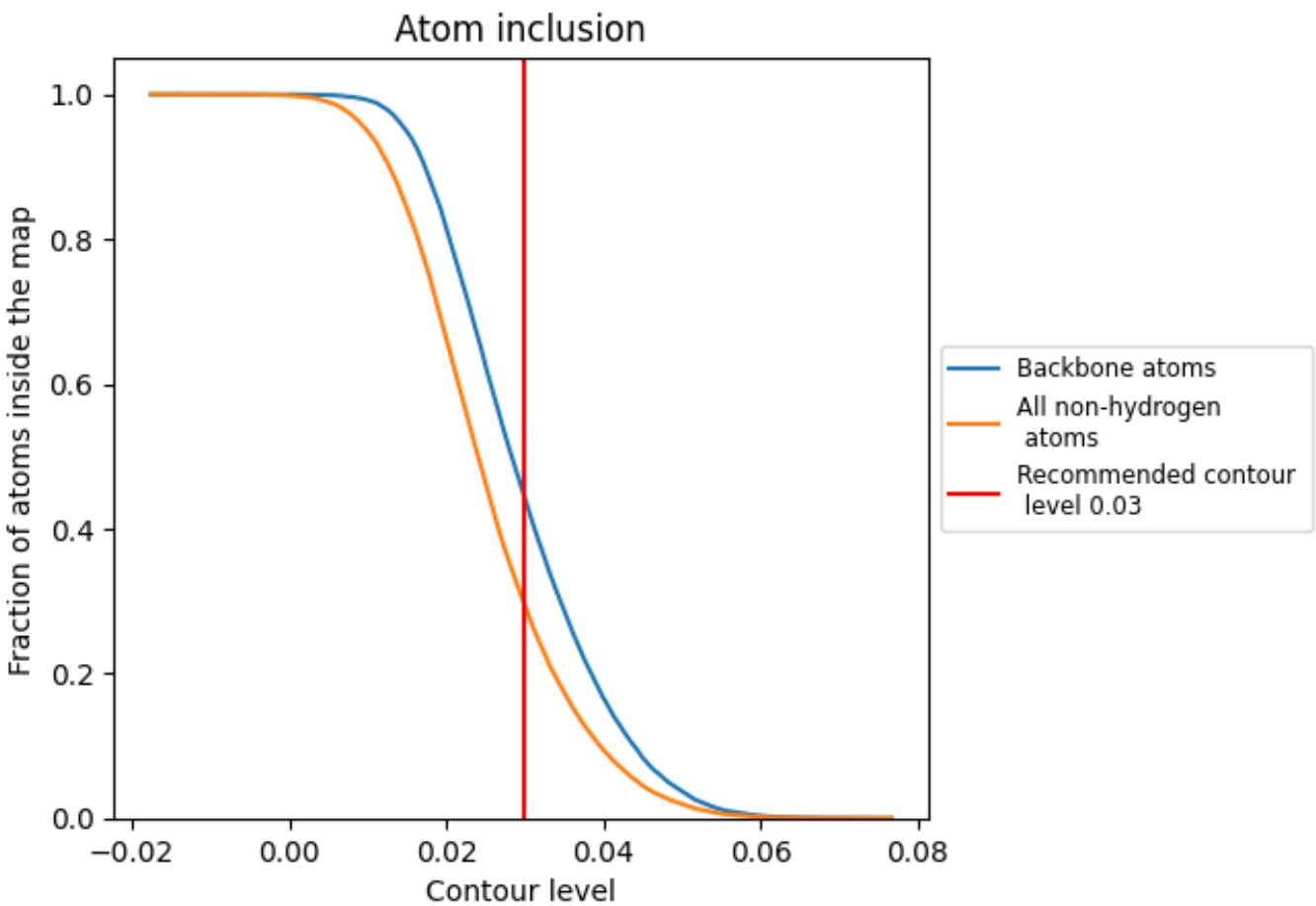
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 44% of all backbone atoms, 29% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2933	0.1320
A	0.3888	0.1540
B	0.3820	0.1470
C	0.5958	0.1560
D	0.1444	0.1000
E	0.2041	0.1230
F	0.3203	0.1380
G	0.0000	0.1940
H	0.0000	0.2760
I	0.0000	0.1120
J	0.0000	0.0750