Full wwPDB EM Validation Report (i)

Nov 21, 2022 – 03:39 AM EST

PDB ID	:	7RBT
EMDB ID	:	EMD-24401
Title	:	cryo-EM structure of human Gastric inhibitory polypeptide receptor GIPR bound to tirzepatide
Authors	:	Sun, B.; Kobilka, B.K.; Sloop, K.W.; Feng, D.; Kobilka, T.S.
Deposited on	:	2021-07-06
Resolution	:	3.08 Å(reported)
Based on initial model	:	6VCB

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:

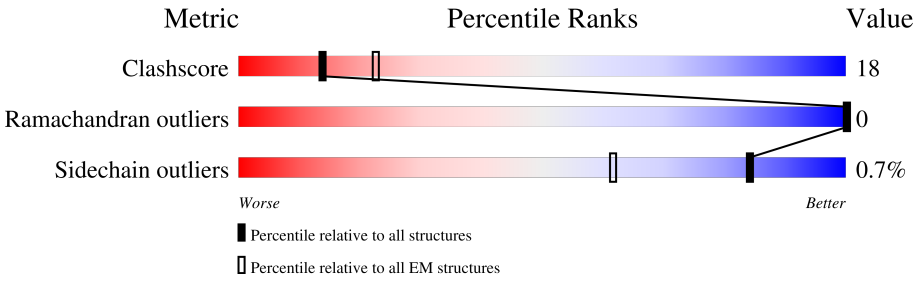
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.08 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	373	7%, 41%, 17%, •, 41%
2	B	350	8%, 59%, 38%, •
3	E	297	11%, 55%, 23%, 22%
4	G	71	35%, 59%, 21%, 20%
5	N	160	7%, 51%, 29%, 20%
6	P	39	18%, 56%, 26%, 18%
7	R	463	24%, 52%, 30%, 18%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 10881 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 Isoform Gnas-2 of Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	220	1792	1138	323	324	7	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	initiating methionine	UNP P63092-2
A	9	GLY	-	expression tag	UNP P63092-2
A	10	CYS	-	expression tag	UNP P63092-2
A	11	THR	-	expression tag	UNP P63092-2
A	12	LEU	-	expression tag	UNP P63092-2
A	13	SER	-	expression tag	UNP P63092-2
A	14	ALA	-	expression tag	UNP P63092-2
A	15	GLU	-	expression tag	UNP P63092-2
A	16	ASP	-	expression tag	UNP P63092-2
A	17	LYS	-	expression tag	UNP P63092-2
A	18	ALA	-	expression tag	UNP P63092-2
A	19	ALA	-	expression tag	UNP P63092-2
A	20	VAL	-	expression tag	UNP P63092-2
A	21	GLU	-	expression tag	UNP P63092-2
A	22	ARG	-	expression tag	UNP P63092-2
A	23	SER	-	expression tag	UNP P63092-2
A	24	LYS	-	expression tag	UNP P63092-2
A	25	MET	-	expression tag	UNP P63092-2

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	339	2581	1591	462	507	21	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MET	-	expression tag	UNP P62873
B	-8	HIS	-	expression tag	UNP P62873
B	-7	HIS	-	expression tag	UNP P62873
B	-6	HIS	-	expression tag	UNP P62873
B	-5	HIS	-	expression tag	UNP P62873
B	-4	HIS	-	expression tag	UNP P62873
B	-3	HIS	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873

- Molecule 3 is a protein called Single-chain variable fragment 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	232	1748	1116	292	330	10	0	0

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	57	436	273	77	83	3	0	0

- Molecule 5 is a protein called nanobody 35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	N	128	969	602	169	192	6	0	0

- Molecule 6 is a protein called Tirzepatide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	P	32	246	162	37	47	0	0

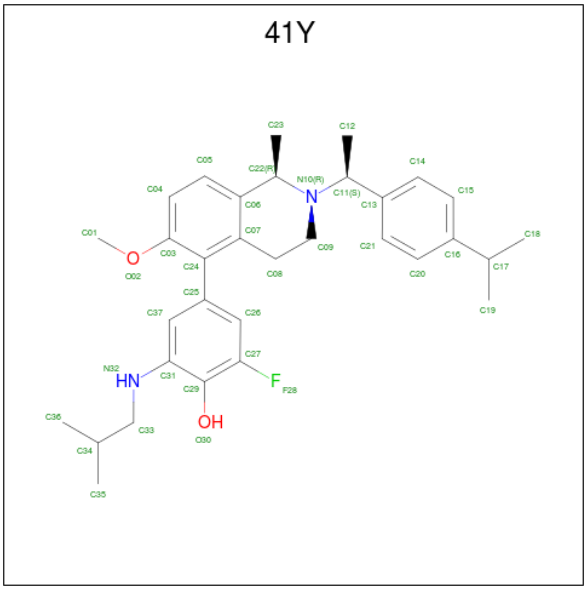
- Molecule 7 is a protein called Gastric inhibitory polypeptide receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	R	378	3072	2001	541	514	16	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	4	ASP	-	expression tag	UNP P48546
R	5	TYR	-	expression tag	UNP P48546
R	6	LYS	-	expression tag	UNP P48546
R	7	ASP	-	expression tag	UNP P48546
R	8	ASP	-	expression tag	UNP P48546
R	9	ASP	-	expression tag	UNP P48546
R	10	ASP	-	expression tag	UNP P48546
R	11	ALA	-	expression tag	UNP P48546
R	12	ALA	-	expression tag	UNP P48546
R	13	ALA	-	expression tag	UNP P48546
R	14	LEU	-	expression tag	UNP P48546
R	15	GLU	-	expression tag	UNP P48546
R	16	VAL	-	expression tag	UNP P48546
R	17	LEU	-	expression tag	UNP P48546
R	18	PHE	-	expression tag	UNP P48546
R	19	GLN	-	expression tag	UNP P48546
R	20	GLY	-	expression tag	UNP P48546
R	21	PRO	-	expression tag	UNP P48546

- Molecule 8 is 2-fluoro-4-[(1R)-6-methoxy-1-methyl-2-{(1S)-1-[4-(propan-2-yl)phenyl]ethyl}-1,2,3,4-tetrahydroisoquinolin-5-yl]-6-[(2-methylpropyl)amino]phenol (three-letter code: 41Y) (formula: $C_{32}H_{41}FN_2O_2$).



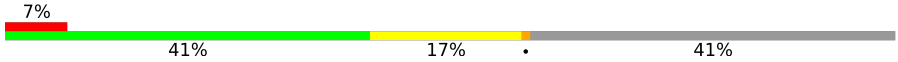
Mol	Chain	Residues	Atoms					AltConf
			Total	C	F	N	O	
8	R	1	37	32	1	2	2	0

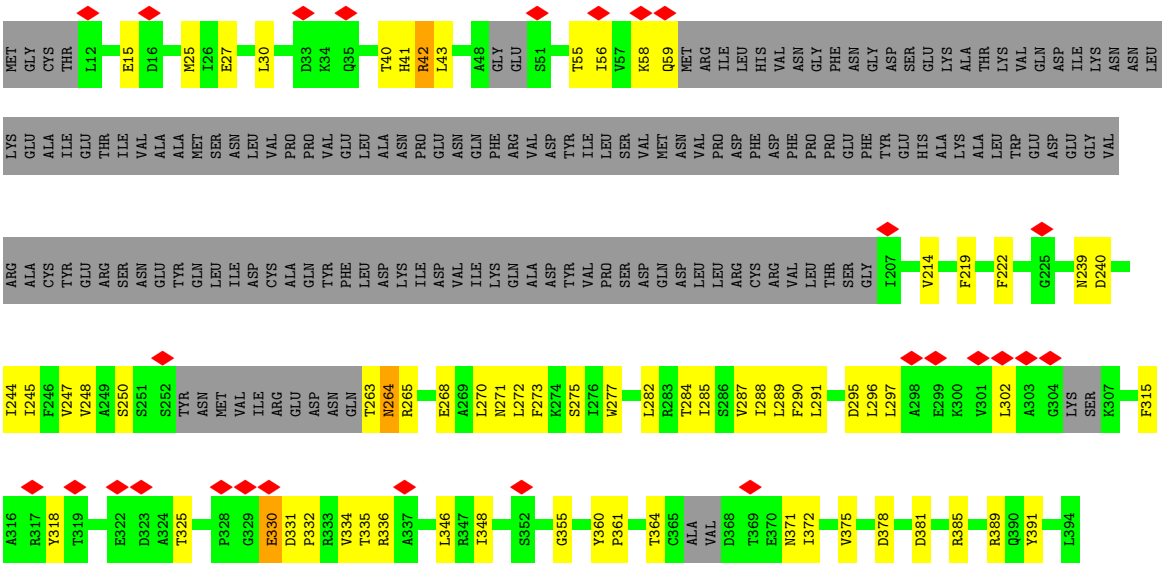
3 Residue-property plots (i)

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: Isoform Gnas-2 of Guanine nucleotide-binding protein G(s) subunit alpha isoforms short

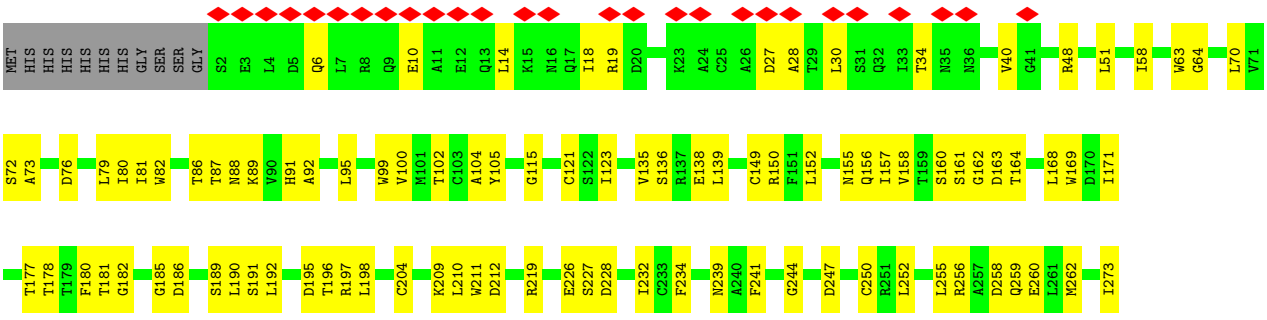
Chain A:

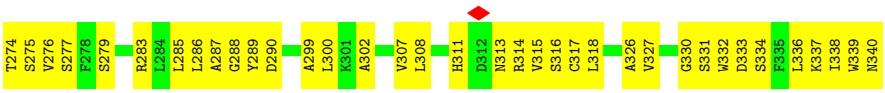




• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

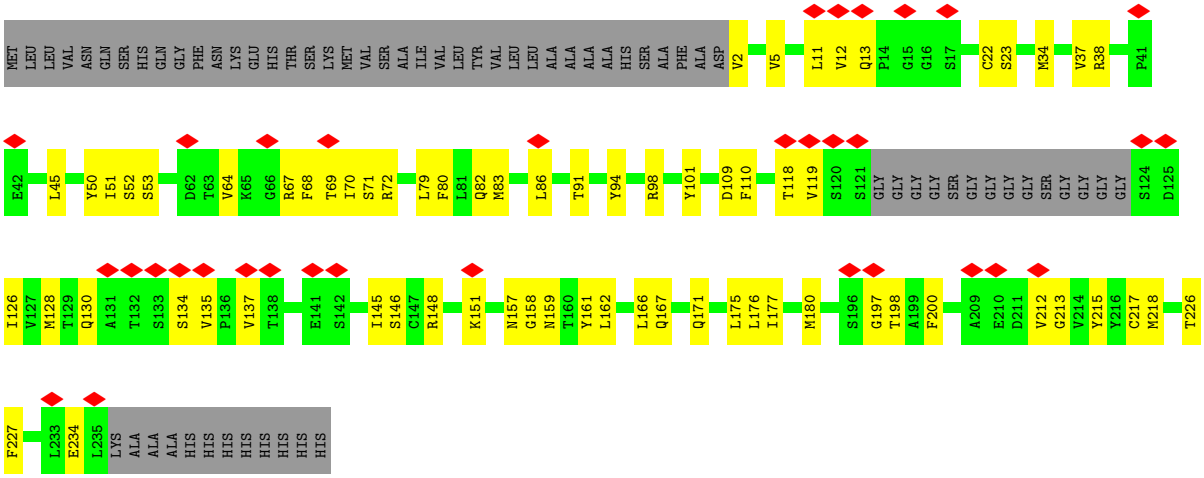
Chain B:





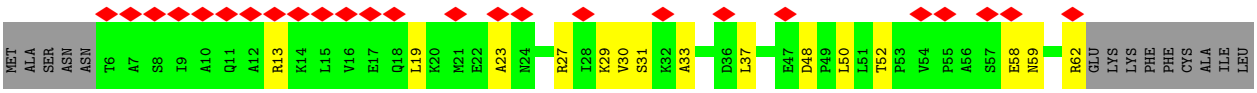
• Molecule 3: Single-chain variable fragment 16

Chain E:



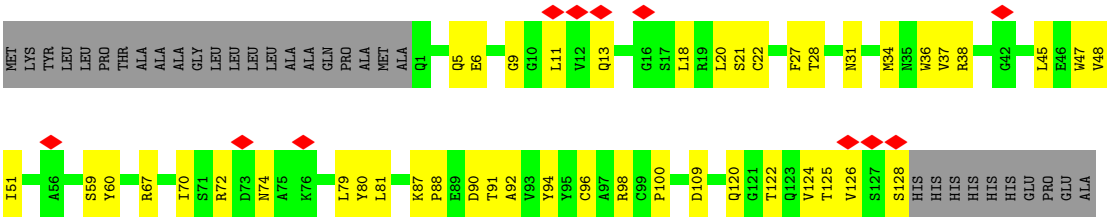
• Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G:



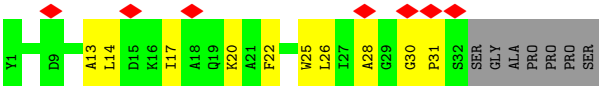
• Molecule 5: nanobody 35

Chain N:



• Molecule 6: Tirzepatide

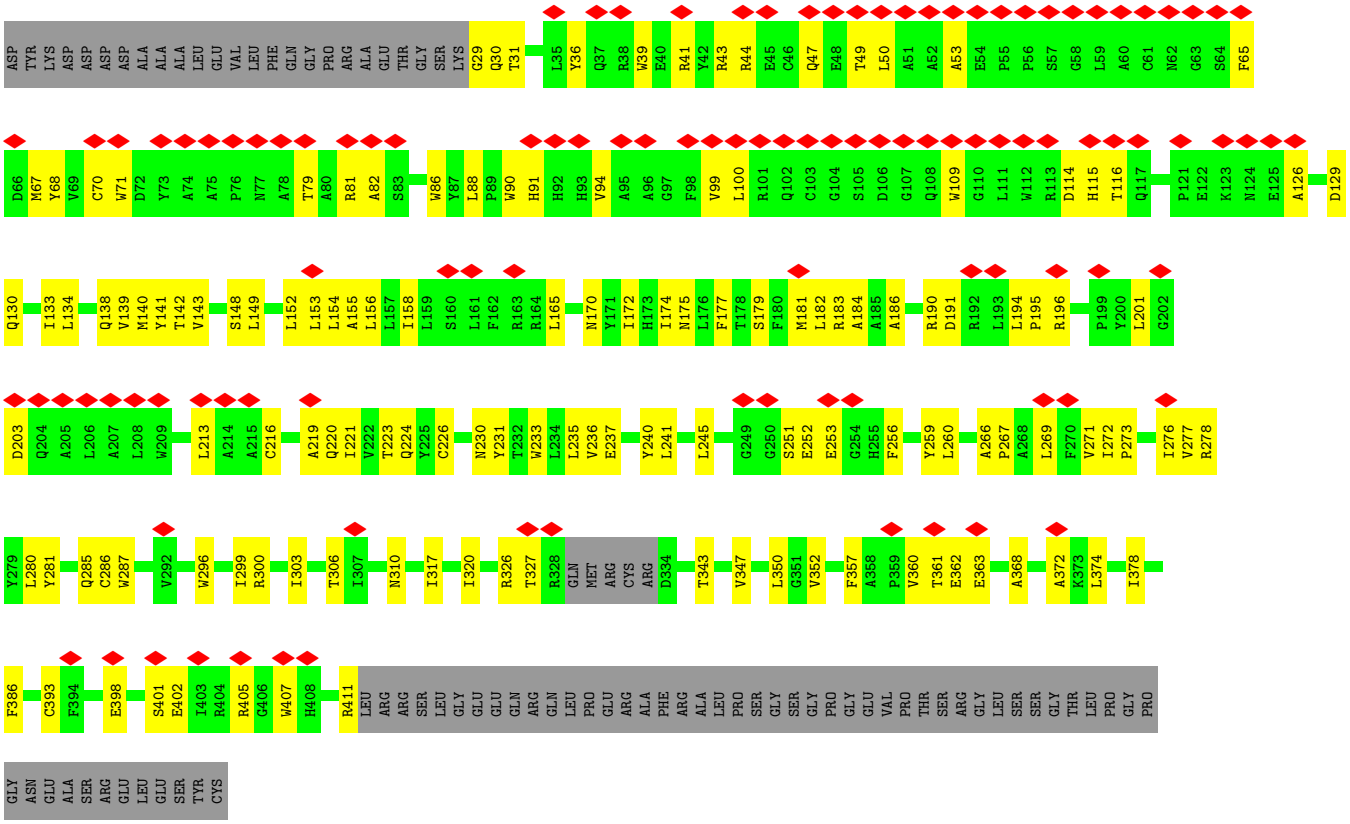
Chain P:



• Molecule 7: Gastric inhibitory polypeptide receptor

Chain R:

24%
52%
30%
18%


ASP TYR LYS ASP ASP ASP ASP ALA ALA ALA LEU GLU VAL LEU PHE GLN GLY PRO ARG ALA GLU THR GLY SER LYS G29 Q30 T31 L35 Y36 Q37 R38 W39 E40 R41 Y42 R43 R44 E45 C46 Q47 E48 T49 L50 A51 A52 A53 E54 P55 P56 S57 G58 L59 A60 C61 N62 G63 S64 F65
D66 M67 Y68 V69 C70 W71 D72 Y73 A74 A75 P76 N77 A78 T79 A80 R81 A82 S83 W86 Y87 L88 P89 W90 H91 H92 H93 V94 A95 A96 G97 F98 V99 L100 R101 Q102 C103 G104 S105 D106 G107 Q108 W109 G110 L111 W112 R113 D114 H115 T116 Q117 P121 E122 K123 N124 E125 A126 D129
Q130 I133 L134 Q138 V139 M140 Y141 T142 V143 S148 L149 L152 L153 L154 A155 L156 L157 I158 L159 S160 L161 F162 R163 R164 L165 N170 Y171 I172 H173 I174 N175 L176 F177 T178 S179 F180 M181 L182 R183 A184 A185 A186 R190 D191 R192 L193 L194 P195 R196 P199 Y200 L201 G202
D203 Q204 A205 L206 A207 L208 W209 L213 A214 A215 C216 A219 Q220 I221 V222 T223 Q224 Y225 C226 N230 Y231 T232 W233 L234 L235 V236 E237 Y240 L241 L245 G249 G250 S251 E252 E253 G254 H255 F256 Y259 L260 A266 P267 A268 L269 F270 V271 I272 P273 I276 V277 R278
Y279 L280 Y281 Q285 C286 W287 V292 W296 I299 R300 I303 T306 I307 N310 I317 I320 R326 T327 R328 GLN MET ARG CYS ARG D334 T343 V347 L350 G351 V352 F357 A358 P359 V360 T361 E362 E363 A368 A372 K373 L374 I378
F386 C393 F394 E398 S401 E402 I403 R404 R405 G406 W407 H408 R411 LEU ARG ARG SER LEU GLY GLU GLU GLN ARG GLN LEU PRO GLU ARG ALA PHE ARG ALA LEU PRO SER GLY SER GLY PRO GLY GLU VAL PRO THR SER ARG GLY LEU SER SER GLY THR LEU PRO GLY PRO
GLY ASN GLU ALA SER ARG GLU LEU GLU SER TYR CYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	259349	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	53.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.091	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	249.6, 249.6, 249.6	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	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: AIB, 41Y

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	0.38	0/1824	0.48	0/2454
2	B	0.36	0/2627	0.54	0/3564
3	E	0.37	0/1792	0.50	0/2434
4	G	0.32	0/442	0.55	0/597
5	N	0.38	0/989	0.51	0/1341
6	P	0.41	0/240	0.45	0/325
7	R	0.40	0/3158	0.51	0/4301
All	All	0.38	0/11072	0.51	0/15016

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1792	0	1752	55	0
2	B	2581	0	2473	120	0
3	E	1748	0	1673	53	0
4	G	436	0	448	19	0
5	N	969	0	927	41	0
6	P	246	0	242	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	R	3072	0	3060	104	0
8	R	37	0	0	0	0
All	All	10881	0	10575	379	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 18.

All (379) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:LEU:HD21	2:B:157:ILE:HD11	1.59	0.84
6:P:26:LEU:HD21	7:R:68:TYR:HB3	1.61	0.82
7:R:190:ARG:NH2	7:R:191:ASP:OD1	2.13	0.81
2:B:139:LEU:HD12	2:B:139:LEU:O	1.82	0.80
3:E:82:GLN:NE2	3:E:83:MET:O	2.15	0.78
7:R:310:ASN:OD1	7:R:350:LEU:HD22	1.84	0.78
2:B:210:LEU:HD13	2:B:255:LEU:HD11	1.63	0.77
1:A:289:LEU:HD21	1:A:291:LEU:HD21	1.64	0.77
3:E:166:LEU:HB2	3:E:176:LEU:HD11	1.68	0.75
7:R:245:LEU:HD13	7:R:320:ILE:HD11	1.69	0.73
7:R:49:THR:O	7:R:53:ALA:N	2.23	0.71
2:B:195:ASP:O	2:B:196:THR:OG1	2.09	0.71
6:P:26:LEU:HD21	7:R:68:TYR:CB	2.20	0.71
7:R:278:ARG:HE	7:R:287:TRP:HA	1.57	0.70
1:A:27:GLU:OE2	2:B:89:LYS:NZ	2.25	0.70
2:B:27:ASP:OD1	2:B:28:ALA:N	2.25	0.69
2:B:244:GLY:HA2	2:B:273:ILE:HD11	1.73	0.69
2:B:58:ILE:HD11	2:B:330:GLY:HA3	1.73	0.69
2:B:123:ILE:O	2:B:136:SER:N	2.26	0.69
3:E:130:GLN:NE2	3:E:146:SER:O	2.25	0.69
2:B:160:SER:HB3	2:B:190:LEU:HD23	1.76	0.68
5:N:47:TRP:NE1	5:N:49:SER:O	2.26	0.68
7:R:343:THR:O	7:R:347:VAL:HG23	1.94	0.68
7:R:213:LEU:HD22	7:R:285:GLN:O	1.94	0.68
2:B:262:MET:CE	2:B:302:ALA:HB2	2.25	0.67
5:N:9:GLY:HA2	5:N:124:VAL:HG22	1.75	0.67
3:E:166:LEU:HD13	3:E:215:TYR:CE1	2.29	0.67
1:A:290:PHE:CD2	1:A:364:THR:HG21	2.30	0.66
2:B:274:THR:O	2:B:275:SER:OG	2.14	0.66
2:B:87:THR:O	2:B:87:THR:HG22	1.94	0.66
2:B:258:ASP:OD2	4:G:27:ARG:NH1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:ASP:OD1	4:G:29:LYS:NZ	2.27	0.66
1:A:214:VAL:HG11	1:A:372:ILE:HG21	1.78	0.66
2:B:182:GLY:O	2:B:209:LYS:NZ	2.28	0.65
2:B:189:SER:OG	2:B:232:ILE:HG22	1.97	0.65
7:R:90:TRP:O	7:R:94:VAL:HG22	1.97	0.65
2:B:95:LEU:HD13	2:B:100:VAL:HG11	1.78	0.65
2:B:58:ILE:HD11	2:B:330:GLY:CA	2.27	0.65
3:E:167:GLN:NE2	3:E:171:GLN:O	2.30	0.64
2:B:307:VAL:O	2:B:308:LEU:HD23	1.98	0.63
5:N:13:GLN:NE2	5:N:128:SER:O	2.32	0.63
7:R:31:THR:HG21	7:R:285:GLN:NE2	2.14	0.63
3:E:71:SER:O	3:E:80:PHE:N	2.31	0.62
4:G:52:THR:O	4:G:52:THR:HG23	1.99	0.62
5:N:6:GLU:OE2	5:N:96:CYS:N	2.32	0.62
3:E:137:VAL:N	3:E:234:GLU:O	2.29	0.62
4:G:19:LEU:O	4:G:23:ALA:N	2.31	0.62
6:P:26:LEU:HD21	7:R:68:TYR:CG	2.34	0.62
7:R:190:ARG:HE	7:R:223:THR:HG21	1.65	0.62
2:B:262:MET:HE2	2:B:302:ALA:HB2	1.81	0.61
2:B:286:LEU:HB3	2:B:318:LEU:HD21	1.81	0.61
1:A:391:TYR:CE2	7:R:241:LEU:HD13	2.35	0.61
2:B:164:THR:HG22	2:B:185:GLY:O	2.00	0.61
2:B:79:LEU:HD22	2:B:95:LEU:HD11	1.83	0.60
1:A:295:ASP:OD1	1:A:296:LEU:N	2.35	0.60
5:N:120:GLN:OE1	5:N:120:GLN:N	2.34	0.60
7:R:50:LEU:HD11	7:R:70:CYS:HB2	1.83	0.60
1:A:263:THR:OG1	1:A:264:ASN:N	2.34	0.60
5:N:9:GLY:HA2	5:N:18:LEU:HD21	1.84	0.60
7:R:129:ASP:OD1	7:R:130:GLN:N	2.34	0.60
7:R:194:LEU:HD22	7:R:219:ALA:HB2	1.83	0.60
2:B:80:ILE:HG22	2:B:92:ALA:HA	1.85	0.59
7:R:156:LEU:HD13	7:R:177:PHE:HB2	1.83	0.59
1:A:284:THR:O	1:A:284:THR:HG22	2.03	0.59
2:B:244:GLY:CA	2:B:273:ILE:HD11	2.33	0.59
2:B:283:ARG:O	2:B:299:ALA:HB3	2.02	0.59
3:E:166:LEU:HD11	3:E:213:GLY:HA3	1.83	0.59
7:R:360:VAL:HG13	7:R:360:VAL:O	2.02	0.59
2:B:51:LEU:HD23	2:B:82:TRP:CD2	2.38	0.59
7:R:280:LEU:HD12	7:R:281:TYR:CD1	2.38	0.59
7:R:194:LEU:HD23	7:R:216:CYS:HA	1.86	0.58
5:N:70:ILE:HD13	5:N:81:LEU:HD13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LEU:HD21	1:A:361:PRO:HG2	1.84	0.58
7:R:194:LEU:HD22	7:R:219:ALA:CB	2.32	0.58
5:N:49:SER:CB	5:N:70:ILE:HD11	2.33	0.58
2:B:210:LEU:CD1	2:B:255:LEU:HD21	2.34	0.57
7:R:300:ARG:HG2	7:R:303:ILE:HD11	1.86	0.57
7:R:29:GLY:O	7:R:30:GLN:NE2	2.36	0.57
1:A:287:VAL:HG23	1:A:287:VAL:O	2.04	0.57
3:E:157:ASN:OD1	3:E:158:GLY:N	2.38	0.57
2:B:80:ILE:HD11	2:B:82:TRP:CZ2	2.39	0.57
7:R:186:ALA:HB1	7:R:223:THR:HA	1.87	0.57
2:B:232:ILE:HD11	2:B:241:PHE:CE1	2.39	0.57
2:B:150:ARG:HG3	2:B:192:LEU:HD13	1.86	0.56
1:A:42:ARG:O	1:A:43:LEU:HD23	2.05	0.56
1:A:277:TRP:HZ3	1:A:287:VAL:HG22	1.68	0.56
2:B:315:VAL:HG23	2:B:315:VAL:O	2.05	0.56
3:E:64:VAL:HG11	3:E:68:PHE:CE2	2.39	0.56
7:R:114:ASP:OD2	7:R:116:THR:OG1	2.24	0.56
7:R:269:LEU:HD23	7:R:269:LEU:O	2.05	0.56
7:R:357:PHE:O	7:R:360:VAL:HG12	2.05	0.56
3:E:162:LEU:HD11	3:E:217:CYS:HB2	1.87	0.55
7:R:182:LEU:HG	7:R:226:CYS:SG	2.47	0.55
2:B:195:ASP:OD2	2:B:197:ARG:NH2	2.39	0.55
1:A:239:ASN:OD1	1:A:240:ASP:N	2.39	0.54
7:R:278:ARG:HE	7:R:287:TRP:CA	2.20	0.54
2:B:102:THR:HG22	2:B:115:GLY:O	2.07	0.54
2:B:34:THR:HG21	2:B:300:LEU:HD12	1.89	0.54
2:B:150:ARG:O	2:B:157:ILE:HG22	2.07	0.54
5:N:20:LEU:HD23	5:N:20:LEU:H	1.71	0.54
7:R:172:ILE:HG22	7:R:237:GLU:OE1	2.07	0.54
3:E:69:THR:O	3:E:82:GLN:N	2.37	0.54
2:B:163:ASP:O	2:B:164:THR:OG1	2.22	0.54
3:E:159:ASN:HB2	3:E:161:TYR:CE1	2.43	0.54
5:N:67:ARG:NH2	5:N:90:ASP:OD2	2.41	0.54
3:E:166:LEU:CB	3:E:176:LEU:HD11	2.38	0.53
7:R:194:LEU:O	7:R:196:ARG:NE	2.41	0.53
3:E:91:THR:HG23	3:E:118:THR:HA	1.89	0.53
1:A:244:ILE:O	1:A:244:ILE:HG22	2.09	0.53
7:R:152:LEU:HD21	7:R:177:PHE:O	2.09	0.53
3:E:98:ARG:NE	3:E:109:ASP:OD1	2.37	0.53
7:R:362:GLU:O	7:R:363:GLU:HG2	2.08	0.53
5:N:28:THR:HG23	5:N:28:THR:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:87:LYS:O	5:N:126:VAL:HG11	2.09	0.53
7:R:235:LEU:HB2	7:R:306:THR:OG1	2.09	0.53
5:N:70:ILE:CD1	5:N:81:LEU:HD13	2.39	0.52
1:A:15:GLU:HG2	3:E:161:TYR:CE2	2.44	0.52
3:E:70:ILE:HG23	3:E:70:ILE:O	2.10	0.52
7:R:172:ILE:HD11	7:R:259:TYR:OH	2.09	0.52
2:B:95:LEU:CD1	2:B:100:VAL:HG11	2.40	0.52
2:B:308:LEU:HD22	2:B:339:TRP:CD1	2.44	0.52
4:G:30:VAL:HG13	4:G:31:SER:N	2.25	0.52
7:R:149:LEU:HD21	7:R:184:ALA:HB3	1.91	0.52
7:R:224:GLN:HE21	7:R:299:ILE:HG21	1.74	0.52
7:R:352:VAL:HG22	7:R:352:VAL:O	2.10	0.52
1:A:330:GLU:OE2	1:A:335:THR:OG1	2.27	0.52
2:B:79:LEU:CD2	2:B:95:LEU:HD21	2.40	0.51
4:G:29:LYS:HD3	4:G:30:VAL:N	2.24	0.51
7:R:266:ALA:N	7:R:267:PRO:CD	2.73	0.51
7:R:165:LEU:O	7:R:165:LEU:HG	2.10	0.51
1:A:355:GLY:O	1:A:389:ARG:NH1	2.43	0.51
3:E:162:LEU:HD12	3:E:218:MET:O	2.10	0.51
7:R:126:ALA:O	7:R:130:GLN:HB2	2.11	0.51
5:N:49:SER:HB2	5:N:70:ILE:HD11	1.93	0.51
5:N:88:PRO:HA	5:N:126:VAL:HG21	1.93	0.51
2:B:30:LEU:O	2:B:34:THR:HG23	2.11	0.50
5:N:20:LEU:HD21	5:N:81:LEU:HD23	1.94	0.50
5:N:34:MET:CB	5:N:79:LEU:HD13	2.40	0.50
2:B:286:LEU:CB	2:B:318:LEU:HD21	2.41	0.50
5:N:36:TRP:HE1	5:N:79:LEU:CD2	2.25	0.50
7:R:175:ASN:OD1	7:R:233:TRP:CE3	2.65	0.50
1:A:315:PHE:O	1:A:336:ARG:NH2	2.44	0.50
7:R:41:ARG:O	7:R:44:ARG:HG2	2.10	0.50
7:R:251:SER:OG	7:R:252:GLU:N	2.44	0.50
7:R:39:TRP:NE1	7:R:67:MET:O	2.44	0.50
2:B:191:SER:OG	2:B:234:PHE:N	2.42	0.50
2:B:326:ALA:HB1	2:B:338:ILE:HG23	1.93	0.50
7:R:99:VAL:HG23	7:R:99:VAL:O	2.11	0.50
7:R:138:GLN:HA	7:R:141:TYR:CE2	2.46	0.49
1:A:214:VAL:O	1:A:214:VAL:HG23	2.12	0.49
2:B:63:TRP:CZ3	2:B:70:LEU:HD23	2.47	0.49
3:E:71:SER:N	3:E:80:PHE:O	2.40	0.49
7:R:361:THR:O	7:R:361:THR:HG22	2.11	0.49
2:B:51:LEU:HD23	2:B:82:TRP:CG	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:ASP:OD1	2:B:314:ARG:NE	2.44	0.49
1:A:288:ILE:HG22	1:A:289:LEU:N	2.28	0.49
2:B:178:THR:HG23	2:B:180:PHE:CE1	2.48	0.49
7:R:71:TRP:HD1	7:R:109:TRP:CZ2	2.30	0.49
2:B:34:THR:HG21	2:B:300:LEU:CD1	2.43	0.49
2:B:64:GLY:HA2	2:B:105:TYR:HD2	1.78	0.49
7:R:245:LEU:HD12	7:R:317:ILE:HD12	1.94	0.49
3:E:197:GLY:O	3:E:198:THR:OG1	2.27	0.49
1:A:372:ILE:HD12	1:A:372:ILE:H	1.78	0.49
2:B:232:ILE:HD11	2:B:241:PHE:CD1	2.48	0.49
2:B:276:VAL:O	2:B:277:SER:OG	2.30	0.49
4:G:29:LYS:HZ2	4:G:31:SER:CB	2.25	0.48
1:A:250:SER:HB2	1:A:297:LEU:HD12	1.94	0.48
1:A:318:TYR:O	1:A:336:ARG:NE	2.45	0.48
5:N:34:MET:HB2	5:N:79:LEU:CD1	2.43	0.48
7:R:172:ILE:HD12	7:R:240:TYR:CD2	2.48	0.48
2:B:64:GLY:HA2	2:B:105:TYR:CD2	2.48	0.48
5:N:91:THR:HG23	5:N:91:THR:O	2.13	0.48
1:A:346:LEU:HD21	1:A:361:PRO:CG	2.43	0.48
2:B:138:GLU:O	2:B:138:GLU:HG2	2.13	0.48
7:R:79:THR:O	7:R:81:ARG:NH1	2.46	0.48
7:R:175:ASN:OD1	7:R:233:TRP:CD2	2.67	0.48
1:A:282:LEU:HD12	1:A:282:LEU:N	2.29	0.48
2:B:313:ASN:HB3	2:B:332:TRP:HB2	1.95	0.48
5:N:37:VAL:CG1	5:N:45:LEU:HD12	2.43	0.48
1:A:270:LEU:HD13	1:A:348:ILE:HD11	1.96	0.48
7:R:233:TRP:CE3	7:R:236:VAL:HG21	2.49	0.48
1:A:302:LEU:HD21	1:A:331:ASP:HB2	1.95	0.48
3:E:145:ILE:HG22	3:E:146:SER:N	2.28	0.48
2:B:150:ARG:HG2	2:B:190:LEU:HD11	1.96	0.48
2:B:276:VAL:HG13	2:B:285:LEU:HD11	1.95	0.48
2:B:135:VAL:HG13	2:B:135:VAL:O	2.13	0.47
7:R:179:SER:OG	7:R:230:ASN:HA	2.14	0.47
1:A:381:ASP:O	1:A:385:ARG:HG3	2.13	0.47
3:E:175:LEU:HD11	3:E:177:ILE:O	2.14	0.47
4:G:30:VAL:O	4:G:33:ALA:N	2.47	0.47
5:N:88:PRO:HA	5:N:126:VAL:HG11	1.96	0.47
2:B:6:GLN:O	2:B:10:GLU:HG3	2.15	0.47
2:B:287:ALA:HB3	2:B:289:TYR:HE1	1.79	0.47
2:B:317:CYS:SG	2:B:330:GLY:N	2.87	0.47
3:E:64:VAL:HG12	3:E:67:ARG:HH21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:212:VAL:HG23	3:E:212:VAL:O	2.15	0.47
4:G:58:GLU:N	4:G:58:GLU:OE2	2.47	0.47
4:G:62:ARG:HH11	4:G:62:ARG:HG3	1.78	0.47
1:A:289:LEU:CD2	1:A:291:LEU:HD21	2.39	0.47
2:B:250:CYS:SG	2:B:273:ILE:HD13	2.54	0.47
2:B:276:VAL:CG1	2:B:285:LEU:HD11	2.45	0.47
7:R:65:PHE:CE2	7:R:67:MET:HA	2.49	0.47
3:E:50:TYR:OH	3:E:52:SER:HB3	2.15	0.47
6:P:30:GLY:N	6:P:31:PRO:HD2	2.29	0.47
2:B:177:THR:HG22	2:B:177:THR:O	2.14	0.47
5:N:37:VAL:HG11	5:N:45:LEU:HD12	1.97	0.47
7:R:82:ALA:HB3	7:R:99:VAL:HG22	1.97	0.47
7:R:140:MET:O	7:R:143:VAL:HG12	2.15	0.46
7:R:36:TYR:CE2	7:R:201:LEU:HD12	2.49	0.46
7:R:156:LEU:HD11	7:R:174:ILE:HG23	1.97	0.46
1:A:248:VAL:O	1:A:248:VAL:HG13	2.15	0.46
3:E:128:MET:HE1	3:E:226:THR:O	2.16	0.46
5:N:38:ARG:HG3	5:N:92:ALA:HB3	1.98	0.46
2:B:152:LEU:HD22	2:B:196:THR:HB	1.97	0.46
1:A:364:THR:HG22	1:A:371:ASN:ND2	2.31	0.46
6:P:26:LEU:CD2	7:R:68:TYR:CG	2.98	0.46
7:R:153:LEU:HD23	7:R:153:LEU:O	2.15	0.46
1:A:325:THR:HG22	1:A:325:THR:O	2.15	0.46
2:B:150:ARG:CG	2:B:190:LEU:HD11	2.46	0.46
6:P:13:AIB:O	6:P:17:ILE:HG22	2.16	0.46
2:B:168:LEU:HB3	2:B:178:THR:HG22	1.98	0.46
2:B:227:SER:OG	2:B:228:ASP:N	2.43	0.46
5:N:72:ARG:NE	5:N:74:ASN:OD1	2.35	0.46
2:B:198:LEU:HD12	2:B:210:LEU:HD11	1.97	0.45
7:R:303:ILE:O	7:R:306:THR:HG22	2.16	0.45
7:R:402:GLU:OE2	7:R:405:ARG:NH1	2.46	0.45
7:R:233:TRP:CZ2	7:R:260:LEU:HD12	2.50	0.45
2:B:279:SER:HG	4:G:48:ASP:CG	2.20	0.45
2:B:327:VAL:CG2	4:G:50:LEU:HD11	2.46	0.45
6:P:26:LEU:O	6:P:26:LEU:HD23	2.16	0.45
2:B:161:SER:OG	2:B:162:GLY:N	2.50	0.45
2:B:307:VAL:HG12	2:B:308:LEU:N	2.31	0.45
3:E:2:VAL:HG12	3:E:2:VAL:O	2.17	0.45
3:E:5:VAL:O	3:E:23:SER:N	2.42	0.45
7:R:100:LEU:H	7:R:100:LEU:HD23	1.81	0.45
7:R:231:TYR:HB3	7:R:306:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:233:TRP:CE3	7:R:236:VAL:CG2	2.99	0.45
7:R:326:ARG:HG3	7:R:327:THR:N	2.32	0.45
1:A:273:PHE:CE2	1:A:287:VAL:HG21	2.52	0.45
3:E:126:ILE:HG12	3:E:151:LYS:HB3	1.98	0.45
3:E:180:MET:O	3:E:180:MET:HG2	2.16	0.45
7:R:88:LEU:HD23	7:R:90:TRP:H	1.82	0.45
2:B:40:VAL:CG2	2:B:283:ARG:HE	2.30	0.45
2:B:337:LYS:HB3	2:B:339:TRP:CZ3	2.51	0.45
5:N:9:GLY:CA	5:N:124:VAL:HG22	2.44	0.45
2:B:121:CYS:HB3	2:B:139:LEU:HD11	1.99	0.45
2:B:290:ASP:OD2	2:B:314:ARG:NH1	2.50	0.45
7:R:398:GLU:O	7:R:401:SER:OG	2.27	0.45
2:B:72:SER:O	2:B:79:LEU:HA	2.17	0.44
2:B:158:VAL:HG13	2:B:158:VAL:O	2.16	0.44
2:B:252:LEU:HD23	2:B:252:LEU:O	2.17	0.44
2:B:259:GLN:NE2	2:B:260:GLU:O	2.49	0.44
3:E:11:LEU:HA	3:E:118:THR:HG23	2.00	0.44
5:N:28:THR:HG21	5:N:31:ASN:OD1	2.16	0.44
6:P:26:LEU:HD23	6:P:26:LEU:C	2.38	0.44
7:R:31:THR:HG21	7:R:285:GLN:HE21	1.80	0.44
2:B:155:ASN:O	2:B:171:ILE:N	2.43	0.44
7:R:221:ILE:HD11	7:R:271:VAL:CG1	2.47	0.44
6:P:25:TRP:O	6:P:28:ALA:HB3	2.16	0.44
7:R:115:HIS:O	7:R:115:HIS:CG	2.70	0.44
1:A:282:LEU:HA	1:A:285:ILE:HD13	1.99	0.44
2:B:239:ASN:HB3	2:B:256:ARG:HE	1.82	0.44
5:N:126:VAL:HG23	5:N:126:VAL:O	2.18	0.44
7:R:374:LEU:O	7:R:378:ILE:HG12	2.17	0.44
1:A:277:TRP:CZ3	1:A:287:VAL:HG22	2.51	0.44
7:R:368:ALA:O	7:R:372:ALA:HB3	2.17	0.44
1:A:360:TYR:HD2	1:A:378:ASP:HB3	1.83	0.44
2:B:95:LEU:HD13	2:B:100:VAL:CG1	2.46	0.44
2:B:279:SER:OG	4:G:48:ASP:OD1	2.36	0.44
2:B:311:HIS:CE1	2:B:331:SER:HG	2.30	0.44
7:R:44:ARG:HA	7:R:47:GLN:OE1	2.18	0.44
2:B:274:THR:HG22	2:B:288:GLY:O	2.18	0.43
1:A:25:MET:HE1	3:E:53:SER:O	2.19	0.43
1:A:41:HIS:HB2	1:A:219:PHE:CD1	2.53	0.43
5:N:11:LEU:HA	5:N:125:THR:OG1	2.18	0.43
7:R:149:LEU:HD22	7:R:181:MET:SD	2.59	0.43
7:R:233:TRP:HA	7:R:236:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:276:ILE:HG13	7:R:277:VAL:N	2.33	0.43
3:E:51:ILE:HG23	3:E:51:ILE:O	2.17	0.43
7:R:154:LEU:O	7:R:158:ILE:HG12	2.18	0.43
1:A:248:VAL:CG1	1:A:291:LEU:HD23	2.48	0.43
1:A:268:GLU:O	1:A:271:ASN:OD1	2.37	0.43
2:B:283:ARG:O	2:B:299:ALA:CB	2.66	0.43
5:N:38:ARG:NH1	5:N:48:VAL:HG22	2.34	0.43
7:R:139:VAL:O	7:R:142:THR:HG22	2.18	0.43
2:B:252:LEU:HD23	2:B:252:LEU:C	2.39	0.43
7:R:220:GLN:O	7:R:223:THR:HG22	2.19	0.43
2:B:333:ASP:O	2:B:334:SER:CB	2.66	0.43
2:B:156:GLN:HB2	2:B:169:TRP:O	2.17	0.43
3:E:22:CYS:HB3	3:E:79:LEU:HB3	1.99	0.43
3:E:34:MET:O	3:E:50:TYR:HD1	2.01	0.43
3:E:130:GLN:OE1	3:E:217:CYS:SG	2.76	0.43
1:A:56:ILE:HD12	1:A:56:ILE:H	1.83	0.43
2:B:123:ILE:HD11	2:B:157:ILE:HD13	2.00	0.43
3:E:162:LEU:HD22	3:E:200:PHE:CG	2.54	0.43
2:B:58:ILE:O	2:B:316:SER:OG	2.37	0.43
3:E:70:ILE:HA	3:E:80:PHE:O	2.18	0.43
7:R:183:ARG:CD	7:R:230:ASN:HD22	2.32	0.43
2:B:104:ALA:HB2	2:B:149:CYS:O	2.19	0.43
3:E:218:MET:HG3	3:E:227:PHE:CE1	2.54	0.43
1:A:245:ILE:HD11	1:A:375:VAL:HG21	2.00	0.42
2:B:186:ASP:O	2:B:204:CYS:N	2.51	0.42
3:E:134:SER:O	3:E:135:VAL:HG13	2.19	0.42
4:G:13:ARG:HG2	4:G:13:ARG:HH11	1.84	0.42
1:A:272:LEU:O	1:A:275:SER:OG	2.28	0.42
3:E:12:VAL:HG22	3:E:13:GLN:N	2.34	0.42
7:R:86:TRP:HB2	7:R:91:HIS:ND1	2.35	0.42
2:B:87:THR:O	2:B:87:THR:CG2	2.64	0.42
2:B:86:THR:OG1	2:B:88:ASN:OD1	2.23	0.42
3:E:72:ARG:HB3	3:E:79:LEU:HD12	2.01	0.42
7:R:183:ARG:HH11	7:R:230:ASN:HD22	1.67	0.42
2:B:181:THR:HG22	2:B:182:GLY:N	2.34	0.42
2:B:212:ASP:OD2	2:B:219:ARG:NH1	2.43	0.42
3:E:109:ASP:OD1	3:E:110:PHE:N	2.52	0.42
4:G:52:THR:O	4:G:52:THR:CG2	2.67	0.42
5:N:5:GLN:O	5:N:22:CYS:HA	2.19	0.42
5:N:59:SER:OG	5:N:60:TYR:N	2.52	0.42
7:R:139:VAL:HA	7:R:142:THR:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ILE:HD13	1:A:247:VAL:HG21	2.02	0.42
1:A:222:PHE:CE2	2:B:99:TRP:HZ2	2.37	0.42
2:B:18:ILE:HD11	4:G:23:ALA:HA	2.01	0.42
2:B:73:ALA:HB1	2:B:100:VAL:HG21	2.01	0.42
2:B:81:ILE:HD13	2:B:91:HIS:HB2	2.02	0.42
3:E:51:ILE:CG2	3:E:79:LEU:HD11	2.49	0.42
5:N:51:ILE:HD13	5:N:72:ARG:CB	2.49	0.42
7:R:286:CYS:O	7:R:287:TRP:HB2	2.19	0.42
1:A:27:GLU:OE2	2:B:89:LYS:CE	2.67	0.42
2:B:72:SER:OG	2:B:336:LEU:HD11	2.20	0.42
1:A:15:GLU:OE2	3:E:101:TYR:CD2	2.73	0.42
1:A:244:ILE:O	1:A:245:ILE:C	2.56	0.42
3:E:137:VAL:HG22	3:E:234:GLU:O	2.20	0.42
5:N:38:ARG:NH2	5:N:94:TYR:OH	2.52	0.42
5:N:98:ARG:NH1	5:N:100:PRO:O	2.53	0.42
7:R:133:ILE:HG23	7:R:134:LEU:HD12	2.01	0.42
2:B:48:ARG:HE	2:B:340:ASN:HB3	1.85	0.42
1:A:331:ASP:OD1	1:A:332:PRO:HD2	2.20	0.41
2:B:327:VAL:HG23	4:G:50:LEU:HD11	2.02	0.41
3:E:37:VAL:HG11	3:E:45:LEU:HD12	2.02	0.41
7:R:148:SER:HA	7:R:386:PHE:HB2	2.02	0.41
7:R:253:GLU:O	7:R:256:PHE:HB3	2.19	0.41
7:R:296:TRP:HE1	7:R:300:ARG:HE	1.67	0.41
5:N:6:GLU:HB3	5:N:122:THR:HG23	2.02	0.41
6:P:14:LEU:HA	6:P:17:ILE:HG22	2.02	0.41
7:R:273:PRO:HA	7:R:276:ILE:HG12	2.01	0.41
2:B:247:ASP:OD1	2:B:247:ASP:C	2.58	0.41
3:E:146:SER:OG	3:E:148:ARG:NH2	2.53	0.41
7:R:190:ARG:O	7:R:195:PRO:CD	2.68	0.41
1:A:239:ASN:ND2	2:B:332:TRP:CZ3	2.89	0.41
2:B:340:ASN:ND2	4:G:59:ASN:OD1	2.54	0.41
5:N:34:MET:HB2	5:N:79:LEU:HD13	2.01	0.41
5:N:36:TRP:NE1	5:N:79:LEU:CD2	2.83	0.41
7:R:231:TYR:CD2	7:R:303:ILE:HG22	2.56	0.41
2:B:252:LEU:HD11	4:G:37:LEU:HD21	2.01	0.41
1:A:30:LEU:HD12	2:B:89:LYS:HE2	2.02	0.41
1:A:331:ASP:O	1:A:334:VAL:HB	2.20	0.41
2:B:19:ARG:HB2	2:B:19:ARG:HH11	1.85	0.41
5:N:70:ILE:HD13	5:N:81:LEU:CD1	2.51	0.41
7:R:155:ALA:HB1	7:R:393:CYS:HB2	2.02	0.41
7:R:272:ILE:N	7:R:273:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:407:TRP:O	7:R:411:ARG:HG2	2.20	0.41
3:E:166:LEU:HD11	3:E:213:GLY:CA	2.47	0.41
2:B:158:VAL:CG1	2:B:192:LEU:HD11	2.51	0.40
5:N:21:SER:HB3	5:N:80:TYR:HD1	1.86	0.40
2:B:180:PHE:O	2:B:211:TRP:CH2	2.74	0.40
2:B:226:GLU:HG2	5:N:27:PHE:HA	2.02	0.40
7:R:280:LEU:HD12	7:R:281:TYR:N	2.36	0.40
1:A:58:LYS:O	1:A:59:GLN:C	2.60	0.40
2:B:14:LEU:O	2:B:18:ILE:HG12	2.22	0.40
3:E:166:LEU:HD13	3:E:215:TYR:CD1	2.56	0.40
7:R:43:ARG:HG3	7:R:65:PHE:CE2	2.57	0.40
7:R:170:ASN:O	7:R:174:ILE:HG12	2.22	0.40
1:A:55:THR:HG22	1:A:371:ASN:OD1	2.22	0.40
1:A:265:ARG:HA	1:A:268:GLU:OE1	2.22	0.40
2:B:79:LEU:HD22	2:B:95:LEU:HD21	2.03	0.40
2:B:262:MET:HE3	2:B:302:ALA:HB2	1.99	0.40
3:E:38:ARG:HG2	3:E:94:TYR:CE2	2.56	0.40
3:E:86:LEU:HD13	3:E:119:VAL:HG21	2.04	0.40
6:P:22:PHE:CD2	7:R:201:LEU:HD13	2.57	0.40
7:R:300:ARG:HA	7:R:303:ILE:HG12	2.02	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	208/373 (56%)	186 (89%)	22 (11%)	0	100	100
2	B	337/350 (96%)	301 (89%)	36 (11%)	0	100	100
3	E	228/297 (77%)	214 (94%)	14 (6%)	0	100	100
4	G	55/71 (78%)	54 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	N	126/160 (79%)	113 (90%)	13 (10%)	0	100	100
6	P	28/39 (72%)	28 (100%)	0	0	100	100
7	R	374/463 (81%)	337 (90%)	37 (10%)	0	100	100
All	All	1356/1753 (77%)	1233 (91%)	123 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/334 (57%)	185 (98%)	4 (2%)	53	77
2	B	277/291 (95%)	276 (100%)	1 (0%)	91	95
3	E	186/239 (78%)	186 (100%)	0	100	100
4	G	46/58 (79%)	46 (100%)	0	100	100
5	N	105/129 (81%)	104 (99%)	1 (1%)	76	89
6	P	24/29 (83%)	23 (96%)	1 (4%)	30	61
7	R	318/389 (82%)	317 (100%)	1 (0%)	92	96
All	All	1145/1469 (78%)	1137 (99%)	8 (1%)	84	92

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	42	ARG
1	A	264	ASN
1	A	330	GLU
2	B	76	ASP
5	N	109	ASP
6	P	20	LYS
7	R	203	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	362	HIS
7	R	224	GLN
7	R	230	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)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
6	AIB	P	13	6	1,5,6	1.05	0	2,7,9	1.13	0
6	AIB	P	2	6	1,5,6	1.23	0	2,7,9	1.14	0

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
6	AIB	P	13	6	-	0/2/3/6	-
6	AIB	P	2	6	-	0/2/3/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	P	13	AIB	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
8	41Y	R	501	-	39,40,40	2.73	13 (33%)	53,58,58	1.80	11 (20%)

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
8	41Y	R	501	-	-	8/23/36/36	0/4/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	R	501	41Y	C11-N10	-10.01	1.34	1.48
8	R	501	41Y	C24-C25	-6.17	1.38	1.50
8	R	501	41Y	C07-C06	-5.88	1.31	1.40
8	R	501	41Y	C09-C08	4.08	1.59	1.51
8	R	501	41Y	C09-N10	-4.06	1.40	1.47
8	R	501	41Y	C23-C22	3.71	1.60	1.52
8	R	501	41Y	C05-C06	3.47	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	R	501	41Y	C13-C11	3.30	1.58	1.52
8	R	501	41Y	C31-N32	3.19	1.46	1.37
8	R	501	41Y	C12-C11	3.17	1.59	1.52
8	R	501	41Y	C08-C07	3.07	1.56	1.51
8	R	501	41Y	C24-C07	2.41	1.45	1.40
8	R	501	41Y	O02-C03	2.38	1.40	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	R	501	41Y	F28-C27-C29	5.07	120.89	117.13
8	R	501	41Y	C26-C27-C29	-5.01	119.87	123.79
8	R	501	41Y	C09-N10-C22	3.92	116.06	110.45
8	R	501	41Y	C12-C11-C13	-3.69	103.94	113.24
8	R	501	41Y	O02-C03-C24	3.66	120.45	115.44
8	R	501	41Y	C26-C25-C24	-3.19	115.40	120.57
8	R	501	41Y	C23-C22-C06	-2.72	106.00	111.87
8	R	501	41Y	C08-C09-N10	2.70	116.06	110.32
8	R	501	41Y	O02-C03-C04	-2.56	119.98	124.37
8	R	501	41Y	C09-N10-C11	2.41	116.48	112.58
8	R	501	41Y	C37-C25-C24	2.32	124.33	120.57

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	R	501	41Y	C12-C11-N10-C09
8	R	501	41Y	C13-C11-N10-C09
8	R	501	41Y	C29-C31-N32-C33
8	R	501	41Y	C37-C31-N32-C33
8	R	501	41Y	C04-C03-O02-C01
8	R	501	41Y	C24-C03-O02-C01
8	R	501	41Y	C13-C11-N10-C22
8	R	501	41Y	C34-C33-N32-C31

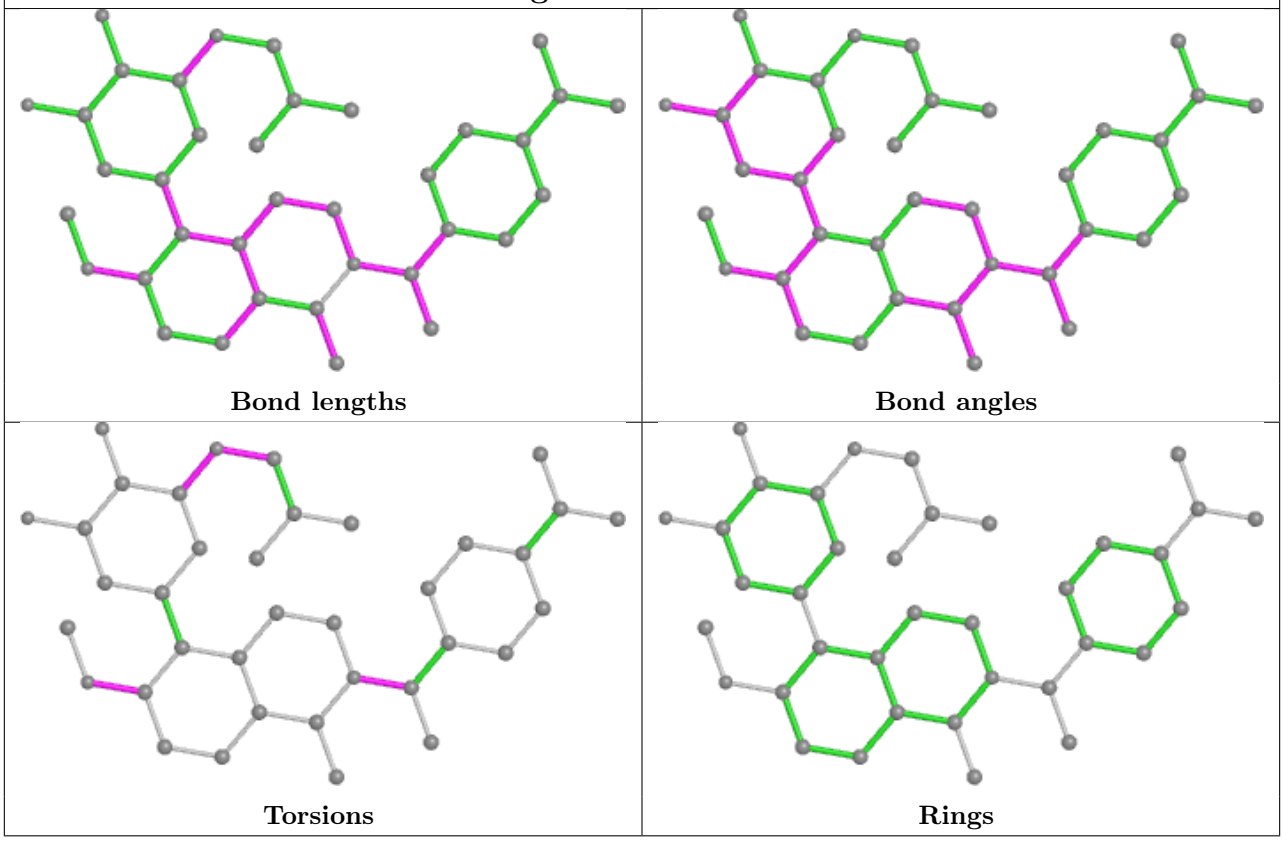
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

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

Ligand 41Y R 501



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.

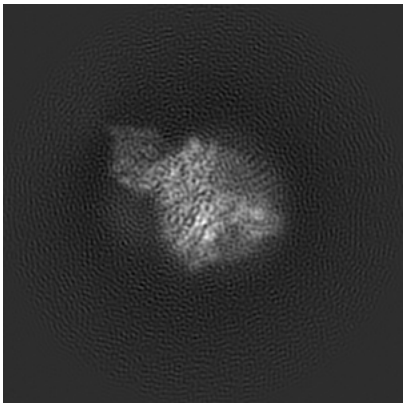
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-24401. These allow visual inspection of the internal detail of the map and identification of artifacts.

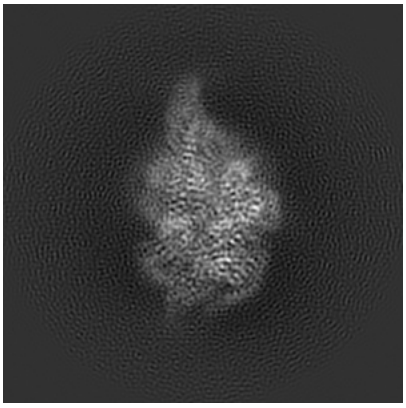
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

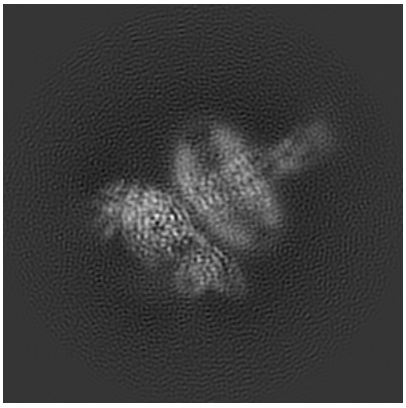
6.1.1 Primary map



X



Y

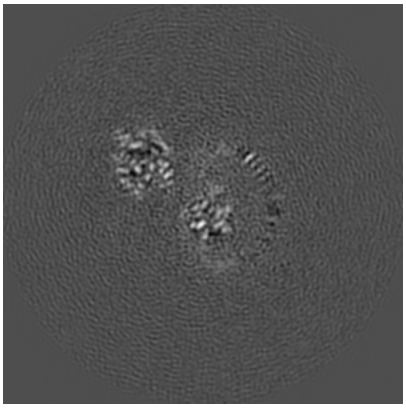


Z

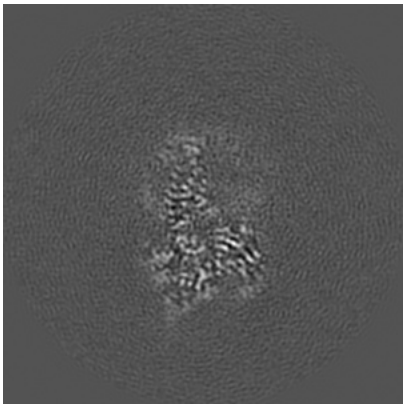
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

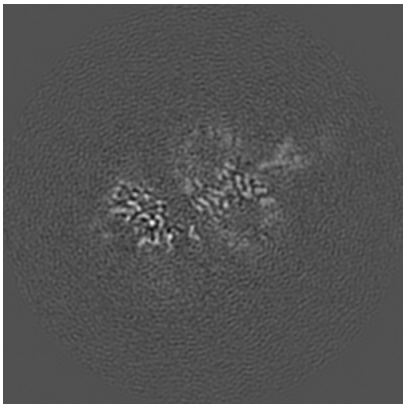
6.2.1 Primary map



X Index: 150



Y Index: 150

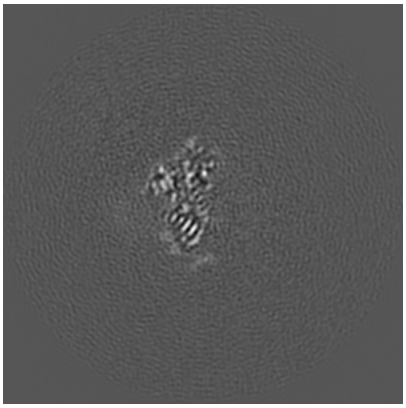


Z Index: 150

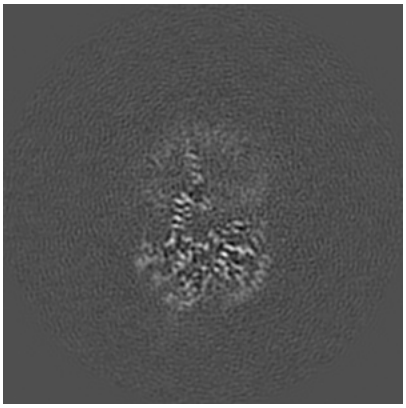
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

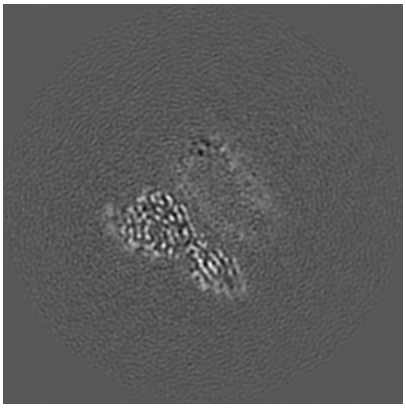
6.3.1 Primary map



X Index: 120



Y Index: 146



Z Index: 175

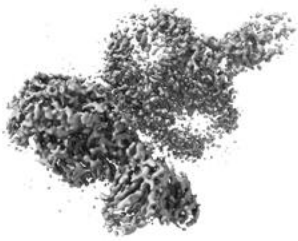
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

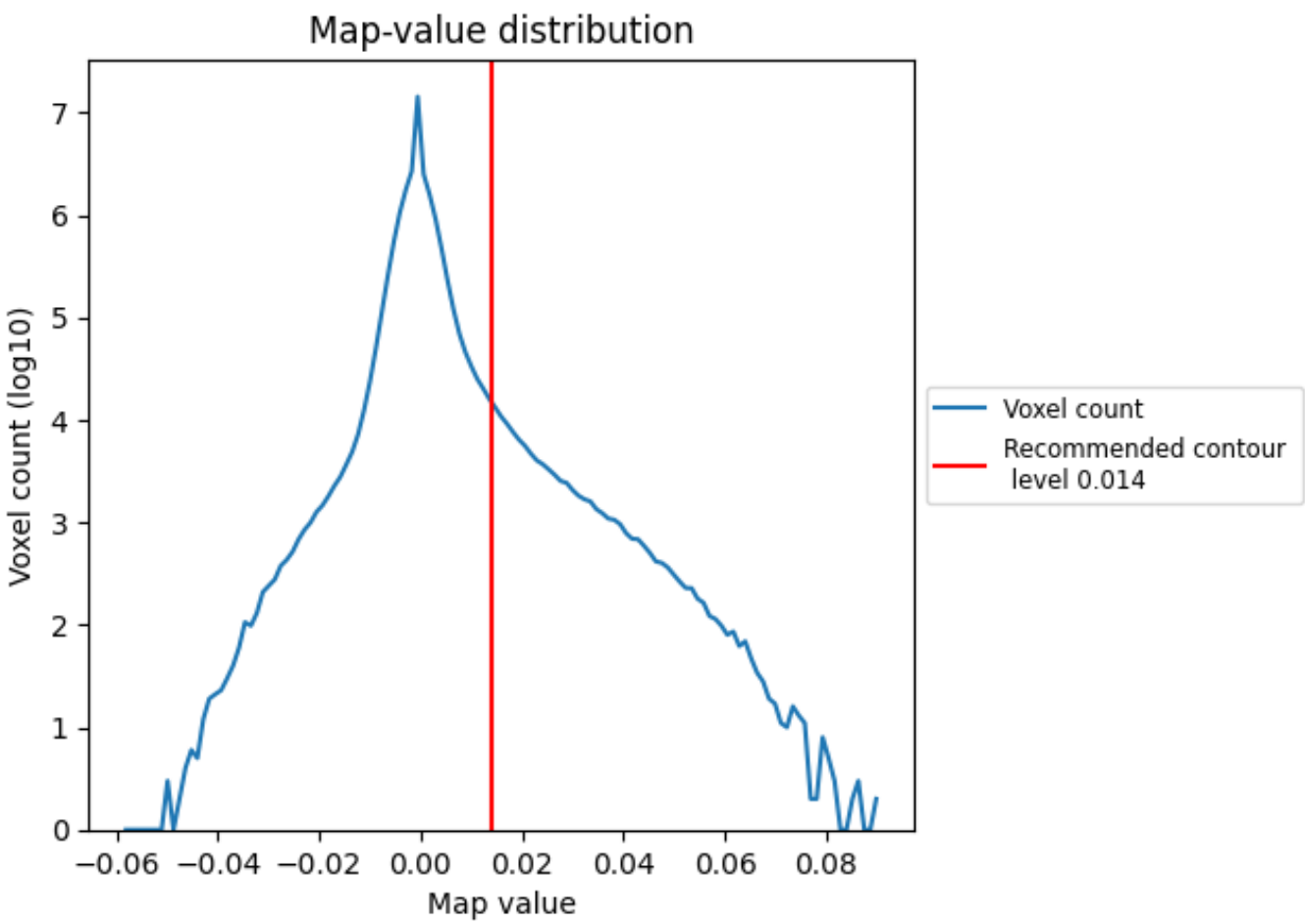
6.5 Mask visualisation (i)

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

7 Map analysis (i)

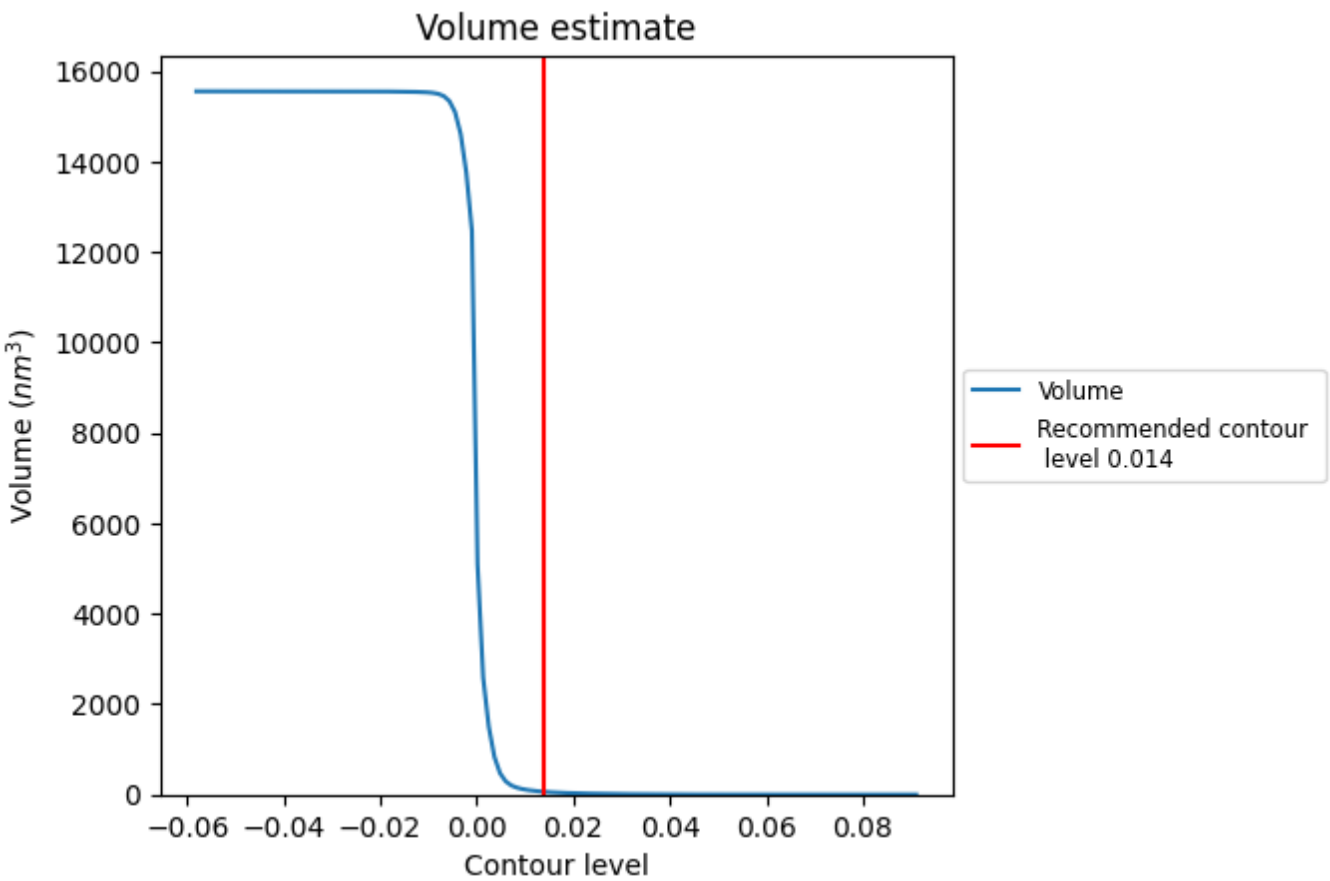
This section contains the results of statistical analysis of the map.

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.

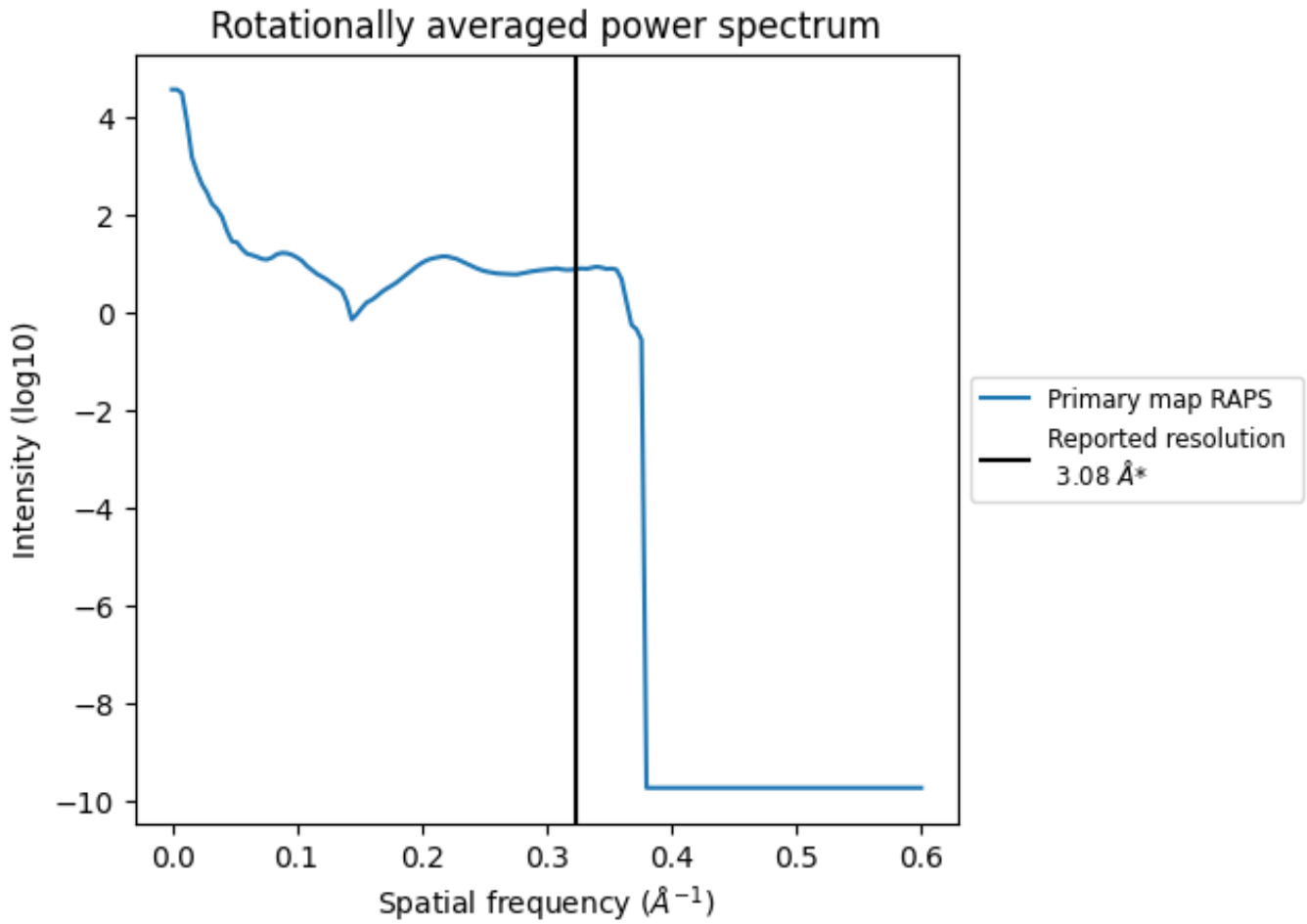
7.2 Volume estimate (i)



The volume at the recommended contour level is 61 nm^3; this corresponds to an approximate mass of 55 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 0.325 Å^{-1}

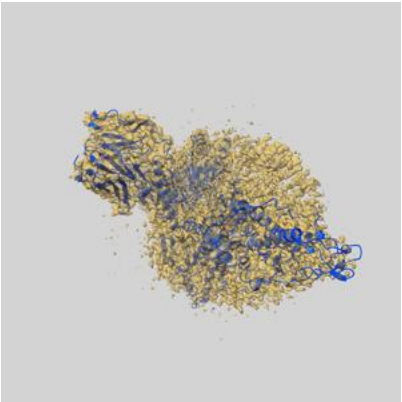
8 Fourier-Shell correlation (i)

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

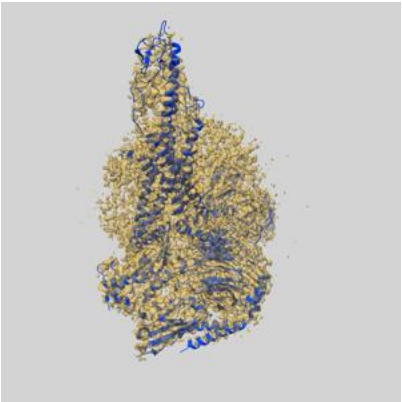
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-24401 and PDB model 7RBT. Per-residue inclusion information can be found in section 3 on page 6.

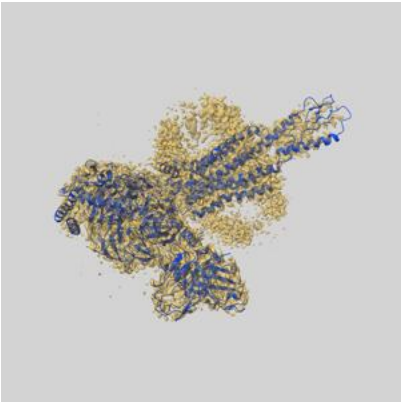
9.1 Map-model overlay (i)



X



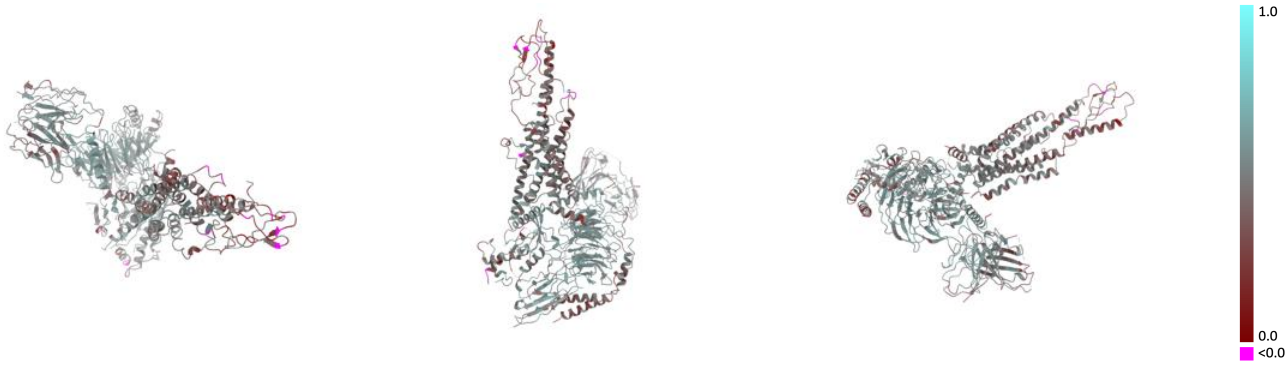
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 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.

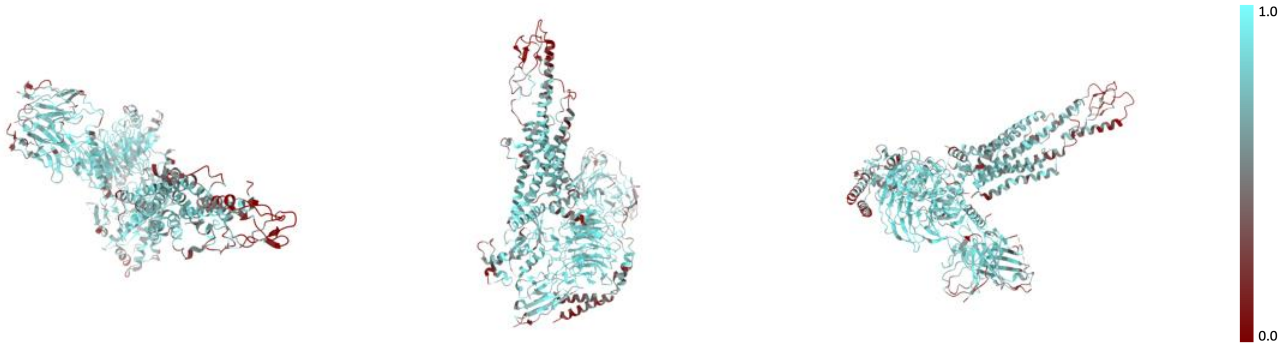
9.2 Q-score mapped to coordinate model (i)



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.

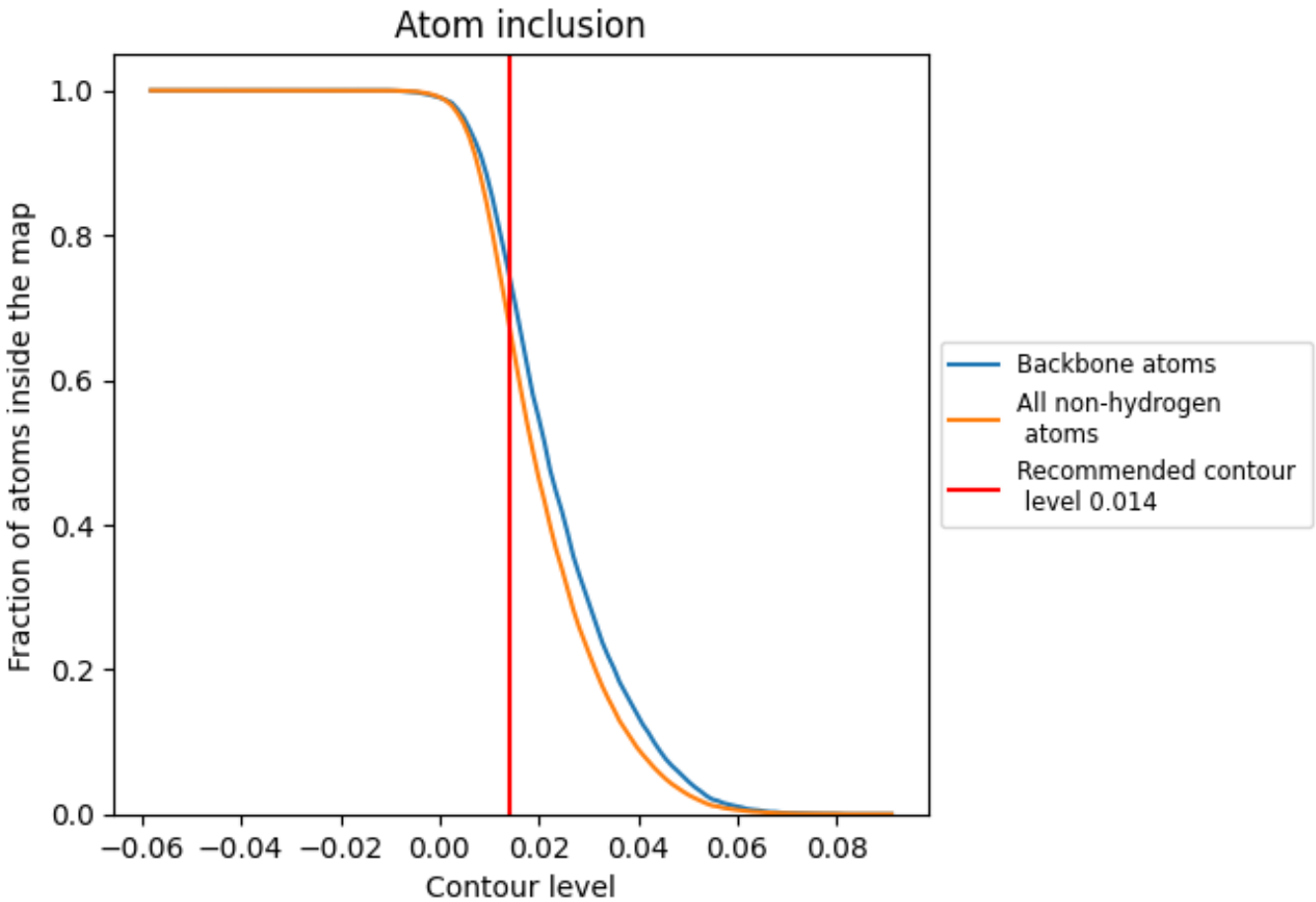
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.014).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 68% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6782	0.4790
A	0.7256	0.4970
B	0.7913	0.5320
E	0.6988	0.4980
G	0.4918	0.4130
N	0.7230	0.5240
P	0.6790	0.4690
R	0.5566	0.4090