Full wwPDB EM Validation Report ⓘ

May 18, 2025 – 07:29 AM EDT

PDB ID	:	9E7H / pdb_00009e7h
EMDB ID	:	EMD-47669
Title	:	CryoEM structure of BchN-BchB bound to Pchlide from the DPOR under turnover complex dataset
Authors	:	Kashyap, R.; Antony, E.
Deposited on	:	2024-11-01
Resolution	:	3.29 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 ⓘ 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 ⓘ) were used in the production of this report:

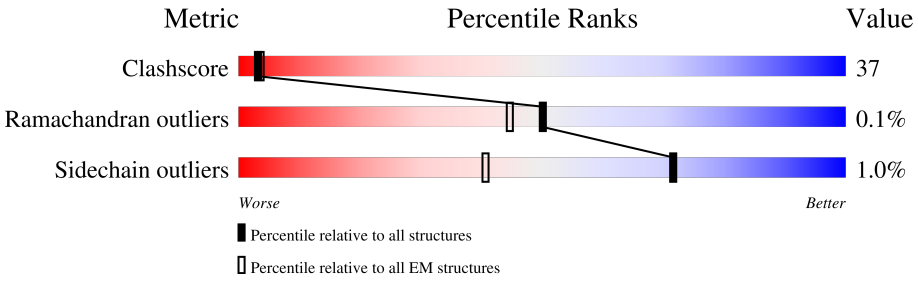
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.29 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	428	45% 48% 6%
1	C	428	12% 47% 43% 9%
2	B	536	36% 40% 22%
2	D	536	33% 44% 22%

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
3	SF4	A	501	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SF4	C	501	-	-	X	-
4	PMR	A	502	X	-	-	-
4	PMR	B	601	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12612 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.

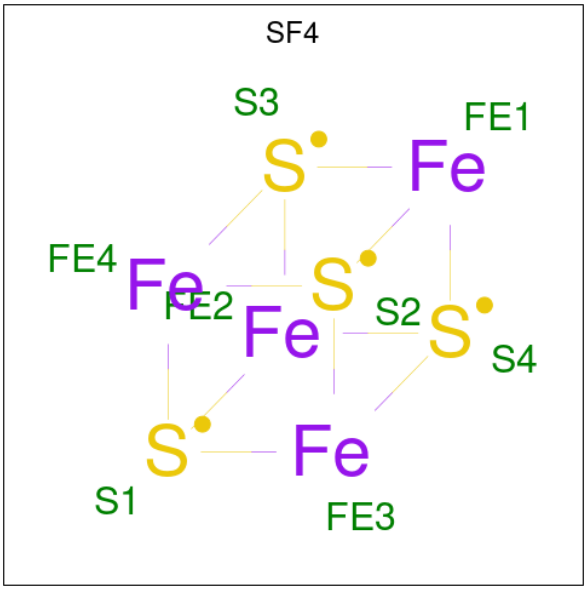
- Molecule 1 is a protein called Light-independent protochlorophyllide reductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	402	Total	C	N	O	S	1	0
			3063	1943	553	557	10		
1	C	389	Total	C	N	O	S	2	0
			2972	1891	535	536	10		

- Molecule 2 is a protein called Light-independent protochlorophyllide reductase subunit B.

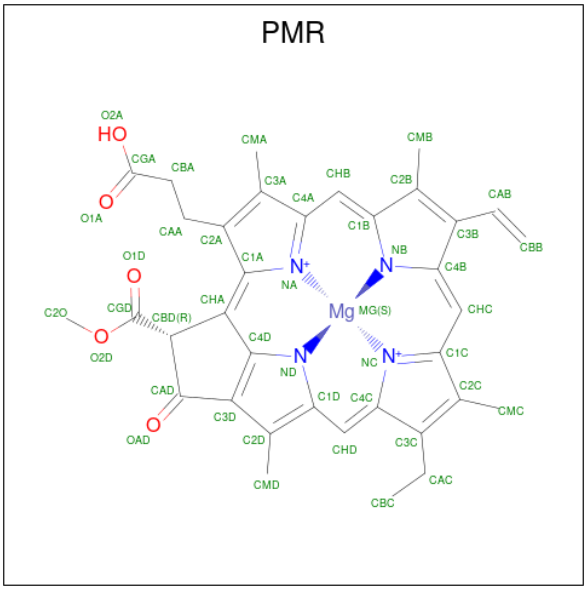
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	419	Total	C	N	O	S	1	0
			3241	2058	565	596	22		
2	D	418	Total	C	N	O	S	1	0
			3228	2046	563	598	21		

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Fe S 8 4 4	0
3	C	1	Total Fe S 8 4 4	0

- Molecule 4 is Protochlorophyllide (CCD ID: PMR) (formula: $C_{35}H_{32}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C Mg N O 45 35 1 4 5	0
4	B	1	Total C Mg N O 45 35 1 4 5	0

- Molecule 5 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

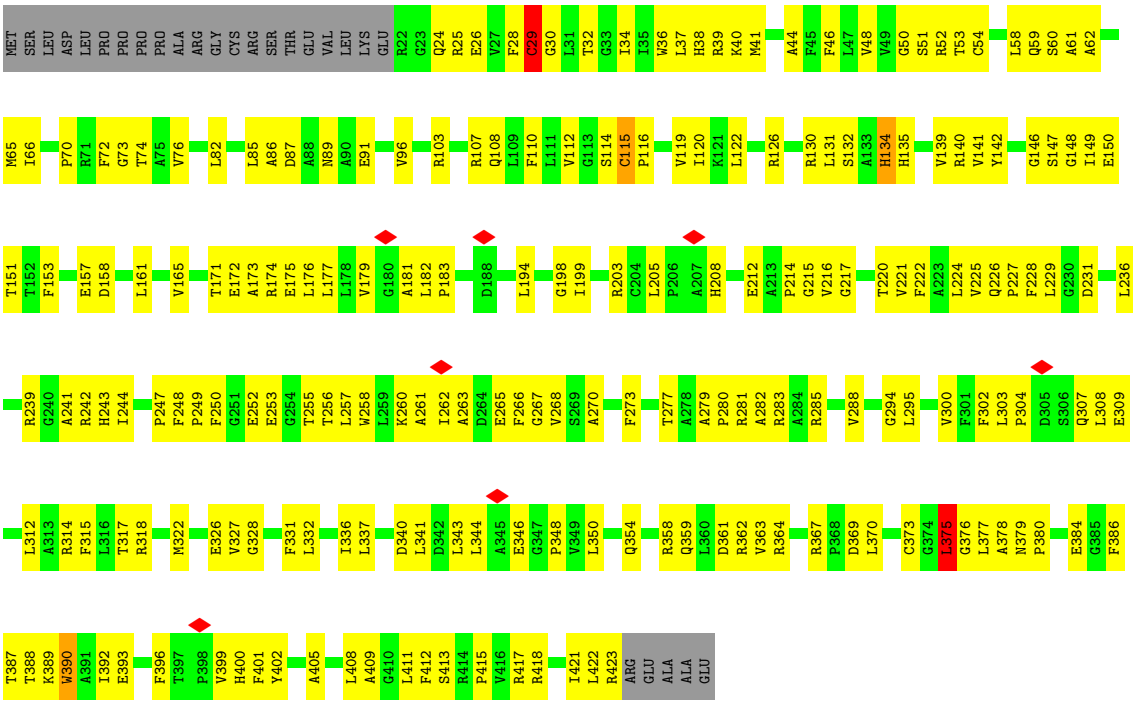
Mol	Chain	Residues	Atoms	AltConf
5	D	2	Total Cu 2 2	0

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.

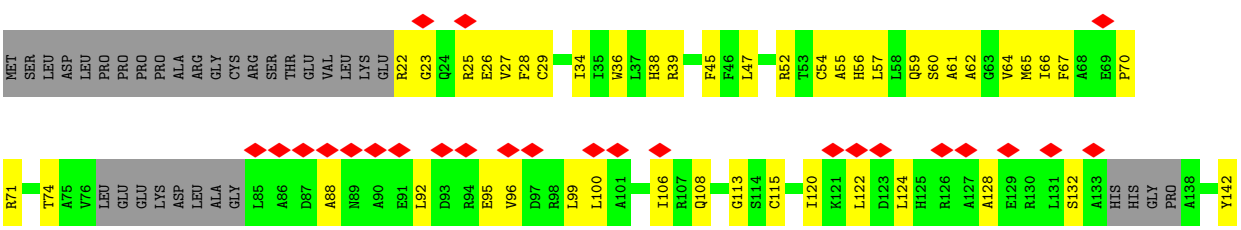
• Molecule 1: Light-independent protochlorophyllide reductase subunit N

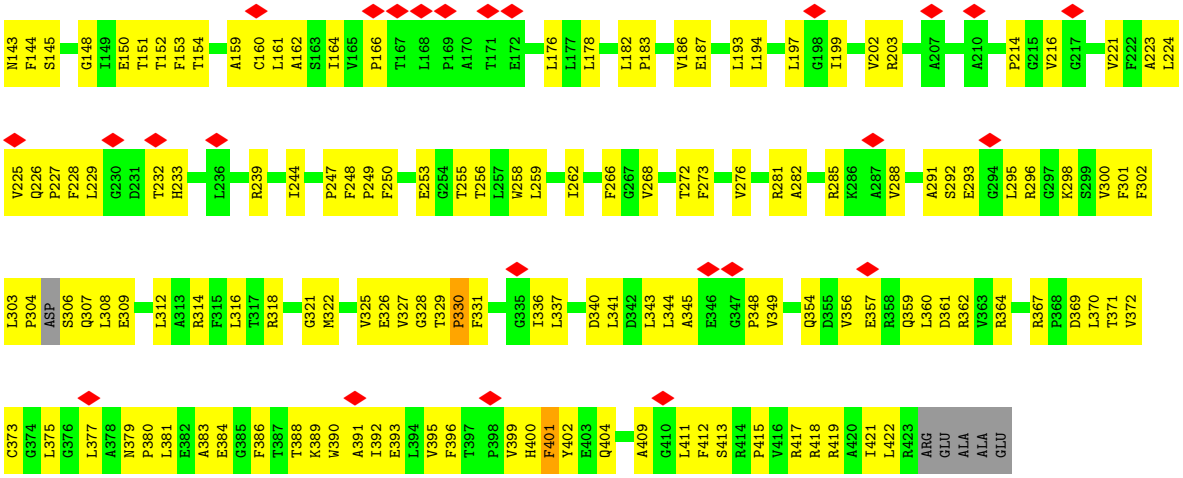
Chain A:



• Molecule 1: Light-independent protochlorophyllide reductase subunit N

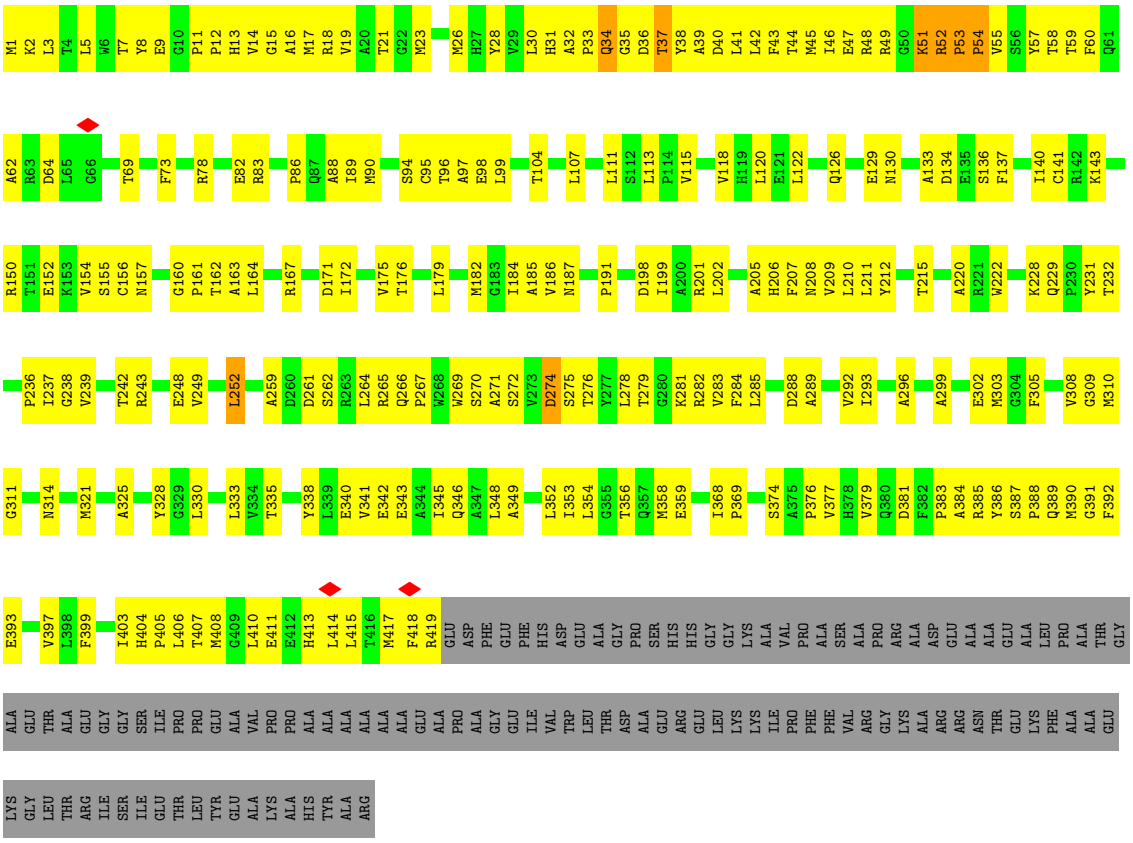
Chain C:





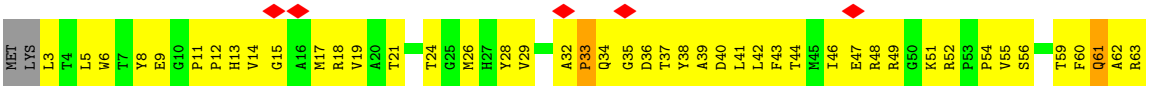
• Molecule 2: Light-independent protochlorophyllide reductase subunit B

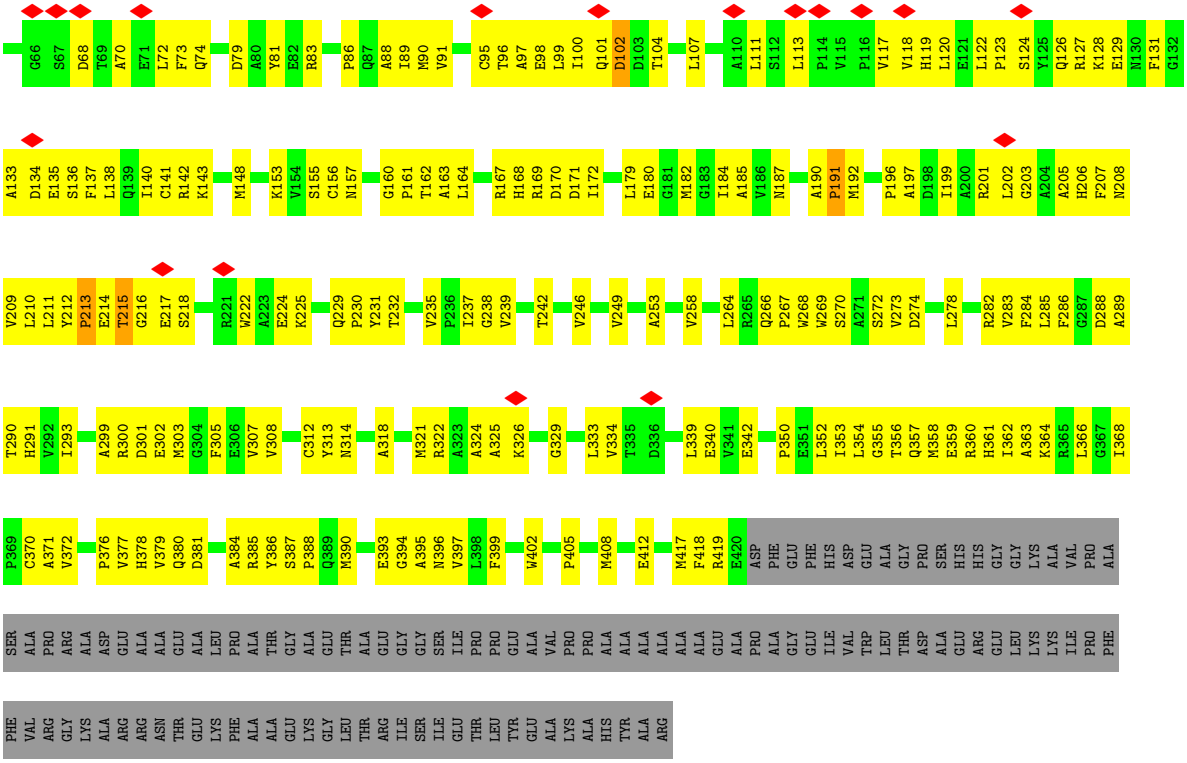
Chain B:



• Molecule 2: Light-independent protochlorophyllide reductase subunit B

Chain D:




G66 S67 D68 T69 A70 E71 L72 F73 Q74 D79 A80 Y81 E82 R83 P86 Q87 A88 I89 M90 V91 C95 T96 A97 E98 L99 I100 Q101 D102 D103 T104 L107 A110 L111 S112 L113 P114 V115 P116 V117 V118 H119 L120 E121 L122 P123 S124 Y125 Q126 R127 K128 E129 N130 F131 G132
A133 D134 E135 S136 F137 L138 Q139 T140 C141 R142 K143 M148 K153 V154 S155 C156 N157 G160 P161 T162 A163 L164 R167 H168 R169 D170 D171 I172 L179 E180 G181 M182 G183 I184 A185 V186 N187 A190 P191 M192 P196 A197 D198 I199 A200 R201 L202 G203 A204 A205 H206 F207 N208
V209 L210 L211 Y212 P213 E214 T215 G216 E217 S218 R221 W222 A223 E224 K225 Q229 P230 Y231 T232 V235 P236 I237 G238 V239 T242 V246 V249 A253 V258 L264 R265 Q266 P267 W268 W269 S270 A271 S272 V273 D274 L278 R282 V283 F284 L285 F286 G287 D288 A289
T290 H291 V292 I293 A299 R300 D301 E302 M303 G304 F305 E306 V307 V308 C312 Y313 N314 A318 M321 R322 A323 A324 A325 K326 G329 L333 V334 T335 D336 L339 E340 V341 E342 P350 E351 L352 I353 L354 G355 T356 Q357 M358 E359 R360 H361 I362 A363 K364 R365 L366 G367 I368
P369 C370 A371 V372 P376 V377 H378 V379 Q380 D381 A384 R385 Y386 S387 P388 Q389 M390 E393 G394 A395 N396 V397 L398 F399 W402 P405 M408 E412 M417 F418 R419 E420 ASP PHE GLU PHE HIS ASP GLU ALA GLY PRO SER HIS HIS GLY GLY LYS ALA VAL PRO ALA
SER ALA PRO ARG ALA ASP GLU ALA ALA GLU ALA LEU PRO ALA THR GLY ALA GLU THR ALA GLU GLY GLY SER ILE PRO PRO GLU ALA VAL PRO PRO ALA ALA ALA ALA ALA ALA GLU ALA PRO ALA GLY GLU ILE VAL TRP LEU THR ASP ALA GLU ARG GLU LEU LYS LYS ILE PRO PHE
PHE VAL ARG GLY LYS ALA ARG ARG ASN THR GLU LYS PHE ALA ALA GLU LYS GLY LEU THR ARG ILE SER ILE GLU THR LEU TYR GLU ALA LYS ALA HIS TYR ALA ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69816	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.460	Depositor
Minimum map value	-0.689	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.0954	Depositor
Map size (Å)	393.6, 393.6, 393.6	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PMR, SF4, CU

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	0.23	0/3132	0.56	2/4257 (0.0%)
1	C	1.77	2/3039 (0.1%)	1.14	7/4126 (0.2%)
2	B	0.25	0/3321	0.59	3/4514 (0.1%)
2	D	0.44	4/3306 (0.1%)	0.90	9/4494 (0.2%)
All	All	0.91	6/12798 (0.0%)	0.83	21/17391 (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	1
2	B	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	330	PRO	N-CD	96.18	2.82	1.47
2	D	33	PRO	CB-CG	-11.64	0.91	1.49
2	D	191	PRO	CB-CG	-11.00	0.94	1.49
1	C	330	PRO	CG-CD	-9.35	1.19	1.50
2	D	191	PRO	CG-CD	-7.80	1.24	1.50
2	D	33	PRO	CG-CD	-7.67	1.24	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	330	PRO	N-CD-CG	-56.26	18.81	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	330	PRO	CA-N-CD	-24.93	77.10	112.00
2	D	191	PRO	CB-CG-CD	22.92	179.44	106.10
2	D	33	PRO	CB-CG-CD	18.81	166.29	106.10
2	D	33	PRO	N-CD-CG	-18.64	75.23	103.20
2	D	33	PRO	CA-CB-CG	-18.48	69.39	104.50
2	D	191	PRO	N-CD-CG	-16.97	77.74	103.20
2	D	191	PRO	CA-CB-CG	-15.80	74.48	104.50
1	C	330	PRO	CA-CB-CG	-14.78	76.43	104.50
2	B	53	PRO	N-CA-C	-14.57	92.92	110.70
2	B	54	PRO	CB-CA-C	9.71	127.57	111.56
2	D	213	PRO	N-CA-CB	8.73	112.42	103.25
2	D	33	PRO	CA-N-CD	-7.63	101.32	112.00
1	C	329	THR	C-N-CD	7.54	155.89	125.00
2	D	191	PRO	CA-N-CD	-7.05	102.13	112.00
1	C	336	ILE	N-CA-C	-6.56	106.34	112.83
1	C	330	PRO	N-CA-CB	-6.33	97.46	103.41
1	A	375	LEU	CA-CB-CG	5.96	137.15	116.30
1	C	402	TYR	CB-CA-C	-5.67	110.02	116.54
1	A	29	CYS	N-CA-C	-5.62	102.14	110.46
2	B	54	PRO	N-CA-CB	-5.02	97.98	103.25

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	375	LEU	Peptide
2	B	52	ARG	Sidechain

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	3063	0	3075	252	0
1	C	2972	0	2994	248	0
2	B	3241	0	3210	237	0
2	D	3228	0	3189	265	0
3	A	8	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	8	0	0	12	0
4	A	45	0	31	7	0
4	B	45	0	31	12	0
5	D	2	0	0	0	0
All	All	12612	0	12530	926	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 37.

All (926) 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:D:90:MET:HE3	2:D:120:LEU:CD1	1.36	1.53
2:B:418:PHE:CE2	1:C:39:ARG:NH1	1.91	1.38
1:C:115:CYS:SG	3:C:501:SF4:FE4	1.16	1.37
1:C:186:VAL:HG23	1:C:404:GLN:NE2	1.38	1.36
1:A:115:CYS:SG	3:A:501:SF4:FE4	1.21	1.30
1:C:393:GLU:OE2	1:C:411:LEU:HD13	1.38	1.22
1:C:54:CYS:SG	3:C:501:SF4:FE3	1.33	1.20
1:C:253:GLU:OE2	1:C:318:ARG:NH1	1.77	1.15
2:D:90:MET:HE3	2:D:120:LEU:HD11	1.24	1.11
2:D:90:MET:CE	2:D:120:LEU:HD13	1.80	1.11
2:D:90:MET:CE	2:D:120:LEU:CD1	2.29	1.11
1:C:393:GLU:OE1	1:C:411:LEU:HD22	1.51	1.09
2:D:213:PRO:HA	2:D:217:GLU:HB2	1.37	1.05
1:C:56:HIS:ND1	2:D:38:TYR:OH	1.89	1.05
2:B:45:MET:SD	2:D:274:ASP:OD1	2.16	1.03
2:D:90:MET:HE3	2:D:120:LEU:HD13	1.08	1.03
1:C:186:VAL:CG2	1:C:404:GLN:NE2	2.21	1.02
1:C:62:ALA:HB1	1:C:65:MET:HB3	1.40	0.99
1:C:66:ILE:HD12	2:D:6:TRP:CE3	1.98	0.97
1:C:115:CYS:HG	3:C:501:SF4:FE4	0.71	0.95
1:C:400:HIS:O	1:C:404:GLN:OE1	1.84	0.94
2:B:49:ARG:HH12	2:B:163:ALA:HB1	1.31	0.94
1:C:186:VAL:HG23	1:C:404:GLN:HE22	1.14	0.94
2:B:419:ARG:HD3	1:C:65:MET:HE3	1.47	0.92
2:B:41:LEU:O	2:B:45:MET:HB2	1.69	0.92
1:A:29:CYS:SG	3:A:501:SF4:FE1	1.63	0.90
2:B:90:MET:HE2	2:B:120:LEU:HD11	1.56	0.88
1:A:61:ALA:HB1	4:A:502:PMR:HBCB	1.55	0.88
1:A:171:THR:HG22	1:A:172:GLU:N	1.86	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:ILE:HD12	2:D:6:TRP:HE3	1.34	0.88
1:A:29:CYS:HG	3:A:501:SF4:FE1	0.57	0.86
1:C:186:VAL:CG2	1:C:404:GLN:CD	2.47	0.86
1:A:199:ILE:HG22	1:A:268:VAL:HG21	1.57	0.85
1:A:390[A]:TRP:CZ2	1:A:393:GLU:OE1	2.29	0.85
1:C:186:VAL:HG23	1:C:404:GLN:CD	2.01	0.85
1:C:197:LEU:HD11	1:C:273:PHE:HD2	1.39	0.85
1:A:194:LEU:HD22	1:A:199:ILE:HD11	1.59	0.84
2:B:403:ILE:HG22	2:D:380:GLN:HE22	1.43	0.83
1:C:381:LEU:HD12	1:C:386:PHE:HD2	1.43	0.83
1:A:171:THR:HG22	1:A:172:GLU:H	1.39	0.83
1:A:390[A]:TRP:CE2	1:A:393:GLU:OE1	2.31	0.83
1:C:393:GLU:OE1	1:C:411:LEU:CD2	2.25	0.83
2:B:15:GLY:HA2	2:B:18:ARG:HD3	1.61	0.83
1:A:54:CYS:SG	3:A:501:SF4:FE3	1.68	0.83
2:D:239:VAL:HG21	2:D:267:PRO:HD3	1.61	0.82
2:D:28:TYR:HB3	2:D:55:VAL:HG22	1.61	0.82
2:B:171:ASP:OD2	2:B:212:TYR:OH	1.95	0.82
2:B:210:LEU:HD13	2:B:220:ALA:CB	2.11	0.81
2:B:418:PHE:HE2	1:C:39:ARG:HH12	1.25	0.81
1:C:54:CYS:HG	3:C:501:SF4:FE3	0.98	0.81
1:C:259:LEU:HB3	1:C:273:PHE:HE2	1.46	0.81
2:D:213:PRO:CA	2:D:217:GLU:HB2	2.10	0.81
2:B:18:ARG:HG2	2:B:164:LEU:HB3	1.62	0.81
1:C:330:PRO:HG3	1:C:331:PHE:N	1.89	0.81
1:A:171:THR:CG2	1:A:172:GLU:H	1.94	0.80
2:D:29:VAL:HA	2:D:56:SER:HB2	1.62	0.80
2:D:123:PRO:HD2	2:D:127:ARG:HG3	1.61	0.80
2:B:210:LEU:HD13	2:B:220:ALA:HB2	1.62	0.80
2:B:385:ARG:NH2	2:D:387:SER:OG	2.17	0.78
1:C:56:HIS:CG	2:D:38:TYR:OH	2.37	0.78
1:C:55:ALA:HB2	1:C:74:THR:HG21	1.67	0.77
1:A:327:VAL:HG22	1:A:348:PRO:HB2	1.65	0.77
4:B:601:PMR:HMCA	1:C:61:ALA:HB1	1.67	0.77
1:C:38:HIS:ND1	1:C:71:ARG:HG2	2.00	0.77
1:C:176:LEU:HD21	1:C:262:ILE:HD12	1.67	0.76
2:D:299:ALA:HA	2:D:303:MET:HB2	1.65	0.76
1:A:317:THR:HA	1:A:322:MET:H	1.50	0.76
1:A:226:GLN:HB2	1:A:229:LEU:HD13	1.66	0.76
1:C:70:PRO:HD2	2:D:5:LEU:HD23	1.68	0.76
2:D:289:ALA:O	2:D:293:ILE:HG13	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ASN:ND2	2:B:44:THR:O	2.18	0.76
2:B:171:ASP:OD1	2:B:389:GLN:N	2.16	0.76
2:D:73:PHE:HD2	2:D:102:ASP:OD1	1.68	0.75
1:A:171:THR:HG22	1:A:173:ALA:H	1.51	0.75
2:B:23:MET:HE1	2:B:140:ILE:HG21	1.67	0.74
2:B:208:ASN:ND2	2:B:229:GLN:OE1	2.20	0.74
2:B:283:VAL:HG12	2:B:352:LEU:HB3	1.69	0.74
2:D:73:PHE:HD2	2:D:102:ASP:CG	1.94	0.74
1:C:203:ARG:HE	1:C:214:PRO:HA	1.51	0.74
1:A:115:CYS:SG	3:A:501:SF4:S3	2.86	0.74
2:B:38:TYR:HA	2:B:41:LEU:HD13	1.67	0.73
2:B:418:PHE:CD2	1:C:39:ARG:NH1	2.56	0.73
2:D:167:ARG:HD3	2:D:387:SER:HB3	1.69	0.73
1:C:314:ARG:HD3	1:C:343:LEU:HB3	1.70	0.73
1:C:361:ASP:HA	1:C:364:ARG:HD2	1.68	0.73
1:A:222:PHE:HB3	1:A:236:LEU:HD22	1.70	0.73
1:C:56:HIS:CE1	2:D:38:TYR:OH	2.40	0.73
1:C:47:LEU:HD22	1:C:99:LEU:HD11	1.70	0.73
2:D:90:MET:CE	2:D:120:LEU:CD2	2.66	0.73
2:D:90:MET:HG2	2:D:118:VAL:HG12	1.71	0.73
1:A:176:LEU:HB3	1:A:266:PHE:HE2	1.55	0.72
2:D:14:VAL:HG13	2:D:129:GLU:HG3	1.70	0.72
2:D:266:GLN:NE2	2:D:395:ALA:O	2.21	0.72
2:B:292:VAL:HG13	2:B:321:MET:HE3	1.72	0.71
1:A:280:PRO:HB2	1:A:402:TYR:HD2	1.56	0.71
1:C:389:LYS:HB2	1:C:415:PRO:HG3	1.70	0.71
1:A:171:THR:CG2	1:A:172:GLU:N	2.51	0.71
2:D:169:ARG:NH1	2:D:170:ASP:OD1	2.24	0.71
2:B:118:VAL:HG12	2:B:143:LYS:HD2	1.72	0.71
1:A:115:CYS:SG	3:A:501:SF4:S2	2.89	0.71
1:C:381:LEU:HD12	1:C:386:PHE:CD2	2.26	0.71
2:D:73:PHE:CD2	2:D:102:ASP:OD1	2.44	0.71
2:B:47:GLU:OE1	2:B:49:ARG:NH1	2.24	0.70
2:B:171:ASP:HB3	2:B:390:MET:HB2	1.72	0.70
2:D:288:ASP:OD2	2:D:291:HIS:ND1	2.19	0.70
1:C:381:LEU:HG	1:C:386:PHE:HB2	1.73	0.70
2:B:415:LEU:HG	1:C:64:VAL:HB	1.73	0.70
2:D:35:GLY:H	2:D:37:THR:HG22	1.56	0.70
2:D:187:ASN:ND2	2:D:201:ARG:O	2.24	0.69
1:A:96:VAL:HG11	1:A:131:LEU:HD11	1.74	0.69
2:B:293:ILE:HG13	2:B:321:MET:HE2	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:LEU:HD13	1:C:99:LEU:HG	1.74	0.69
2:B:411:GLU:O	2:B:415:LEU:HB2	1.92	0.69
2:B:40:ASP:HA	2:B:53:PRO:HG2	1.74	0.69
1:A:359:GLN:O	1:A:363:VAL:HG23	1.91	0.69
1:C:115:CYS:SG	3:C:501:SF4:S3	2.90	0.69
1:C:253:GLU:HA	1:C:256:THR:HB	1.75	0.69
1:C:312:LEU:HD13	1:C:412:PHE:HZ	1.57	0.69
2:D:9:GLU:HB3	2:D:129:GLU:H	1.58	0.69
1:A:307:GLN:NE2	1:A:331:PHE:O	2.26	0.69
2:B:48:ARG:NH2	2:D:269:TRP:O	2.26	0.68
2:D:182:MET:HA	2:D:258:VAL:HB	1.74	0.68
2:D:357:GLN:NE2	2:D:381:ASP:OD2	2.27	0.68
1:C:302:PHE:HB2	1:C:327:VAL:HG12	1.76	0.68
2:B:384:ALA:O	2:D:396:ASN:ND2	2.26	0.68
1:A:370:LEU:HD11	1:A:389:LYS:HB3	1.74	0.68
1:A:295:LEU:HD22	1:A:322:MET:HE1	1.75	0.68
2:B:152:GLU:N	2:B:152:GLU:OE1	2.27	0.67
2:D:117:VAL:HG13	2:D:143:LYS:HD2	1.77	0.67
2:D:142:ARG:HG2	2:D:143:LYS:HE3	1.76	0.67
2:D:378:HIS:HD2	2:D:380:GLN:H	1.42	0.67
2:D:28:TYR:O	2:D:56:SER:N	2.27	0.67
2:D:91:VAL:HG22	2:D:119:HIS:HB2	1.76	0.67
2:D:100:ILE:HG23	2:D:101:GLN:NE2	2.09	0.67
2:B:17:MET:HE1	2:B:39:ALA:CB	2.25	0.67
1:A:222:PHE:HE1	1:A:243:HIS:HB2	1.57	0.67
1:C:259:LEU:HB3	1:C:273:PHE:CE2	2.30	0.67
1:A:65:MET:HE3	1:A:72:PHE:HZ	1.59	0.67
1:A:85:LEU:O	1:A:89:ASN:ND2	2.27	0.67
1:A:221:VAL:HG12	1:A:242:ARG:HB3	1.76	0.66
1:C:298:LYS:HD3	1:C:369:ASP:HB2	1.77	0.66
1:A:263:ALA:O	1:A:267:GLY:N	2.24	0.66
2:B:404:HIS:HA	2:D:380:GLN:HE21	1.60	0.66
1:A:26:GLU:OE1	1:A:376:GLY:N	2.29	0.66
1:A:203:ARG:HB3	1:A:214:PRO:HB3	1.78	0.66
2:D:88:ALA:HA	2:D:113:LEU:HD13	1.76	0.66
1:C:247:PRO:O	1:C:258:TRP:HB2	1.96	0.66
2:B:60:PHE:CG	2:B:69:THR:OG1	2.48	0.66
2:B:413:HIS:HA	2:B:417:MET:CE	2.26	0.66
1:C:186:VAL:HG21	1:C:404:GLN:CD	2.21	0.66
2:D:18:ARG:HG2	2:D:43:PHE:HE1	1.61	0.66
1:A:36:TRP:HE1	1:A:157:GLU:HG3	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:HD11	1:A:341:LEU:HD11	1.77	0.66
1:C:27:VAL:HG11	1:C:330:PRO:HB3	1.78	0.66
2:B:182:MET:HE1	2:B:249:VAL:CG2	2.26	0.66
1:A:34:ILE:HD11	1:A:112:VAL:HG11	1.76	0.65
1:C:115:CYS:SG	3:C:501:SF4:S1	2.94	0.65
1:A:52:ARG:NH1	2:B:7:THR:OG1	2.26	0.65
2:B:13:HIS:O	2:B:17:MET:HG3	1.97	0.65
2:B:414:LEU:HB3	2:B:419:ARG:HH21	1.62	0.65
2:B:264:LEU:HD22	2:B:392:PHE:CD1	2.32	0.65
1:A:40:LYS:NZ	1:A:182:LEU:O	2.25	0.65
1:A:116:PRO:O	1:A:120:ILE:HG13	1.96	0.65
2:B:338:TYR:HB2	2:B:358:MET:HE2	1.79	0.64
1:A:253:GLU:HB3	1:A:318:ARG:HH12	1.62	0.64
1:C:52:ARG:O	1:C:56:HIS:HB3	1.98	0.64
2:B:281:LYS:HB2	2:B:305:PHE:HB3	1.79	0.64
1:C:29:CYS:SG	3:C:501:SF4:S4	2.95	0.64
1:C:128:ALA:O	1:C:132:SER:OG	2.12	0.64
1:A:277:THR:HA	1:A:280:PRO:HG2	1.80	0.63
1:C:316:LEU:HD22	1:C:322:MET:HE2	1.79	0.63
1:C:178:LEU:HD13	1:C:194:LEU:HD11	1.79	0.63
1:A:36:TRP:NE1	1:A:157:GLU:OE1	2.31	0.63
2:B:310:MET:HE2	2:B:325:ALA:HA	1.80	0.63
1:C:150:GLU:HG3	2:D:62:ALA:HB2	1.81	0.63
1:C:393:GLU:OE2	1:C:411:LEU:CD1	2.32	0.63
2:D:322:ARG:HH12	2:D:334:VAL:HG11	1.63	0.63
2:B:17:MET:HE1	2:B:39:ALA:HB1	1.81	0.63
2:D:33:PRO:HA	2:D:59:THR:HA	1.80	0.63
1:A:227:PRO:HD3	1:A:250:PHE:HE2	1.64	0.63
1:A:253:GLU:HG2	1:A:318:ARG:HH22	1.62	0.63
1:A:62:ALA:HB1	1:A:65:MET:HB3	1.80	0.63
2:B:292:VAL:HG13	2:B:321:MET:CE	2.29	0.62
1:C:255:THR:HG21	1:C:401[A]:PHE:CD1	2.34	0.62
1:C:223:ALA:HB2	1:C:262:ILE:HD11	1.80	0.62
1:A:375:LEU:HD12	1:A:378:ALA:HB2	1.81	0.62
2:B:30:LEU:HD22	2:B:32:ALA:HB2	1.82	0.62
2:D:9:GLU:HB2	2:D:128:LYS:HB3	1.80	0.62
2:B:32:ALA:HB1	2:B:36:ASP:HB2	1.80	0.62
2:B:46:ILE:HA	2:B:379:VAL:HG12	1.81	0.62
2:B:288:ASP:N	2:B:374:SER:OG	2.29	0.62
2:D:312:CYS:SG	2:D:313:TYR:N	2.73	0.62
1:A:393:GLU:OE2	1:A:411:LEU:HD11	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:PHE:HB2	2:B:64:ASP:HB2	1.82	0.62
2:B:274:ASP:HB3	4:B:601:PMR:HAA	1.80	0.62
2:B:342:GLU:O	2:B:346:GLN:HG3	2.00	0.62
2:D:184:ILE:HD12	2:D:207:PHE:HE1	1.64	0.62
2:B:16:ALA:HB1	2:B:120:LEU:HD13	1.82	0.62
2:D:14:VAL:O	2:D:18:ARG:HG3	1.98	0.62
1:C:327:VAL:HG22	1:C:348:PRO:HB2	1.82	0.61
2:B:160:GLY:O	2:B:215:THR:OG1	2.14	0.61
1:C:197:LEU:HD11	1:C:273:PHE:CD2	2.28	0.61
1:A:318:ARG:HD2	1:A:343:LEU:HD22	1.81	0.61
1:C:292:SER:HB3	1:C:409:ALA:HB1	1.82	0.61
1:A:244:ILE:HG12	1:A:262:ILE:HA	1.81	0.61
1:A:53:THR:HG23	2:B:11:PRO:HG3	1.83	0.61
1:A:302:PHE:HB3	1:A:309:GLU:HG2	1.83	0.61
1:C:360:LEU:HD12	1:C:364:ARG:NE	2.16	0.61
1:A:379:ASN:HB3	2:D:268:TRP:HH2	1.64	0.61
2:B:415:LEU:HD21	1:C:67:PHE:HB2	1.82	0.61
1:C:375:LEU:HD21	2:D:41:LEU:HD11	1.83	0.61
3:C:501:SF4:FE2	2:D:36:ASP:OD1	1.52	0.61
2:B:414:LEU:HB3	2:B:419:ARG:NH2	2.16	0.61
1:A:396:PHE:HE2	4:A:502:PMR:HACA	1.64	0.61
1:A:390[A]:TRP:NE1	1:A:393:GLU:OE1	2.33	0.60
2:B:212:TYR:CZ	2:B:390:MET:HE3	2.35	0.60
2:B:265:ARG:HB3	2:B:269:TRP:HD1	1.65	0.60
1:A:224:LEU:O	1:A:258:TRP:NE1	2.34	0.60
2:D:205:ALA:O	2:D:229:GLN:NE2	2.34	0.60
1:C:371:THR:CG2	1:C:381:LEU:HD21	2.31	0.60
2:D:90:MET:HE1	2:D:120:LEU:CD2	2.30	0.60
2:D:360:ARG:HA	2:D:370:CYS:SG	2.41	0.60
1:C:108:GLN:HA	1:C:142:TYR:HE1	1.67	0.60
1:C:393:GLU:CD	1:C:411:LEU:HD13	2.22	0.60
2:D:44:THR:HA	2:D:49:ARG:H	1.66	0.60
2:B:28:TYR:HA	2:B:90:MET:O	2.02	0.59
2:D:318:ALA:HB1	2:D:322:ARG:HH22	1.67	0.59
1:C:421:ILE:HG13	1:C:422:LEU:HD12	1.84	0.59
1:C:54:CYS:SG	3:C:501:SF4:S1	3.00	0.59
2:D:90:MET:CE	2:D:120:LEU:HD22	2.31	0.59
2:B:44:THR:CG2	2:B:53:PRO:HD3	2.32	0.59
2:B:73:PHE:CE2	2:B:104:THR:HB	2.38	0.59
1:C:227:PRO:HA	1:C:248:PHE:CE2	2.38	0.59
2:D:15:GLY:HA2	2:D:18:ARG:HE	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100:ILE:CG2	2:D:101:GLN:NE2	2.65	0.59
1:A:110:PHE:CE1	1:A:142:TYR:HB2	2.37	0.59
2:D:96:THR:HG23	2:D:97:ALA:H	1.67	0.59
2:D:141:CYS:SG	2:D:202:LEU:HD22	2.42	0.59
1:A:379:ASN:OD1	2:D:273:VAL:HG23	2.02	0.59
2:B:39:ALA:HA	2:B:42:LEU:HD12	1.84	0.59
2:B:198:ASP:OD1	2:B:201:ARG:NH2	2.36	0.59
1:C:393:GLU:CD	1:C:411:LEU:HD22	2.27	0.59
2:B:248:GLU:O	2:B:252:LEU:HG	2.02	0.59
2:D:179:LEU:HD11	2:D:209:VAL:HG21	1.85	0.59
1:A:212:GLU:HG3	1:A:212:GLU:O	2.02	0.59
1:A:281:ARG:HG3	1:A:402:TYR:CZ	2.38	0.59
2:B:18:ARG:HH11	2:B:129:GLU:HG2	1.66	0.59
2:B:126:GLN:O	2:B:126:GLN:NE2	2.34	0.59
2:D:70:ALA:HA	2:D:102:ASP:OD2	2.02	0.58
2:D:213:PRO:HA	2:D:217:GLU:CB	2.23	0.58
1:A:51:SER:H	1:A:116:PRO:HG2	1.68	0.58
1:A:165:VAL:HG11	1:A:236:LEU:HB2	1.85	0.58
2:B:150:ARG:NH2	2:B:228:LYS:O	2.36	0.58
1:C:292:SER:HB2	1:C:295:LEU:HD12	1.85	0.58
2:B:157:ASN:ND2	2:B:187:ASN:OD1	2.35	0.58
2:B:276:THR:O	2:B:279:THR:OG1	2.22	0.58
2:D:133:ALA:HB1	2:D:162:THR:HG21	1.85	0.58
2:B:78:ARG:O	2:B:82:GLU:HG2	2.02	0.58
4:B:601:PMR:HMDB	4:B:601:PMR:HBCB	1.85	0.58
2:B:17:MET:SD	2:B:55:VAL:HG11	2.44	0.58
2:D:157:ASN:HD21	2:D:187:ASN:HD22	1.51	0.58
1:A:247:PRO:HD2	1:A:257:LEU:HB3	1.85	0.58
1:A:327:VAL:HG11	1:A:344:LEU:HD21	1.85	0.58
1:A:225:VAL:HG13	1:A:249:PRO:HG2	1.86	0.58
2:B:266:GLN:NE2	2:B:302:GLU:OE1	2.31	0.58
1:C:325:VAL:HG22	1:C:326:GLU:H	1.68	0.58
1:A:379:ASN:HB3	2:D:268:TRP:CH2	2.38	0.58
2:B:187:ASN:O	2:B:201:ARG:NH1	2.33	0.58
1:C:296:ARG:HA	1:C:321:GLY:H	1.68	0.58
1:C:115:CYS:SG	3:C:501:SF4:S2	3.01	0.57
1:C:148:GLY:O	2:D:34:GLN:NE2	2.37	0.57
1:C:360:LEU:HD12	1:C:364:ARG:HE	1.69	0.57
2:D:90:MET:CE	2:D:120:LEU:HD11	2.14	0.57
2:D:40:ASP:OD2	2:D:52:ARG:NH2	2.31	0.57
1:A:36:TRP:HE1	1:A:157:GLU:CG	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:HD22	1:A:350:LEU:HG	1.86	0.57
2:B:8:TYR:OH	2:B:359:GLU:OE2	2.20	0.57
1:C:392:ILE:HD12	1:C:392:ILE:H	1.69	0.57
2:D:378:HIS:CD2	2:D:380:GLN:H	2.23	0.57
2:B:310:MET:CE	2:B:325:ALA:HA	2.33	0.57
1:A:28:PHE:HZ	2:B:41:LEU:HD21	1.69	0.57
1:A:59:GLN:HA	1:A:66:ILE:HG21	1.86	0.57
2:B:207:PHE:HA	2:B:229:GLN:HB3	1.86	0.57
2:B:335:THR:OG1	2:B:340:GLU:OE1	2.18	0.57
2:B:419:ARG:HH12	1:C:39:ARG:NH2	2.03	0.57
1:C:166:PRO:O	1:C:239:ARG:NH1	2.38	0.57
1:C:250:PHE:CZ	1:C:308:LEU:HD22	2.39	0.57
2:B:418:PHE:HE2	1:C:39:ARG:NH1	1.77	0.57
1:A:226:GLN:HG2	1:A:400:HIS:NE2	2.20	0.57
2:B:12:PRO:HB2	2:B:122:LEU:CD1	2.35	0.57
2:B:12:PRO:HB2	2:B:122:LEU:HD13	1.87	0.57
2:B:52:ARG:O	2:B:53:PRO:C	2.48	0.57
1:A:375:LEU:HD11	1:A:390[B]:TRP:HA	1.87	0.56
2:B:53:PRO:O	2:B:55:VAL:N	2.38	0.56
1:C:360:LEU:HD22	1:C:377:LEU:HD12	1.86	0.56
2:B:155:SER:HB2	2:B:205:ALA:HA	1.87	0.56
1:C:307:GLN:CG	1:C:330:PRO:HD2	2.35	0.56
1:A:36:TRP:HB3	1:A:396:PHE:CE1	2.41	0.56
1:A:161:LEU:HD21	1:A:181:ALA:HB2	1.87	0.56
2:B:285:LEU:HG	2:B:354:LEU:HD12	1.86	0.56
1:C:224:LEU:HD11	1:C:233:HIS:HB2	1.87	0.56
1:C:227:PRO:HG2	1:C:308:LEU:CD2	2.35	0.56
1:C:359:GLN:HA	1:C:362:ARG:HD3	1.87	0.56
2:D:196:PRO:HA	2:D:199:ILE:HG22	1.86	0.56
2:D:288:ASP:OD1	2:D:288:ASP:N	2.38	0.56
1:A:114:SER:HB3	1:A:116:PRO:HD2	1.88	0.56
1:A:375:LEU:HB2	1:A:378:ALA:HB2	1.87	0.56
4:B:601:PMR:HMBB	1:C:60:SER:HB2	1.87	0.56
2:B:413:HIS:HA	2:B:417:MET:HE2	1.86	0.56
2:D:11:PRO:O	2:D:14:VAL:HG12	2.05	0.56
1:A:244:ILE:HG12	1:A:262:ILE:HG12	1.88	0.56
2:D:148:MET:N	2:D:203:GLY:HA3	2.20	0.56
1:A:44:ALA:HB2	1:A:108:GLN:HG3	1.86	0.56
2:D:68:ASP:O	2:D:72:LEU:HD23	2.06	0.56
2:D:131:PHE:HA	2:D:134:ASP:HB3	1.88	0.56
1:A:115:CYS:HG	3:A:501:SF4:FE4	0.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:VAL:HG21	2:B:211:LEU:HD21	1.88	0.56
1:A:199:ILE:CG2	1:A:268:VAL:HG21	2.32	0.55
2:B:94:SER:H	2:B:97:ALA:HB3	1.71	0.55
2:D:90:MET:HE1	2:D:120:LEU:HD21	1.88	0.55
1:C:371:THR:HG21	1:C:381:LEU:HD21	1.87	0.55
1:A:65:MET:HE3	1:A:72:PHE:CZ	2.39	0.55
2:B:17:MET:CE	2:B:39:ALA:HB1	2.35	0.55
2:D:59:THR:O	2:D:61[B]:GLN:NE2	2.40	0.55
2:D:355:GLY:O	2:D:372:VAL:HA	2.06	0.55
2:D:357:GLN:HA	2:D:360:ARG:HB3	1.87	0.55
2:D:207:PHE:HA	2:D:229:GLN:HB2	1.86	0.55
1:A:40:LYS:HD3	1:A:183:PRO:HA	1.88	0.55
1:A:87:ASP:O	1:A:91:GLU:HG2	2.06	0.55
2:B:49:ARG:HH12	2:B:163:ALA:CB	2.12	0.55
1:A:308:LEU:HD23	1:A:312:LEU:HD11	1.89	0.55
1:A:369:ASP:O	1:A:387:THR:HB	2.06	0.55
1:C:67:PHE:CZ	2:D:6:TRP:CZ3	2.95	0.55
2:D:360:ARG:HD2	2:D:364:LYS:HD2	1.88	0.55
2:B:413:HIS:HA	2:B:417:MET:HE1	1.89	0.55
2:B:276:THR:HG23	1:C:418:ARG:HB2	1.89	0.55
4:B:601:PMR:HBD	4:B:601:PMR:HBAA	1.88	0.55
2:D:301:ASP:OD1	2:D:302:GLU:N	2.40	0.54
1:A:303:LEU:HB2	1:A:373:CYS:HB3	1.89	0.54
2:D:211:LEU:O	2:D:390:MET:HE1	2.06	0.54
1:A:421:ILE:HG13	1:A:422:LEU:HD12	1.89	0.54
2:B:48:ARG:O	2:D:268:TRP:NE1	2.28	0.54
1:C:29:CYS:HB3	2:D:35:GLY:HA3	1.89	0.54
1:A:26:GLU:CD	1:A:377:LEU:HD13	2.33	0.54
2:B:133:ALA:HB1	2:B:162:THR:HG21	1.89	0.54
2:D:190:ALA:HB1	2:D:199:ILE:HD12	1.89	0.54
1:C:341:LEU:HD12	1:C:341:LEU:H	1.72	0.54
1:A:108:GLN:HA	1:A:140:ARG:O	2.08	0.54
1:A:242:ARG:HH22	1:A:265:GLU:HB3	1.72	0.54
2:B:179:LEU:HD11	2:B:209:VAL:HG21	1.89	0.54
2:D:137:PHE:CE2	2:D:191:PRO:HA	2.43	0.54
2:D:408:MET:O	2:D:412:GLU:HB2	2.07	0.54
1:C:360:LEU:HD11	1:C:364:ARG:NH2	2.23	0.54
1:A:260:LYS:HA	1:A:273:PHE:CZ	2.42	0.54
1:A:261:ALA:O	1:A:265:GLU:HG2	2.08	0.54
2:B:299:ALA:HA	2:B:303:MET:HB2	1.90	0.54
2:D:312:CYS:HB3	2:D:321:MET:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:LEU:HA	1:A:315:PHE:CE2	2.43	0.54
2:B:17:MET:HG2	2:B:28:TYR:CE2	2.43	0.54
4:A:502:PMR:HHC	2:B:41:LEU:HD22	1.89	0.53
1:C:100:LEU:HA	1:C:106:ILE:HD11	1.89	0.53
1:A:60:SER:HB3	4:A:502:PMR:HMBB	1.90	0.53
2:B:269:TRP:HB3	2:B:399:PHE:CZ	2.44	0.53
1:C:47:LEU:HD11	2:D:3:LEU:HD21	1.90	0.53
2:D:51:LYS:HE3	2:D:54:PRO:HG3	1.90	0.53
2:B:328:TYR:HB2	2:B:330:LEU:HD13	1.90	0.53
1:C:418:ARG:HD3	1:C:419:ARG:N	2.23	0.53
1:A:62:ALA:HB3	1:A:66:ILE:HG23	1.90	0.53
1:A:390[A]:TRP:HE3	1:A:390[A]:TRP:H	1.54	0.53
1:C:306:SER:OG	1:C:309:GLU:OE2	2.24	0.53
2:B:31:HIS:CE1	2:B:69:THR:HG23	2.43	0.53
2:B:278:LEU:HB3	2:B:305:PHE:CD2	2.43	0.53
1:C:153:PHE:HE2	1:C:395:VAL:HG21	1.74	0.53
1:A:255:THR:HG21	1:A:401:PHE:HA	1.90	0.53
2:B:17:MET:HG2	2:B:28:TYR:CD2	2.44	0.53
2:D:333:LEU:HD21	2:D:340:GLU:HB3	1.89	0.53
1:A:346:GLU:OE1	1:A:346:GLU:N	2.37	0.53
2:B:45:MET:SD	2:D:274:ASP:CG	2.91	0.53
2:B:209:VAL:HA	2:B:232:THR:HG23	1.90	0.53
2:B:377:VAL:HB	2:B:381:ASP:HB2	1.89	0.53
1:C:193:LEU:O	1:C:197:LEU:HD23	2.08	0.53
1:A:96:VAL:HG11	1:A:131:LEU:CD1	2.39	0.53
1:C:249:PRO:O	1:C:400:HIS:ND1	2.33	0.53
1:C:390[A]:TRP:NE1	1:C:393:GLU:HB2	2.23	0.53
2:D:102:ASP:O	2:D:104:THR:OG1	2.25	0.53
1:A:216:VAL:HA	1:A:220:THR:HG21	1.91	0.53
2:B:49:ARG:NH1	2:B:163:ALA:HB1	2.13	0.53
4:B:601:PMR:HMAB	2:D:46:ILE:HD13	1.91	0.53
2:D:161:PRO:O	2:D:192:MET:HB2	2.09	0.53
2:D:239:VAL:HG22	2:D:264:LEU:HD11	1.91	0.53
2:D:184:ILE:HD12	2:D:207:PHE:CE1	2.43	0.52
1:A:39:ARG:NH1	2:D:418:PHE:O	2.42	0.52
1:A:373:CYS:O	1:A:375:LEU:HD22	2.09	0.52
2:B:348:LEU:HD12	2:B:348:LEU:O	2.09	0.52
1:C:144:PHE:HE1	1:C:159:ALA:HB3	1.73	0.52
2:B:419:ARG:CD	1:C:65:MET:HB2	2.40	0.52
1:C:288:VAL:HG13	1:C:409:ALA:HB2	1.91	0.52
2:D:213:PRO:CB	2:D:217:GLU:HB2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:284:PHE:HE2	2:D:286:PHE:HB2	1.74	0.52
1:A:65:MET:HG3	2:D:418:PHE:CD2	2.45	0.52
1:C:182:LEU:HD12	1:C:186:VAL:HG13	1.89	0.52
2:D:224:GLU:HB2	2:D:230:PRO:HA	1.91	0.52
1:C:28:PHE:CE1	1:C:392:ILE:HD11	2.44	0.52
2:D:8:TYR:O	2:D:376:PRO:HB3	2.09	0.52
1:A:314:ARG:HG3	1:A:315:PHE:N	2.25	0.52
1:C:367:ARG:O	1:C:367:ARG:HG3	2.10	0.52
2:D:155:SER:H	2:D:206:HIS:CD2	2.28	0.52
1:A:194:LEU:O	1:A:198:GLY:N	2.27	0.52
2:B:19:VAL:HG21	2:B:136:SER:HB2	1.91	0.52
2:B:274:ASP:OD1	2:D:48:ARG:HD3	2.10	0.52
2:B:415:LEU:HD11	2:D:361:HIS:HD2	1.75	0.52
1:A:295:LEU:HD11	1:A:412:PHE:HB3	1.90	0.52
1:C:56:HIS:HA	1:C:59:GLN:HB3	1.92	0.52
1:C:162:ALA:O	1:C:166:PRO:HD3	2.09	0.52
1:C:226:GLN:HG2	1:C:229:LEU:HG	1.91	0.52
1:C:312:LEU:HD22	1:C:412:PHE:HE2	1.75	0.52
2:D:19:VAL:HG11	2:D:136:SER:HB3	1.92	0.52
1:A:70:PRO:HD2	2:B:5:LEU:HD21	1.91	0.52
1:A:396:PHE:CE2	4:A:502:PMR:HACA	2.43	0.52
4:B:601:PMR:HMC	1:C:392:ILE:HG21	1.92	0.52
2:D:180:GLU:OE1	2:D:180:GLU:HA	2.10	0.52
1:A:107:ARG:O	1:A:140:ARG:N	2.43	0.51
2:B:17:MET:HE1	2:B:39:ALA:HB3	1.92	0.51
1:C:255:THR:HG23	1:C:281:ARG:NH1	2.25	0.51
2:D:278:LEU:HD12	2:D:305:PHE:CZ	2.45	0.51
1:A:203:ARG:HD3	1:A:215:GLY:H	1.75	0.51
2:B:156:CYS:SG	2:B:179:LEU:HD13	2.51	0.51
2:B:210:LEU:HD13	2:B:220:ALA:HB3	1.92	0.51
2:B:356:THR:HB	2:B:376:PRO:HG2	1.91	0.51
2:B:388:PRO:HD2	2:B:397:VAL:HG21	1.91	0.51
1:C:45:PHE:HD2	1:C:106:ILE:HG21	1.74	0.51
1:C:57:LEU:HD13	2:D:38:TYR:HB2	1.93	0.51
1:C:95:GLU:O	1:C:99:LEU:HD12	2.09	0.51
1:A:135:HIS:HB3	1:A:139:VAL:HB	1.91	0.51
1:C:153:PHE:CE2	1:C:306:SER:HA	2.44	0.51
2:D:171:ASP:CG	2:D:390:MET:HG3	2.35	0.51
1:A:270:ALA:HA	1:A:273:PHE:HB2	1.92	0.51
1:C:161:LEU:HD12	1:C:229:LEU:HD11	1.92	0.51
1:C:375:LEU:HD21	2:D:41:LEU:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:99:LEU:HD13	2:D:124:SER:HB2	1.91	0.51
1:A:288:VAL:HG13	1:A:409:ALA:HB2	1.93	0.51
1:A:312:LEU:HA	1:A:315:PHE:CZ	2.46	0.51
2:B:259:ALA:HB1	2:B:392:PHE:HE2	1.76	0.51
2:B:262:SER:O	2:B:265:ARG:NH2	2.44	0.51
1:C:96:VAL:HA	1:C:99:LEU:HD13	1.93	0.51
2:D:288:ASP:HA	2:D:314:ASN:OD1	2.09	0.51
2:B:18:ARG:NE	2:B:164:LEU:O	2.44	0.51
2:B:48:ARG:C	2:D:268:TRP:HE1	2.16	0.51
2:B:270:SER:O	2:B:275:SER:HB2	2.11	0.51
1:A:179:VAL:HA	1:A:205:LEU:HB3	1.93	0.51
2:B:35:GLY:C	2:B:37:THR:H	2.19	0.51
2:B:95:CYS:SG	2:B:96:THR:N	2.84	0.51
1:C:302:PHE:CD1	1:C:309:GLU:HG3	2.46	0.51
1:A:114:SER:C	1:A:147:SER:HB3	2.36	0.50
4:B:601:PMR:HBB	1:C:61:ALA:HB2	1.93	0.50
2:D:46:ILE:HD13	2:D:379:VAL:HB	1.91	0.50
1:A:312:LEU:HD22	1:A:412:PHE:CE2	2.47	0.50
1:C:176:LEU:HD22	1:C:199:ILE:HG21	1.92	0.50
1:C:293:GLU:OE1	1:C:293:GLU:N	2.39	0.50
2:D:137:PHE:CZ	2:D:191:PRO:HA	2.46	0.50
1:A:304:PRO:HD3	1:A:359:GLN:HE22	1.75	0.50
2:B:419:ARG:HD2	1:C:65:MET:HA	1.92	0.50
2:D:74:GLN:HE21	2:D:107:LEU:HB2	1.75	0.50
2:D:278:LEU:HD12	2:D:305:PHE:CE1	2.47	0.50
2:B:31:HIS:HE1	2:B:69:THR:HG23	1.76	0.50
1:C:307:GLN:CG	1:C:330:PRO:CD	2.89	0.50
1:A:337:LEU:O	1:A:341:LEU:N	2.39	0.50
1:A:282:ALA:O	1:A:285:ARG:HG3	2.11	0.50
1:C:306:SER:HB3	1:C:391:ALA:HB1	1.92	0.50
2:B:137:PHE:CD1	2:B:191:PRO:HB3	2.47	0.50
2:B:236:PRO:O	2:B:391:GLY:N	2.42	0.50
2:B:264:LEU:HD22	2:B:392:PHE:HD1	1.76	0.50
1:C:380:PRO:O	1:C:384:GLU:HG3	2.11	0.50
1:A:217:GLY:O	1:A:220:THR:OG1	2.29	0.50
1:A:399:VAL:HB	1:A:408:LEU:HD22	1.93	0.50
2:B:35:GLY:C	2:B:37:THR:N	2.70	0.50
2:D:358:MET:O	2:D:362:ILE:HG13	2.12	0.50
2:D:360:ARG:HD3	2:D:370:CYS:SG	2.52	0.50
1:A:116:PRO:HD3	3:A:501:SF4:S1	2.52	0.50
1:A:248:PHE:CZ	1:A:336:ILE:HG22	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:383:PRO:HG2	2:B:387:SER:HB2	1.94	0.50
2:B:415:LEU:HD11	2:D:361:HIS:CD2	2.47	0.50
2:D:81:TYR:CD1	2:D:111:LEU:HD13	2.47	0.50
2:D:184:ILE:HD11	2:D:253:ALA:HB2	1.94	0.50
1:C:36:TRP:HB2	1:C:396:PHE:CE1	2.47	0.49
2:D:187:ASN:O	2:D:201:ARG:NH2	2.45	0.49
1:A:224:LEU:HB3	1:A:248:PHE:HE1	1.77	0.49
1:A:405:ALA:O	1:A:408:LEU:HB3	2.13	0.49
1:A:422:LEU:HD21	2:D:270:SER:O	2.12	0.49
2:D:90:MET:HE3	2:D:120:LEU:CG	2.32	0.49
1:A:179:VAL:HG13	1:A:205:LEU:HG	1.94	0.49
1:C:418:ARG:HD3	1:C:418:ARG:C	2.36	0.49
1:A:263:ALA:HB1	1:A:268:VAL:HB	1.94	0.49
1:A:375:LEU:HD11	1:A:390[A]:TRP:HA	1.94	0.49
1:A:29:CYS:SG	3:A:501:SF4:S4	3.10	0.49
1:A:30:GLY:N	1:A:146:GLY:O	2.45	0.49
1:A:158:ASP:HB2	1:A:229:LEU:HA	1.95	0.49
1:A:227:PRO:CD	1:A:250:PHE:HE2	2.24	0.49
2:B:33:PRO:HG3	2:B:60:PHE:CZ	2.48	0.49
1:C:56:HIS:CE1	2:D:42:LEU:HD21	2.47	0.49
2:D:377:VAL:HG21	2:D:381:ASP:HB2	1.94	0.49
1:C:249:PRO:HB2	1:C:401[B]:PHE:CD1	2.48	0.49
1:A:153:PHE:CZ	1:A:392:ILE:HG13	2.48	0.49
2:B:182:MET:HE1	2:B:249:VAL:HG23	1.94	0.49
1:A:384:GLU:N	1:A:384:GLU:OE1	2.46	0.49
2:B:167:ARG:O	2:B:212:TYR:OH	2.31	0.49
2:D:157:ASN:OD1	2:D:202:LEU:HG	2.12	0.49
1:A:25:ARG:N	2:B:59:THR:OG1	2.43	0.49
1:A:242:ARG:NH2	1:A:265:GLU:HB3	2.28	0.49
1:A:280:PRO:HB2	1:A:402:TYR:CD2	2.43	0.49
2:B:271:ALA:HB2	1:C:422:LEU:HB3	1.95	0.49
1:C:88:ALA:HB1	1:C:122:LEU:HD21	1.94	0.49
2:D:74:GLN:NE2	2:D:107:LEU:H	2.11	0.49
2:D:47:GLU:HB2	2:D:164:LEU:HD12	1.95	0.48
2:B:33:PRO:HG2	2:B:96:THR:HB	1.94	0.48
1:C:249:PRO:HB2	1:C:401[B]:PHE:HD1	1.76	0.48
2:D:284:PHE:CE2	2:D:286:PHE:HB2	2.48	0.48
1:A:303:LEU:HD13	1:A:359:GLN:NE2	2.28	0.48
2:B:9:GLU:OE2	2:B:130:ASN:ND2	2.46	0.48
2:B:243:ARG:HG3	2:B:243:ARG:HH11	1.78	0.48
2:D:61[A]:GLN:CD	2:D:61[A]:GLN:H	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:356:THR:HG22	2:D:376:PRO:HD2	1.95	0.48
1:A:158:ASP:OD2	1:A:231:ASP:HB2	2.13	0.48
1:A:312:LEU:HD22	1:A:412:PHE:HE2	1.77	0.48
1:C:124:LEU:HB2	1:C:143:ASN:HB2	1.94	0.48
2:D:61[A]:GLN:HB2	2:D:63:ARG:HD2	1.95	0.48
1:A:252:GLU:O	1:A:256:THR:OG1	2.18	0.48
1:A:400:HIS:HB3	1:A:401:PHE:CD1	2.48	0.48
2:D:169:ARG:NH2	2:D:384:ALA:O	2.47	0.48
1:A:222:PHE:HD2	1:A:236:LEU:CD2	2.26	0.48
1:A:216:VAL:HG11	1:A:236:LEU:HD11	1.96	0.48
1:A:370:LEU:CD1	1:A:389:LYS:HB3	2.41	0.48
2:B:21:THR:O	2:B:49:ARG:NH2	2.47	0.48
2:D:74:GLN:HE21	2:D:107:LEU:H	1.62	0.48
2:D:321:MET:HE3	2:D:321:MET:HB3	1.68	0.48
1:A:24:GLN:HB3	2:B:57:TYR:O	2.14	0.48
2:D:235:VAL:HG12	2:D:237:ILE:HG13	1.96	0.48
1:A:74:THR:HG22	1:A:74:THR:O	2.13	0.48
2:D:6:TRP:CD1	2:D:6:TRP:C	2.92	0.48
2:D:21:THR:HG22	2:D:49:ARG:HH11	1.78	0.48
2:D:322:ARG:HB3	2:D:326:LYS:NZ	2.29	0.48
2:D:371:ALA:HB2	2:D:405:PRO:HG3	1.94	0.48
1:A:85:LEU:HD23	1:A:89:ASN:ND2	2.28	0.48
2:B:340:GLU:HA	2:B:343:GLU:OE1	2.14	0.48
1:C:308:LEU:HB3	1:C:312:LEU:HG	1.95	0.48
1:C:381:LEU:HG	1:C:386:PHE:CB	2.42	0.48
2:D:222:TRP:CD1	2:D:225:LYS:HZ1	2.32	0.48
1:A:34:ILE:HA	1:A:37:LEU:HB2	1.95	0.47
1:A:255:THR:HB	1:A:402:TYR:CE1	2.49	0.47
2:B:34:GLN:HB3	2:B:59:THR:HB	1.95	0.47
1:C:38:HIS:CE1	1:C:71:ARG:H	2.33	0.47
1:C:326:GLU:HG2	1:C:349:VAL:HB	1.96	0.47
2:D:18:ARG:HB3	2:D:163:ALA:O	2.14	0.47
2:D:313:TYR:OH	2:D:376:PRO:HD3	2.13	0.47
2:B:31:HIS:NE2	2:B:69:THR:O	2.48	0.47
1:C:303:LEU:HB3	1:C:373:CYS:HA	1.94	0.47
1:A:115:CYS:SG	3:A:501:SF4:S1	3.11	0.47
1:A:358:ARG:HB2	1:A:362:ARG:HH21	1.79	0.47
1:C:162:ALA:HB2	1:C:232:THR:HA	1.96	0.47
1:A:225:VAL:HG12	1:A:400:HIS:CD2	2.50	0.47
1:A:250:PHE:HB3	1:A:315:PHE:CE2	2.50	0.47
2:B:303:MET:HE3	2:B:399:PHE:HD1	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PRO:HA	1:A:248:PHE:CE2	2.49	0.47
1:A:373:CYS:SG	1:A:375:LEU:HB3	2.54	0.47
2:B:284:PHE:C	2:B:285:LEU:HD12	2.40	0.47
1:C:380:PRO:HA	1:C:383:ALA:HB3	1.96	0.47
2:D:38:TYR:HA	2:D:41:LEU:HD13	1.96	0.47
2:D:210:LEU:HD23	2:D:211:LEU:N	2.29	0.47
1:A:418:ARG:O	1:A:422:LEU:HB2	2.14	0.47
2:B:410:LEU:O	2:B:414:LEU:HD12	2.15	0.47
1:C:183:PRO:O	1:C:187:GLU:N	2.46	0.47
1:C:326:GLU:HA	1:C:349:VAL:H	1.80	0.47
1:C:399:VAL:HA	1:C:404:GLN:O	2.15	0.47
2:D:131:PHE:CD1	2:D:135:GLU:HG2	2.49	0.47
2:D:213:PRO:O	2:D:214:GLU:C	2.56	0.47
1:A:400:HIS:HB3	1:A:401:PHE:HD1	1.79	0.47
2:B:419:ARG:CD	1:C:65:MET:HE3	2.33	0.47
1:C:258:TRP:CE3	1:C:259:LEU:HG	2.50	0.47
2:D:95:CYS:HA	2:D:98:GLU:O	2.14	0.47
2:D:213:PRO:HB3	2:D:217:GLU:HB2	1.97	0.47
1:A:126:ARG:HH21	1:A:130:ARG:HH22	1.63	0.47
2:B:52:ARG:O	2:B:54:PRO:N	2.48	0.47
2:B:278:LEU:HB3	2:B:305:PHE:HD2	1.79	0.47
1:A:150:GLU:N	1:A:150:GLU:OE2	2.48	0.47
2:B:407:THR:OG1	2:D:380:GLN:NE2	2.48	0.47
2:D:238:GLY:O	2:D:242:THR:N	2.41	0.47
2:D:353:ILE:O	2:D:353:ILE:HG22	2.15	0.47
1:A:263:ALA:HB3	1:A:273:PHE:CZ	2.49	0.47
1:A:389:LYS:HB2	1:A:415:PRO:HG2	1.96	0.47
2:B:408:MET:O	2:B:411:GLU:HG2	2.15	0.47
1:C:74:THR:H	2:D:3:LEU:HD23	1.78	0.47
1:C:178:LEU:HD11	1:C:258:TRP:CZ2	2.50	0.47
1:A:149:ILE:O	2:B:62:ALA:N	2.44	0.46
2:B:26:MET:HE3	2:B:90:MET:HB2	1.97	0.46
2:B:311:GLY:HA3	2:B:333:LEU:HB3	1.97	0.46
1:C:153:PHE:CD2	1:C:154:THR:HG23	2.49	0.46
1:C:356:VAL:HA	1:C:359:GLN:HB3	1.96	0.46
1:A:48:VAL:HG21	1:A:58:LEU:HD11	1.98	0.46
2:B:28:TYR:CZ	2:B:120:LEU:HD12	2.50	0.46
2:B:284:PHE:HD1	2:B:353:ILE:HG13	1.79	0.46
2:D:131:PHE:HD1	2:D:135:GLU:HG2	1.81	0.46
2:B:38:TYR:O	2:B:41:LEU:N	2.47	0.46
2:B:338:TYR:CB	2:B:358:MET:HE2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:VAL:O	1:C:360:LEU:HD23	2.15	0.46
1:C:357:GLU:HB3	2:D:83:ARG:NH1	2.30	0.46
1:C:377:LEU:O	1:C:380:PRO:HD2	2.15	0.46
2:D:161:PRO:O	2:D:191:PRO:HB2	2.16	0.46
1:A:119:VAL:HG11	2:B:99:LEU:HB3	1.97	0.46
1:A:354:GLN:HB3	1:A:359:GLN:NE2	2.30	0.46
2:B:113:LEU:HD23	2:B:113:LEU:H	1.80	0.46
2:B:345:ILE:HD12	2:B:368:ILE:HD11	1.96	0.46
1:C:194:LEU:HB3	1:C:199:ILE:HD13	1.97	0.46
1:A:37:LEU:HB3	1:A:46:PHE:CZ	2.50	0.46
1:A:175:GLU:OE1	1:A:203:ARG:HD2	2.14	0.46
1:A:222:PHE:CB	1:A:236:LEU:HD22	2.44	0.46
1:A:227:PRO:HA	1:A:248:PHE:CZ	2.49	0.46
1:A:244:ILE:HG21	1:A:262:ILE:HG13	1.96	0.46
2:B:199:ILE:HA	2:B:202:LEU:HD13	1.96	0.46
2:B:272:SER:O	2:B:276:THR:OG1	2.32	0.46
2:D:163:ALA:HA	2:D:192:MET:CE	2.46	0.46
2:B:352:LEU:HD22	2:B:406:LEU:HG	1.97	0.46
1:C:199:ILE:HA	1:C:266:PHE:CE2	2.50	0.46
2:D:89:ILE:HG12	2:D:113:LEU:CD1	2.45	0.46
2:D:155:SER:HA	2:D:185:ALA:HB3	1.97	0.46
1:A:228:PHE:HB3	1:A:307:GLN:HB2	1.97	0.46
2:B:175:VAL:HG21	2:B:211:LEU:CD2	2.45	0.46
1:C:372:VAL:HB	1:C:389:LYS:HB3	1.97	0.46
1:A:312:LEU:HD13	1:A:412:PHE:HZ	1.81	0.46
2:B:387:SER:OG	2:D:385:ARG:NH2	2.41	0.46
1:C:202:VAL:HG23	1:C:203:ARG:H	1.81	0.46
2:D:70:ALA:HA	2:D:102:ASP:CG	2.40	0.46
2:D:303:MET:HE1	2:D:399:PHE:HD1	1.80	0.46
2:D:388:PRO:O	2:D:394:GLY:HA2	2.16	0.46
1:C:301:PHE:HE1	1:C:359:GLN:HE21	1.64	0.46
2:D:81:TYR:CD1	2:D:86:PRO:HD2	2.51	0.46
2:B:46:ILE:HD13	2:B:379:VAL:HG13	1.96	0.46
1:C:330:PRO:HG3	1:C:331:PHE:H	1.76	0.46
2:D:33:PRO:HD3	2:D:60:PHE:CE1	2.51	0.46
2:D:88:ALA:CA	2:D:113:LEU:HD13	2.44	0.46
2:D:246:VAL:HA	2:D:249:VAL:HG22	1.97	0.46
2:D:300:ARG:HH21	2:D:307:VAL:HB	1.81	0.46
2:D:361:HIS:HA	2:D:364:LYS:HD3	1.98	0.46
4:B:601:PMR:HBD	4:B:601:PMR:CBA	2.45	0.45
1:C:29:CYS:HB2	1:C:148:GLY:HA3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:322:ARG:NH1	2:D:334:VAL:HG11	2.30	0.45
1:A:54:CYS:SG	3:A:501:SF4:S1	3.14	0.45
1:A:302:PHE:CG	1:A:309:GLU:HB3	2.51	0.45
2:B:2:LYS:HE3	2:B:3:LEU:H	1.81	0.45
2:B:51:LYS:O	2:B:52:ARG:C	2.59	0.45
2:D:90:MET:HG2	2:D:118:VAL:CG1	2.44	0.45
1:A:73:GLY:HA2	2:B:3:LEU:HD21	1.99	0.45
1:A:326:GLU:HG3	1:A:328:GLY:H	1.81	0.45
1:C:381:LEU:CD1	1:C:386:PHE:CD2	2.98	0.45
1:A:174:ARG:HH12	1:A:242:ARG:NH2	2.15	0.45
1:A:226:GLN:HG2	1:A:400:HIS:CE1	2.52	0.45
1:C:65:MET:HG3	1:C:70:PRO:HG3	1.99	0.45
1:C:360:LEU:CD1	1:C:364:ARG:HH21	2.29	0.45
1:C:371:THR:O	1:C:371:THR:HG22	2.16	0.45
1:C:413:SER:O	1:C:417:ARG:HG2	2.16	0.45
1:A:228:PHE:HE2	1:A:308:LEU:HD12	1.82	0.45
2:B:210:LEU:CD1	2:B:220:ALA:HB2	2.40	0.45
1:C:34:ILE:HD11	1:C:144:PHE:HE2	1.82	0.45
2:D:284:PHE:HB2	2:D:350:PRO:HG2	1.99	0.45
1:A:222:PHE:HD2	1:A:236:LEU:HD23	1.81	0.45
1:A:390[B]:TRP:CE3	1:A:392:ILE:HB	2.52	0.45
2:B:212:TYR:CZ	2:B:390:MET:CE	3.00	0.45
1:C:92:LEU:O	1:C:95:GLU:HG3	2.17	0.45
1:C:186:VAL:HG21	1:C:400:HIS:O	2.16	0.45
1:C:256:THR:OG1	1:C:281:ARG:HD2	2.16	0.45
1:C:340:ASP:O	1:C:344:LEU:HB2	2.16	0.45
2:B:31:HIS:HD2	2:B:58:THR:OG1	2.00	0.45
2:B:220:ALA:HB1	2:B:231:TYR:HB2	1.99	0.45
2:D:161:PRO:HB2	2:D:172:ILE:HD11	1.99	0.45
2:D:318:ALA:HB1	2:D:322:ARG:NH2	2.30	0.45
2:B:14:VAL:O	2:B:18:ARG:HG3	2.17	0.45
1:C:186:VAL:HG21	1:C:404:GLN:OE1	2.16	0.45
1:A:86:ALA:HA	1:A:89:ASN:HD21	1.82	0.45
1:A:390[A]:TRP:HZ3	1:A:415:PRO:HG3	1.81	0.45
1:C:389:LYS:HD2	1:C:390[A]:TRP:H	1.81	0.45
2:B:86:PRO:O	2:B:115:VAL:HG11	2.17	0.45
4:B:601:PMR:CMC	1:C:392:ILE:HG21	2.47	0.45
1:C:306:SER:C	1:C:308:LEU:H	2.25	0.45
1:A:76:VAL:O	2:B:1:MET:HA	2.17	0.44
1:A:294:GLY:HA2	1:A:413:SER:HB2	2.00	0.44
1:C:227:PRO:HG2	1:C:308:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:PRO:HD2	1:C:258:TRP:HA	1.98	0.44
1:A:36:TRP:HE3	1:A:396:PHE:CE1	2.35	0.44
2:B:239:VAL:HG22	2:B:264:LEU:HD21	1.99	0.44
2:B:269:TRP:CZ3	2:D:48:ARG:HB2	2.52	0.44
1:C:312:LEU:HD22	1:C:412:PHE:CE2	2.52	0.44
1:C:377:LEU:CD2	1:C:380:PRO:HB2	2.47	0.44
2:D:32:ALA:HB1	2:D:36:ASP:HB2	2.00	0.44
2:D:138:LEU:HD13	2:D:218:SER:HB3	1.98	0.44
2:D:283:VAL:HG22	2:D:352:LEU:HB3	1.98	0.44
2:D:342:GLU:OE2	2:D:362:ILE:HG23	2.17	0.44
2:D:372:VAL:HG21	2:D:381:ASP:OD1	2.17	0.44
4:B:601:PMR:HMB	2:D:46:ILE:HG12	1.99	0.44
1:C:25:ARG:HD2	1:C:25:ARG:HA	1.79	0.44
1:C:303:LEU:HD23	1:C:304:PRO:HD2	1.99	0.44
1:A:390[B]:TRP:CD1	2:D:273:VAL:HG11	2.52	0.44
2:B:134:ASP:HB2	2:B:215:THR:HA	1.99	0.44
1:C:108:GLN:HA	1:C:142:TYR:CE1	2.49	0.44
2:D:136:SER:O	2:D:140:ILE:HG23	2.17	0.44
1:A:222:PHE:CE1	1:A:243:HIS:HB2	2.45	0.44
1:A:236:LEU:HD23	1:A:241:ALA:HB3	2.00	0.44
1:A:379:ASN:HB2	1:A:380:PRO:HD3	1.99	0.44
1:C:120:ILE:HB	1:C:122:LEU:HD23	2.00	0.44
1:C:377:LEU:HD23	1:C:380:PRO:HB2	1.99	0.44
2:D:207:PHE:HB2	2:D:230:PRO:O	2.18	0.44
2:B:309:GLY:H	2:B:330:LEU:HD23	1.82	0.44
1:C:360:LEU:CD1	1:C:364:ARG:NH2	2.80	0.44
2:D:89:ILE:HG12	2:D:113:LEU:HD11	1.99	0.44
1:A:242:ARG:HH12	1:A:265:GLU:HB3	1.82	0.44
1:A:421:ILE:O	1:A:423:ARG:NH2	2.45	0.44
1:C:197:LEU:HD13	1:C:268:VAL:HG11	1.99	0.44
1:C:248:PHE:HZ	1:C:337:LEU:HD22	1.83	0.44
2:D:90:MET:CE	2:D:120:LEU:CG	2.95	0.44
2:D:100:ILE:HG12	2:D:100:ILE:O	2.18	0.44
2:D:197:ALA:O	2:D:201:ARG:HG3	2.18	0.44
1:A:255:THR:HB	1:A:402:TYR:HE1	1.82	0.44
2:B:176:THR:HG23	2:B:186:VAL:HG21	1.99	0.44
2:B:393:GLU:OE1	2:D:386:TYR:N	2.49	0.44
2:D:74:GLN:OE1	2:D:104:THR:HB	2.18	0.44
2:D:370:CYS:O	2:D:405:PRO:HB3	2.18	0.44
1:A:66:ILE:HA	1:A:70:PRO:HG3	2.00	0.43
2:B:238:GLY:O	2:B:242:THR:OG1	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:275:SER:OG	2:D:48:ARG:NH2	2.50	0.43
1:C:74:THR:O	2:D:3:LEU:HA	2.18	0.43
1:C:304:PRO:HG3	1:C:354:GLN:OE1	2.18	0.43
1:C:360:LEU:HD11	1:C:364:ARG:HH21	1.82	0.43
2:D:208:ASN:O	2:D:231:TYR:HA	2.18	0.43
1:A:148:GLY:HA2	1:A:151:THR:O	2.19	0.43
1:A:295:LEU:CD2	1:A:322:MET:HE1	2.47	0.43
1:A:318:ARG:CD	1:A:343:LEU:HD22	2.47	0.43
1:A:367:ARG:HA	1:A:386:PHE:HE1	1.83	0.43
1:A:389:LYS:HD3	1:A:412:PHE:HA	1.99	0.43
1:C:389:LYS:HD2	1:C:390[B]:TRP:H	1.83	0.43
2:D:148:MET:H	2:D:203:GLY:HA3	1.83	0.43
2:D:266:GLN:OE1	2:D:303:MET:HE2	2.17	0.43
1:A:132:SER:OG	1:A:141:VAL:HG12	2.17	0.43
1:A:300:VAL:HB	1:A:322:MET:HE2	2.00	0.43
1:C:250:PHE:CE2	1:C:308:LEU:HD22	2.52	0.43
1:C:255:THR:HG23	1:C:281:ARG:HH11	1.83	0.43
2:D:46:ILE:O	2:D:379:VAL:HG23	2.18	0.43
2:D:184:ILE:HD11	2:D:253:ALA:CB	2.47	0.43
1:A:28:PHE:CZ	2:B:41:LEU:HD21	2.51	0.43
1:A:308:LEU:CD2	1:A:312:LEU:HD11	2.48	0.43
1:C:54:CYS:SG	3:C:501:SF4:S4	3.03	0.43
1:C:176:LEU:HD12	1:C:221:VAL:HG23	2.01	0.43
1:C:224:LEU:HD23	1:C:224:LEU:HA	1.87	0.43
1:C:248:PHE:CZ	1:C:337:LEU:HB3	2.54	0.43
1:C:291:ALA:HB3	1:C:409:ALA:HB3	1.99	0.43
1:C:381:LEU:HB3	1:C:388:THR:OG1	2.18	0.43
2:D:18:ARG:O	2:D:163:ALA:HB3	2.19	0.43
2:D:352:LEU:HD11	2:D:405:PRO:HG2	2.01	0.43
2:B:265:ARG:HB3	2:B:269:TRP:CD1	2.51	0.43
2:D:325:ALA:O	2:D:329:GLY:N	2.52	0.43
1:A:28:PHE:CE1	4:A:502:PMR:HMCB	2.54	0.43
2:B:239:VAL:O	2:B:243:ARG:HG2	2.19	0.43
2:B:341:VAL:O	2:B:345:ILE:HG23	2.17	0.43
1:C:113:GLY:H	1:C:145:SER:HA	1.83	0.43
1:A:26:GLU:CD	1:A:375:LEU:H	2.26	0.43
1:A:36:TRP:CD1	1:A:157:GLU:OE1	2.72	0.43
1:A:317:THR:HA	1:A:322:MET:N	2.27	0.43
2:B:94:SER:O	2:B:98:GLU:HG3	2.19	0.43
2:D:161:PRO:HA	2:D:168:HIS:ND1	2.33	0.43
1:A:82:LEU:HD23	1:A:82:LEU:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLU:HA	1:A:256:THR:HB	2.00	0.43
1:A:379:ASN:ND2	2:D:272:SER:HB3	2.34	0.43
1:C:194:LEU:O	1:C:197:LEU:HB2	2.19	0.43
2:D:13:HIS:HE1	2:D:39:ALA:HB3	1.84	0.43
1:A:224:LEU:HB3	1:A:248:PHE:CE1	2.53	0.43
1:A:364:ARG:HA	1:A:386:PHE:CZ	2.54	0.43
2:B:89:ILE:HD12	2:B:89:ILE:HA	1.85	0.43
2:B:184:ILE:H	2:B:184:ILE:HD12	1.84	0.43
2:B:184:ILE:HD12	2:B:184:ILE:N	2.33	0.43
2:B:369:PRO:HB3	2:B:405:PRO:O	2.18	0.43
2:B:385:ARG:HB3	2:D:397:VAL:HA	2.00	0.43
1:C:26:GLU:O	1:C:375:LEU:HB3	2.18	0.43
1:C:227:PRO:HA	1:C:248:PHE:CD2	2.53	0.43
1:C:272:THR:O	1:C:276:VAL:HG22	2.18	0.43
2:D:356:THR:HG23	2:D:359:GLU:OE2	2.19	0.43
2:D:377:VAL:CG2	2:D:381:ASP:HB2	2.48	0.43
1:A:314:ARG:NE	1:A:340:ASP:OD1	2.52	0.43
1:A:378:ALA:HA	1:A:388:THR:HG21	2.01	0.43
1:C:160:CYS:O	1:C:164:ILE:HG13	2.19	0.43
2:D:24:THR:O	2:D:24:THR:OG1	2.36	0.43
1:A:41:MET:H	1:A:41:MET:HG2	1.67	0.42
1:A:134:HIS:CE1	1:A:135:HIS:ND1	2.87	0.42
1:C:92:LEU:HD22	1:C:122:LEU:HD12	2.01	0.42
1:C:151:THR:HG22	1:C:152:THR:N	2.35	0.42
1:C:250:PHE:CZ	1:C:308:LEU:CD2	3.01	0.42
2:D:90:MET:HB3	2:D:120:LEU:HD13	2.01	0.42
1:A:41:MET:HA	1:A:208:HIS:HA	2.01	0.42
2:B:259:ALA:HB1	2:B:392:PHE:CE2	2.54	0.42
2:B:265:ARG:O	2:B:269:TRP:HB2	2.19	0.42
2:B:386:TYR:CD2	2:D:386:TYR:HD2	2.37	0.42
1:A:34:ILE:O	1:A:38:HIS:ND1	2.48	0.42
2:B:155:SER:HA	2:B:185:ALA:O	2.19	0.42
1:C:64:VAL:HA	1:C:67:PHE:CD2	2.54	0.42
1:C:66:ILE:CD1	2:D:6:TRP:CE3	2.87	0.42
2:D:160:GLY:HA2	2:D:216:GLY:HA3	2.00	0.42
1:A:29:CYS:O	1:A:32:THR:HG22	2.19	0.42
2:B:21:THR:HG21	2:B:43:PHE:CD1	2.54	0.42
2:B:208:ASN:HD22	2:B:229:GLN:HB2	1.85	0.42
2:B:314:ASN:OD1	2:B:314:ASN:N	2.53	0.42
1:C:221:VAL:HB	1:C:244:ILE:HD11	2.01	0.42
2:D:213:PRO:HD2	2:D:290:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:312:CYS:HB3	2:D:321:MET:CE	2.48	0.42
1:A:153:PHE:CE2	1:A:392:ILE:HA	2.55	0.42
1:A:199:ILE:HD13	1:A:199:ILE:HG21	1.76	0.42
1:A:309:GLU:CD	1:A:309:GLU:H	2.27	0.42
1:C:52:ARG:O	1:C:56:HIS:CB	2.67	0.42
2:D:126:GLN:C	2:D:127:ARG:HG2	2.45	0.42
2:D:417:MET:O	2:D:417:MET:HG2	2.20	0.42
2:B:2:LYS:HD2	2:B:2:LYS:HA	1.86	0.42
4:B:601:PMR:CHC	1:C:390[B]:TRP:HH2	2.33	0.42
1:C:92:LEU:O	1:C:96:VAL:HG23	2.20	0.42
2:D:134:ASP:HB2	2:D:215:THR:HA	2.00	0.42
2:B:271:ALA:HB1	1:C:418:ARG:HH21	1.84	0.42
1:C:59:GLN:HA	1:C:66:ILE:HG21	2.02	0.42
1:C:389:LYS:HZ2	1:C:411:LEU:C	2.27	0.42
2:B:284:PHE:HB2	2:B:348:LEU:HD11	2.01	0.42
1:C:182:LEU:HD13	1:C:225:VAL:HG11	2.00	0.42
2:D:209:VAL:HA	2:D:232:THR:HG23	2.00	0.42
1:C:176:LEU:HB3	1:C:199:ILE:HD12	2.01	0.42
2:D:79:ASP:OD1	2:D:83:ARG:NH2	2.53	0.42
2:D:237:ILE:HD11	2:D:390:MET:HE3	2.00	0.42
1:A:122:LEU:HD12	1:A:122:LEU:HA	1.84	0.42
1:A:249:PRO:HD3	1:A:258:TRP:CD1	2.55	0.42
1:C:22:ARG:HG3	1:C:23:GLY:H	1.85	0.42
1:C:56:HIS:O	1:C:56:HIS:CD2	2.73	0.42
2:D:17:MET:HB3	2:D:43:PHE:CZ	2.55	0.42
1:A:303:LEU:HB2	1:A:373:CYS:HA	2.02	0.41
1:A:417:ARG:O	1:A:421:ILE:HG12	2.20	0.41
1:C:307:GLN:HG2	1:C:330:PRO:CD	2.50	0.41
2:D:162:THR:C	2:D:192:MET:SD	3.03	0.41
2:D:282:ARG:HB3	2:D:308:VAL:HG21	2.00	0.41
2:D:293:ILE:HG23	2:D:324:ALA:HB2	2.02	0.41
1:A:28:PHE:HA	2:B:35:GLY:HA2	2.02	0.41
1:A:248:PHE:O	1:A:314:ARG:NH2	2.52	0.41
1:A:378:ALA:HB1	2:D:273:VAL:HG21	2.02	0.41
2:B:238:GLY:C	2:B:242:THR:HG1	2.20	0.41
2:B:345:ILE:O	2:B:349:ALA:HA	2.20	0.41
1:C:38:HIS:ND1	1:C:71:ARG:NE	2.68	0.41
1:C:344:LEU:HD23	1:C:345:ALA:N	2.35	0.41
1:C:389:LYS:HD2	1:C:390[A]:TRP:CE3	2.55	0.41
2:D:43:PHE:O	2:D:49:ARG:HB2	2.21	0.41
2:D:380:GLN:OE1	2:D:380:GLN:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:393:GLU:HA	2:D:396:ASN:HB2	2.02	0.41
1:A:304:PRO:HD3	1:A:359:GLN:NE2	2.36	0.41
1:A:361:ASP:CG	2:B:83:ARG:HH12	2.28	0.41
2:B:296:ALA:HB1	2:B:328:TYR:HE2	1.84	0.41
1:C:153:PHE:CE2	1:C:154:THR:HG23	2.55	0.41
2:B:90:MET:HA	2:B:118:VAL:HG22	2.03	0.41
2:B:154:VAL:HA	2:B:206:HIS:ND1	2.35	0.41
2:B:243:ARG:NH2	2:B:261:ASP:OD2	2.53	0.41
1:C:375:LEU:HD23	1:C:375:LEU:HA	1.85	0.41
2:D:90:MET:HE2	2:D:120:LEU:HD13	1.89	0.41
1:A:103:ARG:HD3	2:D:419:ARG:HH22	1.86	0.41
1:C:66:ILE:HD12	2:D:6:TRP:CZ3	2.52	0.41
1:C:300:VAL:HA	1:C:370:LEU:O	2.21	0.41
1:C:344:LEU:HD21	1:C:348:PRO:HG2	2.02	0.41
2:D:300:ARG:NH2	2:D:307:VAL:O	2.54	0.41
2:D:363:ALA:HB1	2:D:368:ILE:O	2.21	0.41
1:A:36:TRP:HB3	1:A:396:PHE:CD1	2.54	0.41
1:A:263:ALA:HB3	1:A:273:PHE:HZ	1.85	0.41
2:B:141:CYS:HB3	2:B:222:TRP:CZ3	2.55	0.41
1:C:223:ALA:HB1	1:C:258:TRP:NE1	2.35	0.41
2:D:156:CYS:SG	2:D:179:LEU:HD13	2.61	0.41
1:A:50:GLY:O	1:A:76:VAL:HA	2.21	0.41
1:A:242:ARG:NH1	1:A:265:GLU:HB3	2.36	0.41
1:A:253:GLU:HG2	1:A:318:ARG:NH2	2.34	0.41
2:B:274:ASP:OD1	2:B:274:ASP:N	2.47	0.41
1:C:54:CYS:SG	3:C:501:SF4:S2	3.18	0.41
1:C:292:SER:O	1:C:292:SER:OG	2.27	0.41
2:D:362:ILE:O	2:D:366:LEU:N	2.54	0.41
2:D:38:TYR:CD2	2:D:38:TYR:C	2.97	0.41
1:A:308:LEU:O	1:A:312:LEU:HG	2.21	0.41
1:A:364:ARG:HA	1:A:386:PHE:HZ	1.86	0.41
1:A:390[B]:TRP:CZ2	4:A:502:PMR:H2O	2.56	0.41
2:B:30:LEU:O	2:B:57:TYR:HA	2.21	0.41
2:B:111:LEU:HD22	2:B:113:LEU:HD22	2.03	0.41
2:B:156:CYS:HB3	2:B:207:PHE:CZ	2.56	0.41
2:B:239:VAL:HG21	2:B:267:PRO:HD3	2.03	0.41
2:B:282:ARG:HB2	2:B:308:VAL:HG21	2.03	0.41
2:B:288:ASP:H	2:B:374:SER:CB	2.33	0.41
2:B:289:ALA:HB2	2:B:314:ASN:HB2	2.03	0.41
2:B:356:THR:HG22	2:B:374:SER:HB3	2.02	0.41
1:C:216:VAL:HG21	1:C:239:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:GLU:HG2	1:C:328:GLY:O	2.21	0.41
1:C:379:ASN:HB3	2:D:44:THR:OG1	2.21	0.41
2:D:26:MET:SD	2:D:90:MET:SD	3.18	0.41
2:D:303:MET:HE3	2:D:402:TRP:CE3	2.56	0.41
2:B:31:HIS:O	2:B:97:ALA:HB2	2.21	0.41
2:B:161:PRO:HB2	2:B:172:ILE:HD12	2.02	0.41
1:A:236:LEU:O	1:A:239:ARG:HB3	2.21	0.40
1:A:279:ALA:O	1:A:283:ARG:HB2	2.20	0.40
2:B:212:TYR:CE2	2:B:390:MET:CE	3.04	0.40
2:D:138:LEU:HD12	2:D:138:LEU:HA	1.86	0.40
2:D:153:LYS:HE2	2:D:153:LYS:HB2	1.86	0.40
2:D:286:PHE:HB3	2:D:359:GLU:CD	2.45	0.40
1:A:175:GLU:HG2	1:A:220:THR:HG22	2.02	0.40
1:A:177:LEU:HD23	1:A:203:ARG:HB2	2.02	0.40
1:C:154:THR:HB	1:C:228:PHE:CD1	2.55	0.40
2:D:285:LEU:HD21	2:D:354:LEU:HD12	2.03	0.40
2:D:339:LEU:HD13	2:D:339:LEU:HA	1.94	0.40
1:A:110:PHE:HA	1:A:142:TYR:O	2.22	0.40
2:B:40:ASP:O	2:B:44:THR:HG23	2.20	0.40
2:B:73:PHE:HD2	2:B:107:LEU:HD12	1.86	0.40
1:C:183:PRO:O	1:C:186:VAL:HG12	2.21	0.40
1:C:302:PHE:HB2	1:C:327:VAL:HA	2.03	0.40
2:D:201:ARG:HE	2:D:201:ARG:HB2	1.57	0.40
1:A:418:ARG:HH11	1:A:422:LEU:HD22	1.87	0.40
2:B:45:MET:CE	2:D:274:ASP:OD1	2.69	0.40
1:C:199:ILE:HA	1:C:266:PHE:CZ	2.57	0.40
1:C:282:ALA:HA	1:C:285:ARG:NH1	2.36	0.40
1:C:303:LEU:HD22	1:C:373:CYS:SG	2.61	0.40
2:D:12:PRO:HB2	2:D:122:LEU:HG	2.03	0.40
2:D:210:LEU:HD12	2:D:231:TYR:CD2	2.57	0.40
1:A:253:GLU:CB	1:A:318:ARG:HH12	2.29	0.40
2:B:88:ALA:HA	2:B:115:VAL:HB	2.02	0.40
2:B:237:ILE:HG12	2:B:389:GLN:O	2.21	0.40
2:D:283:VAL:HG22	2:D:352:LEU:CB	2.52	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	401/428 (94%)	359 (90%)	42 (10%)	0	100 100
1	C	383/428 (90%)	336 (88%)	45 (12%)	2 (0%)	25 56
2	B	418/536 (78%)	382 (91%)	36 (9%)	0	100 100
2	D	417/536 (78%)	370 (89%)	47 (11%)	0	100 100
All	All	1619/1928 (84%)	1447 (89%)	170 (10%)	2 (0%)	50 76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	401[A]	PHE
1	C	401[B]	PHE

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	314/335 (94%)	309 (98%)	5 (2%)	58 76
1	C	305/335 (91%)	305 (100%)	0	100 100
2	B	335/415 (81%)	330 (98%)	5 (2%)	60 77
2	D	334/415 (80%)	329 (98%)	5 (2%)	60 77
All	All	1288/1500 (86%)	1273 (99%)	15 (1%)	71 80

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	CYS
1	A	115	CYS
1	A	134	HIS
1	A	390[A]	TRP
1	A	390[B]	TRP
2	B	34	GLN
2	B	37	THR
2	B	51	LYS
2	B	252	LEU
2	B	274	ASP
2	D	61[A]	GLN
2	D	61[B]	GLN
2	D	102	ASP
2	D	212	TYR
2	D	215	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	89	ASN
1	A	125	HIS
1	A	134	HIS
1	A	226	GLN
1	A	359	GLN
2	B	208	ASN
1	C	196	GLN
1	C	209	HIS
1	C	226	GLN
1	C	379	ASN
1	C	404	GLN
2	D	74	GLN
2	D	101	GLN
2	D	157	ASN
2	D	206	HIS
2	D	208	ASN
2	D	378	HIS
2	D	380	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	SF4	C	501	-	0,12,12	-	-	-		
4	PMR	B	601	-	48,53,53	2.19	10 (20%)	54,89,89	2.88	20 (37%)
3	SF4	A	501	-	0,12,12	-	-	-		
4	PMR	A	502	-	48,53,53	2.22	8 (16%)	54,89,89	2.85	18 (33%)

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	SF4	C	501	-	-	-	0/6/5/5
4	PMR	B	601	-	3/3/16/20	8/15/111/111	-
3	SF4	A	501	-	-	-	0/6/5/5
4	PMR	A	502	-	2/2/16/20	8/15/111/111	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	PMR	C4D-CHA	-7.67	1.35	1.45
4	A	502	PMR	C4D-CHA	-7.47	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	PMR	MG-NB	-6.78	1.92	2.05
4	B	601	PMR	MG-NB	-6.33	1.93	2.05
4	A	502	PMR	MG-NC	-6.12	1.91	2.06
4	A	502	PMR	MG-NA	-6.06	1.91	2.06
4	B	601	PMR	MG-NC	-6.05	1.91	2.06
4	B	601	PMR	MG-NA	-5.80	1.92	2.06
4	A	502	PMR	O2D-CGD	-3.27	1.25	1.33
4	B	601	PMR	O2D-CGD	-3.20	1.25	1.33
4	B	601	PMR	C1B-C2B	-3.09	1.39	1.45
4	A	502	PMR	C1B-C2B	-3.06	1.39	1.45
4	A	502	PMR	C3B-C4B	-3.04	1.40	1.46
4	B	601	PMR	C3B-C4B	-3.01	1.40	1.46
4	A	502	PMR	CHD-C4C	2.29	1.40	1.34
4	B	601	PMR	CHD-C4C	2.29	1.40	1.34
4	B	601	PMR	O2D-C2O	2.07	1.49	1.45
4	B	601	PMR	C4D-ND	-2.02	1.32	1.35

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	502	PMR	C2B-C1B-NB	-10.22	100.01	110.13
4	B	601	PMR	C2B-C1B-NB	-7.70	102.51	110.13
4	B	601	PMR	C1A-NA-C4A	7.20	109.97	106.68
4	A	502	PMR	CHC-C4B-NB	-6.59	115.53	124.80
4	B	601	PMR	C3C-C4C-NC	-6.23	103.23	109.90
4	B	601	PMR	CHC-C4B-C3B	6.03	135.38	125.21
4	A	502	PMR	CHC-C4B-C3B	5.98	135.28	125.21
4	A	502	PMR	CHB-C4A-NA	-5.91	115.07	124.23
4	B	601	PMR	C3A-C4A-NA	-5.83	103.24	110.45
4	A	502	PMR	C3A-C4A-NA	-5.80	103.27	110.45
4	A	502	PMR	CHB-C1B-NB	-5.73	116.74	124.80
4	B	601	PMR	CHB-C4A-C3A	4.55	132.22	125.03
4	B	601	PMR	CHC-C4B-NB	-4.38	118.64	124.80
4	B	601	PMR	O2D-CGD-CBD	4.20	118.57	111.23
4	B	601	PMR	C4A-C3A-C2A	-4.09	102.68	106.98
4	B	601	PMR	CHB-C4A-NA	-4.09	117.89	124.23
4	B	601	PMR	CHB-C1B-NB	-4.07	119.08	124.80
4	A	502	PMR	O2D-CGD-CBD	4.05	118.30	111.23
4	A	502	PMR	CHB-C4A-C3A	3.59	130.70	125.03
4	B	601	PMR	C4D-C3D-CAD	-3.58	101.96	107.75
4	B	601	PMR	CHB-C1B-C2B	3.33	132.41	125.49
4	B	601	PMR	CHC-C1C-C2C	3.27	130.18	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	502	PMR	C4D-C3D-CAD	-3.15	102.66	107.75
4	A	502	PMR	CHB-C1B-C2B	3.05	131.83	125.49
4	B	601	PMR	O2D-CGD-O1D	-3.01	117.98	123.85
4	A	502	PMR	C3C-C4C-NC	-2.89	106.81	109.90
4	A	502	PMR	C1B-CHB-C4A	-2.84	119.98	126.02
4	A	502	PMR	O1D-CGD-CBD	-2.75	119.09	124.52
4	A	502	PMR	O2D-CGD-O1D	-2.67	118.66	123.85
4	A	502	PMR	CMD-C2D-C1D	-2.66	124.56	128.46
4	B	601	PMR	O1D-CGD-CBD	-2.63	119.32	124.52
4	A	502	PMR	C1C-C2C-C3C	-2.55	104.30	106.98
4	B	601	PMR	C2C-C1C-NC	-2.54	107.31	110.45
4	B	601	PMR	C4B-CHC-C1C	-2.45	120.81	126.02
4	B	601	PMR	C1C-C2C-C3C	-2.32	104.54	106.98
4	B	601	PMR	CMB-C2B-C3B	-2.25	122.98	128.43
4	A	502	PMR	CHC-C1C-NC	-2.08	121.00	124.23
4	A	502	PMR	C2C-C1C-NC	-2.06	107.91	110.45

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	502	PMR	NC
4	A	502	PMR	NB
4	B	601	PMR	NB
4	B	601	PMR	NC
4	B	601	PMR	NA

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	502	PMR	C2B-C3B-CAB-CBB
4	A	502	PMR	CHA-CBD-CGD-O1D
4	A	502	PMR	CHA-CBD-CGD-O2D
4	A	502	PMR	CBD-CGD-O2D-C2O
4	A	502	PMR	C3A-C2A-CAA-CBA
4	B	601	PMR	C2B-C3B-CAB-CBB
4	B	601	PMR	CHA-CBD-CGD-O2D
4	B	601	PMR	CBD-CGD-O2D-C2O
4	B	601	PMR	O1D-CGD-O2D-C2O
4	A	502	PMR	O1D-CGD-O2D-C2O
4	A	502	PMR	C2A-CAA-CBA-CGA
4	B	601	PMR	C3A-C2A-CAA-CBA
4	B	601	PMR	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
4	A	502	PMR	C1A-C2A-CAA-CBA
4	B	601	PMR	C2A-CAA-CBA-CGA
4	B	601	PMR	CAA-CBA-CGA-O1A

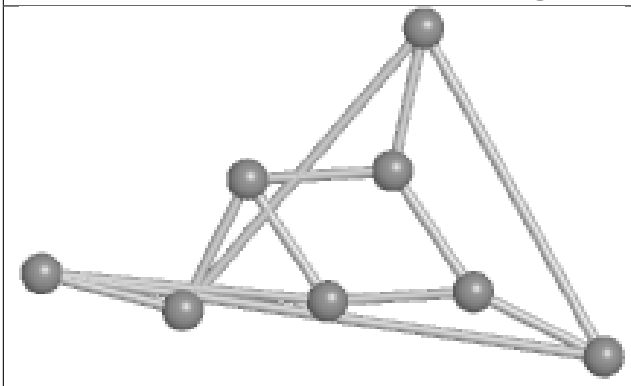
There are no ring outliers.

4 monomers are involved in 42 short contacts:

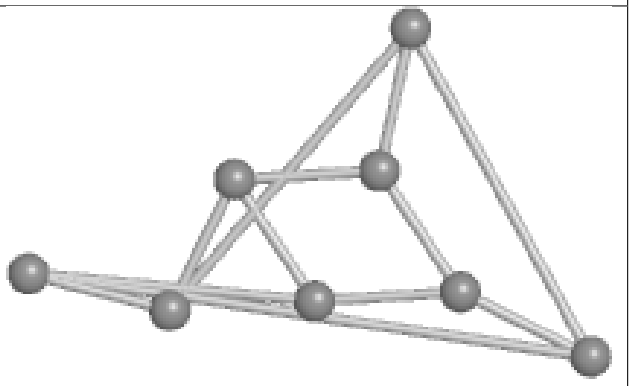
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	SF4	12	0
4	B	601	PMR	12	0
3	A	501	SF4	11	0
4	A	502	PMR	7	0

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.

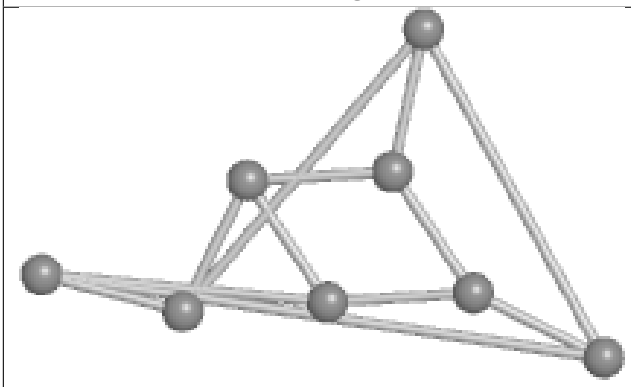
Ligand SF4 C 501



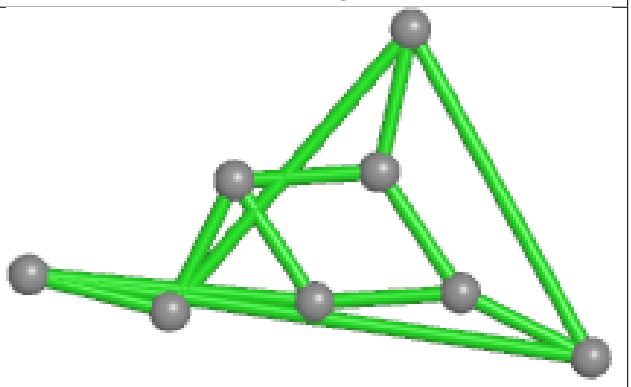
Bond lengths



Bond angles

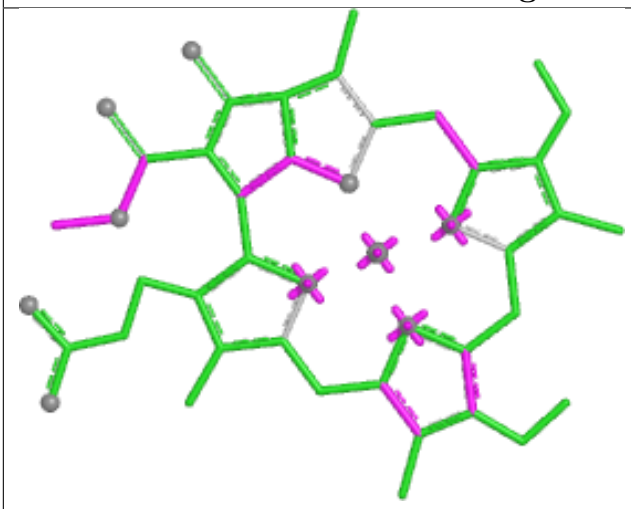


Torsions

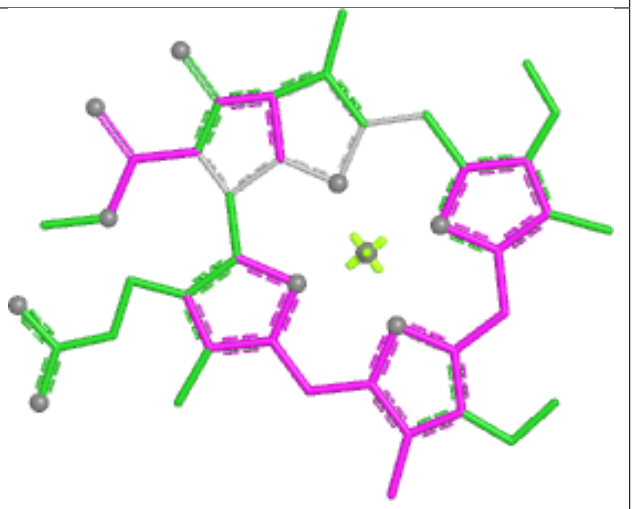


Rings

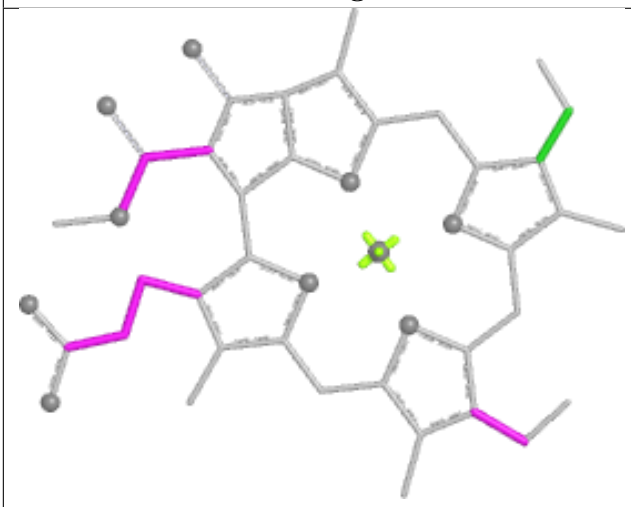
Ligand PMR B 601



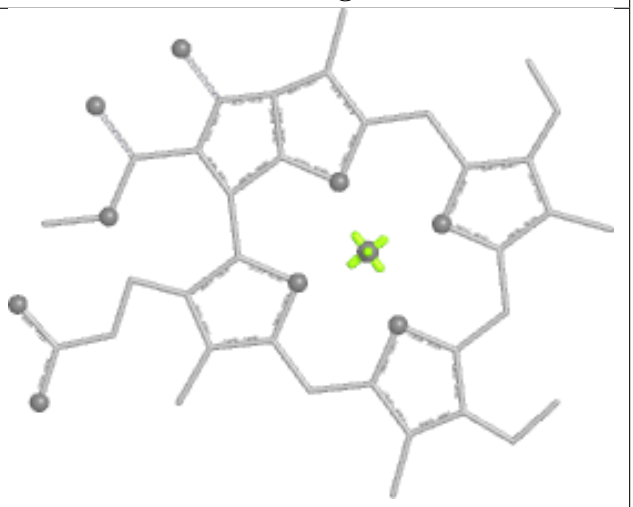
Bond lengths



Bond angles

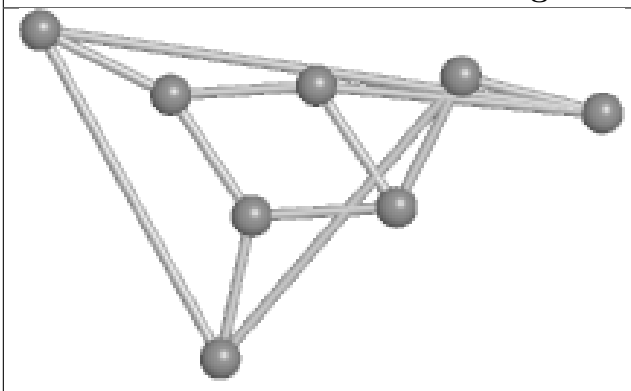


Torsions

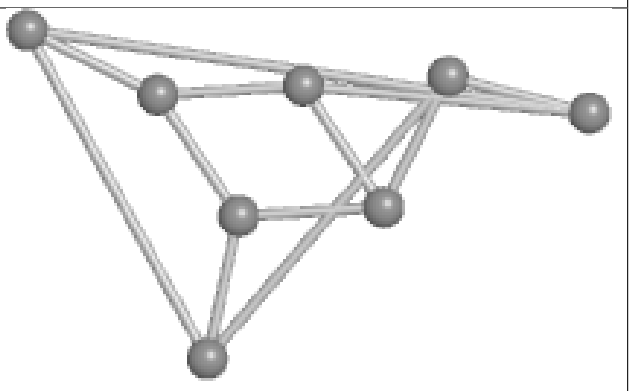


Rings

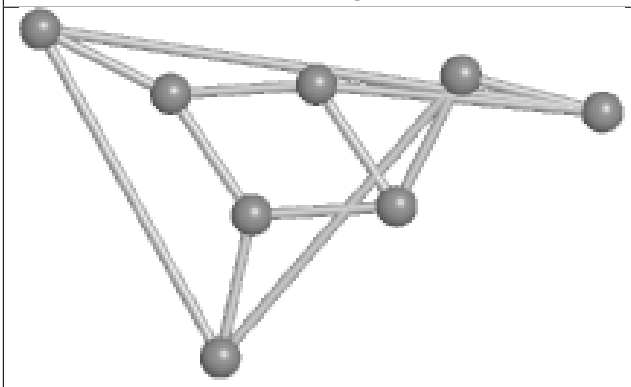
Ligand SF4 A 501



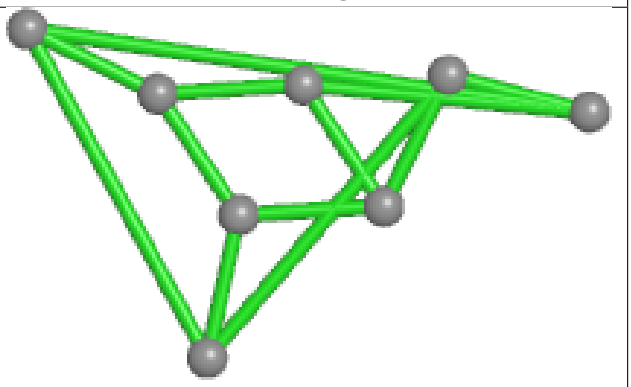
Bond lengths



Bond angles

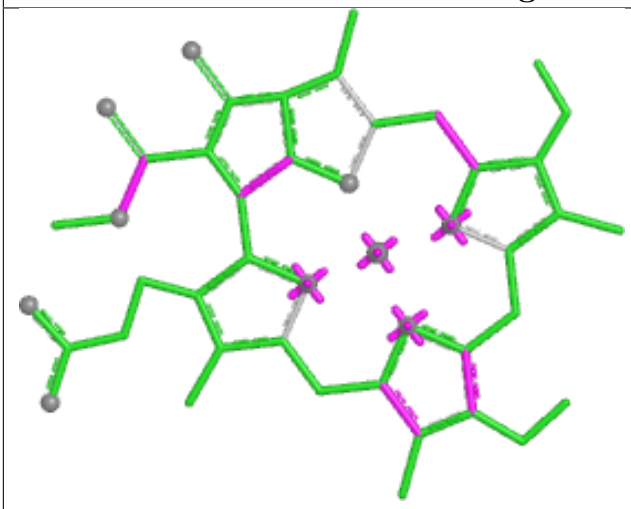


Torsions

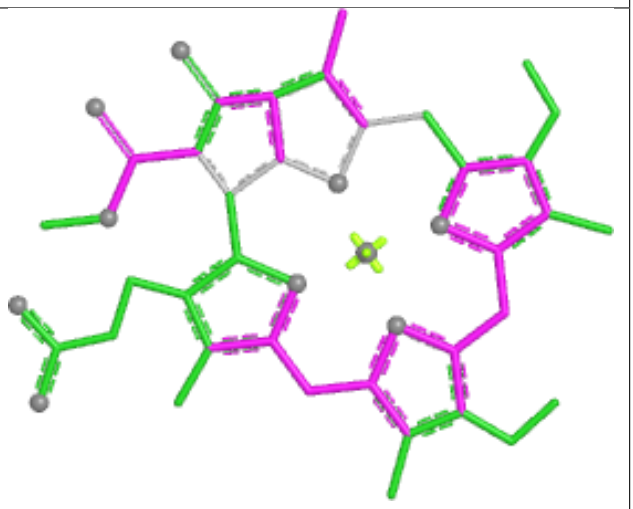


Rings

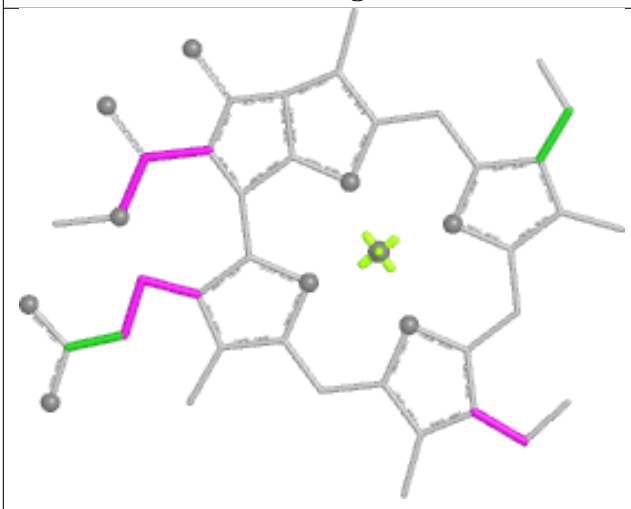
Ligand PMR A 502



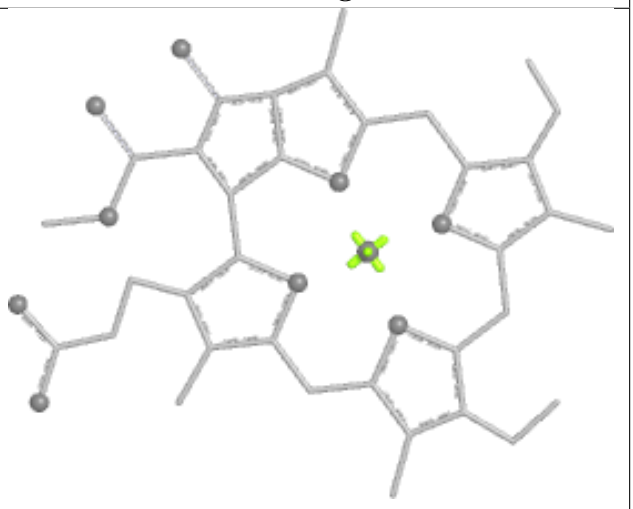
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

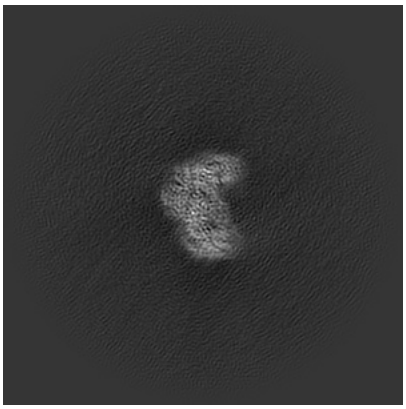
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-47669. These allow visual inspection of the internal detail of the map and identification of artifacts.

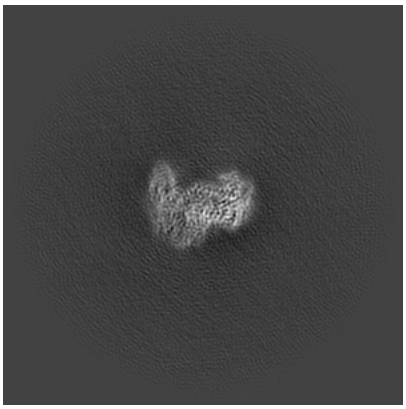
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

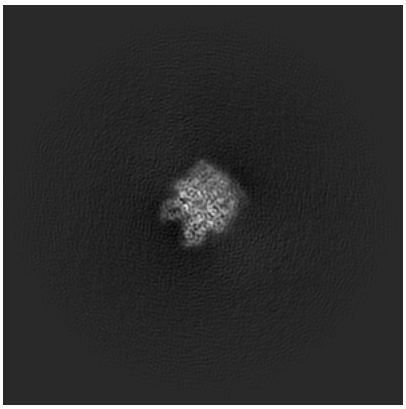
6.1.1 Primary map



X

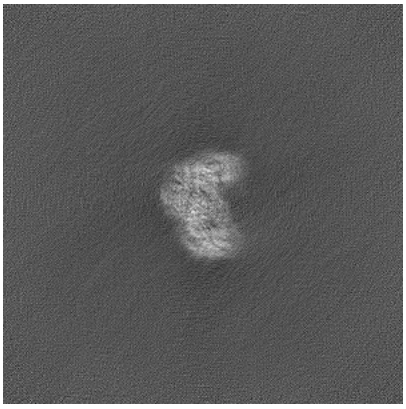


Y

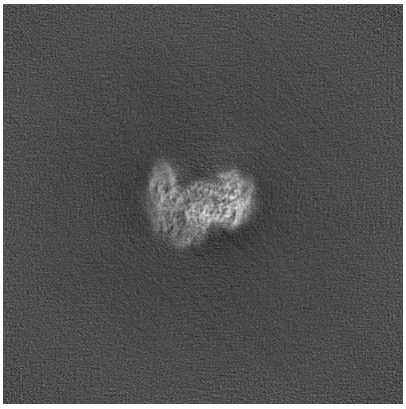


Z

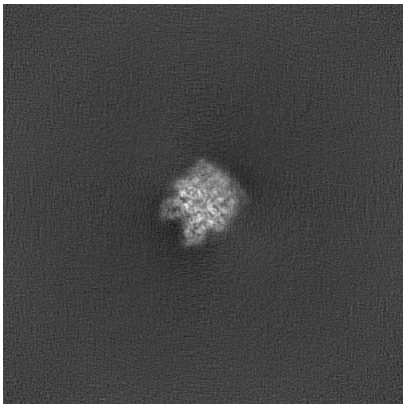
6.1.2 Raw map



X



Y

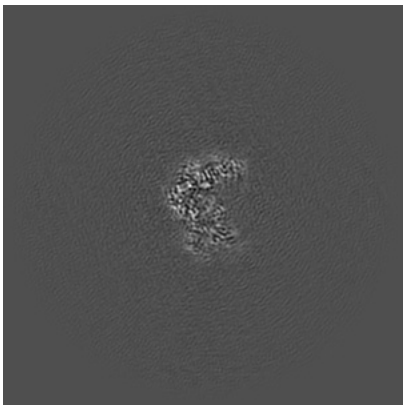


Z

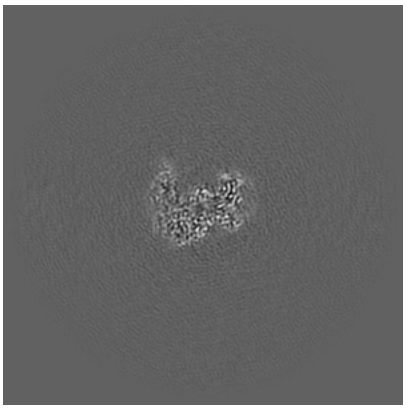
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

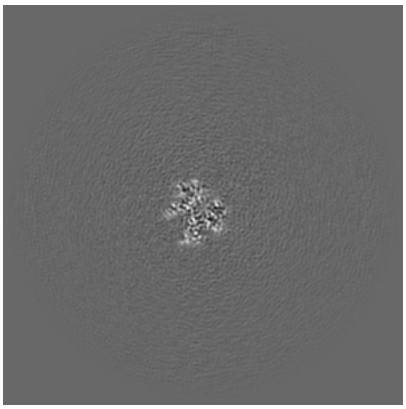
6.2.1 Primary map



X Index: 240

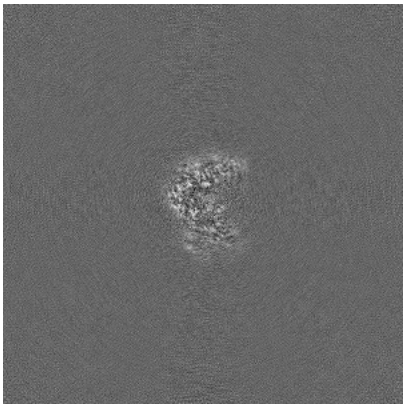


Y Index: 240

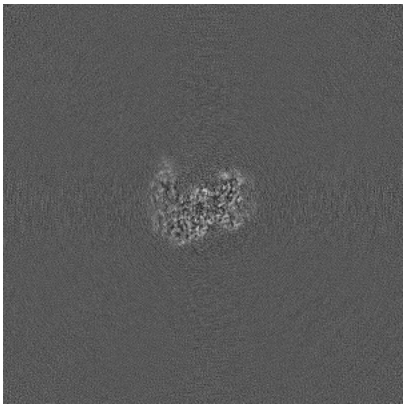


Z Index: 240

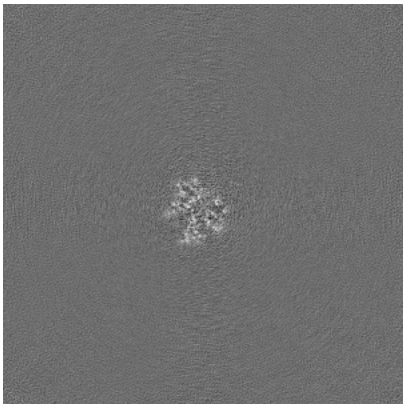
6.2.2 Raw map



X Index: 240



Y Index: 240

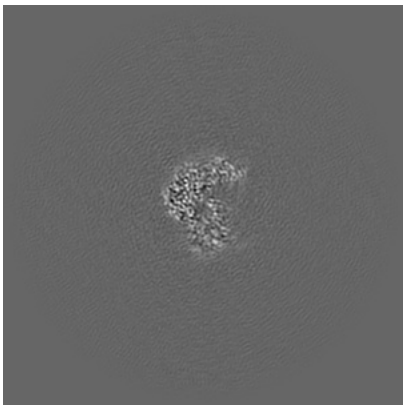


Z Index: 240

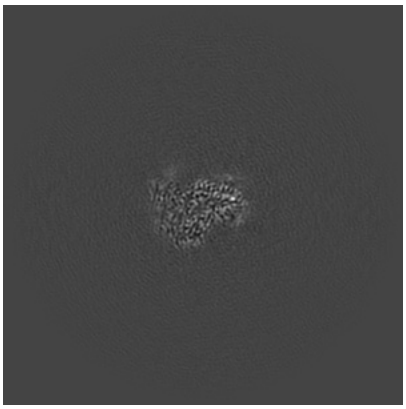
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

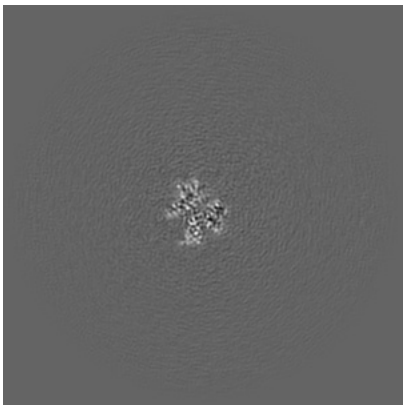
6.3.1 Primary map



X Index: 235

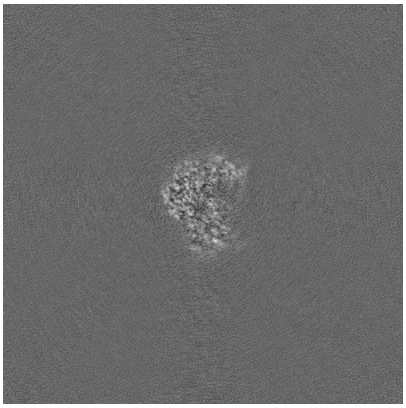


Y Index: 233

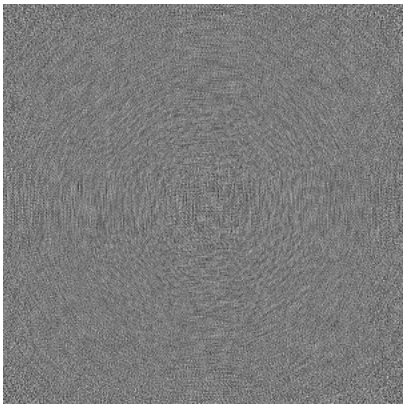


Z Index: 241

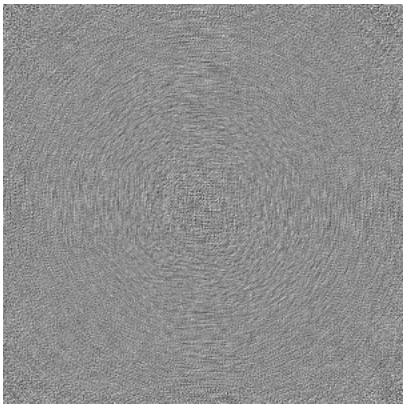
6.3.2 Raw map



X Index: 235



Y Index: 0

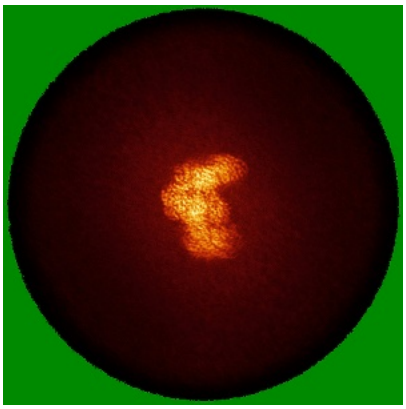


Z Index: 0

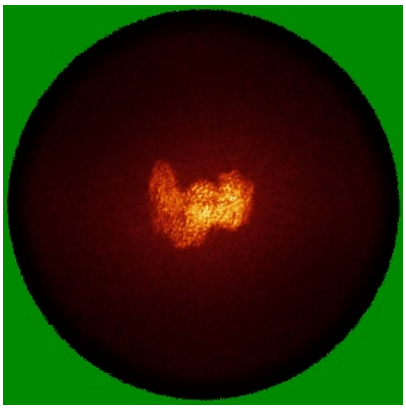
The images above show the largest variance slices of the map in three orthogonal directions.

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

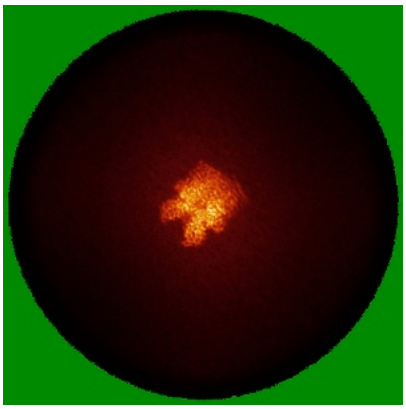
6.4.1 Primary map



X

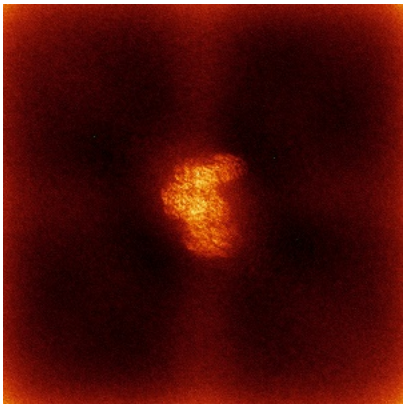


Y

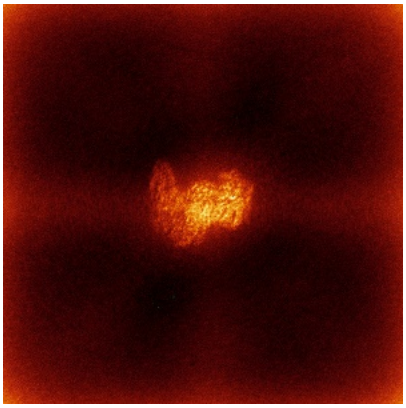


Z

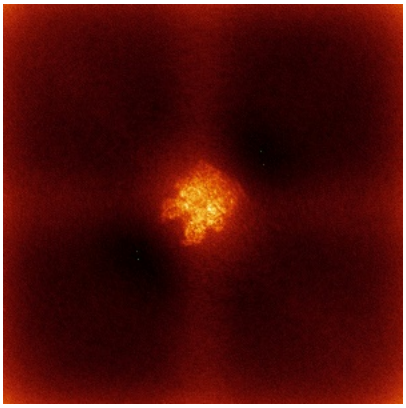
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0954. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

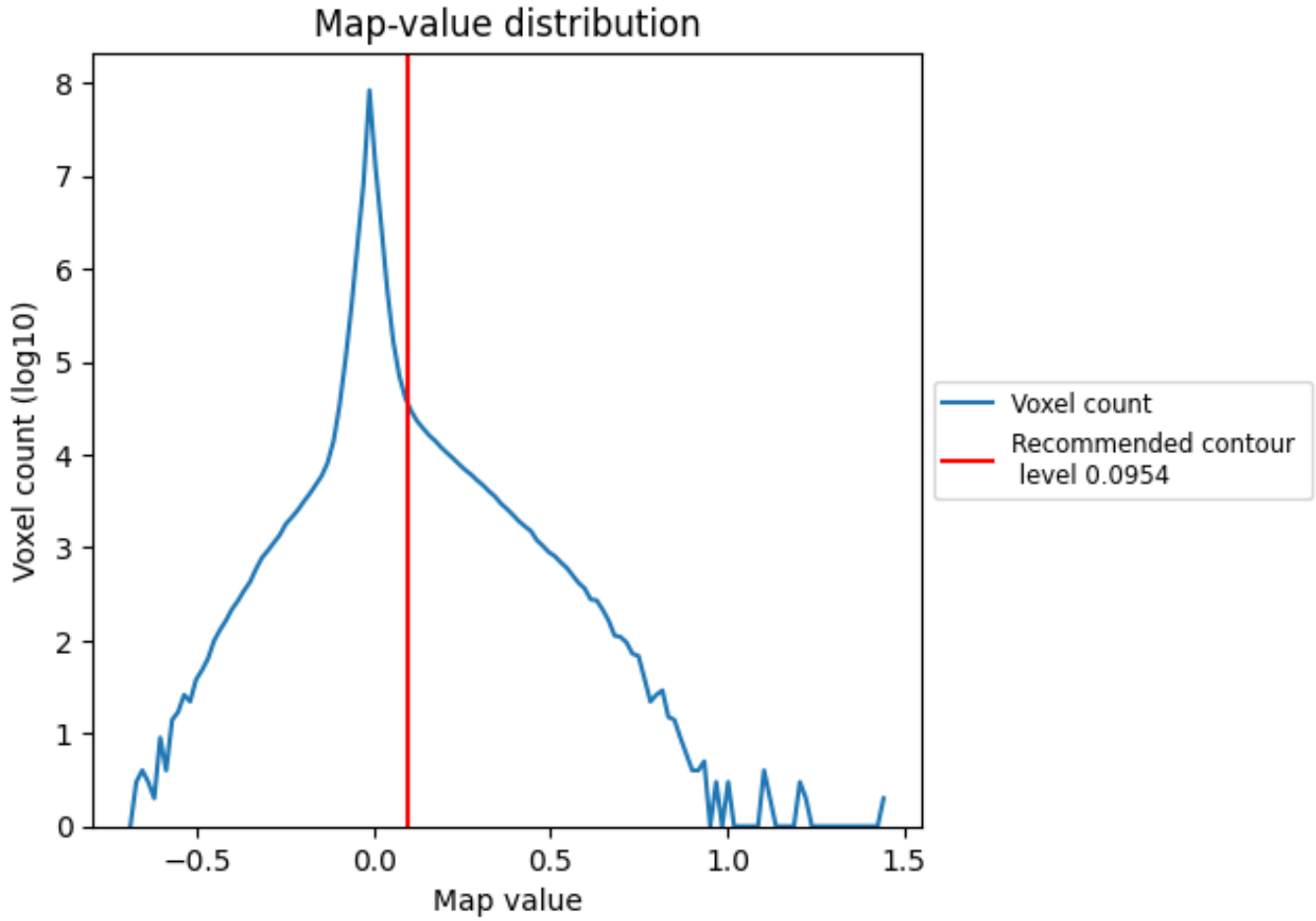
6.6 Mask visualisation (i)

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

7 Map analysis

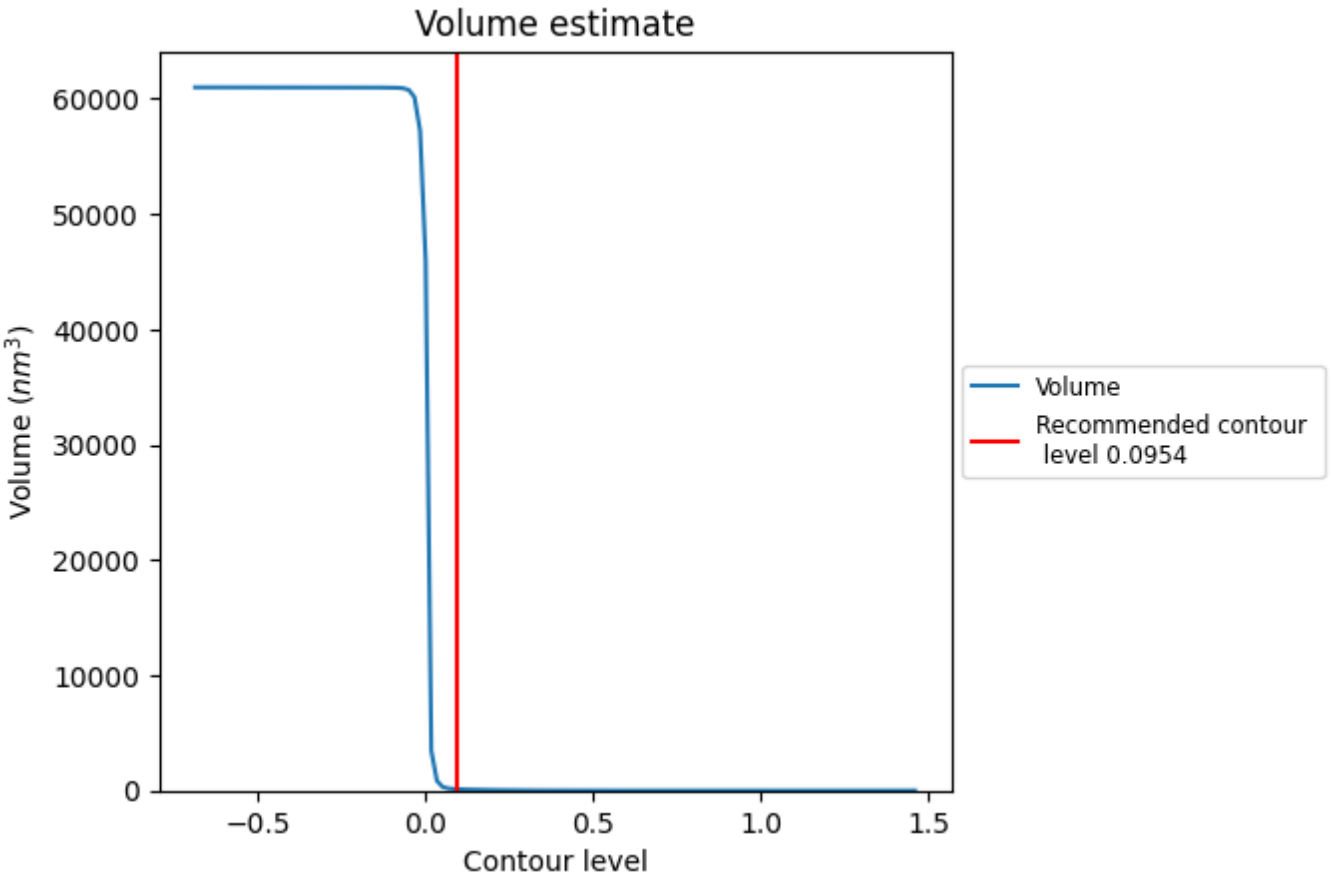
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

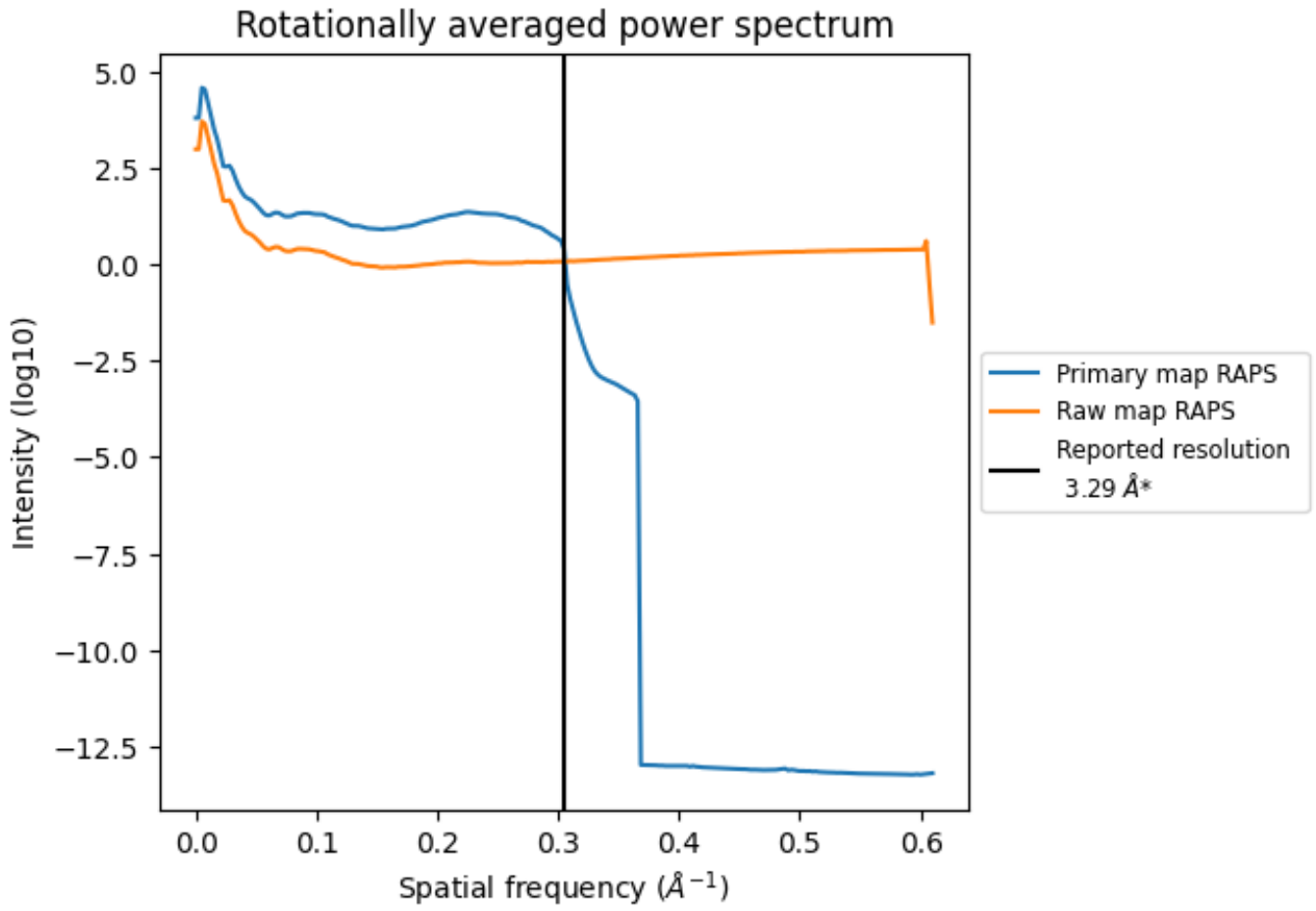
7.2 Volume estimate



The volume at the recommended contour level is 120 nm^3; this corresponds to an approximate mass of 109 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)

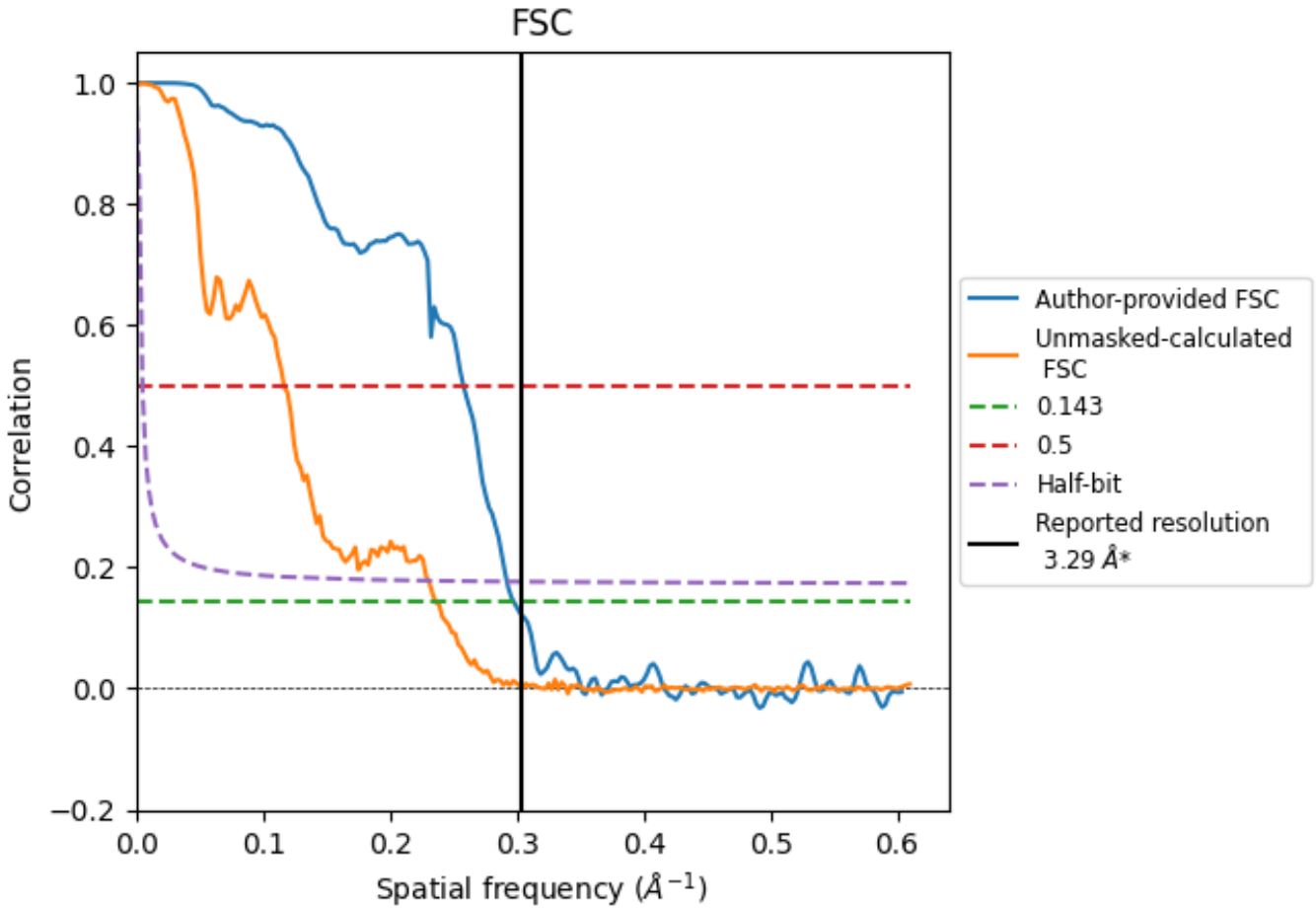


*Reported resolution corresponds to spatial frequency of 0.304 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.304 Å^{-1}

8.2 Resolution estimates (i)

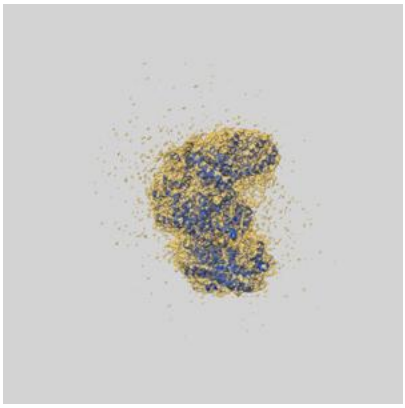
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.29	-	-
Author-provided FSC curve	3.36	3.88	3.42
Unmasked-calculated*	4.24	8.58	4.34

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.24 differs from the reported value 3.29 by more than 10 %

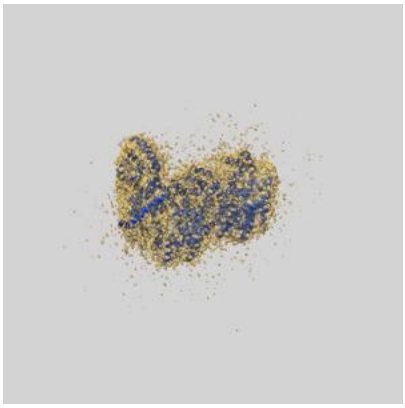
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-47669 and PDB model 9E7H. Per-residue inclusion information can be found in section 3 on page 6.

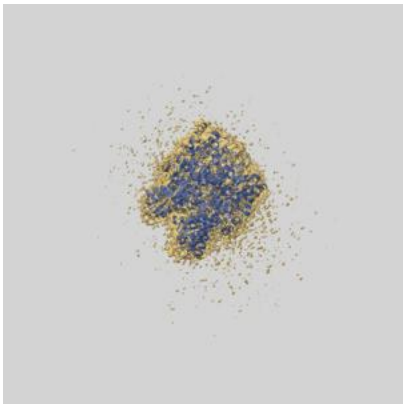
9.1 Map-model overlay



X



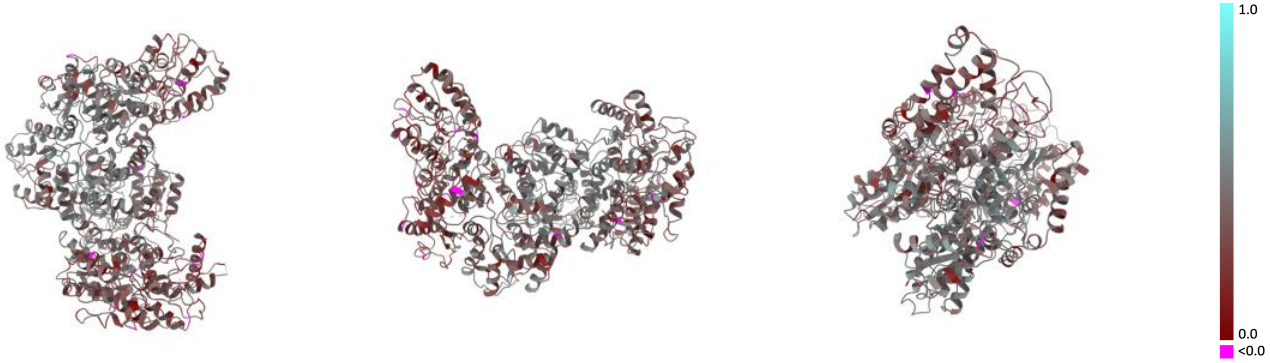
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0954 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

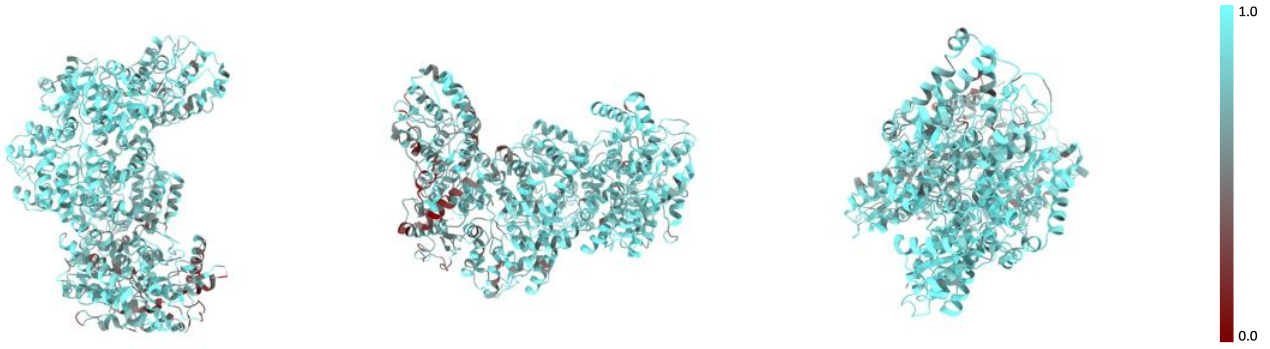
9.2 Q-score mapped to coordinate model



X Y Z

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

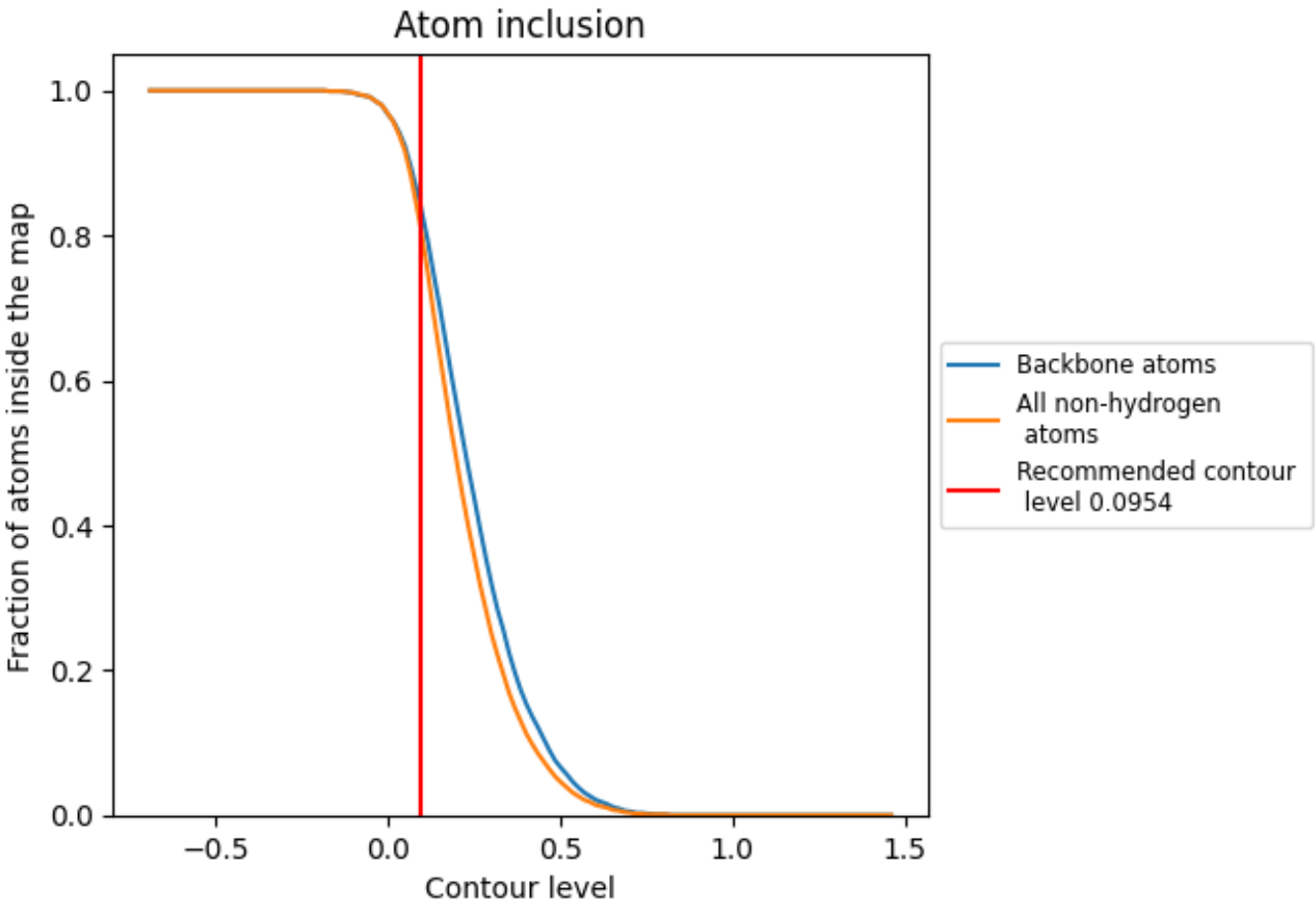
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0954).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0954) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8120	0.3890
A	0.8490	0.3880
B	0.8930	0.4410
C	0.7030	0.3300
D	0.7930	0.3920