Full wwPDB EM Validation Report (i)

Oct 13, 2024 – 09:56 AM EDT

PDB ID	:	7MO9
EMDB ID	:	EMD-23921
Title	:	Cryo-EM map of the c-MET II/HGF I/HGF II (K4 and SPH) sub-complex
Authors	:	Uchikawa, E.; Chen, Z.M.; Xiao, G.Y.; Zhang, X.W.; Bai, X.C.
Deposited on	:	2021-05-01
Resolution	:	4.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

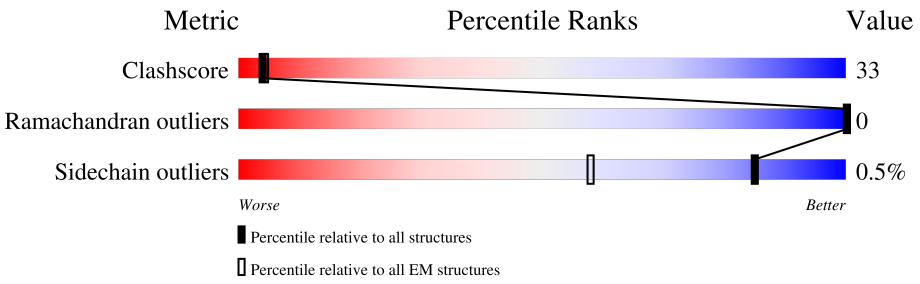
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 4.00 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	728	13% 21% 65%
1	D	728	20% 22% 58%
2	E	1390	25% 24% 51%
3	B	6	50% 67% 33%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9755 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.

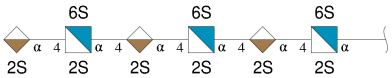
- Molecule 1 is a protein called Hepatocyte growth factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	254	2047	1283	370	373	21	0	0
1	D	305	2287	1443	404	418	22	0	0

- Molecule 2 is a protein called Hepatocyte growth factor receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	688	5324	3373	905	1006	40	0	0

- Molecule 3 is an oligosaccharide called 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose.



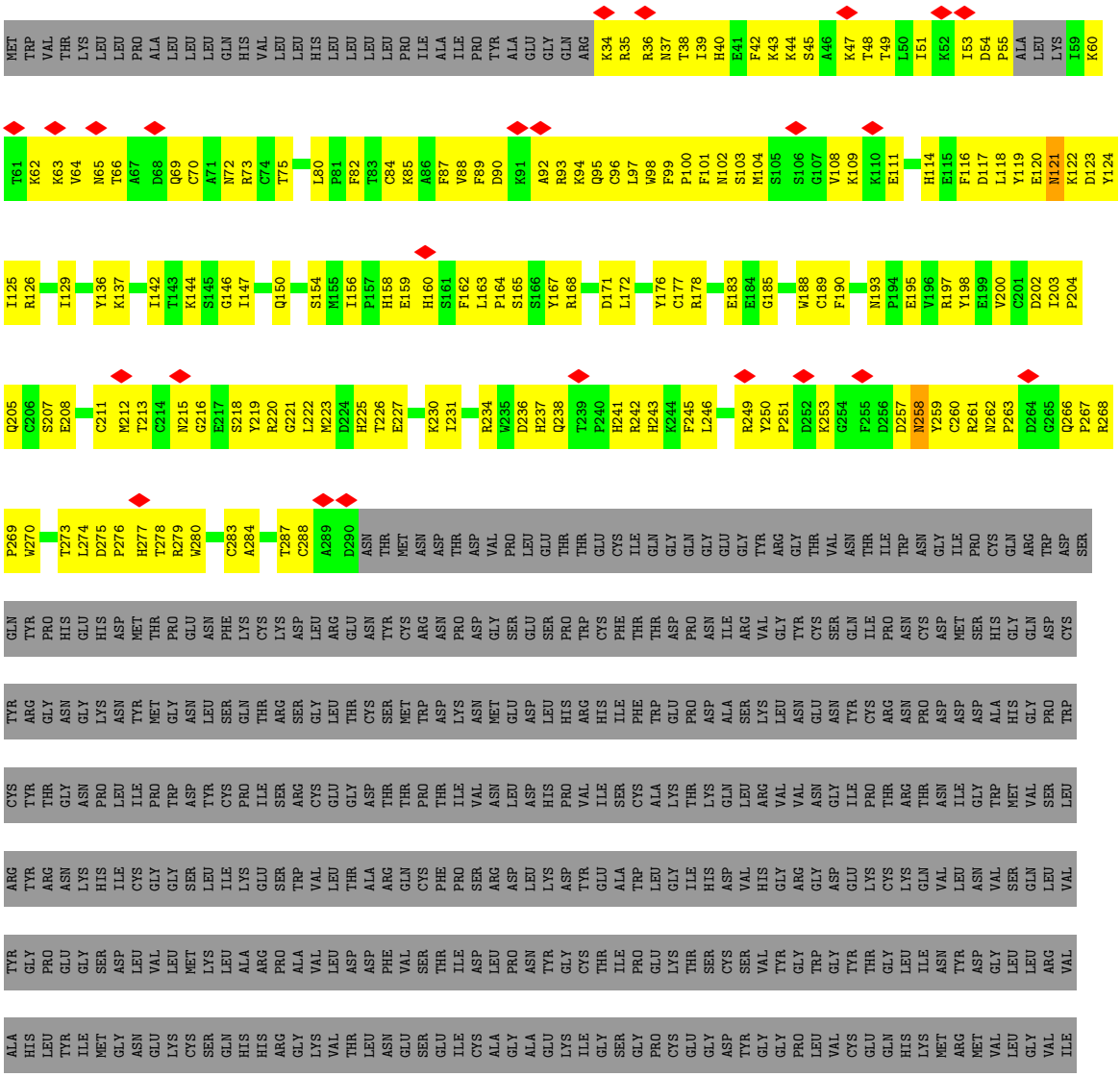
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	6	97	35	3	51	8	0	0

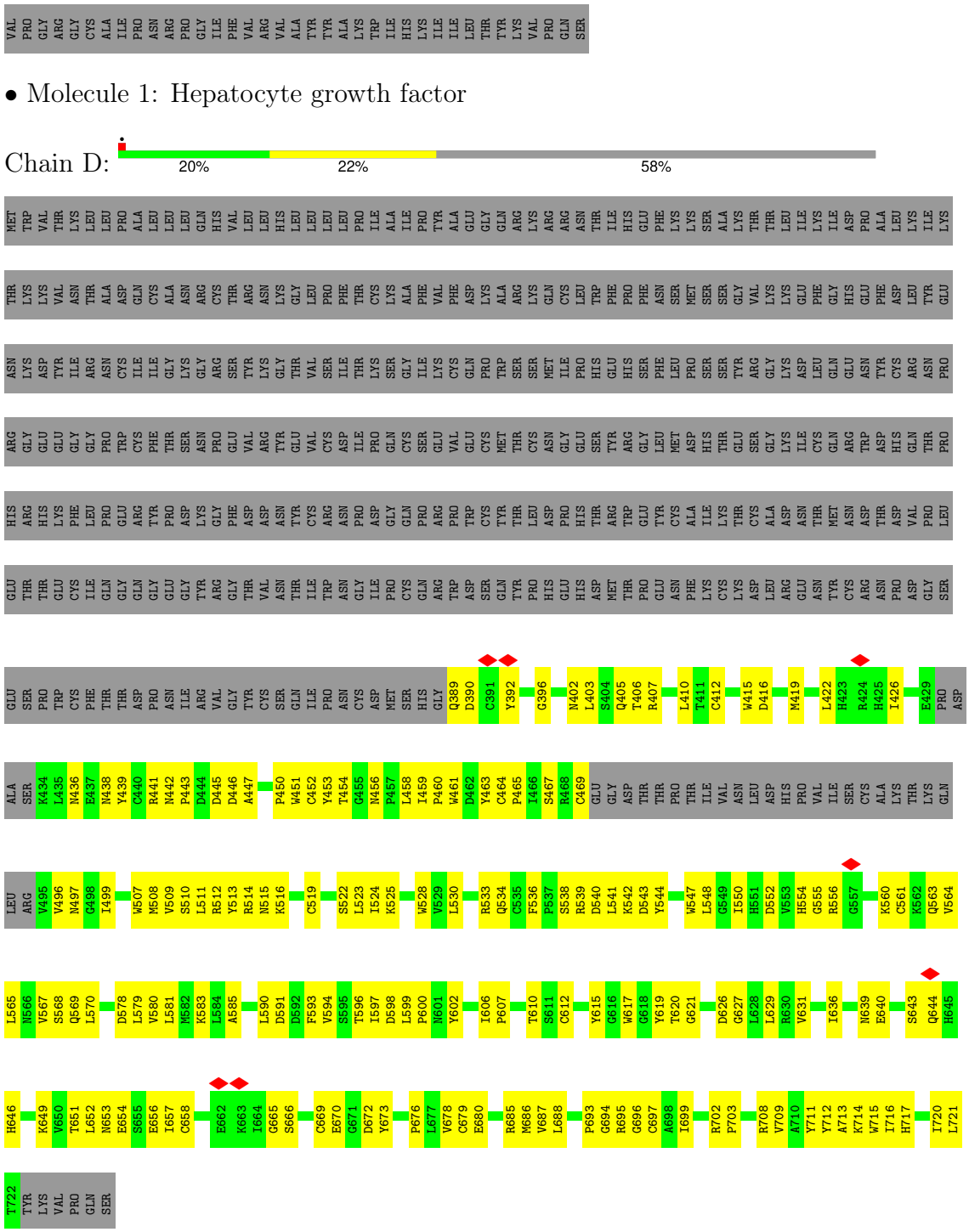
3 Residue-property plots (i)

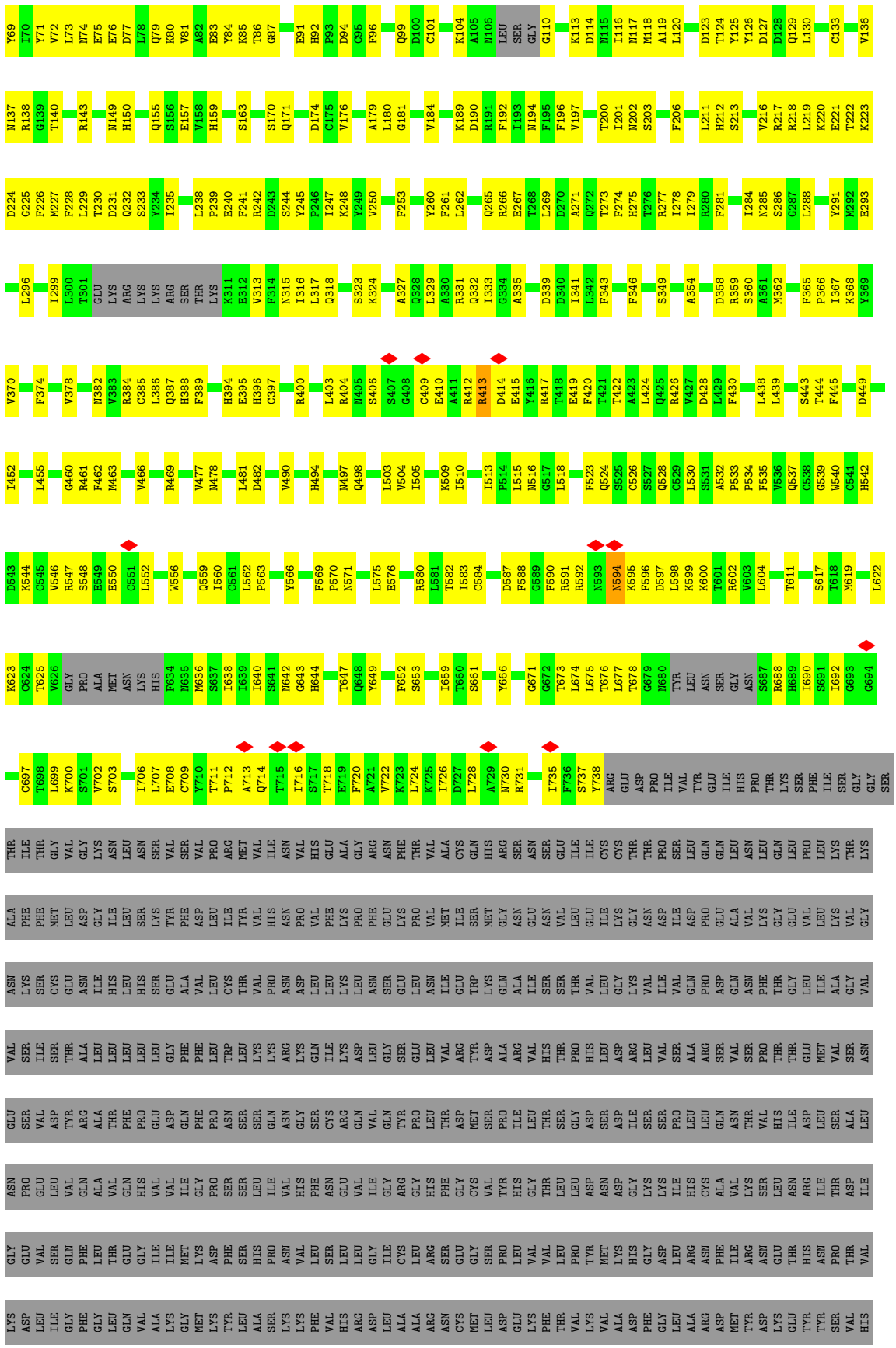
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain A:




VAL PRO GLY ARG GLY CYS ALA ILE PRO ASN ARG PRO GLY ILE PHE VAL ARG VAL ALA TYR TYR ALA LYS TRP ILE HIS LYS ILE ILE LEU THR TYR LYS VAL PRO GLN SER
• Molecule 1: Hepatocyte growth factor
Chain D:
20%
22%
58%
MET TRP VAL THR LYS LEU LEU PRO ALA LEU LEU LEU GLN HIS VAL LEU LEU HIS LEU LEU LEU LEU PRO PRO ILE ALA ILE PRO TYR ALA GLU GLY GLN ARG LYS ARG ARG ASN THR ILE HIS GLU PHE LYS LYS SER ALA LYS THR THR LEU ILE LYS ILE ASP PRO ALA LEU LYS ILE LYS
THR LYS LYS VAL ASN THR ALA ASP GLN CYS ALA ASN ARG CYS THR ARG ASN LYS GLY LEU PRO PHE THR CYS LYS ALA PHE VAL PHE ASP LYS ALA ARG LYS GLN CYS LEU TRP PHE PRO PHE ASN SER MET SER SER SER GLY VAL LYS LYS GLU PHE GLY HIS GLU PHE ASP LEU TYR GLU
ASN LYS ASP TYR ILE ARG ASN CYS ILE ILE GLY LYS GLY ARG SER TYR LYS GLY THR VAL SER ILE THR LYS SER GLY ILE LYS CYS GLN PRO TRP SER SER MET ILE PRO HIS GLU HIS SER PHE LEU PRO SER SER TYR ARG GLY LYS ASP LEU GLN GLU ASN TYR CYS ARG ASN PRO
ARG GLY GLU GLU GLY GLY PRO TRP CYS PHE THR SER ASN PRO GLU VAL ARG TYR GLU VAL CYS ASP ILE PRO GLN CYS SER GLU VAL GLU CYS MET THR CYS ASN GLY GLU SER TYR ARG GLY LEU MET ASP HIS THR GLU SER GLY LYS ILE CYS GLN ARG TRP ASN ASN GLN HIS THR PRO
HIS ARG HIS LYS PHE LEU PRO GLU ARG TYR PRO ASP LYS GLY PHE ASP ASP ASN TYR CYS ARG ASN PRO ASP GLY GLN PRO ARG PRO TRP CYS TYR THR LEU ASP PRO HIS THR ARG TRP GLU TYR CYS ALA ILE LYS THR CYS ALA ASP ASN THR MET ASN ASP THR ASP VAL PRO LEU
GLU THR THR GLU CYS ILE GLN GLY GLN GLY GLU GLY TYR ARG GLY THR VAL ASN THR ILE TRP ASN GLY ILE PRO CYS GLN ARG TRP ASP SER GLN TYR PRO HIS GLU HIS ASP MET THR PRO GLU ASN PHE LYS CYS LYS ASP LEU ARG GLU ASN TYR CYS ARG ASN PRO ASP GLY SER
GLU SER PRO TRP CYS PHE THR THR ASP PRO ASN ILE ARG VAL GLY TYR CYS SER GLN ILE PRO ASN CYS ASP MET SER HIS GLY Q389 D390 C391 Y392 G396 N402 L403 S404 Q405 T406 R407 L410 T411 C412 W415 D416 M419 L422 H423 R424 H425 I426 E429 PRO ASP
ALA SER K434 L435 N436 E437 N438 Y439 C440 R441 N442 P443 D444 D445 D446 A447 P450 W451 C452 Y453 T454 G455 N456 P457 L458 I459 P460 W461 D462 Y463 C464 P465 I466 S467 R468 C469 GLU GLY ASP THR THR PRO THR ILE VAL ASN LEU ASP HIS PRO VAL ILE SER CYS ALA LYS THR LYS GLN
LEU ARG V495 V496 N497 G498 I499 W507 M508 V509 S510 L511 R512 Y513 R514 N515 K516 C519 S522 L523 I524 K525 W528 V529 L530 R533 Q534 C535 F536 P537 S538 R539 D540 L541 K542 D543 Y544 W547 L548 G549 I550 H551 D552 V553 H554 G555 R556 G557 K560 C561 K562 Q563 V564
L565 N566 V567 S568 Q569 L570 D578 L579 V580 L581 M582 K583 L584 A585 L590 D591 D592 F593 V594 S595 T596 I597 D598 L599 P600 N601 Y602 I606 P607 T610 S611 C612 Y615 G616 W617 G618 Y619 T620 G621 D626 G627 L628 L629 R630 V631 I636 N639 E640 S643 Q644 H645
H646 K649 V650 T651 L652 N653 E654 S655 E656 I657 C658 E662 K663 I664 G665 S666 C669 E670 G671 D672 Y673 P676 L677 V678 C679 E680 R685 M686 V687 L688 P693 G694 R695 G696 C697 A698 I699 R702 P703 R708 V709 A710 Y711 Y712 A713 K714 W715 I716 H717 I720 L721
T722 TYR LYS VAL PRO GLN SER
• Molecule 2: Hepatocyte growth factor receptor
Chain E:
25%
24%
51%
MET LYS ALA PRO ALA VAL LEU ALA PRO GLY ILE LEU VAL LEU LEU PHE THR LEU VAL GLN ARG SER ASN GLY GLU C26 K27 E28 A29 L30 A31 K32 M35 N36 V37 N38 M39 K40 Y41 F46 T47 A48 E49 I52 Q53 I56 H60 H61 I62 F63 L64 G65 A66 T67 N68


Y69 I70 Y71 V72 L73 N74 E75 E76 D77 L78 Q79 K80 V81 A82 E83 Y84 K85 T86 G87 E91 H92 P93 D94 C95 F96 Q99 D100 C101 K104 A105 N106 LEU SER GLY G110 K113 D114 N115 I116 N117 M118 A119 L120 D123 T124 Y125 Y126 D127 D128 Q129 L130 C133 V136
N137 R138 G139 T140 R143 N149 H150 Q155 S156 E157 V158 H159 S163 S170 Q171 D174 C175 V176 A179 L180 G181 V184 K189 D190 R191 F192 I193 N194 F195 F196 V197 T200 I201 N202 S203 F206 L211 H212 S213 V216 R217 R218 L219 K220 E221 T222 K223
D224 G225 F226 M227 F228 L229 T230 D231 Q232 S233 Y234 I235 L238 P239 E240 F241 R242 D243 S244 Y245 P246 I247 K248 Y249 V250 F253 Y260 F261 L262 Q265 R266 E267 T268 L269 D270 A271 Q272 T273 F274 H275 T276 R277 I278 I279 R280 F281 I284 N285 S286 G287 L288 Y291 M292 E293
L296 I299 L300 T301 GLU LYS ARG LYS LYS ARG SER THR LYS K311 E312 V313 F314 N315 I316 L317 Q318 S323 K324 A327 Q328 L329 A330 R331 Q332 I333 G334 A335 D339 D340 I341 L342 F343 F346 S349 A354 D358 R359 S360 A361 M362 F365 P366 I367 K368 Y369
V370 F374 V378 N382 V383 R384 C385 L386 Q387 H388 F389 H394 E395 H396 C397 R400 L403 R404 N405 S406 S407 G408 C409 E410 A411 R412 R413 D414 E415 Y416 R417 T418 E419 F420 T421 T422 A423 L424 Q425 R426 V427 D428 L429 F430 L438 L439 S443 T444 F445 D449
I452 L455 G460 R461 F462 M463 V466 R469 V477 N478 L481 D482 V490 H494 N497 Q498 L503 V504 I505 K509 I510 I513 P514 L515 N516 G517 L518 F523 Q524 S525 C526 S527 Q528 C529 L530 S531 A532 P533 P534 F535 V536 Q537 C538 G539 W540 C541 H542
D543 K544 C545 V546 R547 S548 E549 E550 C551 L552 W556 Q559 I560 C561 L562 P563 Y566 F569 P570 N571 L575 E576 R580 L581 T582 I583 C584 D587 F588 G589 F590 R591 R592 N593 N594 K595 F596 D597 L598 K599 K600 T601 R602 V603 L604 T611 S617 T618 M619 L622
K623 C624 T625 V626 GLY PRO ALA MET ASN LYS HIS F634 N635 M636 S637 I638 I639 I640 S641 N642 G643 H644 T647 Q648 Y649 F652 S653 I659 T660 S661 Y666 G671 G672 T673 L674 L675 T676 L677 T678 G679 N680 TYR LEU ASN SER GLY ASN S687 R688 H689 I690 S691 I692 G693 G694
C697 T698 L699 K700 S701 V702 S703 I706 L707 E708 C709 Y710 T711 P712 A713 Q714 T715 I716 S717 T718 E719 F720 A721 V722 K723 L724 K725 I726 D727 L728 A729 N730 R731 I735 F736 S737 Y738 ARG GLU ASP PRO ILE VAL TYR GLU ILE HIS PRO THR LYS SER PHE ILE SER GLY GLY SER
THR ILE THR GLY VAL GLY LYS ASN LEU ASN SER VAL SER VAL PRO ARG MET VAL ILE ASN VAL HIS GLU ALA GLY ARG ASN PHE THR VAL ALA CYS GLN HIS ARG SER ASN SER GLU ILE ILE CYS CYS THR THR PRO SER LEU GLN GLN LEU ASN LEU GLN LEU PRO LEU LYS THR LYS
ALA PHE PHE MET LEU ASP GLY ILE LEU SER LYS TYR PHE ASP LEU ILE TYR VAL HIS ASN PRO VAL PHE LYS PRO PHE GLU LYS PRO VAL MET ILE SER MET GLY ASN GLU ASN VAL LEU GLU ILE LYS GLY ASN ASP ILE ASP PRO GLU ALA VAL LYS GLY GLU VAL LEU LYS VAL GLY
ASN LYS SER CYS GLU ASN ILE HIS LEU HIS SER GLU ALA VAL LEU CYS THR VAL PRO ASN ASP LEU LEU LYS LEU ASN ILE GLU GLU LEU ASN SER GLU LEU TRP LYS GLN ALA ILE SER SER THR VAL LEU GLY LYS VAL ILE VAL GLN PRO ASP GLN ASN PHE THR GLY LEU ILE GLY VAL
VAL SER ILE SER THR ALA LEU LEU LEU LEU GLY PHE PHE LEU TRP LEU LYS LYS ARG LYS GLN ILE LYS ASP LEU GLY SER GLU LEU LEU VAL ARG TYR ASP ALA ARG VAL HIS THR PRO HIS LEU ASP ASP LEU VAL SER PRO THR THR GLU MET VAL ASN
GLU SER VAL ASP TYR ARG ALA THR PHE PRO GLU ASP GLN PHE PRO ASN SER SER GLN ASN GLY SER CYS ARG GLN VAL GLN TYR PRO LEU THR ASP MET SER PRO ILE LEU THR SER GLY ASP SER ASP ILE SER SER PRO LEU LEU GLN GLN VAL THR VAL HIS ILE ASP LEU ILE ILE
ASN PRO GLU LEU VAL GLN ALA VAL HIS VAL ILE ILE GLY PRO SER SER LEU ILE VAL HIS PHE ASN GLU VAL ILE GLY ARG GLY HIS PHE GLY CYS VAL TYR HIS ILE THR GLY LYS LYS ILE HIS CYS ALA VAL LYS SER LEU ASN ARG THR ILE THR ASP ILE
GLY GLU VAL SER GLN PHE GLY MET LYS ASP PHE SER HIS PRO ASN VAL LEU SER LEU LEU GLY ILE CYS LEU ARG SER GLU GLY GLY SER PRO LEU VAL LEU PRO TYR MET LYS HIS GLY ASP LEU LEU ARG ASN PHE ILE ARG ASN GLU THR HIS ASN PRO THR VAL
LYS ASP LEU ILE GLY PHE VAL HIS ARG ASP LEU ALA SER LYS LYS PHE VAL HIS ARG ASN CYS MET LEU ASP GLU LYS PHE THR VAL LYS VAL ALA ASP PHE ALA ALA ARG ASP ASP MET TYR ASP LYS GLU TYR TYR LEU ASP ASP ARG ASP MET TYR SER LEU ASN ARG ILE THR ASP ILE

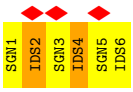
ASN LYS THR GLY ALA LYS LEU LEU PRO VAL LYS TRP MET ALA LEU GLU SER LEU GLN THR GLN LYS PHE THR THR LYS SER ASP VAL TRP SER PHE GLY VAL LEU LEU TRP GLU LEU MET THR ARG GLY ALA PRO PRO TYR PRO ASP VAL ASN THR PHE ASP ILE THR VAL TYR LEU LEU GLN

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

VAL LYS CYS VAL ALA PRO TYR PRO SER LEU LEU SER SER GLU ASP ASN ALA ASP ASP GLU VAL ASP THR ARG PRO ALA SER PHE TRP GLU THR SER

• Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45471	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.077	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	291.6, 291.6, 291.6	wwPDB
Map dimensions	270, 270, 270	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: SGN, IDS

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	0.43	0/2105	0.66	0/2840
1	D	0.45	0/2344	0.63	2/3196 (0.1%)
2	E	0.49	0/5444	0.64	2/7397 (0.0%)
All	All	0.47	0/9893	0.64	4/13433 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	441	ARG	C-N-CA	-5.63	107.62	121.70
1	D	390	ASP	CB-CG-OD2	5.26	123.03	118.30
2	E	413	ARG	CB-CG-CD	-5.21	98.06	111.60
2	E	409	CYS	CA-CB-SG	5.15	123.27	114.00

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	2047	0	1933	169	0
1	D	2287	0	2128	153	0
2	E	5324	0	5126	311	0
3	B	97	0	34	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9755	0	9221	623	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 33.

All (623) 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:E:189:LYS:O	2:E:192:PHE:HB2	1.55	1.04
1:A:36:ARG:O	1:A:72:ASN:ND2	2.01	0.93
1:D:415:TRP:HB2	1:D:438:ASN:H	1.35	0.90
2:E:176:VAL:HA	2:E:217:ARG:HH21	1.35	0.90
2:E:232:GLN:NE2	2:E:415:GLU:OE2	2.08	0.86
2:E:374:PHE:O	2:E:404:ARG:NH1	2.09	0.86
1:D:657:ILE:HG12	1:D:708:ARG:HB2	1.57	0.85
2:E:382:ASN:HD22	2:E:422:THR:HG21	1.40	0.84
1:A:163:LEU:HD23	1:A:167:TYR:HE2	1.41	0.84
1:D:389:GLN:N	1:D:467:SER:HG	1.76	0.84
2:E:118:MET:HE1	2:E:179:ALA:HA	1.60	0.83
1:A:275:ASP:OD1	1:A:277:HIS:ND1	2.10	0.83
2:E:65:GLY:HA3	2:E:117:ASN:HD22	1.41	0.83
2:E:222:THR:OG1	2:E:224:ASP:OD1	1.98	0.82
2:E:424:LEU:HD21	2:E:426:ARG:HH21	1.46	0.80
2:E:428:ASP:OD1	2:E:430:PHE:N	2.13	0.80
1:A:243:HIS:NE2	1:A:245:PHE:O	2.14	0.80
1:A:159:GLU:OE2	2:E:426:ARG:NH1	2.15	0.79
2:E:62:ILE:HD13	2:E:503:LEU:HD21	1.64	0.79
1:D:550:ILE:HD11	1:D:555:GLY:HA2	1.63	0.78
1:D:552:ASP:OD1	1:D:556:ARG:NH2	2.15	0.78
2:E:666:TYR:HA	2:E:737:SER:HB3	1.64	0.78
1:D:653:ASN:OD1	1:D:654:GLU:N	2.16	0.77
1:A:165:SER:HA	1:A:168:ARG:HH12	1.49	0.76
1:D:530:LEU:HD11	1:D:579:LEU:HD11	1.67	0.76
1:A:85:LYS:NZ	1:A:100:PRO:O	2.18	0.76
1:A:147:ILE:HG21	1:A:193:ASN:HB2	1.68	0.76
1:D:534:GLN:NE2	2:E:190:ASP:O	2.19	0.76
2:E:378:VAL:O	2:E:404:ARG:NH2	2.20	0.75
2:E:327:ALA:HB3	2:E:449:ASP:HB2	1.68	0.75
2:E:547:ARG:NH1	2:E:548:SER:H	1.85	0.75
1:D:713:ALA:HA	1:D:716:ILE:HD12	1.67	0.75
2:E:269:LEU:HD11	2:E:387:GLN:HB3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:412:ARG:NH2	2:E:414:ASP:O	2.21	0.74
1:D:640:GLU:O	1:D:644:GLN:NE2	2.18	0.73
1:A:82:PHE:HZ	1:A:98:TRP:HB2	1.53	0.72
1:A:183:GLU:OE1	1:A:185:GLY:N	2.20	0.72
1:A:96:CYS:SG	1:A:98:TRP:NE1	2.63	0.72
1:A:245:PHE:HA	1:A:250:TYR:HE2	1.54	0.72
2:E:217:ARG:HD3	2:E:228:PHE:HE1	1.54	0.72
1:D:602:TYR:HB2	1:D:714:LYS:HD3	1.72	0.71
2:E:358:ASP:HA	2:E:438:LEU:HB2	1.72	0.71
1:D:392:TYR:H	1:D:469:CYS:HB2	1.55	0.71
1:A:43:LYS:HB3	1:A:120:GLU:HB2	1.73	0.71
2:E:537:GLN:O	2:E:547:ARG:NH1	2.24	0.71
1:A:246:LEU:HG	1:A:249:ARG:HH11	1.56	0.71
1:D:524:ILE:HG22	1:D:525:LYS:HD2	1.71	0.71
1:D:534:GLN:HE22	2:E:190:ASP:HB3	1.55	0.70
2:E:386:LEU:HD22	2:E:389:PHE:HB3	1.74	0.70
2:E:590:PHE:HB3	2:E:597:ASP:HB2	1.73	0.70
1:D:513:TYR:OH	1:D:514:ARG:NH2	2.25	0.70
1:A:160:HIS:HB2	1:A:197:ARG:HH22	1.57	0.70
1:D:541:LEU:HD23	1:D:567:VAL:HG12	1.74	0.69
1:D:507:TRP:CD1	1:D:597:ILE:HB	2.28	0.69
1:A:227:GLU:HG3	1:A:284:ALA:HB2	1.75	0.69
1:A:88:VAL:HG23	1:A:99:PHE:CE2	2.28	0.69
1:D:460:PRO:HB2	1:D:461:TRP:HD1	1.58	0.69
1:D:680:GLU:HA	1:D:685:ARG:HA	1.75	0.69
2:E:563:PRO:O	2:E:647:THR:OG1	2.11	0.69
1:A:163:LEU:HD12	1:A:163:LEU:H	1.57	0.68
2:E:571:ASN:O	2:E:653:SER:OG	2.08	0.68
2:E:267:GLU:HG2	2:E:275:HIS:CD2	2.28	0.68
2:E:671:GLY:HA3	2:E:713:ALA:HA	1.75	0.68
1:D:540:ASP:OD1	1:D:541:LEU:N	2.26	0.68
1:A:63:LYS:HD2	1:A:95:GLN:HE22	1.59	0.68
1:A:88:VAL:HG23	1:A:99:PHE:HE2	1.57	0.68
1:A:82:PHE:HD2	1:A:100:PRO:HB3	1.59	0.68
1:D:454:THR:OG1	1:D:459:ILE:O	2.11	0.68
1:D:606:ILE:HD12	1:D:607:PRO:HD2	1.75	0.68
2:E:113:LYS:HG3	2:E:114:ASP:H	1.59	0.67
1:D:600:PRO:HA	1:D:686:MET:HE1	1.76	0.67
2:E:91:GLU:O	2:E:110:GLY:N	2.26	0.67
2:E:343:PHE:HE2	2:E:444:THR:HG21	1.59	0.67
1:A:234:ARG:NH2	1:A:236:ASP:OD2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:678:VAL:HA	1:D:687:VAL:HA	1.77	0.67
2:E:498:GLN:O	2:E:516:ASN:ND2	2.28	0.67
2:E:27:LYS:H	2:E:27:LYS:HD2	1.60	0.66
2:E:332:GLN:OE1	2:E:469:ARG:N	2.27	0.66
1:A:144:LYS:HG2	1:A:202:ASP:HB3	1.77	0.66
1:D:446:ASP:OD1	1:D:447:ALA:N	2.27	0.66
2:E:697:CYS:HB3	2:E:712:PRO:HD3	1.77	0.66
2:E:231:ASP:OD1	2:E:232:GLN:N	2.29	0.66
1:A:177:CYS:C	1:A:178:ARG:HD3	2.15	0.66
1:D:561:CYS:HB3	1:D:593:PHE:CD2	2.31	0.66
2:E:60:HIS:HA	2:E:75:GLU:OE2	1.94	0.66
1:D:524:ILE:HD12	1:D:599:LEU:HD21	1.79	0.65
2:E:211:LEU:O	2:E:212:HIS:ND1	2.29	0.65
2:E:675:LEU:O	2:E:708:GLU:HA	1.96	0.65
2:E:247:ILE:HG22	2:E:265:GLN:HB3	1.78	0.65
2:E:26:CYS:N	2:E:584:CYS:SG	2.70	0.65
1:A:70:CYS:HB3	1:A:98:TRP:NE1	2.12	0.64
1:D:657:ILE:CG1	1:D:708:ARG:HB2	2.25	0.64
1:D:670:GLU:OE2	2:E:221:GLU:N	2.29	0.64
2:E:267:GLU:HG2	2:E:275:HIS:HD2	1.59	0.64
1:D:540:ASP:OD1	1:D:542:LYS:N	2.27	0.64
2:E:119:ALA:HB3	2:E:133:CYS:HB2	1.80	0.64
2:E:213:SER:OG	2:E:235:ILE:O	2.13	0.64
2:E:675:LEU:HD11	2:E:711:THR:HB	1.79	0.64
1:A:188:TRP:HA	1:A:200:VAL:HA	1.79	0.64
2:E:129:GLN:OE1	2:E:143:ARG:NH2	2.22	0.64
2:E:299:ILE:HG22	2:E:313:VAL:HG12	1.80	0.64
2:E:74:ASN:OD1	2:E:75:GLU:N	2.31	0.64
1:A:90:ASP:HB3	1:A:93:ARG:HG2	1.79	0.63
1:D:538:SER:O	1:D:544:TYR:OH	2.11	0.63
2:E:562:LEU:HD12	2:E:563:PRO:HD2	1.79	0.63
2:E:49:GLU:N	2:E:49:GLU:OE1	2.31	0.63
1:A:238:GLN:NE2	1:A:243:HIS:O	2.26	0.63
1:D:606:ILE:HG12	1:D:636:ILE:HG13	1.80	0.63
1:A:63:LYS:HD2	1:A:95:GLN:NE2	2.14	0.62
2:E:68:ASN:HB3	2:E:87:GLY:HA2	1.81	0.62
2:E:261:PHE:HB2	2:E:279:ILE:HB	1.81	0.62
2:E:494:HIS:CD2	2:E:497:ASN:HA	2.34	0.62
2:E:239:PRO:HA	2:E:242:ARG:NE	2.15	0.62
1:A:85:LYS:HB2	1:A:124:TYR:CE2	2.35	0.62
1:D:496:VAL:O	1:D:666:SER:OG	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:VAL:HG11	1:A:116:PHE:HB3	1.81	0.62
1:D:639:ASN:HB3	1:D:652:LEU:HD22	1.82	0.62
1:A:53:ILE:HG12	1:A:109:LYS:NZ	2.15	0.62
1:D:540:ASP:HA	2:E:413:ARG:HH21	1.64	0.62
1:A:158:HIS:CD2	1:A:197:ARG:HA	2.35	0.61
1:D:497:ASN:ND2	1:D:665:GLY:O	2.33	0.61
2:E:230:THR:O	2:E:233:SER:OG	2.14	0.61
1:D:416:ASP:HA	1:D:419:MET:SD	2.40	0.61
1:D:612:CYS:HB2	1:D:679:CYS:HA	1.81	0.61
2:E:220:LYS:HE3	2:E:227:MET:SD	2.40	0.61
2:E:362:MET:HG2	2:E:430:PHE:CE2	2.35	0.61
2:E:46:PHE:HE2	2:E:80:LYS:HB2	1.65	0.61
2:E:244:SER:HB3	2:E:266:ARG:HH22	1.65	0.61
1:A:231:ILE:O	1:A:274:LEU:HD22	2.00	0.61
1:A:66:THR:HG23	1:A:69:GLN:H	1.65	0.61
1:A:150:GLN:NE2	1:A:154:SER:O	2.33	0.61
1:A:250:TYR:HB3	1:A:253:LYS:HD3	1.81	0.61
1:A:262:ASN:ND2	1:A:269:PRO:HA	2.16	0.61
1:A:188:TRP:HB3	1:A:200:VAL:HG22	1.82	0.61
1:A:99:PHE:HB3	1:A:101:PHE:CE1	2.35	0.61
1:A:72:ASN:HA	1:A:75:THR:HG22	1.83	0.60
1:D:422:LEU:O	1:D:426:ILE:N	2.34	0.60
1:A:220:ARG:HH21	1:A:261:ARG:HG3	1.67	0.60
1:A:241:HIS:HB3	1:A:279:ARG:HH21	1.65	0.60
2:E:503:LEU:HB3	2:E:510:ILE:HD11	1.81	0.60
1:A:87:PHE:HB2	1:A:98:TRP:HD1	1.65	0.60
1:D:697:CYS:HB2	2:E:221:GLU:OE1	2.02	0.60
2:E:415:GLU:CD	2:E:415:GLU:H	2.05	0.60
1:D:656:GLU:O	1:D:657:ILE:HD13	2.02	0.60
2:E:196:PHE:CD1	2:E:216:VAL:HG22	2.37	0.60
1:A:259:TYR:HB3	1:A:261:ARG:NH1	2.16	0.59
2:E:149:ASN:OD1	2:E:150:HIS:N	2.35	0.59
1:A:219:TYR:CZ	1:A:221:GLY:HA3	2.37	0.59
1:A:37:ASN:OD1	1:A:38:THR:N	2.36	0.59
1:A:73:ARG:HH22	3:B:2:IDS:H4	1.67	0.59
2:E:590:PHE:CD1	2:E:643:GLY:HA3	2.37	0.59
2:E:403:LEU:HD22	2:E:406:SER:HB2	1.85	0.59
1:A:63:LYS:NZ	1:A:94:LYS:HB2	2.17	0.59
1:D:452:CYS:SG	1:D:453:TYR:N	2.76	0.59
1:D:579:LEU:HD12	1:D:580:VAL:H	1.68	0.59
2:E:238:LEU:HD12	2:E:240:GLU:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLN:NE2	1:A:156:ILE:O	2.35	0.58
1:D:695:ARG:NH1	2:E:125:TYR:HE1	2.00	0.58
1:D:712:TYR:O	1:D:716:ILE:HG13	2.03	0.58
2:E:46:PHE:CE2	2:E:80:LYS:HB2	2.37	0.58
2:E:341:ILE:HD13	2:E:366:PRO:HA	1.85	0.58
1:D:569:GLN:NE2	1:D:570:LEU:O	2.37	0.58
1:A:164:PRO:HA	1:A:172:LEU:HD21	1.84	0.58
1:D:640:GLU:O	1:D:643:SER:OG	2.18	0.58
2:E:69:TYR:CE1	2:E:85:LYS:HD3	2.38	0.58
2:E:623:LYS:HA	2:E:623:LYS:HE2	1.84	0.58
1:A:73:ARG:HB3	1:A:80:LEU:HD21	1.84	0.58
1:A:215:ASN:HD21	1:A:218:SER:H	1.51	0.58
1:A:87:PHE:O	1:A:119:TYR:HB2	2.02	0.58
1:A:102:ASN:OD1	1:A:104:MET:N	2.31	0.58
2:E:358:ASP:OD1	2:E:438:LEU:N	2.36	0.58
2:E:220:LYS:HG2	2:E:225:GLY:O	2.04	0.57
2:E:360:SER:OG	2:E:439:LEU:HG	2.04	0.57
1:D:554:HIS:HB2	1:D:556:ARG:HE	1.69	0.57
1:D:717:HIS:O	1:D:720:ILE:HG22	2.05	0.57
2:E:196:PHE:HD1	2:E:216:VAL:HG22	1.68	0.57
2:E:275:HIS:HE1	2:E:277:ARG:NE	2.02	0.57
2:E:588:PHE:HB2	2:E:619:MET:HA	1.87	0.57
1:A:234:ARG:HE	1:A:237:HIS:CE1	2.23	0.57
1:D:547:TRP:HD1	1:D:564:VAL:HA	1.69	0.57
2:E:382:ASN:ND2	2:E:422:THR:HG21	2.18	0.57
2:E:591:ARG:HG3	2:E:596:PHE:HE1	1.69	0.57
2:E:619:MET:SD	2:E:619:MET:N	2.78	0.57
1:A:207:SER:OG	1:A:208:GLU:OE2	2.16	0.56
2:E:113:LYS:HG3	2:E:114:ASP:N	2.19	0.56
2:E:700:LYS:N	2:E:708:GLU:O	2.38	0.56
1:D:556:ARG:NH2	1:D:626:ASP:O	2.38	0.56
1:D:600:PRO:HG3	1:D:709:VAL:HG23	1.88	0.56
2:E:592:ARG:HB3	2:E:595:LYS:O	2.05	0.56
2:E:659:ILE:HD11	2:E:677:LEU:HD12	1.87	0.56
1:D:643:SER:OG	1:D:644:GLN:NE2	2.39	0.56
2:E:274:PHE:CE2	2:E:354:ALA:HB2	2.41	0.56
2:E:400:ARG:NH1	2:E:414:ASP:HB3	2.20	0.56
1:D:591:ASP:OD1	1:D:593:PHE:N	2.35	0.56
2:E:317:LEU:HA	2:E:346:PHE:HD1	1.71	0.56
2:E:460:GLY:HA3	2:E:482:ASP:O	2.05	0.56
2:E:703:SER:HB3	2:E:706:ILE:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:CYS:HA	1:A:73:ARG:HG2	1.88	0.56
1:A:177:CYS:HB2	1:A:189:CYS:HB3	1.88	0.56
2:E:267:GLU:OE2	2:E:273:THR:HG23	2.06	0.55
2:E:599:LYS:NZ	2:E:600:LYS:HE2	2.21	0.55
1:D:511:LEU:HD11	1:D:536:PHE:HE1	1.71	0.55
2:E:101:CYS:HB2	2:E:104:LYS:HG3	1.88	0.55
2:E:123:ASP:OD2	2:E:129:GLN:NE2	2.39	0.55
1:A:63:LYS:HZ3	1:A:94:LYS:HB2	1.71	0.55
1:D:568:SER:OG	1:D:583:LYS:O	2.18	0.55
1:A:213:THR:O	1:A:216:GLY:N	2.39	0.55
1:A:108:VAL:C	1:A:109:LYS:HD3	2.28	0.55
1:D:626:ASP:OD1	1:D:626:ASP:N	2.40	0.55
2:E:220:LYS:HG2	2:E:225:GLY:C	2.26	0.55
2:E:266:ARG:NH1	2:E:269:LEU:O	2.40	0.55
2:E:394:HIS:NE2	2:E:396:HIS:CE1	2.75	0.55
1:A:125:ILE:HD12	1:A:125:ILE:H	1.70	0.54
1:A:190:PHE:CD1	1:A:198:TYR:HB3	2.41	0.54
2:E:544:LYS:NZ	2:E:546:VAL:HG21	2.22	0.54
1:A:259:TYR:HB3	1:A:261:ARG:HH12	1.71	0.54
2:E:76:GLU:CD	2:E:76:GLU:H	2.10	0.54
1:A:53:ILE:H	1:A:109:LYS:HZ1	1.55	0.54
1:D:396:GLY:H	1:D:445:ASP:HA	1.71	0.54
1:D:560:LYS:HD3	1:D:560:LYS:N	2.23	0.54
2:E:35:MET:HA	2:E:524:GLN:OE1	2.08	0.54
1:A:220:ARG:NH2	1:A:261:ARG:HG3	2.23	0.54
1:A:223:MET:SD	1:A:225:HIS:N	2.75	0.54
1:D:396:GLY:N	1:D:445:ASP:OD1	2.40	0.54
2:E:526:CYS:HA	2:E:540:TRP:CE3	2.42	0.54
1:A:89:PHE:CE1	1:A:96:CYS:HB3	2.42	0.54
1:A:246:LEU:HB2	1:A:249:ARG:HD2	1.89	0.54
2:E:730:ASN:OD1	2:E:731:ARG:N	2.38	0.54
1:A:80:LEU:HD13	1:A:98:TRP:CE3	2.43	0.54
1:A:34:LYS:HG3	1:A:35:ARG:H	1.72	0.54
1:A:70:CYS:HB3	1:A:98:TRP:HE1	1.71	0.54
1:A:163:LEU:HD23	1:A:167:TYR:CE2	2.33	0.54
2:E:181:GLY:N	2:E:200:THR:OG1	2.41	0.54
2:E:674:LEU:HD12	2:E:709:CYS:O	2.08	0.54
1:A:238:GLN:HG3	1:A:242:ARG:HG2	1.89	0.54
1:D:688:LEU:O	1:D:709:VAL:HG22	2.08	0.54
2:E:559:GLN:OE1	2:E:559:GLN:N	2.40	0.53
2:E:659:ILE:HD12	2:E:678:THR:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ASP:O	1:A:178:ARG:NH1	2.41	0.53
1:D:497:ASN:HD22	1:D:666:SER:HA	1.73	0.53
1:D:539:ARG:HH11	1:D:539:ARG:HG2	1.72	0.53
1:A:246:LEU:O	1:A:249:ARG:HG2	2.08	0.53
1:D:708:ARG:HH21	1:D:711:TYR:HB2	1.73	0.53
1:D:415:TRP:HB2	1:D:438:ASN:N	2.16	0.53
1:D:512:ARG:HG3	1:D:512:ARG:HH11	1.73	0.53
1:A:273:THR:OG1	1:A:278:THR:O	2.26	0.53
1:A:183:GLU:CD	1:A:185:GLY:H	2.11	0.53
2:E:80:LYS:NZ	2:E:83:GLU:HB2	2.24	0.53
2:E:241:PHE:CE2	2:E:269:LEU:HD13	2.43	0.53
2:E:267:GLU:CG	2:E:275:HIS:CD2	2.92	0.53
2:E:291:TYR:HB3	2:E:417:ARG:HD2	1.91	0.53
1:D:508:MET:HG3	1:D:629:LEU:HD11	1.90	0.53
2:E:245:TYR:H	2:E:266:ARG:NH2	2.07	0.53
1:D:561:CYS:HB3	1:D:593:PHE:HD2	1.74	0.52
1:A:85:LYS:HZ2	1:A:100:PRO:C	2.13	0.52
1:D:695:ARG:NH1	2:E:125:TYR:CE1	2.77	0.52
2:E:394:HIS:NE2	2:E:396:HIS:HE1	2.07	0.52
1:A:137:LYS:HD2	1:A:171:ASP:HB2	1.90	0.52
2:E:415:GLU:OE1	2:E:415:GLU:N	2.38	0.52
2:E:716:ILE:HG21	2:E:720:PHE:HZ	1.74	0.52
1:A:160:HIS:HB2	1:A:197:ARG:NH2	2.25	0.52
2:E:96:PHE:HB2	2:E:99:GLN:HG2	1.92	0.52
2:E:261:PHE:O	2:E:262:LEU:HD23	2.10	0.52
1:A:53:ILE:H	1:A:109:LYS:NZ	2.08	0.52
1:A:93:ARG:HD2	1:A:95:GLN:HB3	1.92	0.52
1:D:508:MET:HG3	1:D:629:LEU:CD1	2.40	0.52
2:E:673:THR:H	2:E:711:THR:HG22	1.74	0.52
2:E:225:GLY:O	2:E:226:PHE:HD1	1.93	0.52
2:E:417:ARG:HD3	2:E:417:ARG:N	2.24	0.52
1:A:215:ASN:OD1	1:A:218:SER:OG	2.24	0.52
1:D:442:ASN:HB2	1:D:451:TRP:CD1	2.45	0.52
2:E:277:ARG:NH1	2:E:293:GLU:OE1	2.43	0.51
2:E:339:ASP:OD2	2:E:368:LYS:HD3	2.10	0.51
2:E:677:LEU:O	2:E:706:ILE:HD12	2.10	0.51
2:E:730:ASN:CG	2:E:731:ARG:H	2.12	0.51
2:E:235:ILE:HD11	2:E:417:ARG:NH1	2.24	0.51
2:E:546:VAL:HG12	2:E:547:ARG:O	2.10	0.51
1:A:42:PHE:HD2	1:A:119:TYR:HB3	1.75	0.51
2:E:117:ASN:HD21	2:E:120:LEU:HB2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:247:ILE:HG22	2:E:265:GLN:CB	2.41	0.51
1:D:547:TRP:HA	1:D:563:GLN:O	2.10	0.51
1:D:579:LEU:HD12	1:D:580:VAL:N	2.25	0.51
1:D:714:LYS:HE3	1:D:714:LYS:HA	1.91	0.51
2:E:526:CYS:O	2:E:530:LEU:HG	2.11	0.51
1:D:543:ASP:OD1	1:D:543:ASP:N	2.37	0.51
1:A:176:TYR:HB2	1:A:178:ARG:HE	1.76	0.51
1:D:422:LEU:HG	1:D:426:ILE:HB	1.93	0.51
2:E:202:ASN:OD1	2:E:203:SER:N	2.44	0.51
2:E:382:ASN:HD22	2:E:422:THR:CG2	2.18	0.51
2:E:201:ILE:HB	2:E:206:PHE:HE1	1.75	0.51
2:E:253:PHE:CE1	2:E:260:TYR:HB2	2.46	0.51
1:D:717:HIS:O	1:D:721:LEU:HG	2.11	0.50
2:E:69:TYR:HB3	2:E:71:TYR:CE1	2.46	0.50
2:E:77:ASP:HB2	2:E:79:GLN:HG2	1.92	0.50
1:A:40:HIS:HD2	1:A:231:ILE:HG21	1.76	0.50
2:E:218:ARG:HG2	2:E:219:LEU:N	2.22	0.50
2:E:359:ARG:HG2	2:E:359:ARG:HH11	1.75	0.50
2:E:720:PHE:O	2:E:735:ILE:HA	2.11	0.50
2:E:690:ILE:HD13	2:E:724:LEU:HD12	1.92	0.50
2:E:445:PHE:CE1	2:E:452:ILE:HB	2.47	0.50
2:E:494:HIS:NE2	2:E:497:ASN:HA	2.26	0.50
2:E:595:LYS:HD2	2:E:596:PHE:N	2.26	0.50
2:E:296:LEU:HD22	2:E:365:PHE:CE2	2.46	0.50
1:A:43:LYS:NZ	1:A:45:SER:HB3	2.27	0.50
2:E:281:PHE:CE2	2:E:288:LEU:HD23	2.47	0.50
2:E:566:TYR:N	2:E:584:CYS:O	2.42	0.50
1:D:402:ASN:HA	1:D:439:TYR:CD2	2.47	0.50
1:A:80:LEU:HD12	1:A:84:CYS:SG	2.52	0.49
1:A:93:ARG:HH21	1:A:96:CYS:HA	1.77	0.49
2:E:170:SER:HB2	2:E:171:GLN:NE2	2.27	0.49
2:E:174:ASP:O	2:E:176:VAL:HG23	2.12	0.49
2:E:726:ILE:C	2:E:728:LEU:H	2.15	0.49
1:D:510:SER:OG	1:D:547:TRP:HB2	2.11	0.49
2:E:224:ASP:OD1	2:E:224:ASP:N	2.45	0.49
2:E:395:GLU:HG3	2:E:396:HIS:N	2.26	0.49
2:E:452:ILE:HD13	2:E:466:VAL:HA	1.94	0.49
1:D:568:SER:HB3	1:D:585:ALA:HA	1.93	0.49
2:E:56:ILE:HG23	2:E:63:PHE:HD2	1.77	0.49
1:A:38:THR:H	1:A:39:ILE:HD12	1.78	0.49
2:E:271:ALA:O	2:E:273:THR:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:239:PRO:HA	2:E:242:ARG:CZ	2.41	0.49
2:E:659:ILE:HD11	2:E:677:LEU:HB3	1.95	0.49
2:E:194:ASN:HA	2:E:217:ARG:O	2.13	0.49
2:E:638:ILE:HG22	2:E:649:TYR:HD2	1.78	0.49
1:A:136:TYR:O	1:A:137:LYS:HD3	2.13	0.49
1:D:552:ASP:OD2	1:D:555:GLY:N	2.46	0.49
1:D:552:ASP:HA	1:D:627:GLY:O	2.12	0.49
1:A:88:VAL:HG22	1:A:118:LEU:HA	1.95	0.49
1:D:581:LEU:HD23	1:D:715:TRP:CH2	2.47	0.49
1:D:694:GLY:O	1:D:696:GLY:N	2.45	0.49
1:D:708:ARG:HE	1:D:711:TYR:HB2	1.77	0.49
2:E:127:ASP:O	2:E:129:GLN:HG3	2.12	0.49
2:E:550:GLU:OE1	2:E:550:GLU:N	2.46	0.49
2:E:560:ILE:HA	2:E:644:HIS:CE1	2.48	0.49
2:E:676:THR:HA	2:E:707:LEU:O	2.12	0.49
1:A:49:THR:HG23	1:A:111:GLU:OE1	2.13	0.48
1:A:62:LYS:HG3	1:A:64:VAL:HG23	1.95	0.48
1:D:406:THR:HG22	1:D:410:LEU:O	2.13	0.48
1:D:679:CYS:O	1:D:686:MET:N	2.35	0.48
2:E:284:ILE:HG22	2:E:286:SER:H	1.78	0.48
2:E:524:GLN:O	2:E:540:TRP:HH2	1.96	0.48
2:E:611:THR:OG1	2:E:625:THR:O	2.23	0.48
1:A:159:GLU:N	1:A:159:GLU:OE1	2.46	0.48
2:E:335:ALA:HA	2:E:368:LYS:NZ	2.27	0.48
1:D:695:ARG:HH12	2:E:125:TYR:HE1	1.61	0.48
1:A:109:LYS:HB2	1:A:111:GLU:OE2	2.13	0.48
1:D:590:LEU:HD13	1:D:594:VAL:HG23	1.95	0.48
1:D:669:CYS:N	1:D:672:ASP:OD2	2.35	0.48
2:E:590:PHE:HD1	2:E:643:GLY:HA3	1.78	0.48
1:A:39:ILE:HD12	1:A:39:ILE:H	1.79	0.48
1:D:702:ARG:HG3	1:D:702:ARG:HH11	1.78	0.48
2:E:583:ILE:HB	2:E:622:LEU:HB2	1.96	0.48
1:D:519:CYS:HB3	1:D:673:TYR:O	2.13	0.48
1:D:564:VAL:C	1:D:565:LEU:HD12	2.34	0.48
2:E:443:SER:HB2	2:E:490:VAL:HG21	1.94	0.48
2:E:544:LYS:HZ3	2:E:546:VAL:HG21	1.79	0.48
1:A:263:PRO:HD2	1:A:270:TRP:NE1	2.29	0.47
2:E:219:LEU:HD11	2:E:223:LYS:HA	1.96	0.47
2:E:582:THR:O	2:E:583:ILE:HD13	2.14	0.47
1:D:670:GLU:HA	1:D:673:TYR:CZ	2.50	0.47
2:E:30:LEU:HD23	2:E:584:CYS:HB3	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:331:ARG:HB2	2:E:331:ARG:CZ	2.44	0.47
2:E:526:CYS:HB3	2:E:587:ASP:OD2	2.14	0.47
2:E:617:SER:HB2	2:E:622:LEU:HD13	1.97	0.47
1:A:144:LYS:HG3	1:A:200:VAL:O	2.15	0.47
1:A:241:HIS:CB	1:A:279:ARG:HH21	2.27	0.47
1:A:243:HIS:CD2	1:A:245:PHE:H	2.32	0.47
1:A:245:PHE:O	1:A:246:LEU:HD23	2.15	0.47
2:E:137:ASN:O	2:E:140:THR:HG23	2.14	0.47
1:A:88:VAL:HB	1:A:97:LEU:HD21	1.97	0.47
2:E:277:ARG:NH1	2:E:419:GLU:OE2	2.41	0.47
2:E:386:LEU:HD23	2:E:389:PHE:H	1.80	0.47
2:E:677:LEU:HB2	2:E:707:LEU:HB2	1.96	0.47
1:A:129:ILE:N	1:A:204:PRO:O	2.47	0.47
1:D:615:TYR:HB3	1:D:629:LEU:HD21	1.96	0.47
2:E:136:VAL:O	2:E:138:ARG:N	2.41	0.47
2:E:217:ARG:HD3	2:E:228:PHE:CE1	2.42	0.47
2:E:384:ARG:NH1	2:E:387:GLN:OE1	2.41	0.47
2:E:661:SER:O	2:E:677:LEU:HA	2.15	0.47
1:A:136:TYR:C	1:A:137:LYS:HD3	2.34	0.47
1:A:190:PHE:CE1	1:A:198:TYR:HB3	2.50	0.47
1:D:568:SER:OG	1:D:583:LYS:HG3	2.15	0.47
1:D:653:ASN:H	1:D:656:GLU:CD	2.18	0.47
2:E:316:ILE:HG12	2:E:349:SER:HB3	1.97	0.47
2:E:46:PHE:HB3	2:E:510:ILE:HG23	1.97	0.47
1:A:65:ASN:OD1	1:A:66:THR:N	2.48	0.47
1:A:122:LYS:O	1:A:126:ARG:HG3	2.15	0.47
2:E:86:THR:O	2:E:86:THR:OG1	2.24	0.47
2:E:394:HIS:CE1	2:E:395:GLU:HG2	2.50	0.47
2:E:575:LEU:HD12	2:E:576:GLU:N	2.30	0.47
2:E:718:THR:O	2:E:738:TYR:HB2	2.15	0.46
1:A:85:LYS:HZ3	1:A:101:PHE:HA	1.79	0.46
1:A:238:GLN:HG3	1:A:238:GLN:O	2.15	0.46
1:D:514:ARG:HB2	1:D:516:LYS:NZ	2.30	0.46
1:A:51:ILE:HD12	1:A:53:ILE:HD11	1.96	0.46
1:A:137:LYS:HA	1:A:178:ARG:NH1	2.30	0.46
1:A:246:LEU:H	1:A:249:ARG:HD3	1.81	0.46
2:E:547:ARG:CZ	2:E:548:SER:H	2.29	0.46
1:A:109:LYS:HD3	1:A:109:LYS:N	2.31	0.46
1:D:617:TRP:CZ2	1:D:629:LEU:HB2	2.51	0.46
2:E:410:GLU:OE1	2:E:410:GLU:N	2.48	0.46
2:E:530:LEU:HB2	2:E:591:ARG:HE	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:580:ARG:HA	2:E:625:THR:HG22	1.98	0.46
1:D:536:PHE:CE2	1:D:570:LEU:HD21	2.51	0.46
2:E:463:MET:HA	2:E:477:VAL:O	2.16	0.46
1:D:598:ASP:OD1	1:D:686:MET:HB2	2.16	0.46
2:E:181:GLY:N	2:E:200:THR:HG1	2.13	0.46
2:E:562:LEU:HD12	2:E:563:PRO:CD	2.46	0.46
2:E:422:THR:O	2:E:422:THR:OG1	2.28	0.46
2:E:478:ASN:OD1	2:E:478:ASN:O	2.33	0.46
2:E:550:GLU:O	2:E:552:LEU:HD22	2.16	0.46
1:A:123:ASP:HA	1:A:126:ARG:HD3	1.97	0.46
2:E:400:ARG:HH12	2:E:414:ASP:HB3	1.81	0.46
1:A:129:ILE:HG23	1:A:205:GLN:OE1	2.15	0.46
2:E:192:PHE:CZ	2:E:218:ARG:NH1	2.84	0.46
1:A:165:SER:CA	1:A:168:ARG:HH12	2.23	0.45
2:E:211:LEU:HD23	2:E:211:LEU:HA	1.74	0.45
2:E:636:MET:N	2:E:652:PHE:O	2.36	0.45
1:A:222:LEU:HD23	1:A:222:LEU:HA	1.78	0.45
2:E:245:TYR:CE1	2:E:266:ARG:HB2	2.51	0.45
2:E:692:ILE:HD13	2:E:722:VAL:HG22	1.97	0.45
2:E:697:CYS:HB2	2:E:709:CYS:HB3	1.68	0.45
1:D:658:CYS:SG	1:D:703:PRO:HB2	2.56	0.45
2:E:278:ILE:HB	2:E:296:LEU:HD12	1.98	0.45
2:E:323:SER:OG	2:E:324:LYS:N	2.48	0.45
2:E:671:GLY:HA2	2:E:711:THR:HG23	1.97	0.45
1:A:273:THR:HG21	1:A:278:THR:HG23	1.98	0.45
1:D:402:ASN:HA	1:D:439:TYR:CE2	2.51	0.45
1:A:129:ILE:HG22	1:A:204:PRO:O	2.17	0.45
1:D:523:LEU:HG	1:D:596:THR:HG22	1.98	0.45
2:E:260:TYR:HA	2:E:279:ILE:O	2.17	0.45
2:E:343:PHE:CE2	2:E:444:THR:HG21	2.45	0.45
1:A:47:LYS:HA	1:A:114:HIS:HA	1.99	0.45
2:E:157:GLU:OE2	2:E:159:HIS:CE1	2.70	0.45
2:E:403:LEU:HD23	2:E:403:LEU:HA	1.75	0.45
1:A:93:ARG:NE	1:A:95:GLN:O	2.50	0.45
1:A:142:ILE:HD11	1:A:146:GLY:C	2.37	0.45
1:D:512:ARG:HG2	1:D:515:ASN:HA	1.98	0.45
2:E:72:VAL:O	2:E:73:LEU:HD23	2.16	0.45
1:A:260:CYS:O	1:A:261:ARG:NH2	2.49	0.45
1:D:407:ARG:N	1:D:463:TYR:O	2.49	0.45
1:D:533:ARG:HH21	1:D:578:ASP:H	1.65	0.45
2:E:41:TYR:CD2	2:E:518:LEU:HD21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:53:GLN:NE2	2:E:116:ILE:HB	2.31	0.45
2:E:67:THR:HG23	2:E:116:ILE:HG22	1.98	0.45
2:E:114:ASP:N	2:E:114:ASP:OD1	2.50	0.45
2:E:279:ILE:CD1	2:E:293:GLU:HG2	2.47	0.45
1:D:547:TRP:HE1	1:D:564:VAL:HG23	1.81	0.45
2:E:28:GLU:H	2:E:28:GLU:CD	2.20	0.45
2:E:53:GLN:HE21	2:E:116:ILE:HB	1.81	0.45
2:E:540:TRP:HD1	2:E:542:HIS:H	1.62	0.45
1:A:266:GLN:HB3	1:A:267:PRO:HD2	1.99	0.44
1:D:456:ASN:OD1	1:D:458:LEU:N	2.50	0.44
2:E:60:HIS:O	2:E:61:HIS:ND1	2.43	0.44
2:E:72:VAL:HG13	2:E:81:VAL:HG13	1.99	0.44
2:E:563:PRO:HG3	2:E:642:ASN:HD22	1.83	0.44
1:A:220:ARG:NH2	1:A:253:LYS:O	2.46	0.44
1:D:542:LYS:O	1:D:542:LYS:HD3	2.18	0.44
1:D:652:LEU:HD12	1:D:652:LEU:H	1.82	0.44
2:E:445:PHE:CZ	2:E:515:LEU:HB2	2.52	0.44
2:E:494:HIS:HE2	2:E:497:ASN:HA	1.83	0.44
1:A:121:ASN:HB3	1:A:123:ASP:OD1	2.16	0.44
1:A:44:LYS:HD2	1:A:44:LYS:HA	1.74	0.44
1:A:44:LYS:NZ	1:A:117:ASP:HB3	2.33	0.44
1:D:497:ASN:HB2	1:D:666:SER:OG	2.17	0.44
1:D:499:ILE:O	1:D:631:VAL:HG12	2.17	0.44
1:D:530:LEU:HA	1:D:581:LEU:HD13	1.98	0.44
1:D:606:ILE:HG21	1:D:636:ILE:HG21	1.99	0.44
2:E:385:CYS:HB3	2:E:397:CYS:HB3	1.38	0.44
1:A:90:ASP:OD2	1:A:92:ALA:HB3	2.17	0.44
1:A:42:PHE:CD1	1:A:121:ASN:ND2	2.86	0.44
1:A:270:TRP:CE3	1:A:280:TRP:CE3	3.06	0.44
2:E:92:HIS:HE1	2:E:94:ASP:HB2	1.83	0.44
2:E:184:VAL:HG13	2:E:197:VAL:HG12	2.00	0.44
2:E:582:THR:N	2:E:623:LYS:HZ1	2.15	0.44
1:A:54:ASP:OD1	1:A:54:ASP:N	2.46	0.44
2:E:315:ASN:ND2	2:E:349:SER:OG	2.49	0.44
2:E:504:VAL:O	2:E:510:ILE:HD12	2.18	0.44
1:D:552:ASP:O	1:D:555:GLY:N	2.46	0.43
1:D:651:THR:O	1:D:651:THR:OG1	2.32	0.43
2:E:180:LEU:HB2	2:E:200:THR:OG1	2.18	0.43
1:A:234:ARG:HE	1:A:237:HIS:HE1	1.64	0.43
1:A:251:PRO:O	1:A:253:LYS:HD2	2.18	0.43
2:E:68:ASN:OD1	2:E:114:ASP:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:80:LYS:HZ3	2:E:83:GLU:HB2	1.83	0.43
2:E:699:LEU:HD21	2:E:702:VAL:HB	1.99	0.43
1:A:34:LYS:N	3:B:4:IDS:O1S	2.51	0.43
1:D:403:LEU:HD23	1:D:405:GLN:H	1.82	0.43
2:E:130:LEU:HA	2:E:130:LEU:HD12	1.75	0.43
2:E:275:HIS:CE1	2:E:277:ARG:NE	2.84	0.43
2:E:281:PHE:CD2	2:E:288:LEU:HD23	2.53	0.43
2:E:505:ILE:HG13	2:E:510:ILE:HD13	2.00	0.43
2:E:611:THR:HG1	2:E:625:THR:HG1	1.60	0.43
1:A:177:CYS:CB	1:A:189:CYS:HB3	2.47	0.43
2:E:509:LYS:HD3	2:E:509:LYS:HA	1.89	0.43
2:E:724:LEU:HD12	2:E:724:LEU:HA	1.90	0.43
1:A:215:ASN:OD1	1:A:216:GLY:N	2.51	0.43
1:A:227:GLU:CD	1:A:268:ARG:HH21	2.21	0.43
1:A:230:LYS:HE3	1:A:278:THR:HG21	2.00	0.43
2:E:378:VAL:HG21	2:E:420:PHE:CE2	2.54	0.43
2:E:602:ARG:O	2:E:640:ILE:HD12	2.18	0.43
1:D:406:THR:C	1:D:465:PRO:HD3	2.39	0.43
2:E:75:GLU:N	2:E:75:GLU:OE1	2.47	0.43
2:E:126:TYR:OH	2:E:221:GLU:HG2	2.18	0.43
2:E:533:PRO:HB2	2:E:535:PHE:CD1	2.53	0.43
1:A:203:ILE:HD12	1:A:203:ILE:HA	1.92	0.43
1:A:226:THR:HA	1:A:283:CYS:HA	2.01	0.43
1:D:405:GLN:OE1	1:D:406:THR:N	2.52	0.43
2:E:36:ASN:OD1	2:E:36:ASN:N	2.52	0.43
1:A:211:CYS:HB3	1:A:288:CYS:HB3	1.95	0.43
1:A:215:ASN:ND2	1:A:218:SER:H	2.16	0.43
1:D:528:TRP:CH2	1:D:583:LYS:HB3	2.54	0.43
1:D:438:ASN:O	1:D:439:TYR:CD1	2.71	0.43
1:D:513:TYR:O	1:D:516:LYS:NZ	2.50	0.43
1:A:53:ILE:O	1:A:55:PRO:HD3	2.19	0.43
1:A:220:ARG:HE	1:A:261:ARG:HD2	1.83	0.43
1:D:406:THR:OG1	1:D:407:ARG:N	2.52	0.43
1:D:547:TRP:CD1	1:D:564:VAL:HA	2.51	0.43
2:E:384:ARG:HH22	2:E:387:GLN:HG2	1.83	0.43
1:A:212:MET:HE3	1:A:287:THR:HG22	2.01	0.42
1:D:512:ARG:NH2	1:D:547:TRP:CE3	2.87	0.42
1:D:570:LEU:HD23	1:D:570:LEU:HA	1.69	0.42
1:D:673:TYR:CE1	1:D:693:PRO:HG3	2.54	0.42
2:E:455:LEU:HA	2:E:455:LEU:HD23	1.68	0.42
2:E:462:PHE:HE2	2:E:513:ILE:HG21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:530:LEU:HB2	2:E:591:ARG:HH21	1.84	0.42
1:A:48:THR:O	1:A:116:PHE:HB2	2.19	0.42
1:A:241:HIS:NE2	1:A:276:PRO:O	2.51	0.42
1:D:564:VAL:O	1:D:565:LEU:HD12	2.19	0.42
2:E:200:THR:HG22	2:E:247:ILE:O	2.19	0.42
2:E:539:GLY:H	2:E:556:TRP:HE1	1.67	0.42
2:E:591:ARG:HG2	2:E:591:ARG:HH11	1.83	0.42
1:D:412:CYS:HB2	1:D:438:ASN:OD1	2.19	0.42
1:D:708:ARG:NH2	1:D:711:TYR:HB2	2.34	0.42
2:E:99:GLN:NE2	2:E:101:CYS:HB3	2.35	0.42
1:A:82:PHE:CD2	1:A:100:PRO:HB3	2.47	0.42
2:E:335:ALA:HA	2:E:368:LYS:HZ1	1.84	0.42
2:E:690:ILE:HD11	2:E:722:VAL:CG1	2.49	0.42
1:D:451:TRP:HA	1:D:463:TYR:HA	2.01	0.42
1:D:646:HIS:HE1	1:D:695:ARG:HB3	1.84	0.42
2:E:537:GLN:O	2:E:547:ARG:HD2	2.19	0.42
2:E:540:TRP:CD1	2:E:542:HIS:N	2.87	0.42
2:E:671:GLY:HA3	2:E:713:ALA:CA	2.48	0.42
1:A:43:LYS:C	1:A:43:LYS:HD3	2.39	0.42
1:D:649:LYS:NZ	2:E:124:THR:HB	2.34	0.42
1:A:142:ILE:HD11	1:A:146:GLY:HA2	2.02	0.42
1:D:646:HIS:CE1	1:D:695:ARG:HG3	2.55	0.42
1:D:699:ILE:HD12	1:D:699:ILE:H	1.84	0.42
2:E:192:PHE:CE2	2:E:218:ARG:CZ	3.03	0.42
2:E:250:VAL:HG11	2:E:317:LEU:HD22	2.02	0.42
2:E:279:ILE:HD13	2:E:293:GLU:HG2	2.01	0.42
2:E:690:ILE:HD11	2:E:722:VAL:HG12	2.02	0.42
1:D:528:TRP:CZ3	1:D:583:LYS:HB3	2.54	0.42
2:E:598:LEU:HD13	2:E:617:SER:O	2.19	0.42
2:E:726:ILE:C	2:E:728:LEU:N	2.73	0.42
1:D:406:THR:HA	1:D:464:CYS:HA	2.02	0.42
1:D:619:TYR:O	1:D:620:THR:OG1	2.35	0.42
2:E:113:LYS:HE2	2:E:113:LYS:HB2	1.95	0.42
2:E:206:PHE:CG	2:E:242:ARG:NH1	2.88	0.42
2:E:714:GLN:HB2	2:E:738:TYR:CE2	2.55	0.42
1:A:39:ILE:HD12	1:A:39:ILE:N	2.35	0.42
1:D:436:ASN:OD1	1:D:439:TYR:HB2	2.19	0.42
2:E:569:PHE:HA	2:E:570:PRO:HA	1.83	0.42
2:E:640:ILE:CG2	2:E:647:THR:HB	2.50	0.42
1:A:34:LYS:N	3:B:4:IDS:O2S	2.52	0.41
1:D:619:TYR:CZ	1:D:621:GLY:HA2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:238:LEU:HD12	2:E:241:PHE:H	1.85	0.41
2:E:595:LYS:NZ	2:E:596:PHE:O	2.29	0.41
1:A:238:GLN:HG3	1:A:242:ARG:HA	2.01	0.41
2:E:513:ILE:HD12	2:E:513:ILE:N	2.35	0.41
2:E:523:PHE:CD1	2:E:528:GLN:HB3	2.55	0.41
1:A:53:ILE:HG12	1:A:109:LYS:HZ3	1.85	0.41
1:A:257:ASP:HB3	1:A:258:ASN:H	1.74	0.41
1:A:102:ASN:OD1	1:A:103:SER:N	2.53	0.41
2:E:72:VAL:C	2:E:73:LEU:HD23	2.41	0.41
2:E:200:THR:HG22	2:E:248:LYS:HA	2.03	0.41
2:E:367:ILE:HA	2:E:370:VAL:HG12	2.02	0.41
2:E:460:GLY:O	2:E:481:LEU:N	2.45	0.41
2:E:84:TYR:HD1	2:E:155:GLN:HG3	1.85	0.41
2:E:329:LEU:O	2:E:333:ILE:HG12	2.20	0.41
1:A:123:ASP:OD1	1:A:124:TYR:N	2.53	0.41
1:A:160:HIS:ND1	1:A:162:PHE:HE1	2.18	0.41
2:E:39:MET:HG2	2:E:40:LYS:N	2.35	0.41
2:E:48:ALA:HB3	2:E:52:ILE:HD11	2.00	0.41
2:E:592:ARG:O	2:E:594:ASN:N	2.54	0.41
1:D:442:ASN:HA	1:D:443:PRO:HD3	1.92	0.41
2:E:533:PRO:HA	2:E:534:PRO:HD3	1.90	0.41
2:E:706:ILE:O	2:E:707:LEU:HD23	2.21	0.41
1:A:142:ILE:HD12	1:A:142:ILE:HA	1.91	0.41
1:D:522:SER:OG	1:D:676:PRO:HB3	2.21	0.41
1:D:524:ILE:C	1:D:525:LYS:HD2	2.40	0.41
2:E:163:SER:OG	2:E:174:ASP:OD2	2.30	0.41
1:A:60:LYS:HD3	1:A:98:TRP:CZ3	2.55	0.41
1:D:405:GLN:O	1:D:464:CYS:HB2	2.21	0.41
1:D:442:ASN:HD22	1:D:450:PRO:HA	1.86	0.41
1:D:509:VAL:HG22	1:D:548:LEU:HD11	2.03	0.41
1:D:617:TRP:HZ3	1:D:627:GLY:O	2.04	0.41
2:E:190:ASP:O	2:E:192:PHE:HD1	2.04	0.41
2:E:599:LYS:HZ2	2:E:600:LYS:HE2	1.86	0.41
2:E:688:ARG:HA	2:E:726:ILE:HA	2.03	0.41
1:A:94:LYS:N	1:A:94:LYS:HD2	2.36	0.41
1:A:195:GLU:OE1	1:A:195:GLU:N	2.42	0.40
1:D:606:ILE:HD11	1:D:610:THR:HG21	2.03	0.40
2:E:296:LEU:HD23	2:E:424:LEU:HB3	2.02	0.40
2:E:559:GLN:HG2	2:E:560:ILE:H	1.86	0.40
1:A:84:CYS:HA	1:A:100:PRO:HA	2.02	0.40
1:A:215:ASN:HD21	1:A:218:SER:N	2.16	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:442:ASN:HB3	1:D:450:PRO:HA	2.03	0.40
1:D:713:ALA:HA	1:D:716:ILE:CD1	2.45	0.40
2:E:245:TYR:CE2	2:E:388:HIS:HB3	2.56	0.40
2:E:661:SER:O	2:E:677:LEU:HD13	2.21	0.40
1:D:598:ASP:C	1:D:599:LEU:HD22	2.41	0.40
2:E:229:LEU:HA	2:E:229:LEU:HD23	1.66	0.40
2:E:266:ARG:HA	2:E:274:PHE:HD1	1.86	0.40
2:E:285:ASN:OD1	2:E:286:SER:N	2.54	0.40
2:E:532:ALA:HA	2:E:533:PRO:HD3	1.96	0.40
1:A:219:TYR:CE1	1:A:221:GLY:HA3	2.56	0.40
1:D:511:LEU:HD23	1:D:512:ARG:N	2.36	0.40
2:E:318:GLN:OE1	2:E:318:GLN:HA	2.21	0.40
2:E:461:ARG:NH2	2:E:478:ASN:O	2.54	0.40
2:E:598:LEU:HD23	2:E:598:LEU:HA	1.86	0.40
2:E:604:LEU:O	2:E:638:ILE:HD12	2.22	0.40
2:E:699:LEU:HD11	2:E:702:VAL:HB	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	250/728 (34%)	224 (90%)	26 (10%)	0	100	100
1	D	299/728 (41%)	275 (92%)	24 (8%)	0	100	100
2	E	678/1390 (49%)	615 (91%)	63 (9%)	0	100	100
All	All	1227/2846 (43%)	1114 (91%)	113 (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	224/646 (35%)	222 (99%)	2 (1%)	75	83
1	D	235/646 (36%)	235 (100%)	0	100	100
2	E	598/1246 (48%)	595 (100%)	3 (0%)	86	89
All	All	1057/2538 (42%)	1052 (100%)	5 (0%)	85	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	258	ASN
2	E	32	LYS
2	E	38	ASN
2	E	594	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	497	ASN
1	D	644	GLN
1	D	646	HIS
2	E	275	HIS
2	E	396	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

6 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SGN	B	1	3	15,18,20	1.33	1 (6%)	20,26,31	1.53	3 (15%)
3	IDS	B	2	3	16,16,17	1.12	0	16,24,26	1.00	1 (6%)
3	SGN	B	3	3	19,19,20	3.78	4 (21%)	23,29,31	1.54	3 (13%)
3	IDS	B	4	3	16,16,17	1.28	2 (12%)	16,24,26	1.11	1 (6%)
3	SGN	B	5	3	13,13,20	4.17	4 (30%)	12,19,31	2.23	3 (25%)
3	IDS	B	6	3	15,15,17	1.08	0	14,22,26	2.50	6 (42%)

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	SGN	B	1	3	-	3/8/27/31	0/1/1/1
3	IDS	B	2	3	-	1/9/26/29	0/1/1/1
3	SGN	B	3	3	-	3/11/28/31	0/1/1/1
3	IDS	B	4	3	-	0/9/26/29	1/1/1/1
3	SGN	B	5	3	-	5/5/19/31	0/1/1/1
3	IDS	B	6	3	-	6/9/22/29	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5	SGN	O2S-S1	9.95	1.53	1.42
3	B	5	SGN	O1S-S1	9.72	1.53	1.42
3	B	3	SGN	O2S-S1	9.72	1.53	1.42
3	B	3	SGN	O1S-S1	9.35	1.52	1.42
3	B	3	SGN	S1-N2	8.33	1.70	1.59
3	B	5	SGN	S1-N2	3.84	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5	SGN	O4-C4	2.81	1.49	1.43
3	B	1	SGN	C1-C2	-2.54	1.48	1.52
3	B	4	IDS	O2-C2	-2.45	1.43	1.47
3	B	4	IDS	O4-C4	2.21	1.48	1.43
3	B	3	SGN	C4-C5	2.12	1.57	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	6	IDS	C1-O5-C5	-5.91	104.22	113.81
3	B	5	SGN	O1S-S1-O2S	-5.13	108.94	120.36
3	B	6	IDS	C1-C2-C3	-5.08	102.68	109.84
3	B	3	SGN	O1S-S1-O2S	-4.89	109.48	120.36
3	B	5	SGN	C3-C2-N2	3.80	115.31	110.32
3	B	1	SGN	O5-C1-C2	-3.47	105.93	111.29
3	B	1	SGN	C3-C4-C5	3.17	115.97	110.23
3	B	5	SGN	C5-O5-C1	2.76	115.87	111.42
3	B	6	IDS	O6A-C6-C5	-2.71	117.00	122.85
3	B	3	SGN	O5-C5-C6	2.70	113.43	107.59
3	B	2	IDS	O2-C2-C3	2.69	110.70	106.95
3	B	6	IDS	O5-C1-C2	-2.48	104.49	109.51
3	B	4	IDS	O3S-S-O2	2.35	111.77	106.37
3	B	1	SGN	C2-N2-S1	-2.35	110.92	116.99
3	B	3	SGN	O6-C6-C5	2.16	111.41	107.57
3	B	6	IDS	O3S-S-O2	2.15	111.32	106.37
3	B	6	IDS	C4-C3-C2	-2.05	108.15	110.76

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1	SGN	C4-C5-C6-O6
3	B	1	SGN	O5-C5-C6-O6
3	B	2	IDS	C3-C2-O2-S
3	B	3	SGN	C2-N2-S1-O1S
3	B	3	SGN	C2-N2-S1-O3S
3	B	5	SGN	C2-N2-S1-O1S
3	B	5	SGN	C2-N2-S1-O2S
3	B	5	SGN	C2-N2-S1-O3S
3	B	6	IDS	C1-C2-O2-S
3	B	6	IDS	C3-C2-O2-S
3	B	6	IDS	C2-O2-S-O2S

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Mol	Chain	Res	Type	Atoms
3	B	6	IDS	C2-O2-S-O1S
3	B	6	IDS	C2-O2-S-O3S
3	B	5	SGN	C1-C2-N2-S1
3	B	5	SGN	C3-C2-N2-S1
3	B	3	SGN	C2-N2-S1-O2S
3	B	6	IDS	O5-C5-C6-O6A
3	B	1	SGN	C5-C6-O6-S2

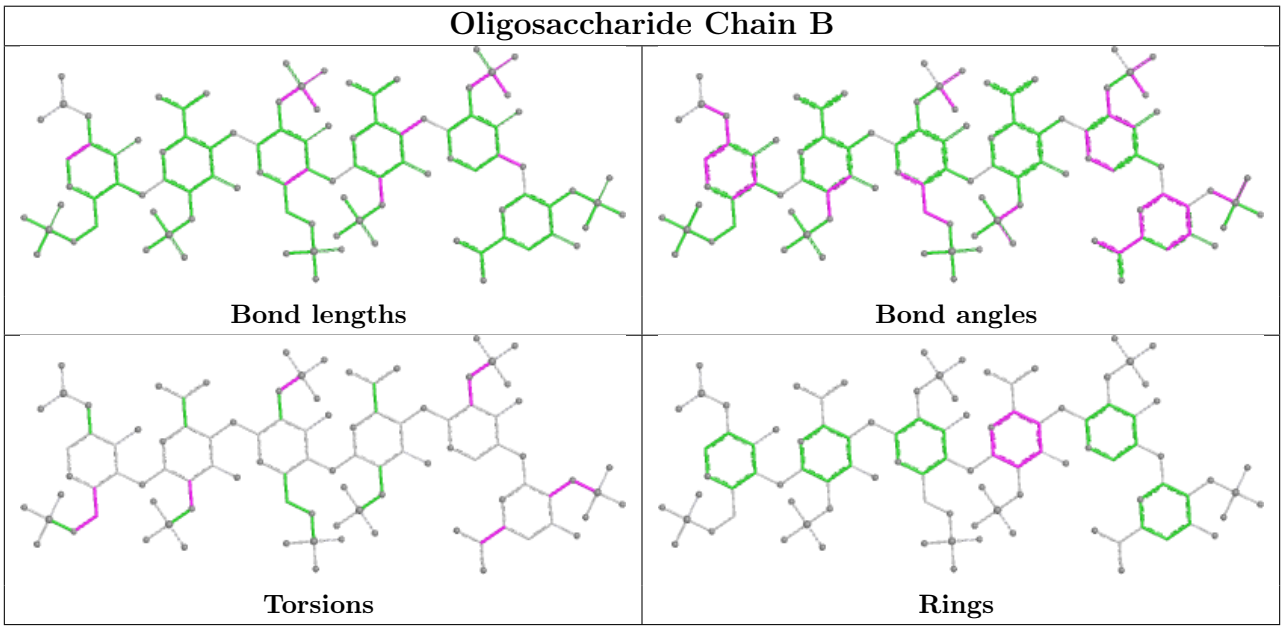
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	4	IDS	C1-C2-C3-C4-C5-O5

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	4	IDS	2	0
3	B	2	IDS	1	0

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



5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

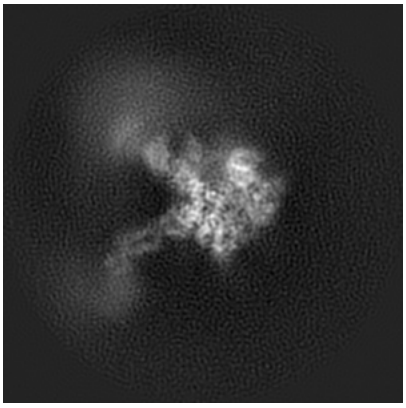
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-23921. These allow visual inspection of the internal detail of the map and identification of artifacts.

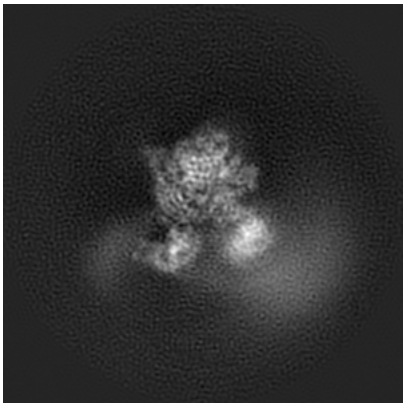
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

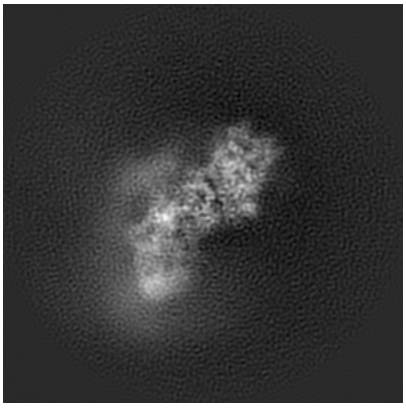
6.1.1 Primary map



X



Y

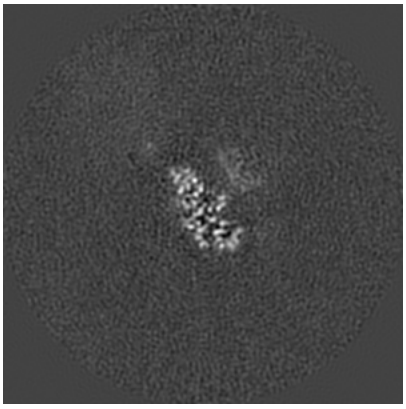


Z

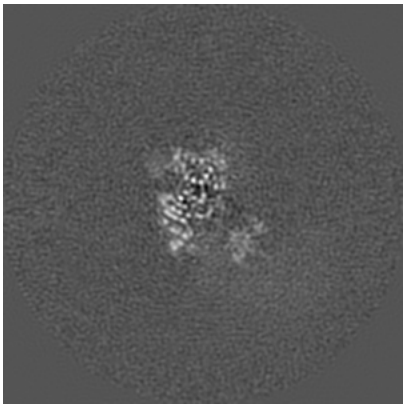
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

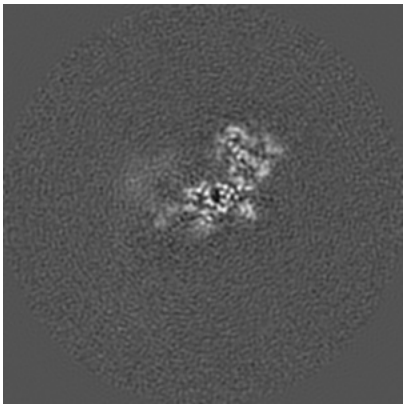
6.2.1 Primary map



X Index: 135



Y Index: 135

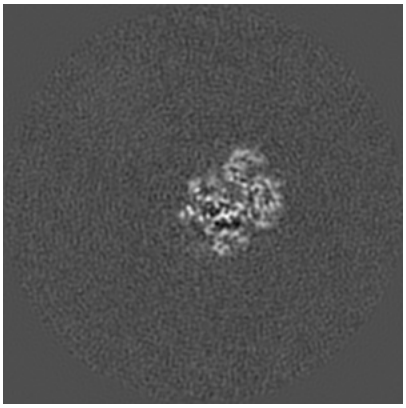


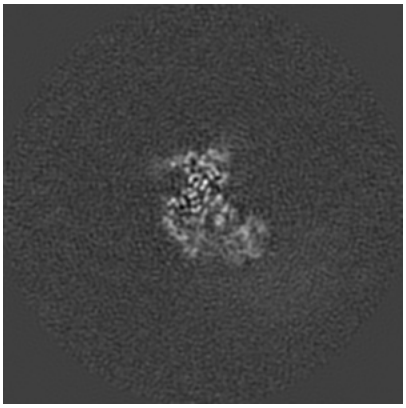
Z Index: 135

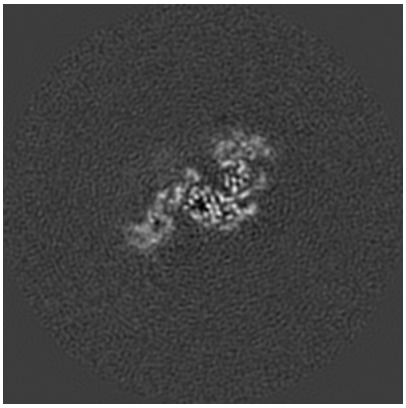
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 155

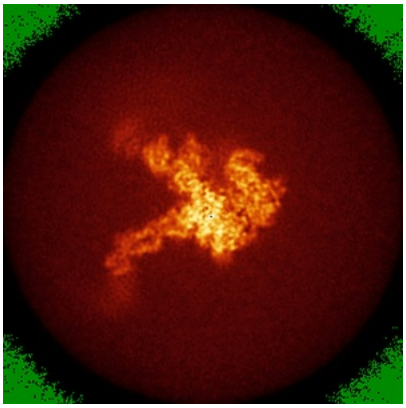

Y Index: 131

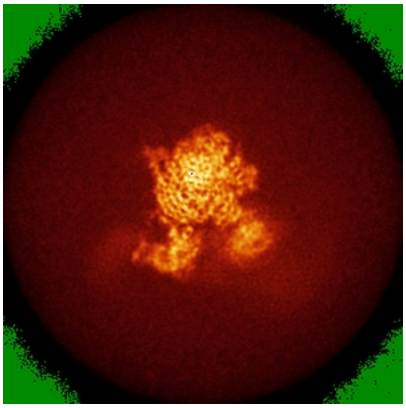

Z Index: 125

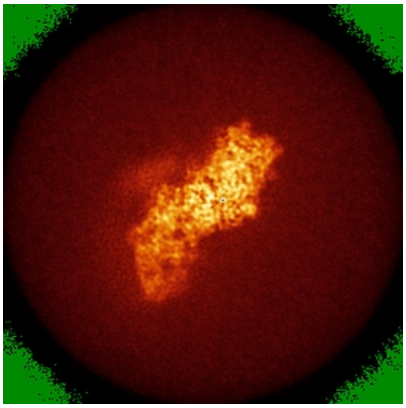
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X


Y


Z

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

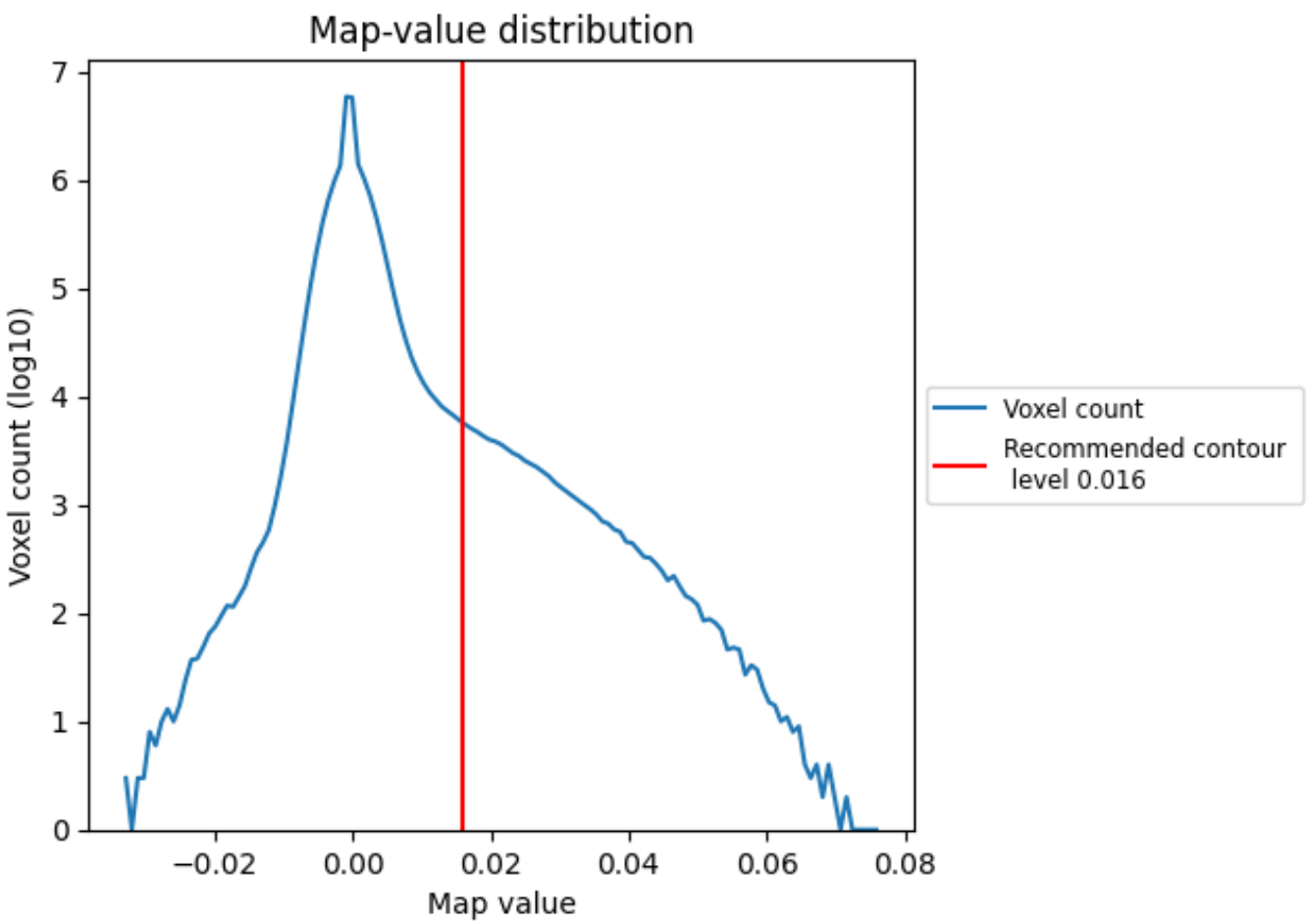
6.6 Mask visualisation (i)

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

7 Map analysis (i)

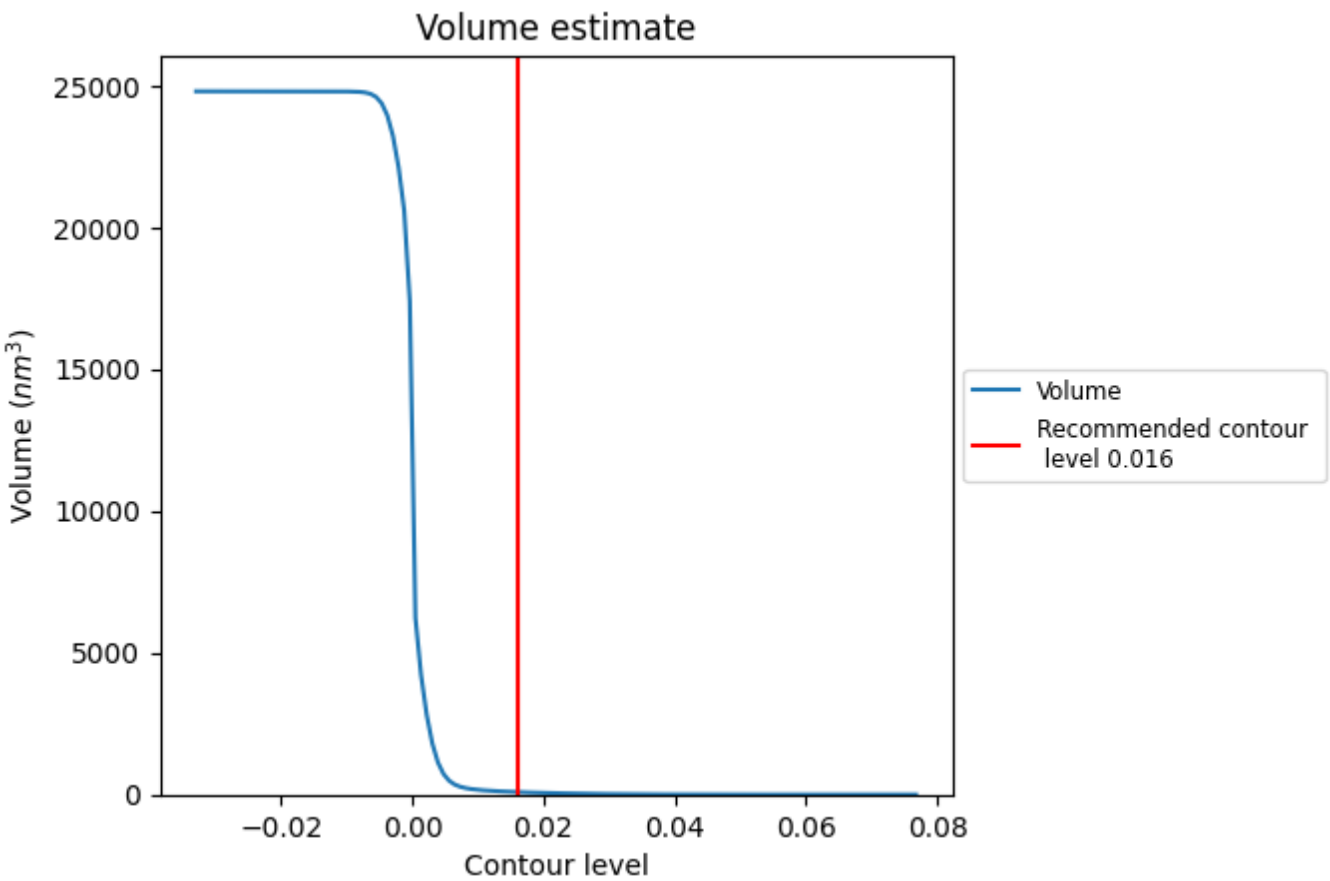
This section contains the results of statistical analysis of the map.

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.

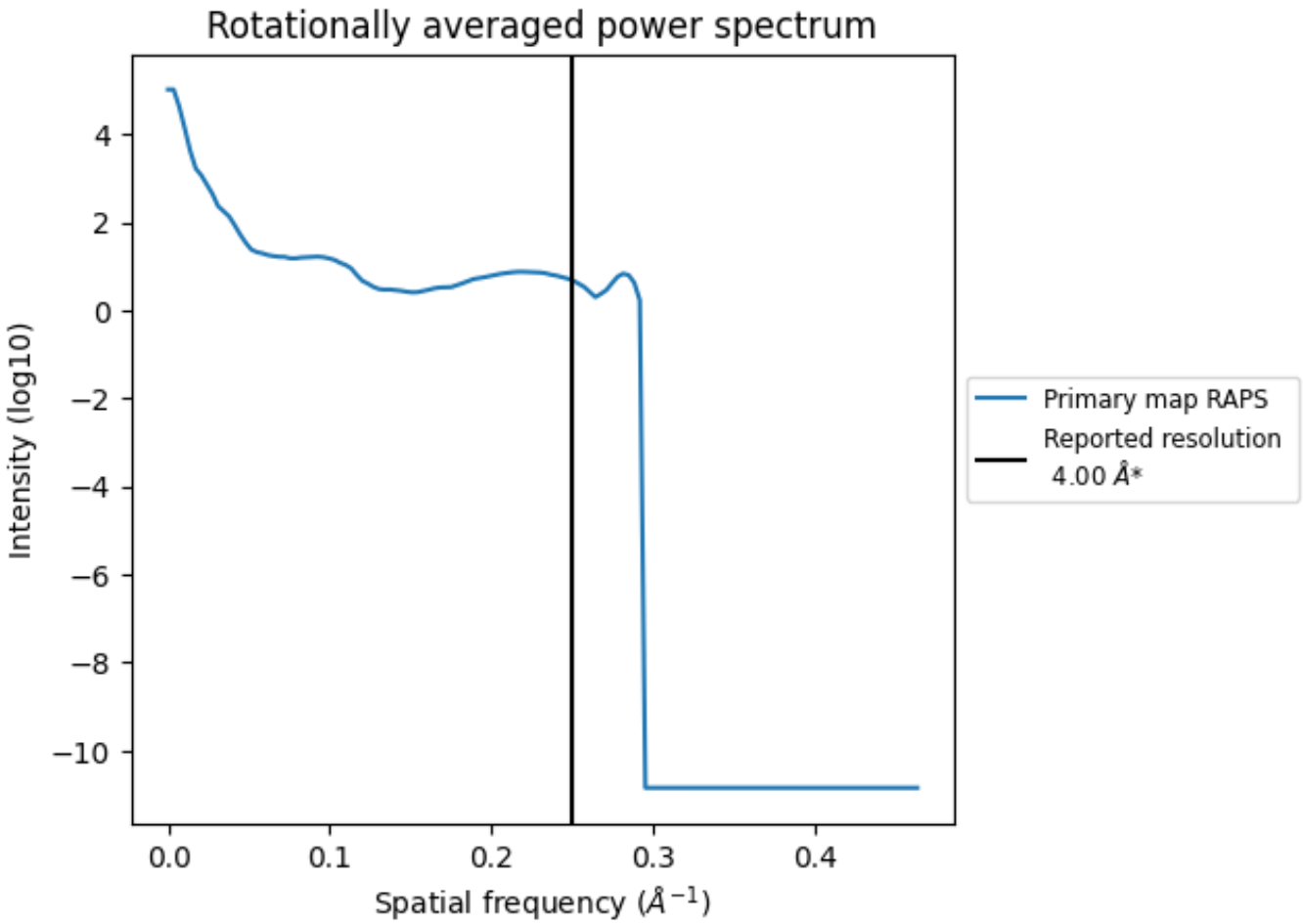
7.2 Volume estimate (i)



The volume at the recommended contour level is 87 nm^3; this corresponds to an approximate mass of 79 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 0.250 Å^{-1}

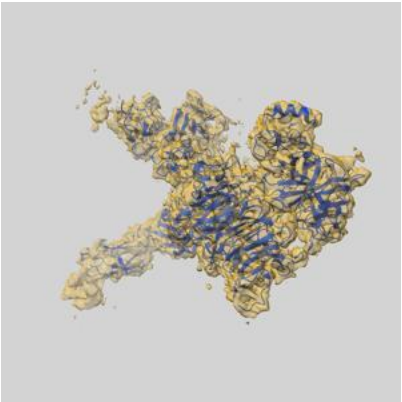
8 Fourier-Shell correlation (i)

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

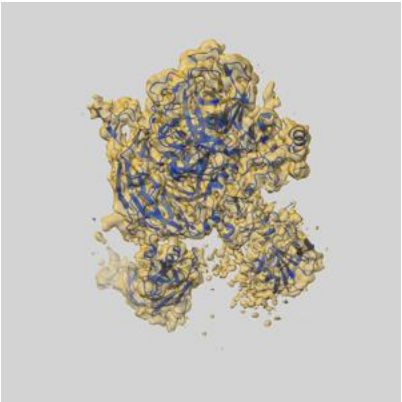
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-23921 and PDB model 7MO9. Per-residue inclusion information can be found in section 3 on page 4.

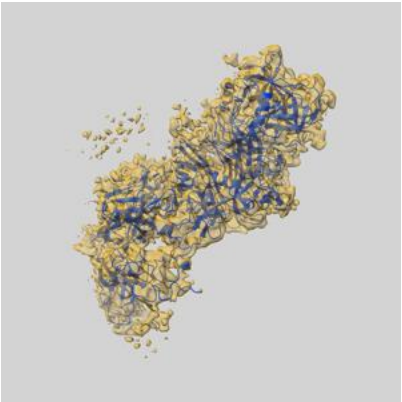
9.1 Map-model overlay (i)



X



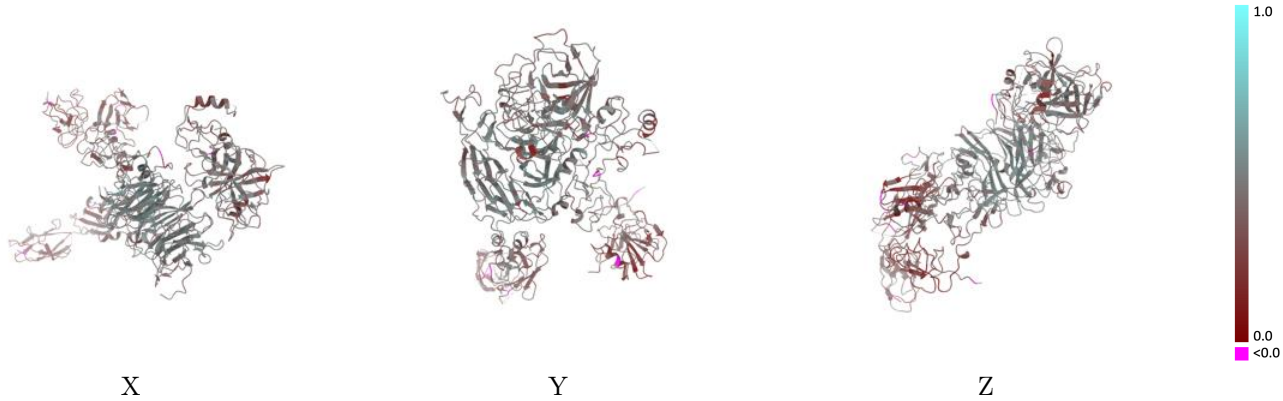
Y



Z

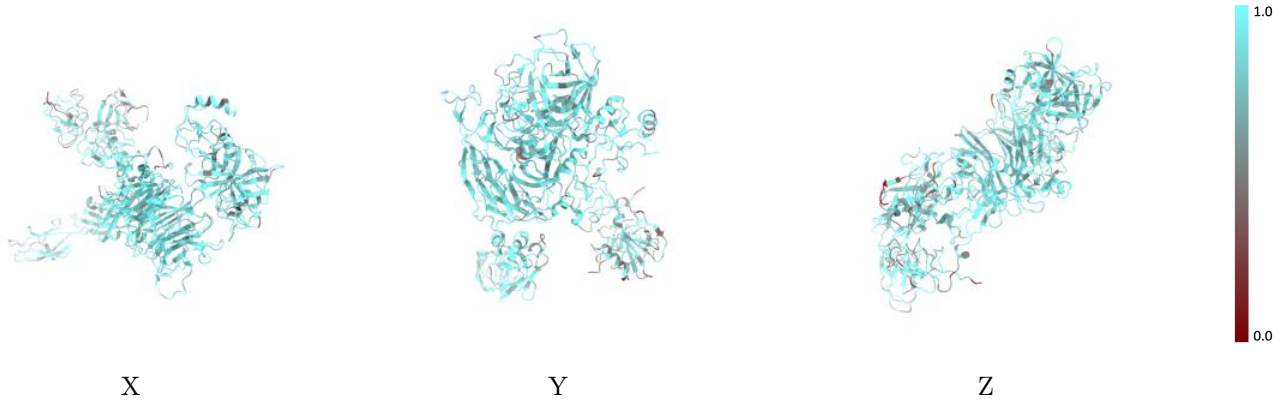
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



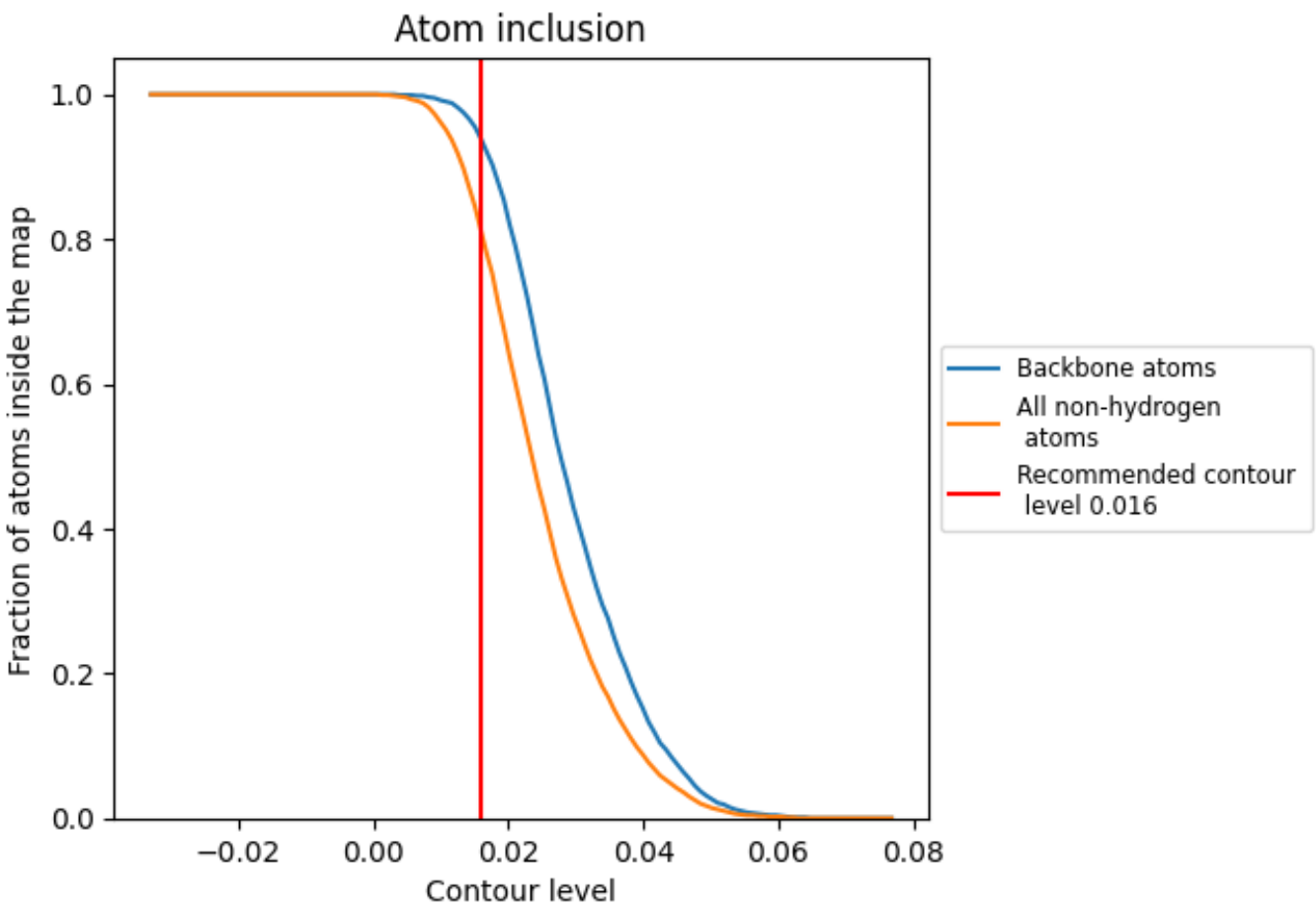
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.016).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 81% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8100	0.4100
A	0.7350	0.3300
B	0.3400	0.3710
D	0.8210	0.4140
E	0.8430	0.4400