Full wwPDB EM Validation Report ⓘ

May 9, 2022 – 10:32 pm BST

PDB ID	:	7ZGU
EMDB ID	:	EMD-14713
Title	:	Human NLRP3-deltaPYD hexamer
Authors	:	Raisch, T.; Machtens, D.A.; Bresch, I.B.; Eberhage, J.; Prumbaum, D.; Reubold, T.F.; Raunser, S.; Eschenburg, S.
Deposited on	:	2022-04-04
Resolution	:	3.40 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 following versions of software and data (see references ⓘ) were used in the production of this report:

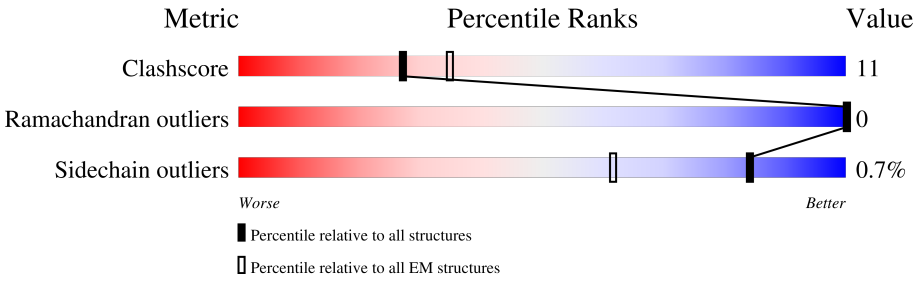
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 3.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	924	28% 65% 23% 12%
1	B	924	29% 65% 22% 12%
1	C	924	27% 65% 22% 12%
1	D	924	32% 65% 22% 12%
1	E	924	32% 65% 23% 12%
1	F	924	32% 65% 22% 12%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 38940 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 NACHT, LRR and PYD domains-containing protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	809	Total	C	N	O	S	0	0
			6463	4125	1098	1185	55		
1	B	809	Total	C	N	O	S	0	0
			6463	4125	1098	1185	55		
1	C	809	Total	C	N	O	S	0	0
			6463	4125	1098	1185	55		
1	D	809	Total	C	N	O	S	0	0
			6463	4125	1098	1185	55		
1	E	809	Total	C	N	O	S	0	0
			6463	4125	1098	1185	55		
1	F	809	Total	C	N	O	S	0	0
			6463	4125	1098	1185	55		

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	125	MET	-	initiating methionine	UNP Q96P20
A	1037	GLY	-	expression tag	UNP Q96P20
A	1038	SER	-	expression tag	UNP Q96P20
A	1039	GLY	-	expression tag	UNP Q96P20
A	1040	GLY	-	expression tag	UNP Q96P20
A	1041	ASP	-	expression tag	UNP Q96P20
A	1042	TYR	-	expression tag	UNP Q96P20
A	1043	LYS	-	expression tag	UNP Q96P20
A	1044	ASP	-	expression tag	UNP Q96P20
A	1045	ASP	-	expression tag	UNP Q96P20
A	1046	ASP	-	expression tag	UNP Q96P20
A	1047	ASP	-	expression tag	UNP Q96P20
A	1048	LYS	-	expression tag	UNP Q96P20
B	125	MET	-	initiating methionine	UNP Q96P20
B	1037	GLY	-	expression tag	UNP Q96P20
B	1038	SER	-	expression tag	UNP Q96P20
B	1039	GLY	-	expression tag	UNP Q96P20
B	1040	GLY	-	expression tag	UNP Q96P20

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1041	ASP	-	expression tag	UNP Q96P20
B	1042	TYR	-	expression tag	UNP Q96P20
B	1043	LYS	-	expression tag	UNP Q96P20
B	1044	ASP	-	expression tag	UNP Q96P20
B	1045	ASP	-	expression tag	UNP Q96P20
B	1046	ASP	-	expression tag	UNP Q96P20
B	1047	ASP	-	expression tag	UNP Q96P20
B	1048	LYS	-	expression tag	UNP Q96P20
C	125	MET	-	initiating methionine	UNP Q96P20
C	1037	GLY	-	expression tag	UNP Q96P20
C	1038	SER	-	expression tag	UNP Q96P20
C	1039	GLY	-	expression tag	UNP Q96P20
C	1040	GLY	-	expression tag	UNP Q96P20
C	1041	ASP	-	expression tag	UNP Q96P20
C	1042	TYR	-	expression tag	UNP Q96P20
C	1043	LYS	-	expression tag	UNP Q96P20
C	1044	ASP	-	expression tag	UNP Q96P20
C	1045	ASP	-	expression tag	UNP Q96P20
C	1046	ASP	-	expression tag	UNP Q96P20
C	1047	ASP	-	expression tag	UNP Q96P20
C	1048	LYS	-	expression tag	UNP Q96P20
D	125	MET	-	initiating methionine	UNP Q96P20
D	1037	GLY	-	expression tag	UNP Q96P20
D	1038	SER	-	expression tag	UNP Q96P20
D	1039	GLY	-	expression tag	UNP Q96P20
D	1040	GLY	-	expression tag	UNP Q96P20
D	1041	ASP	-	expression tag	UNP Q96P20
D	1042	TYR	-	expression tag	UNP Q96P20
D	1043	LYS	-	expression tag	UNP Q96P20
D	1044	ASP	-	expression tag	UNP Q96P20
D	1045	ASP	-	expression tag	UNP Q96P20
D	1046	ASP	-	expression tag	UNP Q96P20
D	1047	ASP	-	expression tag	UNP Q96P20
D	1048	LYS	-	expression tag	UNP Q96P20
E	125	MET	-	initiating methionine	UNP Q96P20
E	1037	GLY	-	expression tag	UNP Q96P20
E	1038	SER	-	expression tag	UNP Q96P20
E	1039	GLY	-	expression tag	UNP Q96P20
E	1040	GLY	-	expression tag	UNP Q96P20
E	1041	ASP	-	expression tag	UNP Q96P20
E	1042	TYR	-	expression tag	UNP Q96P20
E	1043	LYS	-	expression tag	UNP Q96P20

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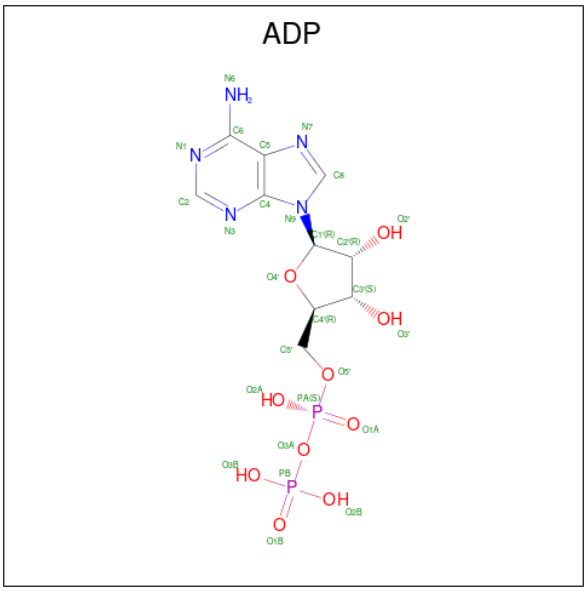
Chain	Residue	Modelled	Actual	Comment	Reference
E	1044	ASP	-	expression tag	UNP Q96P20
E	1045	ASP	-	expression tag	UNP Q96P20
E	1046	ASP	-	expression tag	UNP Q96P20
E	1047	ASP	-	expression tag	UNP Q96P20
E	1048	LYS	-	expression tag	UNP Q96P20
F	125	MET	-	initiating methionine	UNP Q96P20
F	1037	GLY	-	expression tag	UNP Q96P20
F	1038	SER	-	expression tag	UNP Q96P20
F	1039	GLY	-	expression tag	UNP Q96P20
F	1040	GLY	-	expression tag	UNP Q96P20
F	1041	ASP	-	expression tag	UNP Q96P20
F	1042	TYR	-	expression tag	UNP Q96P20
F	1043	LYS	-	expression tag	UNP Q96P20
F	1044	ASP	-	expression tag	UNP Q96P20
F	1045	ASP	-	expression tag	UNP Q96P20
F	1046	ASP	-	expression tag	UNP Q96P20
F	1047	ASP	-	expression tag	UNP Q96P20
F	1048	LYS	-	expression tag	UNP Q96P20

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

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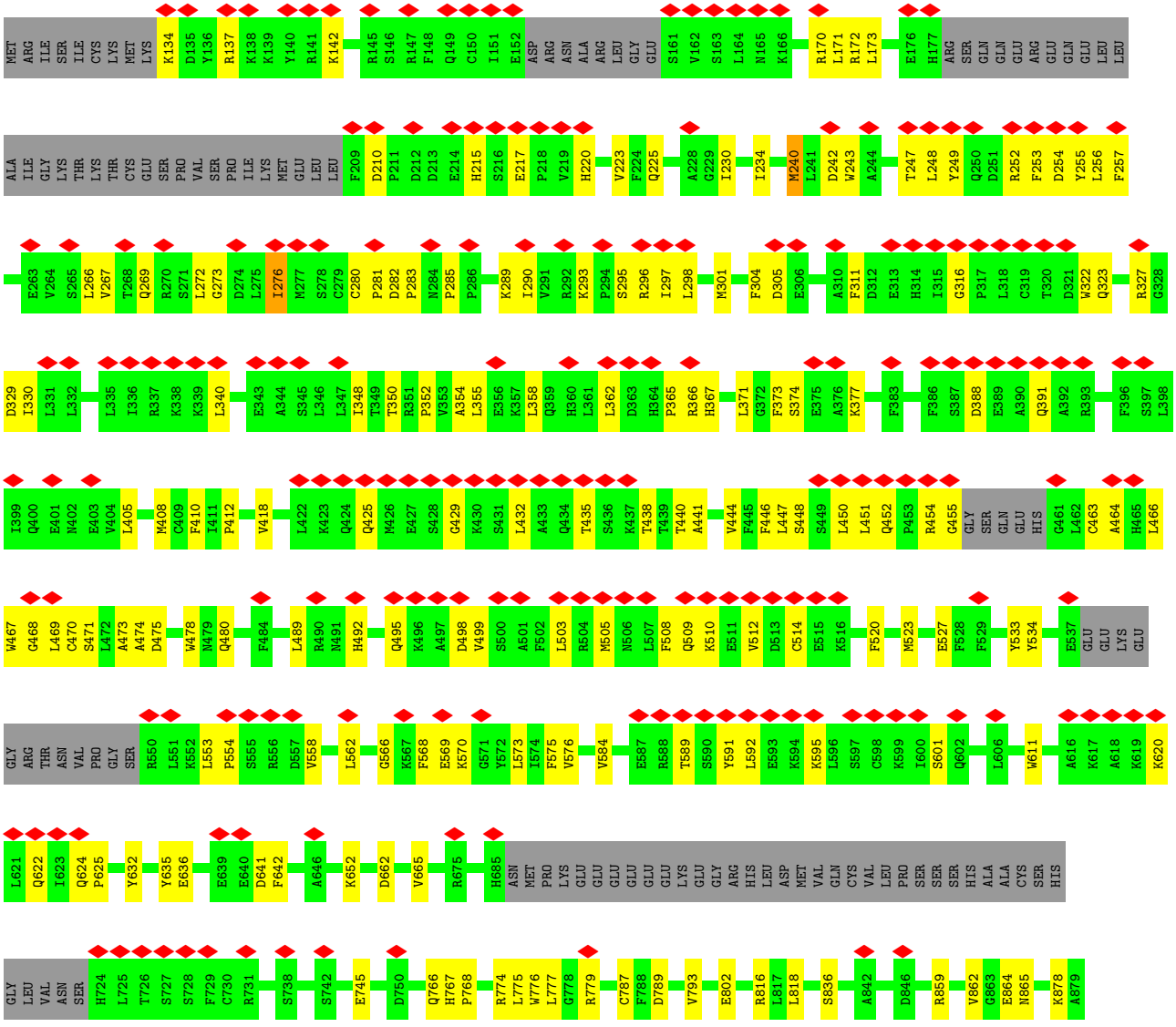
Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

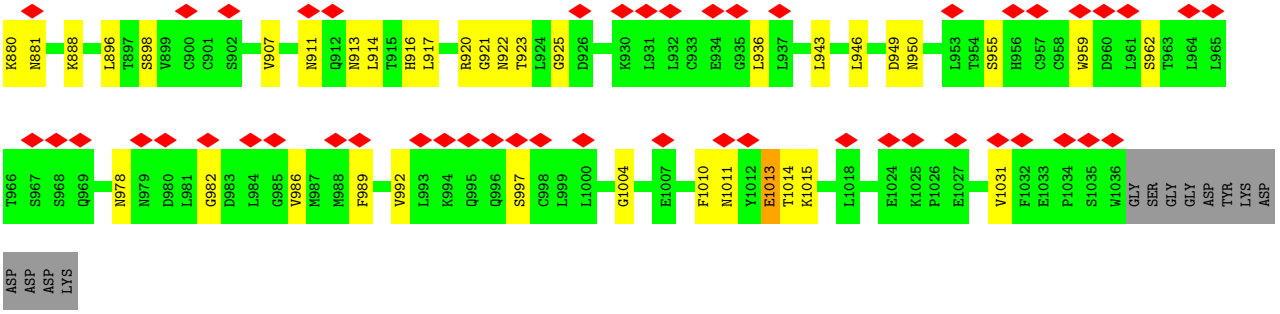
3 Residue-property plots (i)

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: NACHT, LRR and PYD domains-containing protein 3

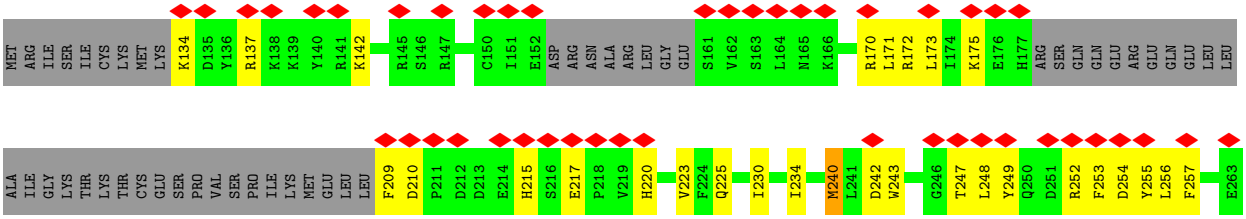
Chain A:

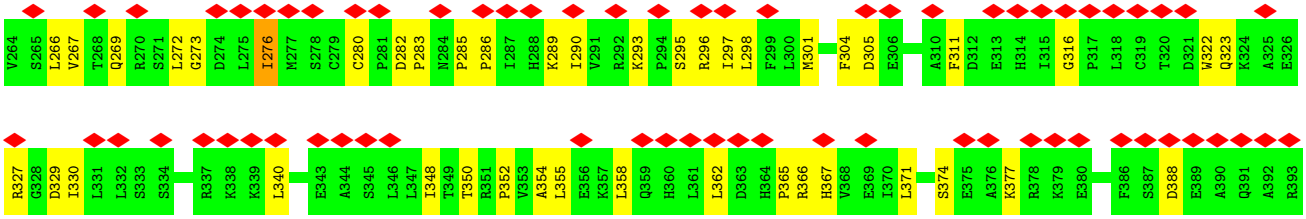


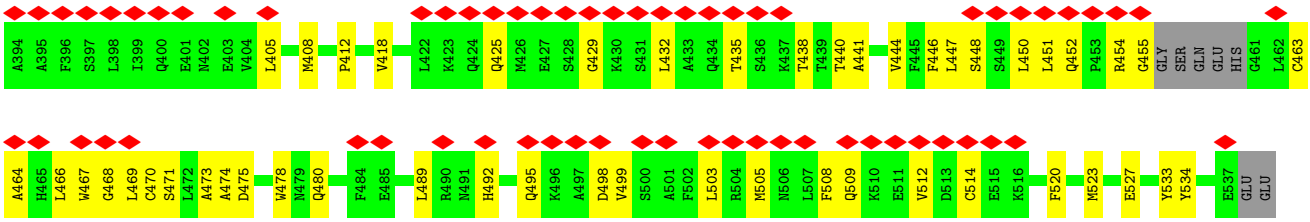


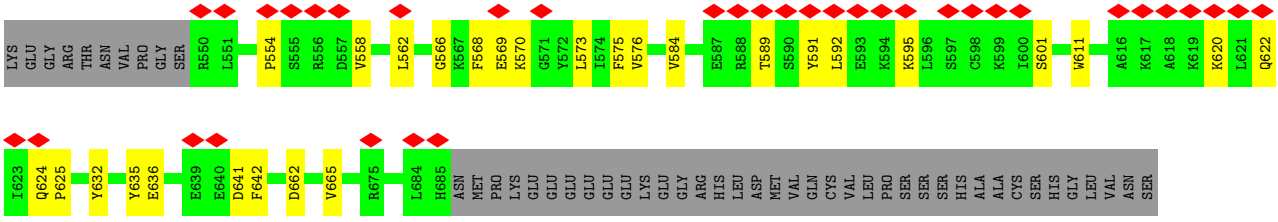
• Molecule 1: NACHT, LRR and PYD domains-containing protein 3

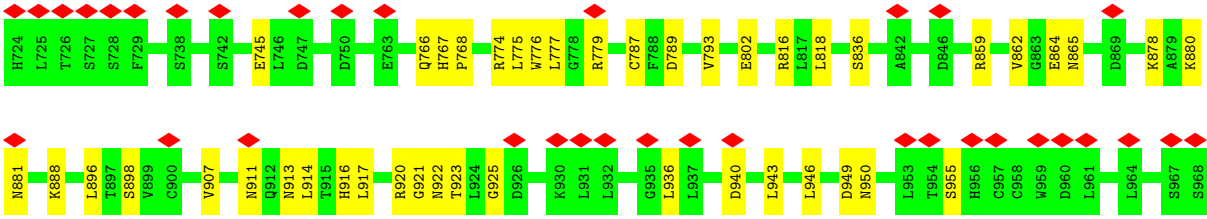
Chain B:

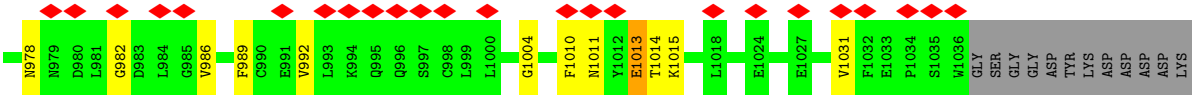






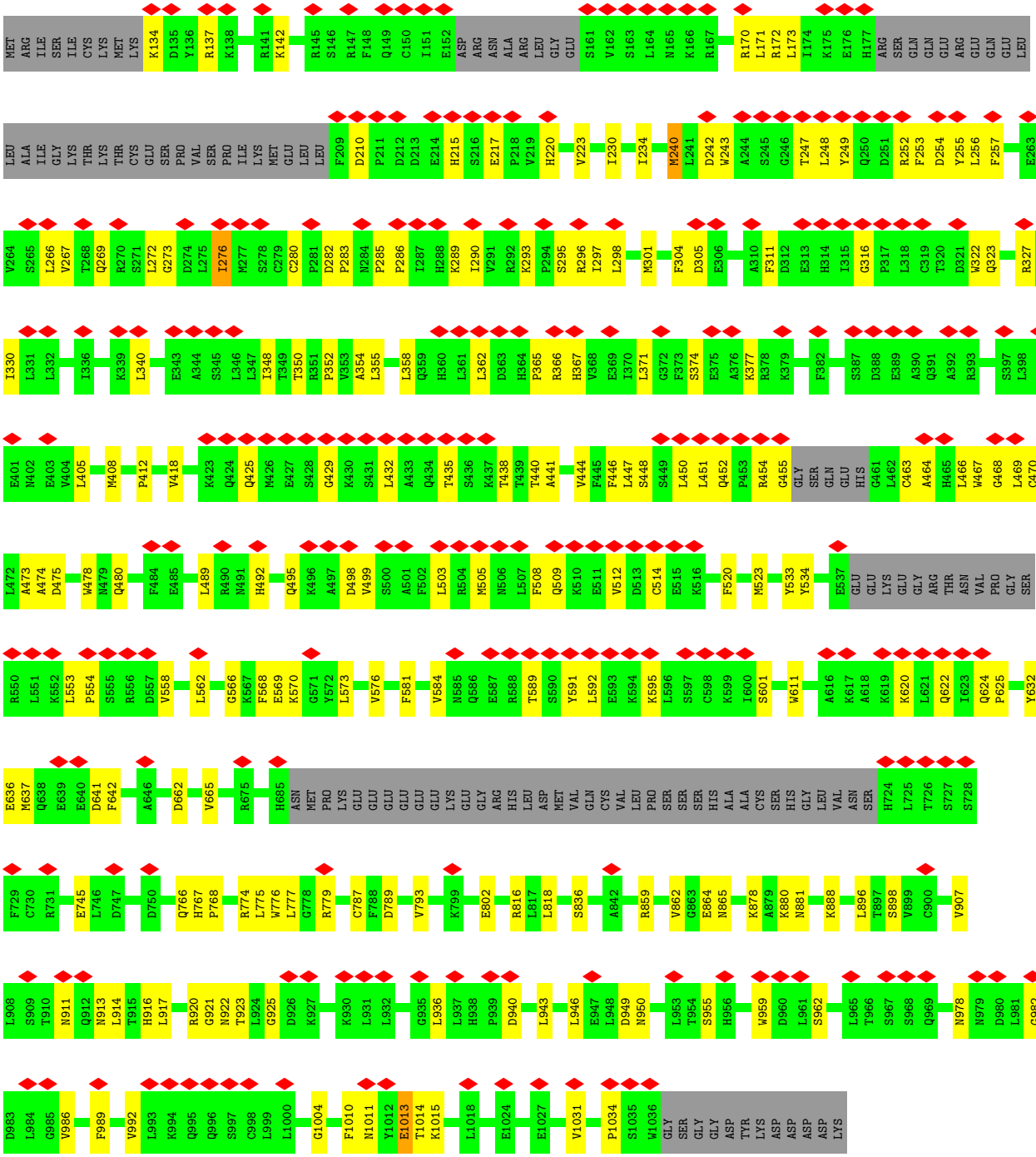






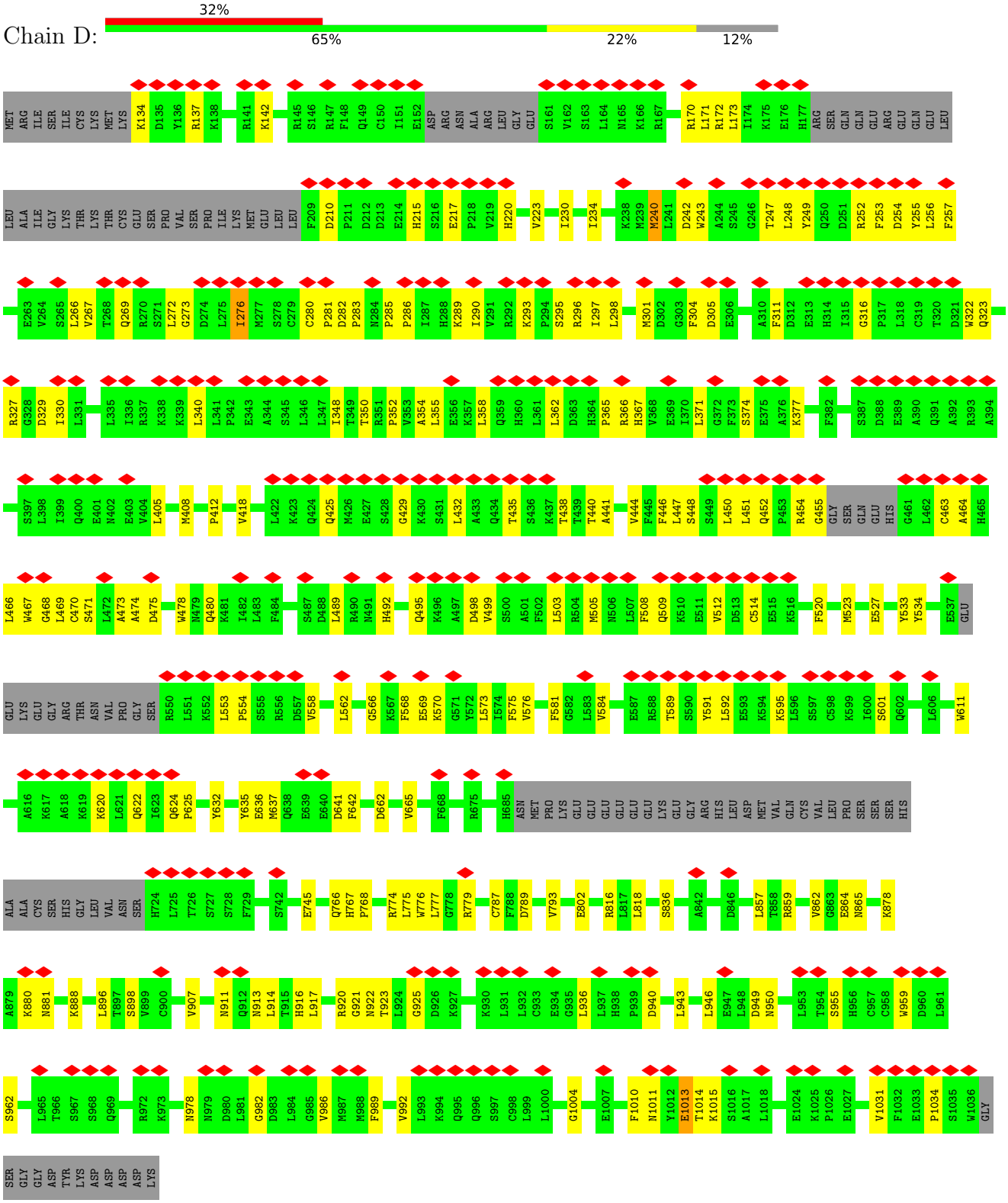
• Molecule 1: NACHT, LRR and PYD domains-containing protein 3

Chain C:



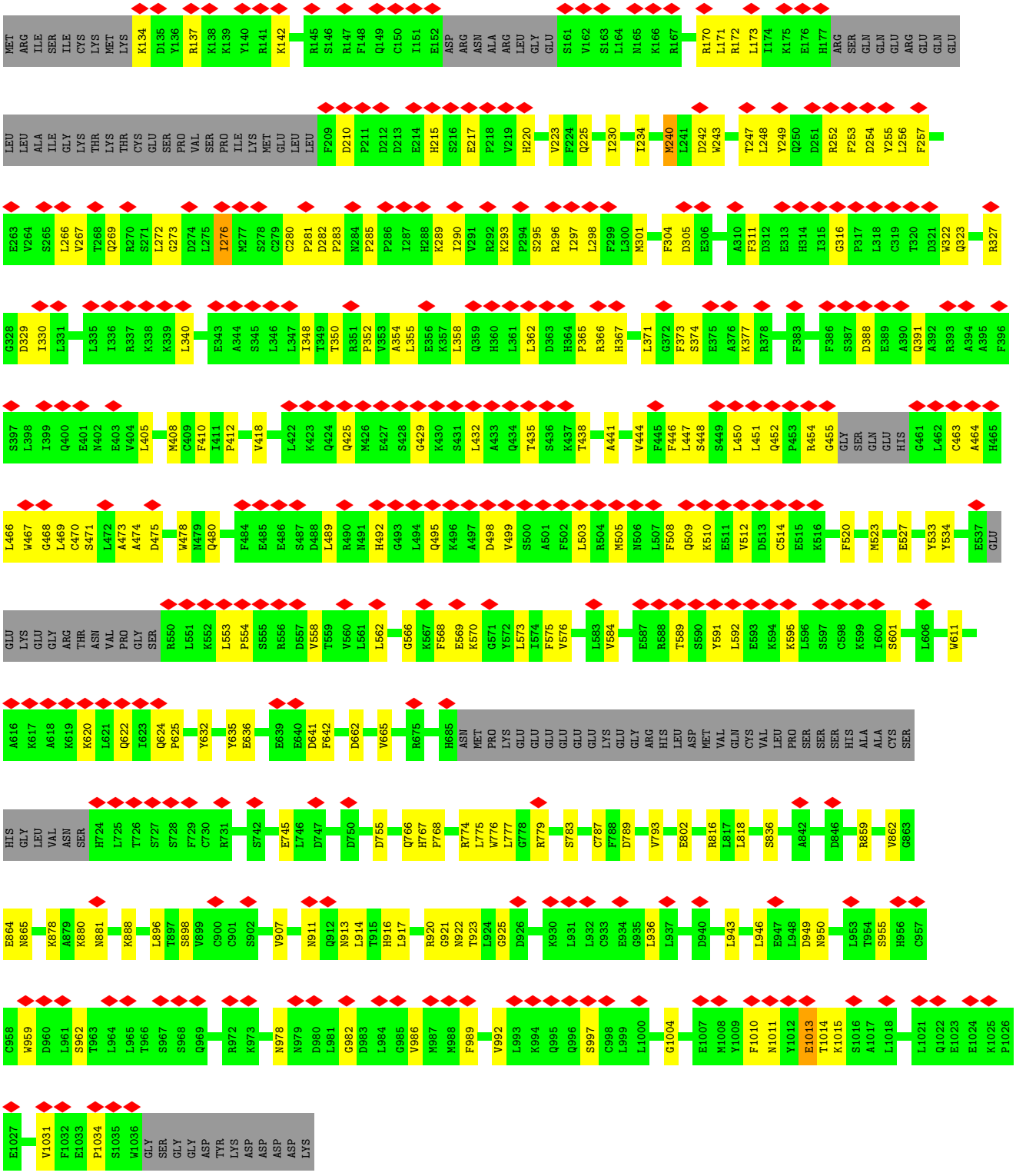
• Molecule 1: NACHT, LRR and PYD domains-containing protein 3

Chain D:



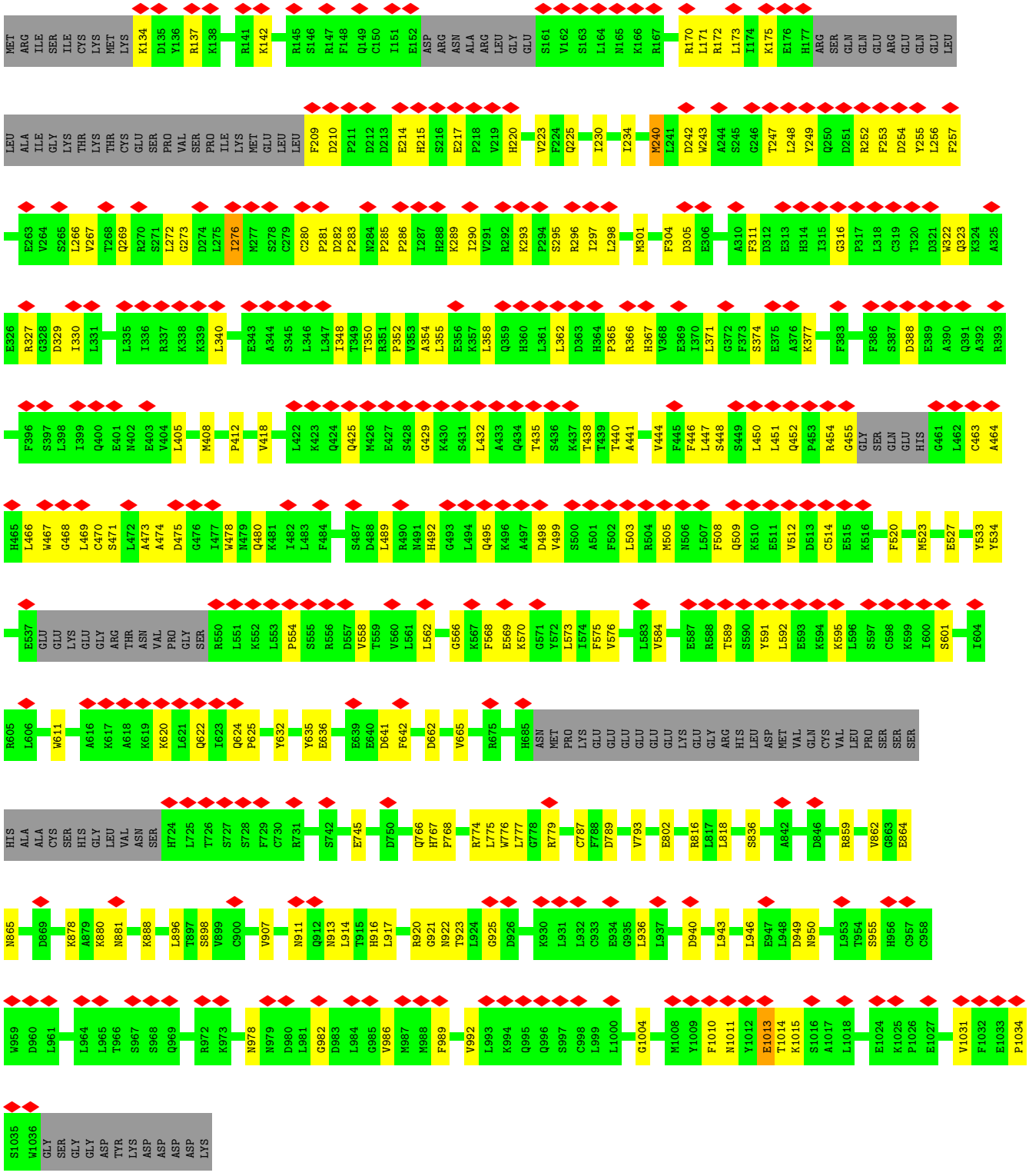
• Molecule 1: NACHT, LRR and PYD domains-containing protein 3

Chain E:



• Molecule 1: NACHT, LRR and PYD domains-containing protein 3

Chain F:


MET ARG ILE SER ILE CYS LYS MET LYS K134 D135 Y136 R137 K138 R141 K142 R145 S146 R147 F148 Q149 C150 I151 E152 ASP ARG ASN ALA ARG LEU GLY GLU S161 V162 S163 L164 N165 K166 R167 R170 L171 R172 L173 I174 K175 E176 H177 ARG SER GLN GLN GLU ARG GLU GLN GLU LEU
LEU ALA ILE GLY LYS THR LYS THR CYS GLU SER PRO VAL SER PRO ILE LYS MET GLU LEU LEU F209 D210 F211 D212 D213 E214 H215 S216 E217 P218 V219 H220 V223 F224 Q225 I230 I234 M240 L241 D242 W243 A244 S245 G246 T247 L248 Y249 Q250 D251 R252 F253 D254 Y255 L256 F257
E263 V264 S265 L266 V267 T268 Q269 R270 S271 L272 G273 D274 L275 I276 M277 S278 C279 C280 P281 D282 P283 N284 P285 P286 I287 H288 K289 I290 V291 R292 K293 P294 S295 R296 I297 L298 M301 F304 D305 E306 A310 F311 D312 E313 H314 I315 G316 P317 L318 C319 T320 D321 W322 Q323 K324 A325
E326 R327 G328 D329 I330 L331 L335 I336 R337 K338 K339 L340 E343 A344 S345 L346 L347 I348 T349 T350 R351 P352 V353 A354 L355 E356 K357 L358 Q359 H360 L361 L362 D363 H364 P365 R366 H367 V368 E369 I370 L371 G372 F373 S374 E375 A376 K377 F383 F386 S387 D388 E389 A390 Q391 A392 R393
F396 S397 L398 I399 Q400 E401 N402 E403 V404 L405 M408 P412 V418 L422 K423 Q424 Q425 M426 E427 S428 G429 K430 S431 L432 A433 Q434 T435 S436 K437 T438 T439 T440 A441 V444 F445 F446 L447 S448 S449 L450 L451 Q452 P453 R454 G455 GLY SER GLN GLU HIS G461 L462 C463 A464
H465 L466 W467 G468 L469 C470 S471 L472 A473 A474 D475 G476 I477 W478 N479 Q480 K481 I482 L483 F484 S487 D488 L489 R490 N491 H492 G493 L494 Q495 K496 A497 D498 V499 S500 A501 F502 L503 R504 M505 N506 L507 F508 Q509 K510 E511 V512 D513 C514 E515 K516 F520 M523 E527 Y533 Y534
E537 GLU GLU LYS GLU GLY ARG THR ASN VAL PRO GLY SER R550 L551 K552 L553 P554 S555 R556 D557 V558 T559 V560 L561 L562 G566 K567 F568 E569 K570 G571 Y572 L573 I574 F575 V576 L583 V584 E587 R588 T589 S590 Y591 L592 E593 K594 K595 L596 S597 C598 K599 I600 S601 I604
R605 L606 W611 A616 K617 A618 K619 K620 L621 Q622 I623 Q624 P625 Y632 Y635 E636 E639 E640 D641 F642 D662 V665 R675 H686 ASN MET PRO LYS GLU GLU GLU GLU GLU LYS GLU GLY ARG HIS LEU ASP MET VAL GLN CYS VAL LEU PRO SER SER SER
HIS ALA ALA CYS SER HIS GLY LEU VAL ASN SER H724 L725 T726 S727 S728 F729 C730 R731 S742 E745 D750 Q766 H767 P768 R774 L775 W776 L777 G778 R779 C787 F788 D789 V793 E802 R816 L817 L818 S836 A842 D846 R859 V862 G863 E864
N865 D869 K878 A879 K880 N881 K888 L896 T897 S898 V899 C900 V907 N911 Q912 N913 L914 T915 H916 L917 R920 G921 N922 T923 L924 G925 D926 K930 L931 L932 C933 E934 G935 L936 L937 D940 L943 L946 E947 L948 D949 N950 L953 T954 S955 H956 C957 C958
W959 D960 L961 L964 L965 T966 S967 S968 Q969 R972 K973 N978 N979 D980 L981 G982 D983 L984 G985 V986 M987 M988 F989 V992 L993 K994 Q995 Q996 S997 C998 L999 L1000 G1004 M1008 Y1009 F1010 N1011 Y1012 E1013 T1014 K1015 S1016 A1017 L1018 E1024 K1025 P1026 E1027 V1031 F1032 E1033 P1034
S1035 W1036 GLY SER GLY GLY ASP TYR LYS ASP ASP ASP ASP LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	124523	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 ($e^-/Å^2$)	99	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.639	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	318.24, 318.24, 318.24	wwPDB
Map dimensions	468, 468, 468	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.68, 0.68, 0.68	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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	0.25	0/6586	0.49	1/8879 (0.0%)
1	B	0.25	0/6586	0.49	1/8879 (0.0%)
1	C	0.25	0/6586	0.49	1/8879 (0.0%)
1	D	0.25	0/6586	0.49	1/8879 (0.0%)
1	E	0.25	0/6586	0.49	1/8879 (0.0%)
1	F	0.25	0/6586	0.49	1/8879 (0.0%)
All	All	0.25	0/39516	0.49	6/53274 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1013	GLU	CA-CB-CG	6.00	126.60	113.40
1	A	1013	GLU	CA-CB-CG	5.99	126.58	113.40
1	B	1013	GLU	CA-CB-CG	5.99	126.57	113.40
1	F	1013	GLU	CA-CB-CG	5.99	126.57	113.40
1	E	1013	GLU	CA-CB-CG	5.98	126.55	113.40
1	C	1013	GLU	CA-CB-CG	5.97	126.53	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	6463	0	6516	146	0
1	B	6463	0	6516	141	0
1	C	6463	0	6516	144	0
1	D	6463	0	6516	148	0
1	E	6463	0	6516	146	0
1	F	6463	0	6516	144	0
2	A	27	0	12	1	0
2	B	27	0	12	1	0
2	C	27	0	12	1	0
2	D	27	0	12	1	0
2	E	27	0	12	1	0
2	F	27	0	12	1	0
All	All	38940	0	39168	853	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 11.

All (853) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:HIS:HE1	1:E:220:HIS:HA	1.39	0.87
1:A:215:HIS:HE1	1:A:220:HIS:HA	1.39	0.87
1:C:215:HIS:HE1	1:C:220:HIS:HA	1.39	0.86
1:D:215:HIS:HE1	1:D:220:HIS:HA	1.40	0.86
1:B:215:HIS:HE1	1:B:220:HIS:HA	1.40	0.85
1:F:215:HIS:HE1	1:F:220:HIS:HA	1.39	0.85
1:B:256:LEU:HG	1:B:298:LEU:HD21	1.61	0.82
1:F:256:LEU:HG	1:F:298:LEU:HD21	1.61	0.82
1:C:256:LEU:HG	1:C:298:LEU:HD21	1.61	0.82
1:D:256:LEU:HG	1:D:298:LEU:HD21	1.61	0.82
1:F:624:GLN:HG2	1:F:625:PRO:HD3	1.62	0.82
1:B:624:GLN:HG2	1:B:625:PRO:HD3	1.62	0.82
1:E:256:LEU:HG	1:E:298:LEU:HD21	1.61	0.81
1:A:256:LEU:HG	1:A:298:LEU:HD21	1.61	0.81
1:E:624:GLN:HG2	1:E:625:PRO:HD3	1.61	0.81
1:A:301:MET:HB3	1:A:348:ILE:HG22	1.64	0.80
1:E:301:MET:HB3	1:E:348:ILE:HG22	1.64	0.80
1:A:624:GLN:HG2	1:A:625:PRO:HD3	1.62	0.80
1:C:624:GLN:HG2	1:C:625:PRO:HD3	1.62	0.80
1:D:624:GLN:HG2	1:D:625:PRO:HD3	1.61	0.80
1:D:978:ASN:HB2	1:E:142:LYS:HE3	1.64	0.80
1:B:480:GLN:HE21	1:B:570:LYS:HA	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:480:GLN:HE21	1:F:570:LYS:HA	1.47	0.80
1:E:475:ASP:HA	1:E:478:TRP:HB2	1.66	0.78
1:E:480:GLN:HE21	1:E:570:LYS:HA	1.47	0.78
1:A:475:ASP:HA	1:A:478:TRP:HB2	1.66	0.78
1:A:480:GLN:HE21	1:A:570:LYS:HA	1.47	0.78
1:D:142:LYS:HE3	1:F:978:ASN:HB2	1.65	0.78
1:B:475:ASP:HA	1:B:478:TRP:HB2	1.66	0.78
1:C:480:GLN:HE21	1:C:570:LYS:HA	1.47	0.78
1:F:475:ASP:HA	1:F:478:TRP:HB2	1.66	0.78
1:D:480:GLN:HE21	1:D:570:LYS:HA	1.47	0.77
1:D:301:MET:HB3	1:D:348:ILE:HG22	1.64	0.77
1:B:301:MET:HB3	1:B:348:ILE:HG22	1.64	0.77
1:F:301:MET:HB3	1:F:348:ILE:HG22	1.64	0.77
1:C:301:MET:HB3	1:C:348:ILE:HG22	1.64	0.77
1:D:475:ASP:HA	1:D:478:TRP:HB2	1.66	0.77
1:C:475:ASP:HA	1:C:478:TRP:HB2	1.66	0.76
1:A:142:LYS:HE3	1:C:978:ASN:HB2	1.65	0.76
1:B:789:ASP:OD1	1:D:816:ARG:NH2	2.20	0.74
1:C:267:VAL:HG23	1:C:269:GLN:HE22	1.52	0.74
1:D:267:VAL:HG23	1:D:269:GLN:HE22	1.52	0.74
1:F:267:VAL:HG23	1:F:269:GLN:HE22	1.52	0.74
1:B:267:VAL:HG23	1:B:269:GLN:HE22	1.52	0.73
1:B:955:SER:HB3	1:B:982:GLY:H	1.54	0.73
1:F:955:SER:HB3	1:F:982:GLY:H	1.54	0.73
1:D:955:SER:HB3	1:D:982:GLY:H	1.54	0.73
1:C:955:SER:HB3	1:C:982:GLY:H	1.54	0.73
1:A:955:SER:HB3	1:A:982:GLY:H	1.54	0.72
1:E:955:SER:HB3	1:E:982:GLY:H	1.54	0.72
1:C:273:GLY:HA2	1:C:276:ILE:HD12	1.72	0.72
1:D:273:GLY:HA2	1:D:276:ILE:HD12	1.72	0.72
1:A:978:ASN:HB2	1:B:142:LYS:HE3	1.71	0.72
1:A:267:VAL:HG23	1:A:269:GLN:HE22	1.52	0.71
1:E:267:VAL:HG23	1:E:269:GLN:HE22	1.52	0.71
1:E:978:ASN:HB2	1:F:142:LYS:HE3	1.72	0.71
1:F:273:GLY:HA2	1:F:276:ILE:HD12	1.72	0.71
1:B:273:GLY:HA2	1:B:276:ILE:HD12	1.72	0.70
1:A:273:GLY:HA2	1:A:276:ILE:HD12	1.72	0.70
1:E:273:GLY:HA2	1:E:276:ILE:HD12	1.72	0.70
1:A:816:ARG:NH2	1:E:789:ASP:OD1	2.28	0.67
1:B:888:LYS:HG2	1:B:916:HIS:HB2	1.77	0.67
1:F:888:LYS:HG2	1:F:916:HIS:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:888:LYS:HG2	1:C:916:HIS:HB2	1.77	0.66
1:D:888:LYS:HG2	1:D:916:HIS:HB2	1.77	0.65
1:A:888:LYS:HG2	1:A:916:HIS:HB2	1.77	0.65
1:E:888:LYS:HG2	1:E:916:HIS:HB2	1.77	0.65
1:B:451:LEU:O	1:B:455:GLY:N	2.30	0.65
1:C:911:ASN:ND2	1:C:913:ASN:OD1	2.30	0.65
1:D:911:ASN:ND2	1:D:913:ASN:OD1	2.30	0.65
1:F:451:LEU:O	1:F:455:GLY:N	2.30	0.65
1:B:362:LEU:HB3	1:B:365:PRO:HG3	1.80	0.64
1:F:362:LEU:HB3	1:F:365:PRO:HG3	1.80	0.64
1:F:438:THR:HG21	1:F:636:GLU:HA	1.80	0.64
1:B:438:THR:HG21	1:B:636:GLU:HA	1.80	0.64
1:A:137:ARG:HG2	1:A:255:TYR:HE1	1.63	0.64
1:B:911:ASN:ND2	1:B:913:ASN:OD1	2.30	0.64
1:D:362:LEU:HB3	1:D:365:PRO:HG3	1.80	0.64
1:B:816:ARG:NH2	1:D:789:ASP:OD1	2.31	0.64
1:A:911:ASN:ND2	1:A:913:ASN:OD1	2.30	0.64
1:E:137:ARG:HG2	1:E:255:TYR:HE1	1.63	0.64
1:C:362:LEU:HB3	1:C:365:PRO:HG3	1.80	0.63
1:F:911:ASN:ND2	1:F:913:ASN:OD1	2.30	0.63
1:E:911:ASN:ND2	1:E:913:ASN:OD1	2.30	0.63
1:D:137:ARG:HG2	1:D:255:TYR:HE1	1.63	0.63
1:D:451:LEU:O	1:D:455:GLY:N	2.30	0.63
1:C:137:ARG:HG2	1:C:255:TYR:HE1	1.63	0.63
1:C:447:LEU:HA	1:C:450:LEU:HB3	1.81	0.63
1:D:775:LEU:HD13	1:D:777:LEU:HD13	1.80	0.63
1:A:451:LEU:O	1:A:455:GLY:N	2.30	0.63
1:C:451:LEU:O	1:C:455:GLY:N	2.30	0.63
1:D:447:LEU:HA	1:D:450:LEU:HB3	1.81	0.63
1:E:451:LEU:O	1:E:455:GLY:N	2.30	0.63
1:B:137:ARG:HG2	1:B:255:TYR:HE1	1.63	0.63
1:D:418:VAL:HG23	1:D:432:LEU:HD22	1.81	0.63
1:B:775:LEU:HD13	1:B:777:LEU:HD13	1.80	0.63
1:C:775:LEU:HD13	1:C:777:LEU:HD13	1.80	0.63
1:E:362:LEU:HB3	1:E:365:PRO:HG3	1.80	0.63
1:A:362:LEU:HB3	1:A:365:PRO:HG3	1.80	0.63
1:C:418:VAL:HG23	1:C:432:LEU:HD22	1.81	0.63
1:F:137:ARG:HG2	1:F:255:TYR:HE1	1.63	0.62
1:F:447:LEU:HA	1:F:450:LEU:HB3	1.81	0.62
1:F:775:LEU:HD13	1:F:777:LEU:HD13	1.80	0.62
1:B:447:LEU:HA	1:B:450:LEU:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:862:VAL:O	1:B:865:ASN:ND2	2.32	0.62
1:C:862:VAL:O	1:C:865:ASN:ND2	2.32	0.62
1:D:862:VAL:O	1:D:865:ASN:ND2	2.32	0.62
1:F:862:VAL:O	1:F:865:ASN:ND2	2.32	0.62
1:C:438:THR:HG21	1:C:636:GLU:HA	1.80	0.62
1:C:943:LEU:HD21	1:C:946:LEU:HB2	1.82	0.62
1:D:943:LEU:HD21	1:D:946:LEU:HB2	1.82	0.62
1:E:775:LEU:HD13	1:E:777:LEU:HD13	1.80	0.62
1:A:775:LEU:HD13	1:A:777:LEU:HD13	1.80	0.62
1:A:943:LEU:HD21	1:A:946:LEU:HB2	1.82	0.62
1:D:438:THR:HG21	1:D:636:GLU:HA	1.80	0.62
1:E:943:LEU:HD21	1:E:946:LEU:HB2	1.82	0.62
1:E:862:VAL:O	1:E:865:ASN:ND2	2.32	0.62
1:E:438:THR:HG21	1:E:636:GLU:HA	1.80	0.62
1:A:862:VAL:O	1:A:865:ASN:ND2	2.32	0.61
1:A:438:THR:HG21	1:A:636:GLU:HA	1.80	0.61
1:A:447:LEU:HA	1:A:450:LEU:HB3	1.81	0.61
1:E:447:LEU:HA	1:E:450:LEU:HB3	1.81	0.61
1:B:418:VAL:HG23	1:B:432:LEU:HD22	1.81	0.61
1:B:978:ASN:HB2	1:C:142:LYS:HE3	1.82	0.61
1:F:943:LEU:HD21	1:F:946:LEU:HB2	1.82	0.61
1:A:215:HIS:CE1	1:A:220:HIS:HA	2.30	0.61
1:B:1004:GLY:HA2	1:B:1031:VAL:HB	1.83	0.61
1:E:215:HIS:CE1	1:E:220:HIS:HA	2.30	0.61
1:F:418:VAL:HG23	1:F:432:LEU:HD22	1.81	0.61
1:F:1004:GLY:HA2	1:F:1031:VAL:HB	1.83	0.61
1:A:418:VAL:HG23	1:A:432:LEU:HD22	1.81	0.61
1:B:943:LEU:HD21	1:B:946:LEU:HB2	1.82	0.61
1:E:418:VAL:HG23	1:E:432:LEU:HD22	1.81	0.61
1:C:1004:GLY:HA2	1:C:1031:VAL:HB	1.83	0.60
1:D:1004:GLY:HA2	1:D:1031:VAL:HB	1.83	0.60
1:F:898:SER:HB3	1:F:925:GLY:HA3	1.84	0.60
1:B:898:SER:HB3	1:B:925:GLY:HA3	1.84	0.60
1:C:789:ASP:OD1	1:F:816:ARG:NH2	2.35	0.60
1:F:170:ARG:NH1	1:F:171:LEU:O	2.35	0.60
1:A:898:SER:HB3	1:A:925:GLY:HA3	1.84	0.60
1:E:898:SER:HB3	1:E:925:GLY:HA3	1.84	0.60
1:A:170:ARG:NH1	1:A:171:LEU:O	2.35	0.60
1:B:170:ARG:NH1	1:B:171:LEU:O	2.35	0.60
1:A:1004:GLY:HA2	1:A:1031:VAL:HB	1.83	0.59
1:B:632:TYR:OH	1:B:662:ASP:OD1	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:ARG:NH1	1:E:171:LEU:O	2.35	0.59
1:E:1004:GLY:HA2	1:E:1031:VAL:HB	1.83	0.59
1:B:766:GLN:HG3	1:B:793:VAL:HG12	1.84	0.59
1:F:632:TYR:OH	1:F:662:ASP:OD1	2.20	0.59
1:C:632:TYR:OH	1:C:662:ASP:OD1	2.20	0.59
1:C:898:SER:HB3	1:C:925:GLY:HA3	1.84	0.59
1:D:632:TYR:OH	1:D:662:ASP:OD1	2.20	0.59
1:C:766:GLN:HG3	1:C:793:VAL:HG12	1.84	0.59
1:D:766:GLN:HG3	1:D:793:VAL:HG12	1.84	0.59
1:D:898:SER:HB3	1:D:925:GLY:HA3	1.84	0.59
1:F:766:GLN:HG3	1:F:793:VAL:HG12	1.84	0.59
1:C:170:ARG:NH1	1:C:171:LEU:O	2.35	0.59
1:D:170:ARG:NH1	1:D:171:LEU:O	2.35	0.59
1:E:766:GLN:HG3	1:E:793:VAL:HG12	1.84	0.59
1:A:766:GLN:HG3	1:A:793:VAL:HG12	1.84	0.59
1:F:215:HIS:CE1	1:F:220:HIS:HA	2.30	0.58
1:B:215:HIS:CE1	1:B:220:HIS:HA	2.30	0.58
1:A:789:ASP:OD1	1:E:816:ARG:NH2	2.36	0.58
1:F:316:GLY:HA3	1:F:330:ILE:HG12	1.86	0.58
1:A:632:TYR:OH	1:A:662:ASP:OD1	2.20	0.58
1:C:215:HIS:CE1	1:C:220:HIS:HA	2.30	0.58
1:C:880:LYS:HB3	1:C:907:VAL:HG12	1.85	0.58
1:D:215:HIS:CE1	1:D:220:HIS:HA	2.30	0.58
1:D:880:LYS:HB3	1:D:907:VAL:HG12	1.85	0.58
1:A:311:PHE:HB3	1:A:568:PHE:HE2	1.69	0.58
1:B:316:GLY:HA3	1:B:330:ILE:HG12	1.86	0.58
1:E:632:TYR:OH	1:E:662:ASP:OD1	2.20	0.58
1:F:242:ASP:OD1	1:F:247:THR:OG1	2.21	0.58
1:E:311:PHE:HB3	1:E:568:PHE:HE2	1.69	0.58
1:D:469:LEU:O	1:D:473:ALA:N	2.34	0.58
1:B:880:LYS:HB3	1:B:907:VAL:HG12	1.85	0.57
1:C:316:GLY:HA3	1:C:330:ILE:HG12	1.86	0.57
1:D:316:GLY:HA3	1:D:330:ILE:HG12	1.86	0.57
1:C:469:LEU:O	1:C:473:ALA:N	2.34	0.57
1:E:242:ASP:OD1	1:E:247:THR:OG1	2.21	0.57
1:F:880:LYS:HB3	1:F:907:VAL:HG12	1.85	0.57
1:C:311:PHE:HB3	1:C:568:PHE:HE2	1.69	0.57
1:A:242:ASP:OD1	1:A:247:THR:OG1	2.21	0.57
1:F:469:LEU:O	1:F:473:ALA:N	2.34	0.57
1:D:311:PHE:HB3	1:D:568:PHE:HE2	1.69	0.57
1:E:316:GLY:HA3	1:E:330:ILE:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ARG:HH12	1:B:374:SER:HB3	1.69	0.57
1:A:316:GLY:HA3	1:A:330:ILE:HG12	1.86	0.57
1:B:311:PHE:HB3	1:B:568:PHE:HE2	1.69	0.57
1:D:172:ARG:HH12	1:D:374:SER:HB3	1.69	0.57
1:A:172:ARG:HH12	1:A:374:SER:HB3	1.69	0.57
1:B:469:LEU:O	1:B:473:ALA:N	2.34	0.57
1:C:495:GLN:HB2	1:C:498:ASP:HB2	1.87	0.56
1:F:311:PHE:HB3	1:F:568:PHE:HE2	1.69	0.56
1:D:495:GLN:HB2	1:D:498:ASP:HB2	1.87	0.56
1:E:172:ARG:HH12	1:E:374:SER:HB3	1.69	0.56
1:F:172:ARG:HH12	1:F:374:SER:HB3	1.69	0.56
1:C:172:ARG:HH12	1:C:374:SER:HB3	1.69	0.56
1:E:469:LEU:O	1:E:473:ALA:N	2.34	0.56
1:C:816:ARG:NH2	1:F:789:ASP:OD1	2.38	0.56
1:A:880:LYS:HB3	1:A:907:VAL:HG12	1.85	0.56
1:C:745:GLU:OE2	1:C:776:TRP:NE1	2.39	0.56
1:A:469:LEU:O	1:A:473:ALA:N	2.34	0.56
1:D:745:GLU:OE2	1:D:776:TRP:NE1	2.39	0.56
1:D:242:ASP:OD1	1:D:247:THR:OG1	2.21	0.56
1:C:242:ASP:OD1	1:C:247:THR:OG1	2.21	0.56
1:E:880:LYS:HB3	1:E:907:VAL:HG12	1.85	0.56
1:A:495:GLN:HB2	1:A:498:ASP:HB2	1.87	0.55
1:F:365:PRO:HG2	1:F:367:HIS:HE2	1.71	0.55
1:E:446:PHE:O	1:E:450:LEU:N	2.39	0.55
1:E:495:GLN:HB2	1:E:498:ASP:HB2	1.87	0.55
1:A:446:PHE:O	1:A:450:LEU:N	2.39	0.55
1:A:745:GLU:OE2	1:A:776:TRP:NE1	2.39	0.55
1:E:745:GLU:OE2	1:E:776:TRP:NE1	2.39	0.55
1:B:365:PRO:HG2	1:B:367:HIS:HE2	1.71	0.55
1:E:290:ILE:HG22	1:E:297:ILE:HD11	1.88	0.55
1:F:495:GLN:HB2	1:F:498:ASP:HB2	1.87	0.55
1:A:290:ILE:HG22	1:A:297:ILE:HD11	1.88	0.55
1:B:495:GLN:HB2	1:B:498:ASP:HB2	1.87	0.55
1:C:290:ILE:HG22	1:C:297:ILE:HD11	1.88	0.55
1:A:327:ARG:NH2	1:A:329:ASP:OD2	2.40	0.55
1:D:290:ILE:HG22	1:D:297:ILE:HD11	1.88	0.55
1:E:327:ARG:NH2	1:E:329:ASP:OD2	2.40	0.55
1:B:290:ILE:HG22	1:B:297:ILE:HD11	1.88	0.54
1:C:896:LEU:O	1:C:923:THR:OG1	2.23	0.54
1:D:896:LEU:O	1:D:923:THR:OG1	2.23	0.54
1:F:290:ILE:HG22	1:F:297:ILE:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:TYR:O	1:A:595:LYS:HE3	2.08	0.54
1:C:446:PHE:O	1:C:450:LEU:N	2.39	0.54
1:E:591:TYR:O	1:E:595:LYS:HE3	2.08	0.54
1:C:327:ARG:NH2	1:C:329:ASP:OD2	2.40	0.54
1:C:365:PRO:HG2	1:C:367:HIS:HE2	1.71	0.54
1:D:446:PHE:O	1:D:450:LEU:N	2.39	0.54
1:D:327:ARG:NH2	1:D:329:ASP:OD2	2.40	0.54
1:D:365:PRO:HG2	1:D:367:HIS:HE2	1.71	0.54
1:A:896:LEU:O	1:A:923:THR:OG1	2.23	0.54
1:E:896:LEU:O	1:E:923:THR:OG1	2.23	0.54
1:B:446:PHE:O	1:B:450:LEU:N	2.39	0.54
1:F:327:ARG:NH2	1:F:329:ASP:OD2	2.40	0.54
1:B:327:ARG:NH2	1:B:329:ASP:OD2	2.40	0.54
1:B:591:TYR:O	1:B:595:LYS:HE3	2.08	0.54
1:E:273:GLY:HA2	1:E:276:ILE:CD1	2.38	0.54
1:A:273:GLY:HA2	1:A:276:ILE:CD1	2.39	0.54
1:F:463:CYS:O	1:F:467:TRP:N	2.35	0.54
1:D:591:TYR:O	1:D:595:LYS:HE3	2.08	0.53
1:F:446:PHE:O	1:F:450:LEU:N	2.39	0.53
1:F:591:TYR:O	1:F:595:LYS:HE3	2.08	0.53
1:A:365:PRO:HG2	1:A:367:HIS:HE2	1.71	0.53
1:A:584:VAL:HG23	1:A:601:SER:HB2	1.89	0.53
1:B:508:PHE:HB2	1:B:520:PHE:HA	1.90	0.53
1:C:463:CYS:O	1:C:467:TRP:N	2.35	0.53
1:C:591:TYR:O	1:C:595:LYS:HE3	2.08	0.53
1:D:508:PHE:HB2	1:D:520:PHE:HA	1.90	0.53
1:C:508:PHE:HB2	1:C:520:PHE:HA	1.90	0.53
1:E:584:VAL:HG23	1:E:601:SER:HB2	1.90	0.53
1:F:508:PHE:HB2	1:F:520:PHE:HA	1.90	0.53
1:A:920:ARG:HG3	1:A:949:ASP:HB2	1.91	0.53
1:B:584:VAL:HG23	1:B:601:SER:HB2	1.89	0.53
1:D:463:CYS:O	1:D:467:TRP:N	2.35	0.53
1:E:920:ARG:HG3	1:E:949:ASP:HB2	1.91	0.53
1:C:444:VAL:HG13	1:C:592:LEU:HG	1.91	0.53
1:D:444:VAL:HG13	1:D:592:LEU:HG	1.91	0.53
1:E:365:PRO:HG2	1:E:367:HIS:HE2	1.72	0.53
1:F:584:VAL:HG23	1:F:601:SER:HB2	1.89	0.53
1:B:444:VAL:HG13	1:B:592:LEU:HG	1.91	0.53
1:F:444:VAL:HG13	1:F:592:LEU:HG	1.91	0.53
1:D:920:ARG:HG3	1:D:949:ASP:HB2	1.91	0.53
1:E:444:VAL:HG13	1:E:592:LEU:HG	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:PRO:HG2	1:F:1034:PRO:O	2.09	0.52
1:A:444:VAL:HG13	1:A:592:LEU:HG	1.91	0.52
1:F:896:LEU:O	1:F:923:THR:OG1	2.23	0.52
1:C:920:ARG:HG3	1:C:949:ASP:HB2	1.91	0.52
1:A:562:LEU:HD13	1:A:611:TRP:HB2	1.91	0.52
1:B:920:ARG:HG3	1:B:949:ASP:HB2	1.91	0.52
1:C:273:GLY:HA2	1:C:276:ILE:CD1	2.38	0.52
1:C:562:LEU:HD13	1:C:611:TRP:HB2	1.91	0.52
1:D:562:LEU:HD13	1:D:611:TRP:HB2	1.92	0.52
1:F:562:LEU:HD13	1:F:611:TRP:HB2	1.91	0.52
1:B:440:THR:OG1	1:B:636:GLU:OE2	2.22	0.52
1:B:562:LEU:HD13	1:B:611:TRP:HB2	1.92	0.52
1:B:896:LEU:O	1:B:923:THR:OG1	2.23	0.52
1:C:584:VAL:HG23	1:C:601:SER:HB2	1.89	0.52
1:D:273:GLY:HA2	1:D:276:ILE:CD1	2.38	0.52
1:D:584:VAL:HG23	1:D:601:SER:HB2	1.89	0.52
1:A:508:PHE:HB2	1:A:520:PHE:HA	1.90	0.52
1:E:508:PHE:HB2	1:E:520:PHE:HA	1.90	0.52
1:E:562:LEU:HD13	1:E:611:TRP:HB2	1.92	0.52
1:F:920:ARG:HG3	1:F:949:ASP:HB2	1.91	0.52
1:C:249:TYR:HE2	1:C:252:ARG:NH1	2.08	0.52
1:E:272:LEU:HD21	1:E:340:LEU:HD21	1.92	0.52
1:F:304:PHE:HB3	1:F:350:THR:HG22	1.92	0.52
1:A:272:LEU:HD21	1:A:340:LEU:HD21	1.92	0.52
1:D:249:TYR:HE2	1:D:252:ARG:NH1	2.08	0.52
1:F:470:CYS:O	1:F:474:ALA:N	2.43	0.52
1:A:249:TYR:HE2	1:A:252:ARG:NH1	2.08	0.52
1:B:223:VAL:HG23	1:B:348:ILE:HG13	1.92	0.52
1:B:273:GLY:HA2	1:B:276:ILE:CD1	2.38	0.52
1:B:304:PHE:HB3	1:B:350:THR:HG22	1.92	0.52
1:B:470:CYS:O	1:B:474:ALA:N	2.43	0.52
1:C:217:GLU:OE1	1:C:366:ARG:NH2	2.43	0.52
1:D:217:GLU:OE1	1:D:366:ARG:NH2	2.43	0.52
1:E:249:TYR:HE2	1:E:252:ARG:NH1	2.08	0.52
1:E:304:PHE:HB3	1:E:350:THR:HG22	1.92	0.52
1:F:440:THR:OG1	1:F:636:GLU:OE2	2.22	0.52
1:A:304:PHE:HB3	1:A:350:THR:HG22	1.92	0.52
1:C:293:LYS:HD3	1:C:295:SER:HB3	1.92	0.52
1:D:293:LYS:HD3	1:D:295:SER:HB3	1.92	0.52
1:B:293:LYS:HD3	1:B:295:SER:HB3	1.92	0.51
1:B:745:GLU:OE2	1:B:776:TRP:NE1	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:VAL:HG23	1:E:348:ILE:HG13	1.92	0.51
1:F:223:VAL:HG23	1:F:348:ILE:HG13	1.92	0.51
1:F:293:LYS:HD3	1:F:295:SER:HB3	1.92	0.51
1:A:293:LYS:HD3	1:A:295:SER:HB3	1.92	0.51
1:C:470:CYS:O	1:C:474:ALA:N	2.43	0.51
1:F:273:GLY:HA2	1:F:276:ILE:CD1	2.38	0.51
1:A:217:GLU:OE1	1:A:366:ARG:NH2	2.43	0.51
1:A:223:VAL:HG23	1:A:348:ILE:HG13	1.92	0.51
1:E:293:LYS:HD3	1:E:295:SER:HB3	1.92	0.51
1:D:470:CYS:O	1:D:474:ALA:N	2.43	0.51
1:F:249:TYR:HE2	1:F:252:ARG:NH1	2.08	0.51
1:F:745:GLU:OE2	1:F:776:TRP:NE1	2.39	0.51
1:B:282:ASP:OD1	1:B:282:ASP:N	2.44	0.51
1:E:217:GLU:OE1	1:E:366:ARG:NH2	2.43	0.51
1:B:249:TYR:HE2	1:B:252:ARG:NH1	2.08	0.51
1:F:282:ASP:N	1:F:282:ASP:OD1	2.44	0.51
1:D:272:LEU:HD21	1:D:340:LEU:HD21	1.92	0.51
1:D:304:PHE:HB3	1:D:350:THR:HG22	1.92	0.51
1:E:470:CYS:O	1:E:474:ALA:N	2.43	0.51
1:A:470:CYS:O	1:A:474:ALA:N	2.43	0.51
1:B:272:LEU:HD21	1:B:340:LEU:HD21	1.92	0.51
1:E:489:LEU:HD21	1:E:499:VAL:HG21	1.93	0.51
1:A:448:SER:O	1:A:452:GLN:N	2.41	0.50
1:A:489:LEU:HD21	1:A:499:VAL:HG21	1.93	0.50
1:B:242:ASP:OD1	1:B:247:THR:OG1	2.21	0.50
1:C:272:LEU:HD21	1:C:340:LEU:HD21	1.92	0.50
1:C:304:PHE:HB3	1:C:350:THR:HG22	1.92	0.50
1:D:936:LEU:HD21	1:D:943:LEU:HD13	1.94	0.50
1:C:936:LEU:HD21	1:C:943:LEU:HD13	1.94	0.50
1:F:272:LEU:HD21	1:F:340:LEU:HD21	1.92	0.50
1:C:440:THR:OG1	1:C:636:GLU:OE2	2.21	0.50
1:A:463:CYS:O	1:A:467:TRP:N	2.35	0.50
1:C:454:ARG:NH1	1:C:505:MET:SD	2.85	0.50
1:D:454:ARG:NH1	1:D:505:MET:SD	2.85	0.50
1:E:451:LEU:HD23	1:E:454:ARG:HE	1.77	0.50
1:A:451:LEU:HD23	1:A:454:ARG:HE	1.77	0.50
1:D:440:THR:OG1	1:D:636:GLU:OE2	2.21	0.50
1:C:489:LEU:HD21	1:C:499:VAL:HG21	1.93	0.50
1:F:936:LEU:HD21	1:F:943:LEU:HD13	1.94	0.50
1:B:489:LEU:HD21	1:B:499:VAL:HG21	1.93	0.50
1:B:936:LEU:HD21	1:B:943:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ASP:OD1	1:C:282:ASP:N	2.44	0.50
1:D:489:LEU:HD21	1:D:499:VAL:HG21	1.94	0.50
1:E:463:CYS:O	1:E:467:TRP:N	2.35	0.50
1:D:282:ASP:N	1:D:282:ASP:OD1	2.44	0.50
1:F:451:LEU:HD23	1:F:454:ARG:HE	1.77	0.50
1:C:223:VAL:HG23	1:C:348:ILE:HG13	1.92	0.49
1:D:467:TRP:HA	1:D:470:CYS:SG	2.53	0.49
1:E:282:ASP:OD1	1:E:282:ASP:N	2.44	0.49
1:A:282:ASP:N	1:A:282:ASP:OD1	2.44	0.49
1:A:936:LEU:HD21	1:A:943:LEU:HD13	1.93	0.49
1:B:451:LEU:HD23	1:B:454:ARG:HE	1.77	0.49
1:B:503:LEU:HD22	1:B:509:GLN:HA	1.95	0.49
1:C:467:TRP:HA	1:C:470:CYS:SG	2.53	0.49
1:F:448:SER:O	1:F:452:GLN:N	2.41	0.49
1:F:454:ARG:NH1	1:F:505:MET:SD	2.85	0.49
1:F:489:LEU:HD21	1:F:499:VAL:HG21	1.94	0.49
1:D:223:VAL:HG23	1:D:348:ILE:HG13	1.92	0.49
1:D:503:LEU:HD22	1:D:509:GLN:HA	1.95	0.49
1:F:503:LEU:HD22	1:F:509:GLN:HA	1.95	0.49
1:A:454:ARG:NH1	1:A:505:MET:SD	2.85	0.49
1:C:503:LEU:HD22	1:C:509:GLN:HA	1.95	0.49
1:D:620:LYS:HG3	1:D:622:GLN:HG3	1.95	0.49
1:E:936:LEU:HD21	1:E:943:LEU:HD13	1.94	0.49
1:B:448:SER:O	1:B:452:GLN:N	2.41	0.49
1:B:454:ARG:NH1	1:B:505:MET:SD	2.85	0.49
1:B:467:TRP:HA	1:B:470:CYS:SG	2.52	0.49
1:C:464:ALA:O	1:C:468:GLY:N	2.42	0.49
1:C:620:LYS:HG3	1:C:622:GLN:HG3	1.95	0.49
1:E:454:ARG:NH1	1:E:505:MET:SD	2.85	0.49
1:F:467:TRP:HA	1:F:470:CYS:SG	2.52	0.49
1:A:503:LEU:HD22	1:A:509:GLN:HA	1.95	0.49
1:A:620:LYS:HG3	1:A:622:GLN:HG3	1.95	0.49
1:B:589:THR:HG21	1:B:592:LEU:HD23	1.95	0.49
1:D:451:LEU:HD23	1:D:454:ARG:HE	1.77	0.49
1:D:464:ALA:O	1:D:468:GLY:N	2.42	0.49
1:E:620:LYS:HG3	1:E:622:GLN:HG3	1.95	0.49
1:F:620:LYS:HG3	1:F:622:GLN:HG3	1.95	0.49
1:A:170:ARG:HH22	1:A:173:LEU:HB3	1.78	0.49
1:A:480:GLN:NE2	1:A:569:GLU:O	2.46	0.49
1:B:243:TRP:CE2	1:B:256:LEU:HD13	2.48	0.49
1:C:451:LEU:HD23	1:C:454:ARG:HE	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:ARG:HH22	1:E:173:LEU:HB3	1.78	0.49
1:E:503:LEU:HD22	1:E:509:GLN:HA	1.95	0.49
1:F:243:TRP:CE2	1:F:256:LEU:HD13	2.48	0.49
1:B:620:LYS:HG3	1:B:622:GLN:HG3	1.95	0.49
1:C:234:ILE:HD11	2:C:1101:ADP:C5	2.48	0.49
1:E:480:GLN:NE2	1:E:569:GLU:O	2.46	0.49
1:F:589:THR:HG21	1:F:592:LEU:HD23	1.95	0.49
1:A:467:TRP:HA	1:A:470:CYS:SG	2.52	0.49
1:B:170:ARG:HH22	1:B:173:LEU:HB3	1.78	0.49
1:D:234:ILE:HD11	2:D:1101:ADP:C5	2.48	0.49
1:F:170:ARG:HH22	1:F:173:LEU:HB3	1.78	0.49
1:C:170:ARG:HH22	1:C:173:LEU:HB3	1.78	0.48
1:D:243:TRP:CE2	1:D:256:LEU:HD13	2.48	0.48
1:E:467:TRP:HA	1:E:470:CYS:SG	2.52	0.48
1:C:243:TRP:CE2	1:C:256:LEU:HD13	2.48	0.48
1:D:170:ARG:HH22	1:D:173:LEU:HB3	1.78	0.48
1:D:589:THR:HG21	1:D:592:LEU:HD23	1.95	0.48
1:A:234:ILE:HD11	2:A:1101:ADP:C5	2.48	0.48
1:A:253:PHE:CD1	1:A:298:LEU:HD22	2.49	0.48
1:B:480:GLN:NE2	1:B:569:GLU:O	2.46	0.48
1:E:253:PHE:CD1	1:E:298:LEU:HD22	2.49	0.48
1:E:1034:PRO:O	1:F:281:PRO:HG2	2.12	0.48
1:F:217:GLU:OE1	1:F:366:ARG:NH2	2.43	0.48
1:A:425:GLN:O	1:A:429:GLY:N	2.33	0.48
1:C:253:PHE:CD1	1:C:298:LEU:HD22	2.49	0.48
1:C:589:THR:HG21	1:C:592:LEU:HD23	1.95	0.48
1:D:253:PHE:CD1	1:D:298:LEU:HD22	2.49	0.48
1:E:234:ILE:HD11	2:E:1101:ADP:C5	2.48	0.48
1:E:425:GLN:O	1:E:429:GLY:N	2.33	0.48
1:F:234:ILE:HD11	2:F:1101:ADP:C5	2.48	0.48
1:F:480:GLN:NE2	1:F:569:GLU:O	2.46	0.48
1:A:435:THR:HG22	1:A:441:ALA:HB1	1.95	0.48
1:C:624:GLN:HG2	1:C:625:PRO:CD	2.41	0.48
1:D:624:GLN:HG2	1:D:625:PRO:CD	2.40	0.48
1:E:435:THR:HG22	1:E:441:ALA:HB1	1.95	0.48
1:E:468:GLY:HA2	1:E:492:HIS:HB3	1.95	0.48
1:A:468:GLY:HA2	1:A:492:HIS:HB3	1.95	0.48
1:A:589:THR:HG21	1:A:592:LEU:HD23	1.95	0.48
1:B:234:ILE:HD11	2:B:1101:ADP:C5	2.48	0.48
1:E:589:THR:HG21	1:E:592:LEU:HD23	1.95	0.48
1:E:989:PHE:HA	1:E:992:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:272:LEU:HD12	1:F:323:GLN:HA	1.96	0.48
1:A:624:GLN:HG2	1:A:625:PRO:CD	2.41	0.48
1:A:989:PHE:HA	1:A:992:VAL:HG22	1.96	0.48
1:C:435:THR:HG22	1:C:441:ALA:HB1	1.95	0.48
1:B:272:LEU:HD12	1:B:323:GLN:HA	1.96	0.48
1:C:896:LEU:HB2	1:C:922:ASN:HB3	1.96	0.48
1:D:435:THR:HG22	1:D:441:ALA:HB1	1.95	0.48
1:C:480:GLN:NE2	1:C:569:GLU:O	2.46	0.48
1:C:989:PHE:HA	1:C:992:VAL:HG22	1.95	0.48
1:D:480:GLN:NE2	1:D:569:GLU:O	2.46	0.48
1:D:896:LEU:HB2	1:D:922:ASN:HB3	1.96	0.48
1:E:624:GLN:HG2	1:E:625:PRO:CD	2.40	0.48
1:F:989:PHE:HA	1:F:992:VAL:HG22	1.95	0.48
1:B:464:ALA:O	1:B:468:GLY:N	2.42	0.47
1:B:468:GLY:HA2	1:B:492:HIS:HB3	1.96	0.47
1:B:836:SER:H	1:B:864:GLU:HB3	1.78	0.47
1:B:989:PHE:HA	1:B:992:VAL:HG22	1.95	0.47
1:C:836:SER:H	1:C:864:GLU:HB3	1.78	0.47
1:E:243:TRP:CE2	1:E:256:LEU:HD13	2.48	0.47
1:B:170:ARG:HH12	1:B:173:LEU:HB2	1.79	0.47
1:D:450:LEU:HD12	1:D:505:MET:HE1	1.96	0.47
1:D:836:SER:H	1:D:864:GLU:HB3	1.78	0.47
1:D:989:PHE:HA	1:D:992:VAL:HG22	1.95	0.47
1:A:170:ARG:HH12	1:A:173:LEU:HB2	1.79	0.47
1:A:243:TRP:CE2	1:A:256:LEU:HD13	2.48	0.47
1:C:450:LEU:HD12	1:C:505:MET:HE1	1.96	0.47
1:F:170:ARG:HH12	1:F:173:LEU:HB2	1.79	0.47
1:F:836:SER:H	1:F:864:GLU:HB3	1.78	0.47
1:A:293:LYS:H	1:A:296:ARG:HH21	1.62	0.47
1:E:170:ARG:HH12	1:E:173:LEU:HB2	1.79	0.47
1:E:293:LYS:H	1:E:296:ARG:HH21	1.62	0.47
1:F:468:GLY:HA2	1:F:492:HIS:HB3	1.95	0.47
1:A:440:THR:OG1	1:A:636:GLU:OE2	2.22	0.47
1:A:896:LEU:HB2	1:A:922:ASN:HB3	1.96	0.47
1:B:253:PHE:CD1	1:B:298:LEU:HD22	2.49	0.47
1:C:272:LEU:HD12	1:C:323:GLN:HA	1.96	0.47
1:B:435:THR:HG22	1:B:441:ALA:HB1	1.95	0.47
1:D:272:LEU:HD12	1:D:323:GLN:HA	1.96	0.47
1:F:435:THR:HG22	1:F:441:ALA:HB1	1.95	0.47
1:A:836:SER:H	1:A:864:GLU:HB3	1.78	0.47
1:B:217:GLU:OE1	1:B:366:ARG:NH2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:836:SER:H	1:E:864:GLU:HB3	1.78	0.47
1:E:896:LEU:HB2	1:E:922:ASN:HB3	1.96	0.47
1:E:992:VAL:O	1:E:997:SER:OG	2.25	0.47
1:F:464:ALA:O	1:F:468:GLY:N	2.42	0.47
1:A:272:LEU:HD12	1:A:323:GLN:HA	1.96	0.47
1:C:134:LYS:HD2	1:C:137:ARG:HD2	1.97	0.47
1:C:558:VAL:O	1:C:562:LEU:HG	2.15	0.47
1:E:272:LEU:HD12	1:E:323:GLN:HA	1.96	0.47
1:F:253:PHE:CD1	1:F:298:LEU:HD22	2.49	0.47
1:C:170:ARG:HH12	1:C:173:LEU:HB2	1.79	0.47
1:D:170:ARG:HH12	1:D:173:LEU:HB2	1.79	0.47
1:D:468:GLY:HA2	1:D:492:HIS:HB3	1.96	0.47
1:D:558:VAL:O	1:D:562:LEU:HG	2.15	0.47
1:F:558:VAL:O	1:F:562:LEU:HG	2.15	0.47
1:B:463:CYS:O	1:B:467:TRP:N	2.35	0.47
1:B:558:VAL:O	1:B:562:LEU:HG	2.15	0.47
1:B:569:GLU:HG3	1:B:570:LYS:HD3	1.97	0.47
1:B:896:LEU:HB2	1:B:922:ASN:HB3	1.96	0.47
1:C:468:GLY:HA2	1:C:492:HIS:HB3	1.96	0.47
1:C:470:CYS:SG	1:C:471:SER:N	2.88	0.47
1:D:134:LYS:HD2	1:D:137:ARG:HD2	1.97	0.47
1:F:569:GLU:HG3	1:F:570:LYS:HD3	1.98	0.47
1:D:448:SER:O	1:D:452:GLN:N	2.41	0.46
1:D:470:CYS:SG	1:D:471:SER:N	2.88	0.46
1:A:992:VAL:O	1:A:997:SER:OG	2.25	0.46
1:A:281:PRO:HG2	1:C:1034:PRO:O	2.15	0.46
1:B:450:LEU:HD12	1:B:505:MET:HE1	1.97	0.46
1:C:448:SER:O	1:C:452:GLN:N	2.41	0.46
1:D:425:GLN:O	1:D:429:GLY:N	2.33	0.46
1:C:569:GLU:HG3	1:C:570:LYS:HD3	1.98	0.46
1:D:569:GLU:HG3	1:D:570:LYS:HD3	1.98	0.46
1:F:450:LEU:HD12	1:F:505:MET:HE1	1.97	0.46
1:F:896:LEU:HB2	1:F:922:ASN:HB3	1.96	0.46
1:A:558:VAL:O	1:A:562:LEU:HG	2.15	0.46
1:B:293:LYS:H	1:B:296:ARG:HH21	1.62	0.46
1:E:405:LEU:HA	1:E:408:MET:HE2	1.97	0.46
1:E:464:ALA:O	1:E:468:GLY:N	2.42	0.46
1:E:558:VAL:O	1:E:562:LEU:HG	2.15	0.46
1:B:470:CYS:SG	1:B:471:SER:N	2.88	0.46
1:C:405:LEU:HA	1:C:408:MET:HE2	1.98	0.46
1:C:425:GLN:O	1:C:429:GLY:N	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:LYS:H	1:D:296:ARG:HH21	1.62	0.46
1:E:573:LEU:HB3	1:E:576:VAL:HB	1.98	0.46
1:F:293:LYS:H	1:F:296:ARG:HH21	1.62	0.46
1:A:464:ALA:O	1:A:468:GLY:N	2.42	0.46
1:A:573:LEU:HB3	1:A:576:VAL:HB	1.98	0.46
1:C:293:LYS:H	1:C:296:ARG:HH21	1.62	0.46
1:B:280:CYS:HB2	1:B:283:PRO:HG3	1.98	0.46
1:F:280:CYS:HB2	1:F:283:PRO:HG3	1.98	0.46
1:A:285:PRO:O	1:A:289:LYS:HG2	2.16	0.46
1:A:569:GLU:HG3	1:A:570:LYS:HD3	1.97	0.46
1:E:285:PRO:O	1:E:289:LYS:HG2	2.16	0.46
1:E:569:GLU:HG3	1:E:570:LYS:HD3	1.98	0.46
1:F:405:LEU:HA	1:F:408:MET:HE2	1.97	0.46
1:F:470:CYS:SG	1:F:471:SER:N	2.88	0.46
1:E:859:ARG:HH11	1:E:888:LYS:HD2	1.81	0.46
1:A:470:CYS:SG	1:A:471:SER:N	2.88	0.45
1:C:859:ARG:HH11	1:C:888:LYS:HD2	1.81	0.45
1:D:405:LEU:HA	1:D:408:MET:HE2	1.98	0.45
1:D:573:LEU:HB3	1:D:576:VAL:HB	1.98	0.45
1:D:859:ARG:HH11	1:D:888:LYS:HD2	1.81	0.45
1:A:859:ARG:HH11	1:A:888:LYS:HD2	1.82	0.45
1:E:470:CYS:SG	1:E:471:SER:N	2.88	0.45
1:B:405:LEU:HA	1:B:408:MET:HE2	1.97	0.45
1:C:573:LEU:HB3	1:C:576:VAL:HB	1.98	0.45
1:B:285:PRO:O	1:B:289:LYS:HG2	2.16	0.45
1:E:280:CYS:HB2	1:E:283:PRO:HG3	1.98	0.45
1:F:285:PRO:O	1:F:289:LYS:HG2	2.16	0.45
1:A:134:LYS:HD2	1:A:137:ARG:HD2	1.97	0.45
1:A:280:CYS:HB2	1:A:283:PRO:HG3	1.98	0.45
1:F:210:ASP:OD1	1:F:210:ASP:N	2.50	0.45
1:A:859:ARG:HD3	1:A:888:LYS:HD2	1.99	0.45
1:E:134:LYS:HD2	1:E:137:ARG:HD2	1.97	0.45
1:E:859:ARG:HD3	1:E:888:LYS:HD2	1.99	0.45
1:F:134:LYS:HD2	1:F:137:ARG:HD2	1.97	0.45
1:A:466:LEU:HA	1:A:469:LEU:HG	1.99	0.45
1:B:210:ASP:OD1	1:B:210:ASP:N	2.50	0.45
1:B:466:LEU:HA	1:B:469:LEU:HG	1.99	0.45
1:C:280:CYS:HB2	1:C:283:PRO:HG3	1.98	0.45
1:D:285:PRO:O	1:D:289:LYS:HG2	2.16	0.45
1:B:921:GLY:HA2	1:B:950:ASN:HB3	1.99	0.45
1:C:285:PRO:O	1:C:289:LYS:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:CYS:HB2	1:D:283:PRO:HG3	1.98	0.45
1:E:466:LEU:HA	1:E:469:LEU:HG	1.99	0.45
1:D:466:LEU:HA	1:D:469:LEU:HG	1.99	0.45
1:F:466:LEU:HA	1:F:469:LEU:HG	1.99	0.45
1:B:573:LEU:HB3	1:B:576:VAL:HB	1.98	0.44
1:B:859:ARG:HH11	1:B:888:LYS:HD2	1.81	0.44
1:C:466:LEU:HA	1:C:469:LEU:HG	1.99	0.44
1:C:921:GLY:HA2	1:C:950:ASN:HB3	2.00	0.44
1:D:921:GLY:HA2	1:D:950:ASN:HB3	1.99	0.44
1:C:210:ASP:OD1	1:C:210:ASP:N	2.50	0.44
1:F:859:ARG:HH11	1:F:888:LYS:HD2	1.81	0.44
1:B:134:LYS:HD2	1:B:137:ARG:HD2	1.97	0.44
1:D:210:ASP:OD1	1:D:210:ASP:N	2.50	0.44
1:F:573:LEU:HB3	1:F:576:VAL:HB	1.98	0.44
1:F:921:GLY:HA2	1:F:950:ASN:HB3	2.00	0.44
1:E:448:SER:O	1:E:452:GLN:N	2.41	0.44
1:A:921:GLY:HA2	1:A:950:ASN:HB3	1.99	0.44
1:C:859:ARG:HD3	1:C:888:LYS:HD2	1.99	0.44
1:D:859:ARG:HD3	1:D:888:LYS:HD2	1.99	0.44
1:A:358:LEU:HB3	1:A:362:LEU:HD11	2.00	0.44
1:C:352:PRO:HA	1:C:355:LEU:HD23	1.99	0.44
1:D:352:PRO:HA	1:D:355:LEU:HD23	1.99	0.44
1:E:210:ASP:OD1	1:E:210:ASP:N	2.50	0.44
1:E:921:GLY:HA2	1:E:950:ASN:HB3	1.99	0.44
1:A:210:ASP:OD1	1:A:210:ASP:N	2.50	0.44
1:C:374:SER:H	1:C:377:LYS:HB2	1.82	0.44
1:D:878:LYS:O	1:D:881:ASN:ND2	2.50	0.44
1:E:358:LEU:HB3	1:E:362:LEU:HD11	2.00	0.44
1:F:352:PRO:HA	1:F:355:LEU:HD23	1.99	0.44
1:C:878:LYS:O	1:C:881:ASN:ND2	2.50	0.44
1:B:352:PRO:HA	1:B:355:LEU:HD23	1.99	0.44
1:D:374:SER:H	1:D:377:LYS:HB2	1.82	0.44
1:E:374:SER:H	1:E:377:LYS:HB2	1.82	0.43
1:F:859:ARG:HD3	1:F:888:LYS:HD2	1.99	0.43
1:A:362:LEU:HD22	1:A:365:PRO:HB3	2.00	0.43
1:A:374:SER:H	1:A:377:LYS:HB2	1.82	0.43
1:E:352:PRO:HA	1:E:355:LEU:HD23	1.99	0.43
1:E:362:LEU:HD22	1:E:365:PRO:HB3	2.00	0.43
1:B:641:ASP:OD1	1:B:642:PHE:N	2.51	0.43
1:B:859:ARG:HD3	1:B:888:LYS:HD2	1.99	0.43
1:C:1010:PHE:HB3	1:C:1014:THR:OG1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:940:ASP:OD1	1:F:940:ASP:N	2.51	0.43
1:A:172:ARG:HB2	1:A:371:LEU:HB2	2.00	0.43
1:A:352:PRO:HA	1:A:355:LEU:HD23	1.99	0.43
1:B:986:VAL:HG21	1:B:1010:PHE:CZ	2.54	0.43
1:C:137:ARG:HG2	1:C:255:TYR:CE1	2.50	0.43
1:D:1010:PHE:HB3	1:D:1014:THR:OG1	2.19	0.43
1:F:566:GLY:HA3	1:F:624:GLN:HG3	2.00	0.43
1:F:589:THR:HB	1:F:592:LEU:HB2	2.00	0.43
1:A:254:ASP:OD1	1:A:254:ASP:N	2.52	0.43
1:B:940:ASP:OD1	1:B:940:ASP:N	2.51	0.43
1:D:137:ARG:HG2	1:D:255:TYR:CE1	2.50	0.43
1:D:254:ASP:OD1	1:D:254:ASP:N	2.52	0.43
1:E:172:ARG:HB2	1:E:371:LEU:HB2	2.00	0.43
1:E:322:TRP:CE3	1:E:323:GLN:HB2	2.54	0.43
1:F:254:ASP:OD1	1:F:254:ASP:N	2.52	0.43
1:F:358:LEU:HB3	1:F:362:LEU:HD11	2.00	0.43
1:F:641:ASP:OD1	1:F:642:PHE:N	2.51	0.43
1:F:986:VAL:HG21	1:F:1010:PHE:CZ	2.54	0.43
1:B:254:ASP:N	1:B:254:ASP:OD1	2.52	0.43
1:B:566:GLY:HA3	1:B:624:GLN:HG3	2.00	0.43
1:D:172:ARG:HB2	1:D:371:LEU:HB2	2.00	0.43
1:D:358:LEU:HB3	1:D:362:LEU:HD11	2.00	0.43
1:E:254:ASP:N	1:E:254:ASP:OD1	2.52	0.43
1:E:305:ASP:OD2	1:E:354:ALA:HB2	2.18	0.43
1:A:322:TRP:CE3	1:A:323:GLN:HB2	2.54	0.43
1:B:358:LEU:HB3	1:B:362:LEU:HD11	2.00	0.43
1:B:374:SER:H	1:B:377:LYS:HB2	1.82	0.43
1:B:589:THR:HB	1:B:592:LEU:HB2	2.00	0.43
1:C:172:ARG:HB2	1:C:371:LEU:HB2	2.00	0.43
1:C:358:LEU:HB3	1:C:362:LEU:HD11	2.00	0.43
1:A:305:ASP:OD2	1:A:354:ALA:HB2	2.18	0.43
1:A:327:ARG:HB3	1:A:330:ILE:HB	2.01	0.43
1:A:573:LEU:HD23	1:A:576:VAL:HG11	2.01	0.43
1:A:878:LYS:O	1:A:881:ASN:ND2	2.50	0.43
1:C:257:PHE:CD2	1:C:297:ILE:HG23	2.54	0.43
1:C:305:ASP:OD2	1:C:354:ALA:HB2	2.18	0.43
1:C:573:LEU:HD23	1:C:576:VAL:HG11	2.01	0.43
1:C:986:VAL:HG21	1:C:1010:PHE:CZ	2.54	0.43
1:D:305:ASP:OD2	1:D:354:ALA:HB2	2.18	0.43
1:D:362:LEU:HD22	1:D:365:PRO:HB3	2.00	0.43
1:D:573:LEU:HD23	1:D:576:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:573:LEU:HD23	1:E:576:VAL:HG11	2.01	0.43
1:A:1010:PHE:HB3	1:A:1014:THR:OG1	2.19	0.43
1:C:362:LEU:HD22	1:C:365:PRO:HB3	2.01	0.43
1:C:512:VAL:HG12	1:C:514:CYS:H	1.84	0.43
1:C:566:GLY:HA3	1:C:624:GLN:HG3	2.00	0.43
1:D:257:PHE:CD2	1:D:297:ILE:HG23	2.54	0.43
1:D:566:GLY:HA3	1:D:624:GLN:HG3	2.00	0.43
1:D:986:VAL:HG21	1:D:1010:PHE:CZ	2.54	0.43
1:E:450:LEU:HD12	1:E:505:MET:HE1	2.01	0.43
1:E:986:VAL:HG21	1:E:1010:PHE:CZ	2.54	0.43
1:E:1010:PHE:HB3	1:E:1014:THR:OG1	2.19	0.43
1:B:172:ARG:HB2	1:B:371:LEU:HB2	2.00	0.43
1:B:305:ASP:OD2	1:B:354:ALA:HB2	2.18	0.43
1:D:512:VAL:HG12	1:D:514:CYS:H	1.84	0.43
1:E:327:ARG:HB3	1:E:330:ILE:HB	2.01	0.43
1:E:878:LYS:O	1:E:881:ASN:ND2	2.50	0.43
1:A:450:LEU:HD12	1:A:505:MET:HE1	2.01	0.42
1:A:641:ASP:OD1	1:A:642:PHE:N	2.51	0.42
1:A:986:VAL:HG21	1:A:1010:PHE:CZ	2.54	0.42
1:B:624:GLN:HG2	1:B:625:PRO:CD	2.41	0.42
1:E:641:ASP:OD1	1:E:642:PHE:N	2.51	0.42
1:F:305:ASP:OD2	1:F:354:ALA:HB2	2.18	0.42
1:A:405:LEU:HA	1:A:408:MET:HE2	2.00	0.42
1:C:322:TRP:CE3	1:C:323:GLN:HB2	2.54	0.42
1:D:322:TRP:CE3	1:D:323:GLN:HB2	2.54	0.42
1:B:362:LEU:HD22	1:B:365:PRO:HB3	2.00	0.42
1:B:878:LYS:O	1:B:881:ASN:ND2	2.50	0.42
1:C:327:ARG:HB3	1:C:330:ILE:HB	2.01	0.42
1:E:755:ASP:OD2	1:E:783:SER:OG	2.31	0.42
1:F:374:SER:H	1:F:377:LYS:HB2	1.82	0.42
1:A:257:PHE:CD2	1:A:297:ILE:HG23	2.54	0.42
1:B:534:TYR:HA	1:B:554:PRO:HB3	2.01	0.42
1:B:787:CYS:HB3	1:B:818:LEU:HG	2.02	0.42
1:B:1010:PHE:HB3	1:B:1014:THR:OG1	2.19	0.42
1:D:589:THR:HB	1:D:592:LEU:HB2	2.00	0.42
1:E:257:PHE:CD2	1:E:297:ILE:HG23	2.54	0.42
1:F:172:ARG:HB2	1:F:371:LEU:HB2	2.00	0.42
1:F:787:CYS:HB3	1:F:818:LEU:HG	2.01	0.42
1:F:878:LYS:O	1:F:881:ASN:ND2	2.50	0.42
1:B:470:CYS:SG	1:B:533:TYR:HB2	2.59	0.42
1:C:534:TYR:HA	1:C:554:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:589:THR:HB	1:C:592:LEU:HB2	2.00	0.42
1:D:327:ARG:HB3	1:D:330:ILE:HB	2.01	0.42
1:D:534:TYR:HA	1:D:554:PRO:HB3	2.01	0.42
1:F:362:LEU:HD22	1:F:365:PRO:HB3	2.00	0.42
1:F:1010:PHE:HB3	1:F:1014:THR:OG1	2.19	0.42
1:A:470:CYS:SG	1:A:533:TYR:HB2	2.59	0.42
1:A:510:LYS:HD2	1:A:510:LYS:HA	1.84	0.42
1:B:774:ARG:HG2	1:B:802:GLU:HB2	2.02	0.42
1:D:470:CYS:SG	1:D:533:TYR:HB2	2.60	0.42
1:E:566:GLY:HA3	1:E:624:GLN:HG3	2.00	0.42
1:F:534:TYR:HA	1:F:554:PRO:HB3	2.01	0.42
1:C:470:CYS:SG	1:C:533:TYR:HB2	2.60	0.42
1:C:787:CYS:HB3	1:C:818:LEU:HG	2.01	0.42
1:D:787:CYS:HB3	1:D:818:LEU:HG	2.01	0.42
1:D:955:SER:HB3	1:D:982:GLY:N	2.30	0.42
1:E:534:TYR:HA	1:E:554:PRO:HB3	2.01	0.42
1:F:243:TRP:HD1	1:F:248:LEU:O	2.03	0.42
1:F:470:CYS:SG	1:F:533:TYR:HB2	2.60	0.42
1:F:624:GLN:HG2	1:F:625:PRO:CD	2.41	0.42
1:F:774:ARG:HG2	1:F:802:GLU:HB2	2.02	0.42
1:A:534:TYR:HA	1:A:554:PRO:HB3	2.01	0.42
1:A:589:THR:HB	1:A:592:LEU:HB2	2.00	0.42
1:A:888:LYS:HE2	1:A:916:HIS:CG	2.55	0.42
1:B:243:TRP:HD1	1:B:248:LEU:O	2.03	0.42
1:D:641:ASP:OD1	1:D:642:PHE:N	2.51	0.42
1:E:470:CYS:SG	1:E:533:TYR:HB2	2.60	0.42
1:F:512:VAL:HG12	1:F:514:CYS:H	1.84	0.42
1:A:566:GLY:HA3	1:A:624:GLN:HG3	2.00	0.42
1:B:635:TYR:CB	1:B:665:VAL:HG23	2.50	0.42
1:B:888:LYS:HE2	1:B:916:HIS:CG	2.55	0.42
1:C:243:TRP:HD1	1:C:248:LEU:O	2.03	0.42
1:C:266:LEU:HD13	1:C:329:ASP:OD1	2.20	0.42
1:C:955:SER:HB3	1:C:982:GLY:N	2.30	0.42
1:D:243:TRP:HD1	1:D:248:LEU:O	2.03	0.42
1:D:266:LEU:HD13	1:D:329:ASP:OD1	2.20	0.42
1:E:243:TRP:HD1	1:E:248:LEU:O	2.03	0.42
1:E:888:LYS:HE2	1:E:916:HIS:CG	2.55	0.42
1:F:322:TRP:CE3	1:F:323:GLN:HB2	2.54	0.42
1:A:358:LEU:HB3	1:A:362:LEU:CD1	2.50	0.42
1:A:767:HIS:ND1	1:A:768:PRO:O	2.53	0.42
1:A:914:LEU:HD21	1:A:917:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:MET:HG3	1:B:256:LEU:HD23	2.01	0.42
1:B:266:LEU:HD13	1:B:329:ASP:OD1	2.20	0.42
1:B:388:ASP:OD1	1:B:388:ASP:N	2.50	0.42
1:B:512:VAL:HG12	1:B:514:CYS:H	1.84	0.42
1:C:230:ILE:HA	1:C:412:PRO:HD2	2.02	0.42
1:C:641:ASP:OD1	1:C:642:PHE:N	2.51	0.42
1:D:888:LYS:HE2	1:D:916:HIS:CG	2.55	0.42
1:E:510:LYS:HD2	1:E:510:LYS:HA	1.84	0.42
1:E:767:HIS:ND1	1:E:768:PRO:O	2.53	0.42
1:E:914:LEU:HD21	1:E:917:LEU:HB2	2.02	0.42
1:F:230:ILE:HA	1:F:412:PRO:HD2	2.02	0.42
1:F:266:LEU:HD13	1:F:329:ASP:OD1	2.20	0.42
1:F:635:TYR:CB	1:F:665:VAL:HG23	2.50	0.42
1:F:888:LYS:HE2	1:F:916:HIS:CG	2.55	0.42
1:A:240:MET:HG3	1:A:256:LEU:HD23	2.01	0.41
1:B:358:LEU:HB3	1:B:362:LEU:CD1	2.50	0.41
1:B:767:HIS:ND1	1:B:768:PRO:O	2.53	0.41
1:C:635:TYR:CB	1:C:665:VAL:HG23	2.50	0.41
1:C:888:LYS:HE2	1:C:916:HIS:CG	2.55	0.41
1:D:230:ILE:HA	1:D:412:PRO:HD2	2.02	0.41
1:E:266:LEU:HD13	1:E:329:ASP:OD1	2.20	0.41
1:E:358:LEU:HB3	1:E:362:LEU:CD1	2.50	0.41
1:E:589:THR:HB	1:E:592:LEU:HB2	2.00	0.41
1:F:240:MET:HG3	1:F:256:LEU:HD23	2.02	0.41
1:F:257:PHE:CD2	1:F:297:ILE:HG23	2.54	0.41
1:A:243:TRP:HD1	1:A:248:LEU:O	2.03	0.41
1:A:257:PHE:HD2	1:A:297:ILE:HG23	1.85	0.41
1:A:622:GLN:O	1:A:625:PRO:HD2	2.21	0.41
1:A:787:CYS:HB3	1:A:818:LEU:HG	2.02	0.41
1:B:257:PHE:CD2	1:B:297:ILE:HG23	2.54	0.41
1:C:257:PHE:HD2	1:C:297:ILE:HG23	1.85	0.41
1:D:257:PHE:HD2	1:D:297:ILE:HG23	1.85	0.41
1:E:787:CYS:HB3	1:E:818:LEU:HG	2.02	0.41
1:F:358:LEU:HB3	1:F:362:LEU:CD1	2.50	0.41
1:F:767:HIS:ND1	1:F:768:PRO:O	2.53	0.41
1:A:266:LEU:HD13	1:A:329:ASP:OD1	2.20	0.41
1:B:230:ILE:HA	1:B:412:PRO:HD2	2.02	0.41
1:B:322:TRP:CE3	1:B:323:GLN:HB2	2.54	0.41
1:B:327:ARG:HB3	1:B:330:ILE:HB	2.01	0.41
1:C:914:LEU:HD21	1:C:917:LEU:HB2	2.02	0.41
1:D:635:TYR:CB	1:D:665:VAL:HG23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:914:LEU:HD21	1:D:917:LEU:HB2	2.02	0.41
1:E:257:PHE:HD2	1:E:297:ILE:HG23	1.85	0.41
1:E:622:GLN:O	1:E:625:PRO:HD2	2.21	0.41
1:F:327:ARG:HB3	1:F:330:ILE:HB	2.01	0.41
1:F:388:ASP:OD1	1:F:388:ASP:N	2.50	0.41
1:F:914:LEU:HD21	1:F:917:LEU:HB2	2.02	0.41
1:D:857:LEU:HD12	1:D:857:LEU:HA	1.89	0.41
1:E:225:GLN:HE22	1:E:367:HIS:HB3	1.86	0.41
1:B:914:LEU:HD21	1:B:917:LEU:HB2	2.02	0.41
1:C:1011:ASN:O	1:C:1015:LYS:HG2	2.21	0.41
1:D:240:MET:HG3	1:D:256:LEU:HD23	2.02	0.41
1:D:1011:ASN:O	1:D:1015:LYS:HG2	2.21	0.41
1:E:240:MET:HG3	1:E:256:LEU:HD23	2.02	0.41
1:F:1011:ASN:O	1:F:1015:LYS:HG2	2.21	0.41
1:F:425:GLN:O	1:F:429:GLY:N	2.33	0.41
1:A:225:GLN:HE22	1:A:367:HIS:HB3	1.86	0.41
1:A:527:GLU:OE1	1:A:575:PHE:HB2	2.21	0.41
1:A:774:ARG:HG2	1:A:802:GLU:HB2	2.02	0.41
1:B:573:LEU:HD23	1:B:576:VAL:HG11	2.01	0.41
1:B:1011:ASN:O	1:B:1015:LYS:HG2	2.21	0.41
1:C:254:ASP:OD1	1:C:254:ASP:N	2.52	0.41
1:E:527:GLU:OE1	1:E:575:PHE:HB2	2.21	0.41
1:E:774:ARG:HG2	1:E:802:GLU:HB2	2.02	0.41
1:F:257:PHE:HD2	1:F:297:ILE:HG23	1.85	0.41
1:B:480:GLN:NE2	1:B:570:LYS:HA	2.27	0.41
1:C:240:MET:HG3	1:C:256:LEU:HD23	2.02	0.41
1:D:774:ARG:HG2	1:D:802:GLU:HB2	2.02	0.41
1:E:959:TRP:O	1:E:962:SER:OG	2.34	0.41
1:F:573:LEU:HD23	1:F:576:VAL:HG11	2.01	0.41
1:A:512:VAL:HG12	1:A:514:CYS:H	1.84	0.41
1:A:959:TRP:O	1:A:962:SER:OG	2.34	0.41
1:B:225:GLN:HE22	1:B:367:HIS:HB3	1.86	0.41
1:B:257:PHE:HD2	1:B:297:ILE:HG23	1.85	0.41
1:B:425:GLN:O	1:B:429:GLY:N	2.33	0.41
1:C:358:LEU:HB3	1:C:362:LEU:CD1	2.50	0.41
1:C:499:VAL:O	1:C:503:LEU:N	2.52	0.41
1:C:774:ARG:HG2	1:C:802:GLU:HB2	2.02	0.41
1:D:358:LEU:HB3	1:D:362:LEU:CD1	2.50	0.41
1:D:499:VAL:O	1:D:503:LEU:N	2.52	0.41
1:D:581:PHE:HD1	1:D:637:MET:HE1	1.86	0.41
1:E:373:PHE:N	1:E:410:PHE:O	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:225:GLN:HE22	1:F:367:HIS:HB3	1.86	0.41
1:A:635:TYR:CB	1:A:665:VAL:HG23	2.50	0.41
1:B:622:GLN:O	1:B:625:PRO:HD2	2.20	0.41
1:C:581:PHE:HD1	1:C:637:MET:HE1	1.86	0.41
1:E:512:VAL:HG12	1:E:514:CYS:H	1.84	0.41
1:F:527:GLU:OE1	1:F:575:PHE:HB2	2.21	0.41
1:A:388:ASP:OD1	1:A:388:ASP:N	2.50	0.40
1:B:527:GLU:OE1	1:B:575:PHE:HB2	2.21	0.40
1:C:635:TYR:HB2	1:C:665:VAL:HG23	2.04	0.40
1:D:553:LEU:HG	1:D:554:PRO:HD2	2.03	0.40
1:D:959:TRP:O	1:D:962:SER:OG	2.34	0.40
1:E:534:TYR:CE1	1:E:554:PRO:HA	2.57	0.40
1:E:635:TYR:CB	1:E:665:VAL:HG23	2.50	0.40
1:E:1011:ASN:O	1:E:1015:LYS:HG2	2.21	0.40
1:A:230:ILE:HA	1:A:412:PRO:HD2	2.02	0.40
1:A:373:PHE:N	1:A:410:PHE:O	2.46	0.40
1:A:534:TYR:CE1	1:A:554:PRO:HA	2.57	0.40
1:A:652:LYS:HE3	1:A:652:LYS:HB2	1.93	0.40
1:A:1011:ASN:O	1:A:1015:LYS:HG2	2.21	0.40
1:C:534:TYR:CE1	1:C:554:PRO:HA	2.57	0.40
1:D:534:TYR:CE1	1:D:554:PRO:HA	2.57	0.40
1:D:635:TYR:HB2	1:D:665:VAL:HG23	2.04	0.40
1:F:286:PRO:HA	1:F:290:ILE:HG12	2.04	0.40
1:F:499:VAL:O	1:F:503:LEU:N	2.52	0.40
1:A:388:ASP:OD1	1:A:391:GLN:NE2	2.49	0.40
1:B:286:PRO:HA	1:B:290:ILE:HG12	2.04	0.40
1:B:499:VAL:O	1:B:503:LEU:N	2.52	0.40
1:C:286:PRO:HA	1:C:290:ILE:HG12	2.04	0.40
1:D:286:PRO:HA	1:D:290:ILE:HG12	2.04	0.40
1:E:230:ILE:HA	1:E:412:PRO:HD2	2.02	0.40
1:E:388:ASP:OD1	1:E:388:ASP:N	2.50	0.40
1:A:553:LEU:HG	1:A:554:PRO:HD2	2.03	0.40
1:C:553:LEU:HG	1:C:554:PRO:HD2	2.04	0.40
1:C:767:HIS:ND1	1:C:768:PRO:O	2.53	0.40
1:D:767:HIS:ND1	1:D:768:PRO:O	2.53	0.40
1:D:940:ASP:OD1	1:D:940:ASP:N	2.51	0.40
1:F:480:GLN:NE2	1:F:570:LYS:HA	2.27	0.40
1:F:622:GLN:O	1:F:625:PRO:HD2	2.21	0.40
1:A:566:GLY:CA	1:A:624:GLN:HG3	2.52	0.40
1:B:175:LYS:HD2	1:B:209:PHE:CD1	2.57	0.40
1:C:566:GLY:CA	1:C:624:GLN:HG3	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:940:ASP:OD1	1:C:940:ASP:N	2.51	0.40
1:C:959:TRP:O	1:C:962:SER:OG	2.34	0.40
1:D:527:GLU:OE1	1:D:575:PHE:HB2	2.21	0.40
1:D:566:GLY:CA	1:D:624:GLN:HG3	2.52	0.40
1:D:622:GLN:O	1:D:625:PRO:HD2	2.21	0.40
1:D:1034:PRO:O	1:E:281:PRO:HG2	2.22	0.40
1:E:388:ASP:OD1	1:E:391:GLN:NE2	2.49	0.40
1:E:553:LEU:HG	1:E:554:PRO:HD2	2.03	0.40
1:E:566:GLY:CA	1:E:624:GLN:HG3	2.52	0.40
1:F:175:LYS:HD2	1:F:209:PHE:CD1	2.57	0.40
1:F:214:GLU:H	1:F:214:GLU:CD	2.25	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	797/924 (86%)	746 (94%)	51 (6%)	0	100	100
1	B	797/924 (86%)	748 (94%)	49 (6%)	0	100	100
1	C	797/924 (86%)	749 (94%)	48 (6%)	0	100	100
1	D	797/924 (86%)	748 (94%)	49 (6%)	0	100	100
1	E	797/924 (86%)	749 (94%)	48 (6%)	0	100	100
1	F	797/924 (86%)	745 (94%)	52 (6%)	0	100	100
All	All	4782/5544 (86%)	4485 (94%)	297 (6%)	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	733/834 (88%)	728 (99%)	5 (1%)	84 92
1	B	733/834 (88%)	728 (99%)	5 (1%)	84 92
1	C	733/834 (88%)	728 (99%)	5 (1%)	84 92
1	D	733/834 (88%)	728 (99%)	5 (1%)	84 92
1	E	733/834 (88%)	728 (99%)	5 (1%)	84 92
1	F	733/834 (88%)	728 (99%)	5 (1%)	84 92
All	All	4398/5004 (88%)	4368 (99%)	30 (1%)	84 92

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	240	MET
1	A	276	ILE
1	A	523	MET
1	A	779	ARG
1	A	1013	GLU
1	B	240	MET
1	B	276	ILE
1	B	523	MET
1	B	779	ARG
1	B	1013	GLU
1	C	240	MET
1	C	276	ILE
1	C	523	MET
1	C	779	ARG
1	C	1013	GLU
1	D	240	MET
1	D	276	ILE
1	D	523	MET
1	D	779	ARG
1	D	1013	GLU
1	E	240	MET
1	E	276	ILE

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Mol	Chain	Res	Type
1	E	523	MET
1	E	779	ARG
1	E	1013	GLU
1	F	240	MET
1	F	276	ILE
1	F	523	MET
1	F	779	ARG
1	F	1013	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	HIS
1	A	269	GLN
1	A	480	GLN
1	A	911	ASN
1	B	215	HIS
1	B	269	GLN
1	B	480	GLN
1	B	911	ASN
1	C	215	HIS
1	C	269	GLN
1	C	480	GLN
1	C	911	ASN
1	D	215	HIS
1	D	269	GLN
1	D	480	GLN
1	D	911	ASN
1	E	215	HIS
1	E	269	GLN
1	E	480	GLN
1	E	911	ASN
1	F	215	HIS
1	F	269	GLN
1	F	480	GLN
1	F	911	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADP	F	1101	-	24,29,29	0.94	1 (4%)	29,45,45	1.47	4 (13%)
2	ADP	C	1101	-	24,29,29	0.95	1 (4%)	29,45,45	1.48	4 (13%)
2	ADP	A	1101	-	24,29,29	0.95	1 (4%)	29,45,45	1.48	4 (13%)
2	ADP	B	1101	-	24,29,29	0.95	1 (4%)	29,45,45	1.47	4 (13%)
2	ADP	E	1101	-	24,29,29	0.95	1 (4%)	29,45,45	1.48	4 (13%)
2	ADP	D	1101	-	24,29,29	0.94	1 (4%)	29,45,45	1.48	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	F	1101	-	-	4/12/32/32	0/3/3/3
2	ADP	C	1101	-	-	4/12/32/32	0/3/3/3
2	ADP	A	1101	-	-	4/12/32/32	0/3/3/3
2	ADP	B	1101	-	-	4/12/32/32	0/3/3/3
2	ADP	E	1101	-	-	4/12/32/32	0/3/3/3
2	ADP	D	1101	-	-	4/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1101	ADP	C5-C4	2.48	1.47	1.40
2	A	1101	ADP	C5-C4	2.48	1.47	1.40
2	B	1101	ADP	C5-C4	2.45	1.47	1.40
2	C	1101	ADP	C5-C4	2.45	1.47	1.40
2	F	1101	ADP	C5-C4	2.44	1.47	1.40
2	E	1101	ADP	C5-C4	2.43	1.47	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1101	ADP	PA-O3A-PB	-3.62	120.41	132.83
2	A	1101	ADP	PA-O3A-PB	-3.61	120.43	132.83
2	E	1101	ADP	PA-O3A-PB	-3.61	120.43	132.83
2	B	1101	ADP	PA-O3A-PB	-3.61	120.44	132.83
2	C	1101	ADP	PA-O3A-PB	-3.61	120.44	132.83
2	F	1101	ADP	PA-O3A-PB	-3.60	120.47	132.83
2	E	1101	ADP	C3'-C2'-C1'	3.29	105.93	100.98
2	A	1101	ADP	C3'-C2'-C1'	3.29	105.92	100.98
2	C	1101	ADP	C3'-C2'-C1'	3.28	105.91	100.98
2	F	1101	ADP	C3'-C2'-C1'	3.27	105.91	100.98
2	B	1101	ADP	C3'-C2'-C1'	3.27	105.90	100.98
2	D	1101	ADP	C3'-C2'-C1'	3.26	105.88	100.98
2	F	1101	ADP	N3-C2-N1	-3.19	123.69	128.68
2	C	1101	ADP	N3-C2-N1	-3.18	123.71	128.68
2	E	1101	ADP	N3-C2-N1	-3.16	123.74	128.68
2	A	1101	ADP	N3-C2-N1	-3.15	123.75	128.68
2	D	1101	ADP	N3-C2-N1	-3.13	123.78	128.68
2	B	1101	ADP	N3-C2-N1	-3.12	123.79	128.68
2	D	1101	ADP	C4-C5-N7	-2.68	106.61	109.40
2	A	1101	ADP	C4-C5-N7	-2.66	106.62	109.40
2	C	1101	ADP	C4-C5-N7	-2.65	106.64	109.40
2	E	1101	ADP	C4-C5-N7	-2.63	106.66	109.40
2	B	1101	ADP	C4-C5-N7	-2.63	106.66	109.40
2	F	1101	ADP	C4-C5-N7	-2.61	106.67	109.40

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1101	ADP	C5'-O5'-PA-O1A
2	E	1101	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	F	1101	ADP	C5'-O5'-PA-O1A
2	A	1101	ADP	C5'-O5'-PA-O3A
2	B	1101	ADP	C5'-O5'-PA-O3A
2	C	1101	ADP	C5'-O5'-PA-O3A
2	D	1101	ADP	C5'-O5'-PA-O3A
2	E	1101	ADP	C5'-O5'-PA-O3A
2	F	1101	ADP	C5'-O5'-PA-O3A
2	A	1101	ADP	C5'-O5'-PA-O2A
2	B	1101	ADP	C5'-O5'-PA-O2A
2	C	1101	ADP	C5'-O5'-PA-O2A
2	A	1101	ADP	C3'-C4'-C5'-O5'
2	B	1101	ADP	C3'-C4'-C5'-O5'
2	C	1101	ADP	C3'-C4'-C5'-O5'
2	D	1101	ADP	C3'-C4'-C5'-O5'
2	E	1101	ADP	C3'-C4'-C5'-O5'
2	F	1101	ADP	C3'-C4'-C5'-O5'
2	A	1101	ADP	O4'-C4'-C5'-O5'
2	C	1101	ADP	O4'-C4'-C5'-O5'
2	E	1101	ADP	O4'-C4'-C5'-O5'
2	F	1101	ADP	O4'-C4'-C5'-O5'
2	B	1101	ADP	O4'-C4'-C5'-O5'
2	D	1101	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

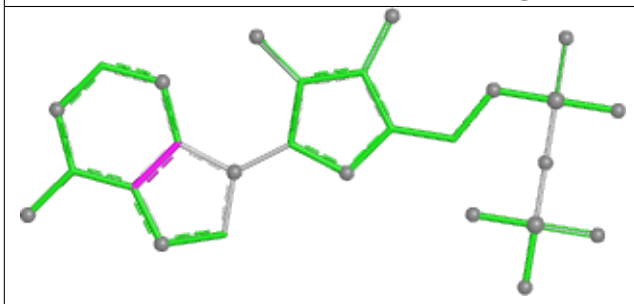
6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1101	ADP	1	0
2	C	1101	ADP	1	0
2	A	1101	ADP	1	0
2	B	1101	ADP	1	0
2	E	1101	ADP	1	0
2	D	1101	ADP	1	0

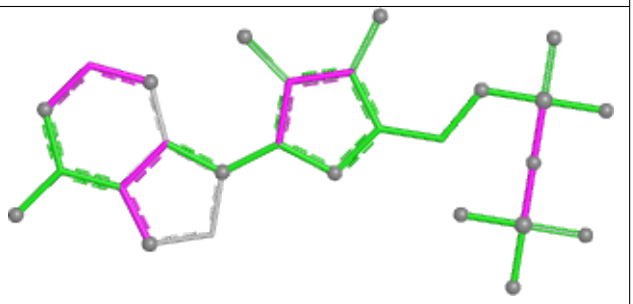
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

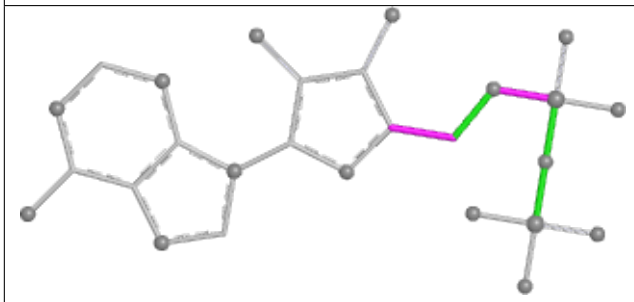
Ligand ADP F 1101



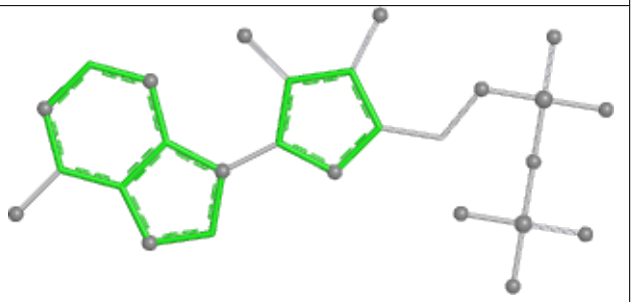
Bond lengths



Bond angles

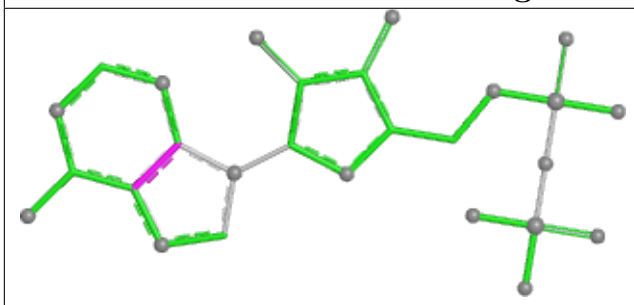


Torsions

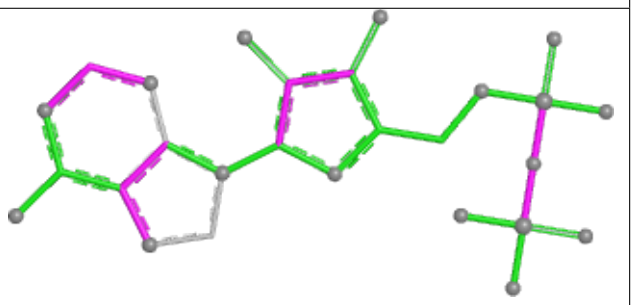


Rings

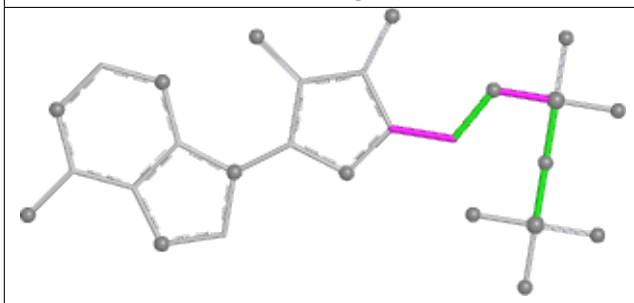
Ligand ADP C 1101



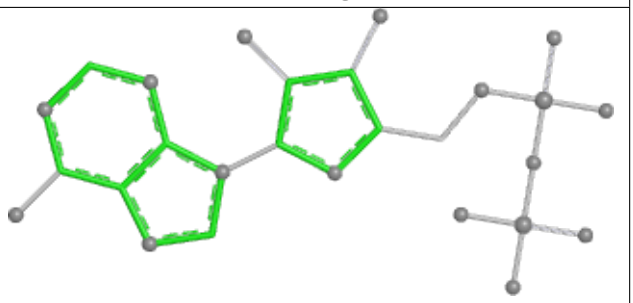
Bond lengths



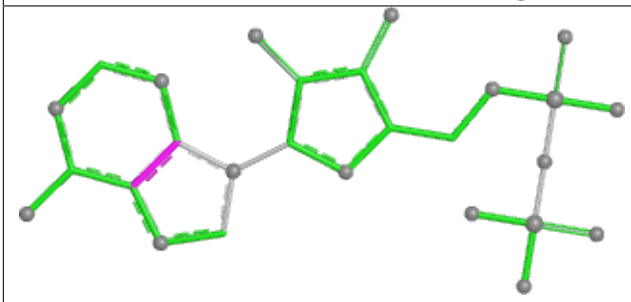
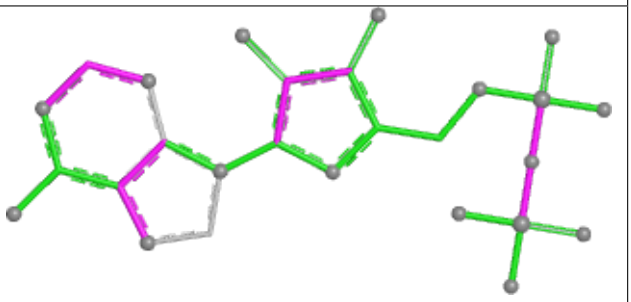
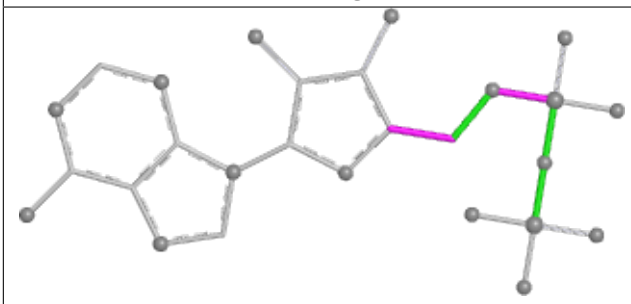
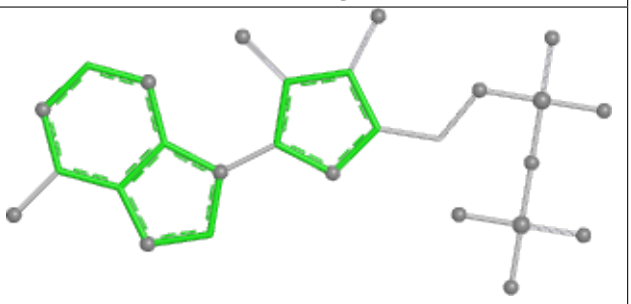
Bond angles

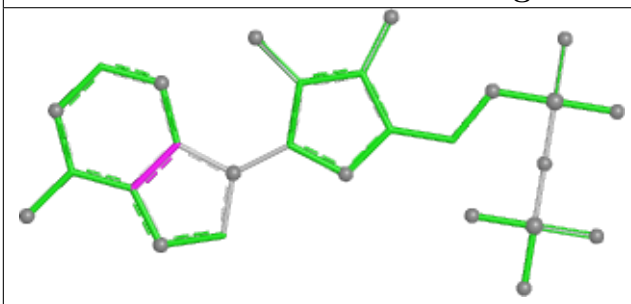
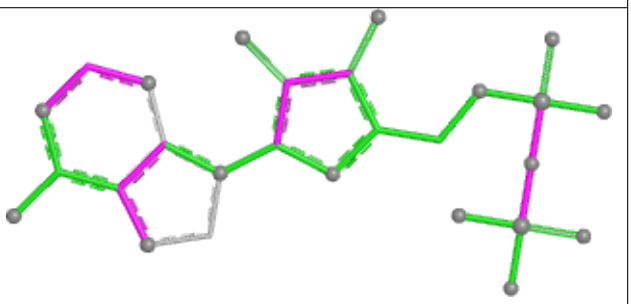
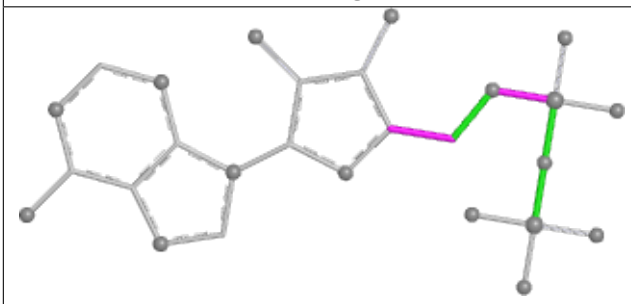
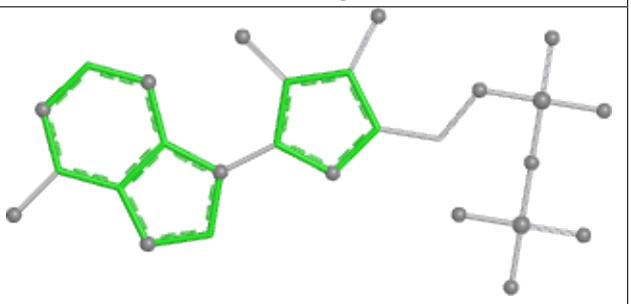


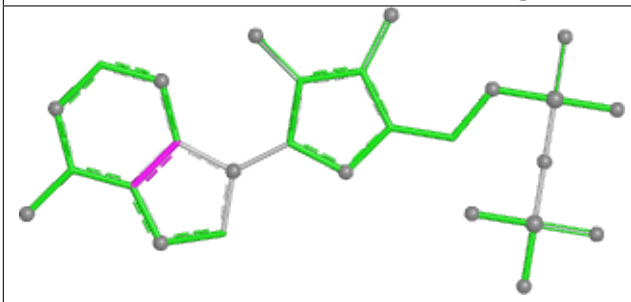
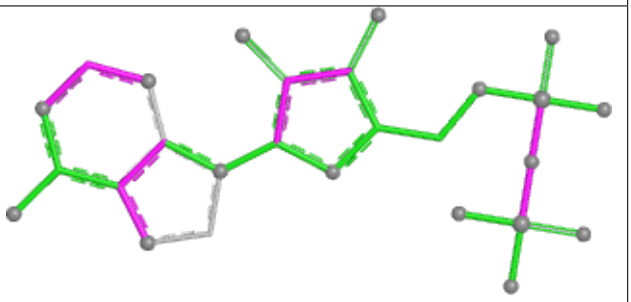
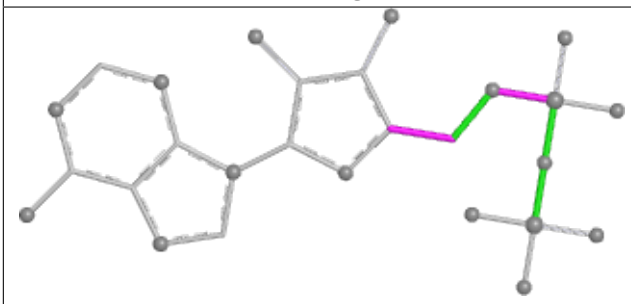
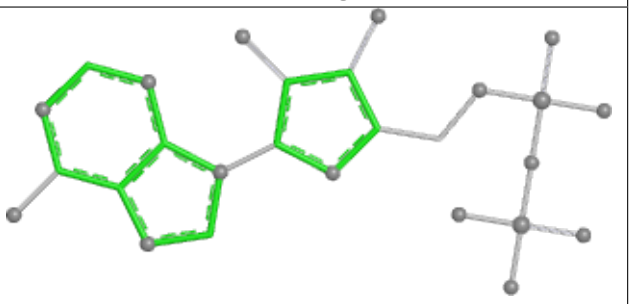
Torsions

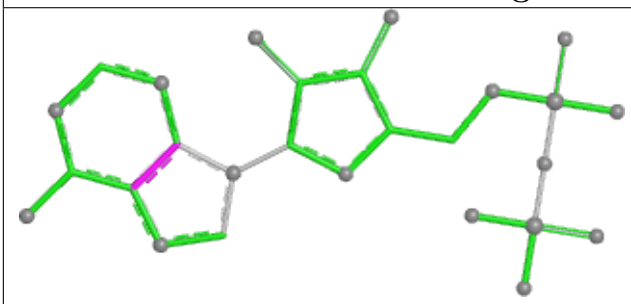
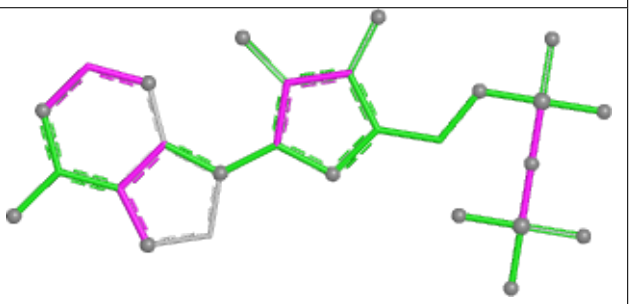
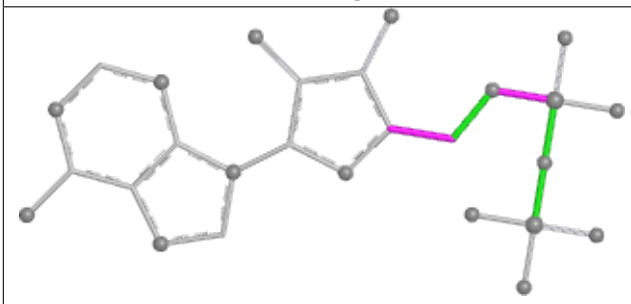
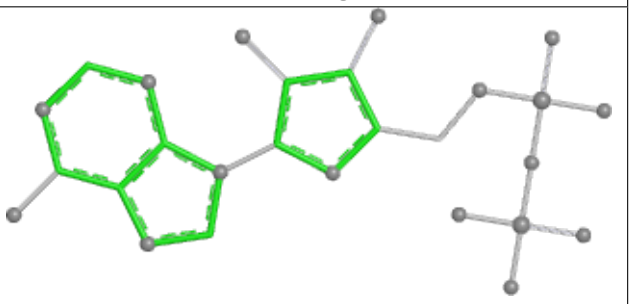


Rings

Ligand ADP A 1101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP B 1101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP E 1101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP D 1101	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

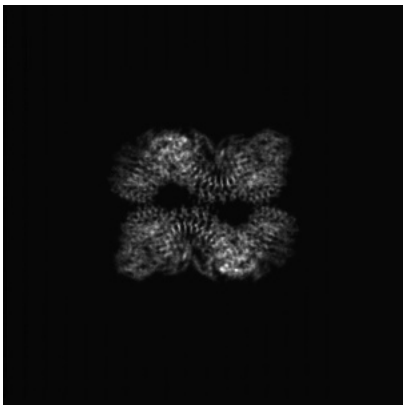
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14713. These allow visual inspection of the internal detail of the map and identification of artifacts.

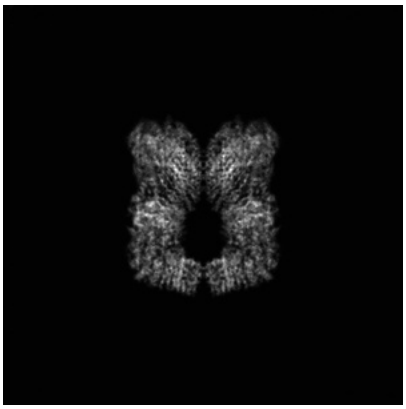
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

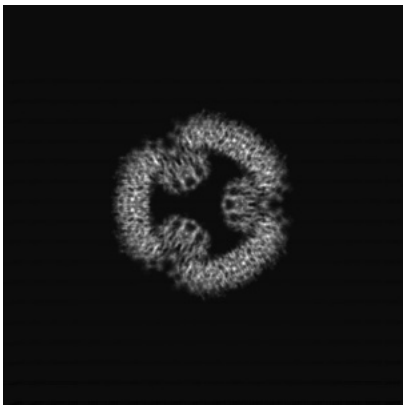
6.1.1 Primary map



X

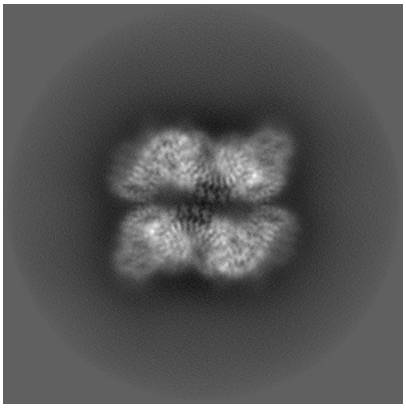


Y

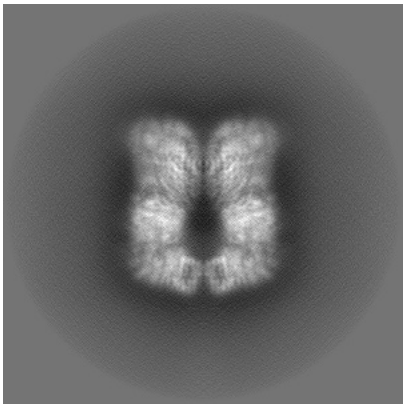


Z

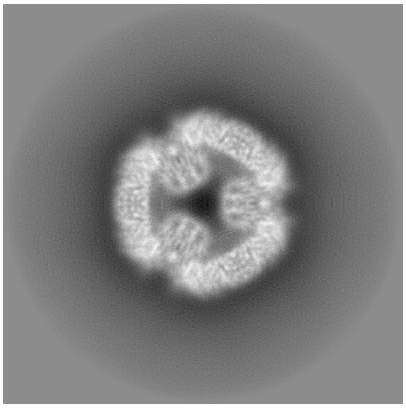
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

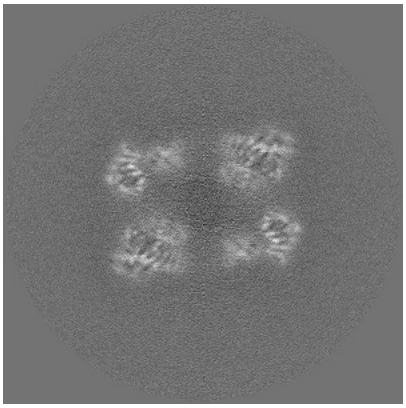
6.2.1 Primary map

X Index: 234

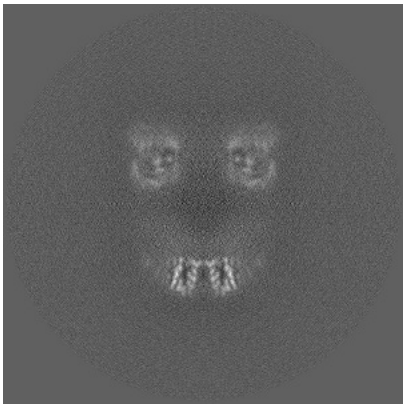
Y Index: 234

Z Index: 234

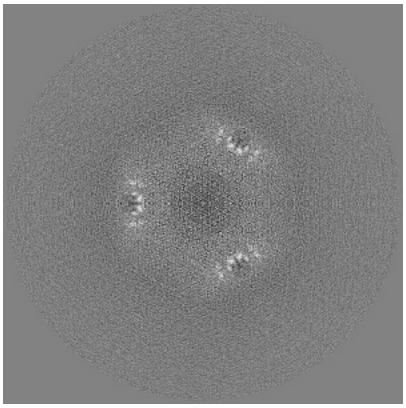
6.2.2 Raw map



X Index: 234



Y Index: 234



Z Index: 234

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

6.3 Largest variance slices (i)

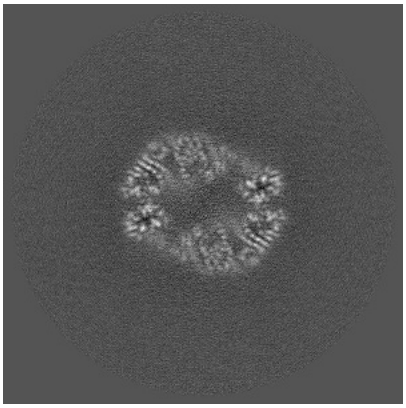
6.3.1 Primary map

X Index: 283

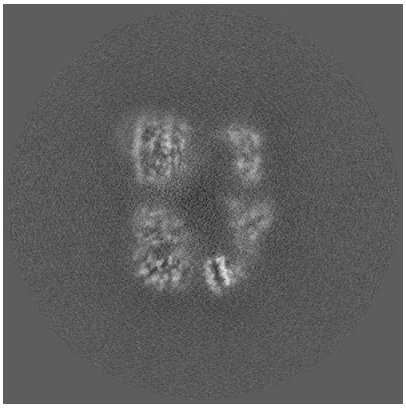
Y Index: 308

Z Index: 258

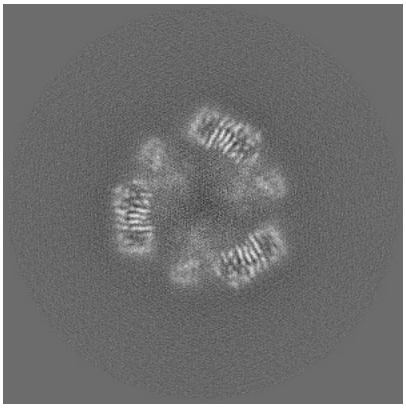
6.3.2 Raw map



X Index: 283



Y Index: 256



Z Index: 209

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

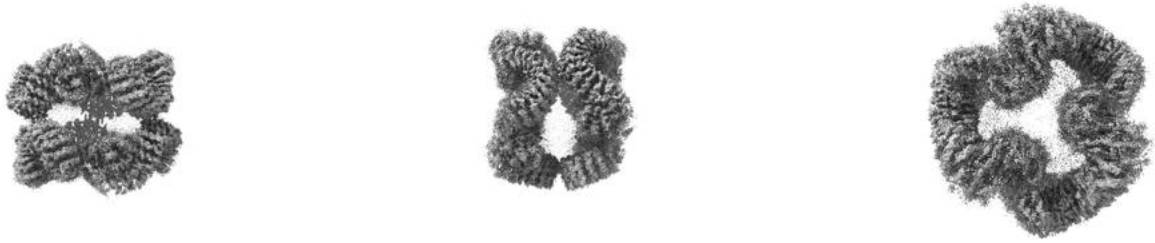
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

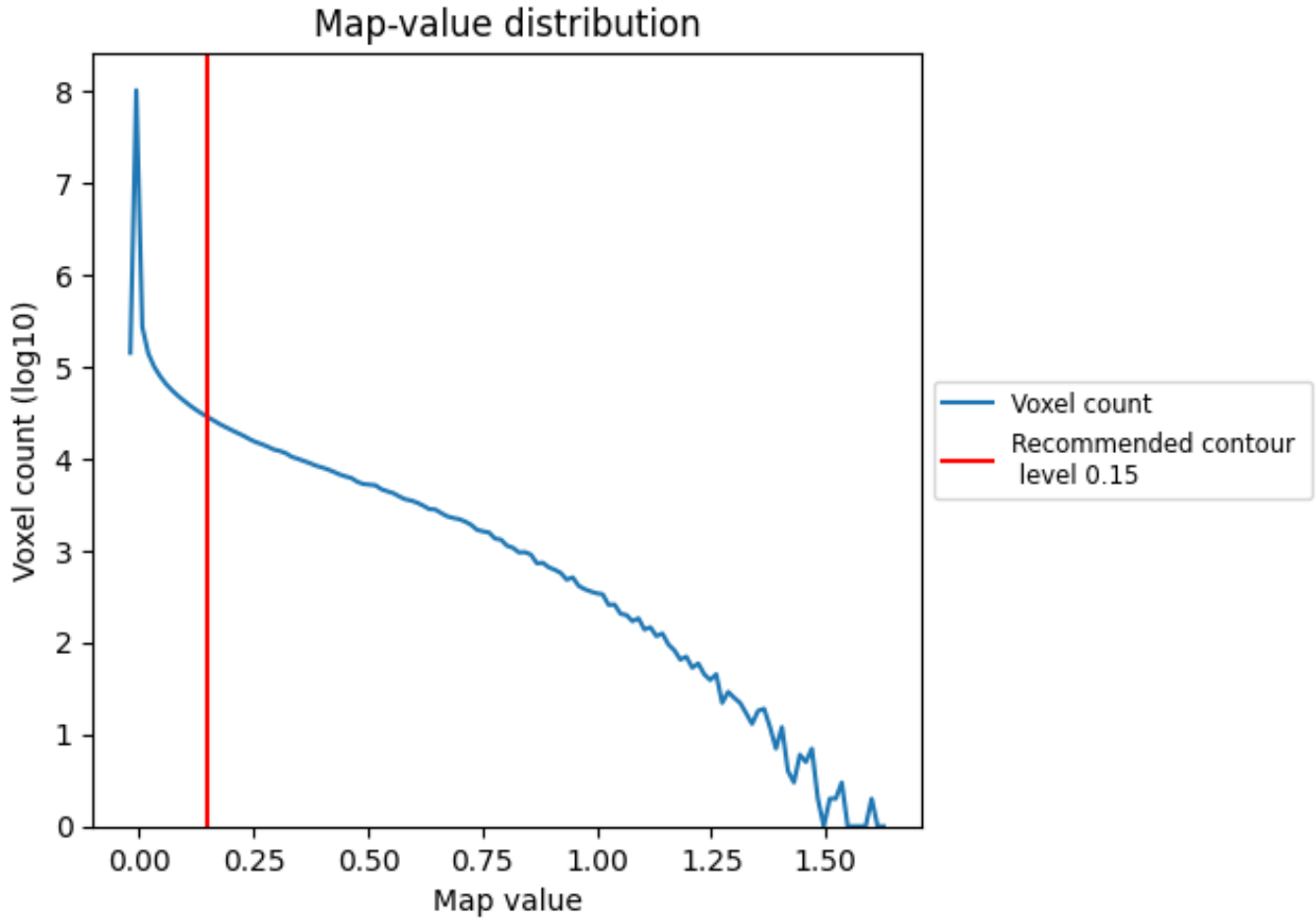
6.5 Mask visualisation (i)

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

7 Map analysis

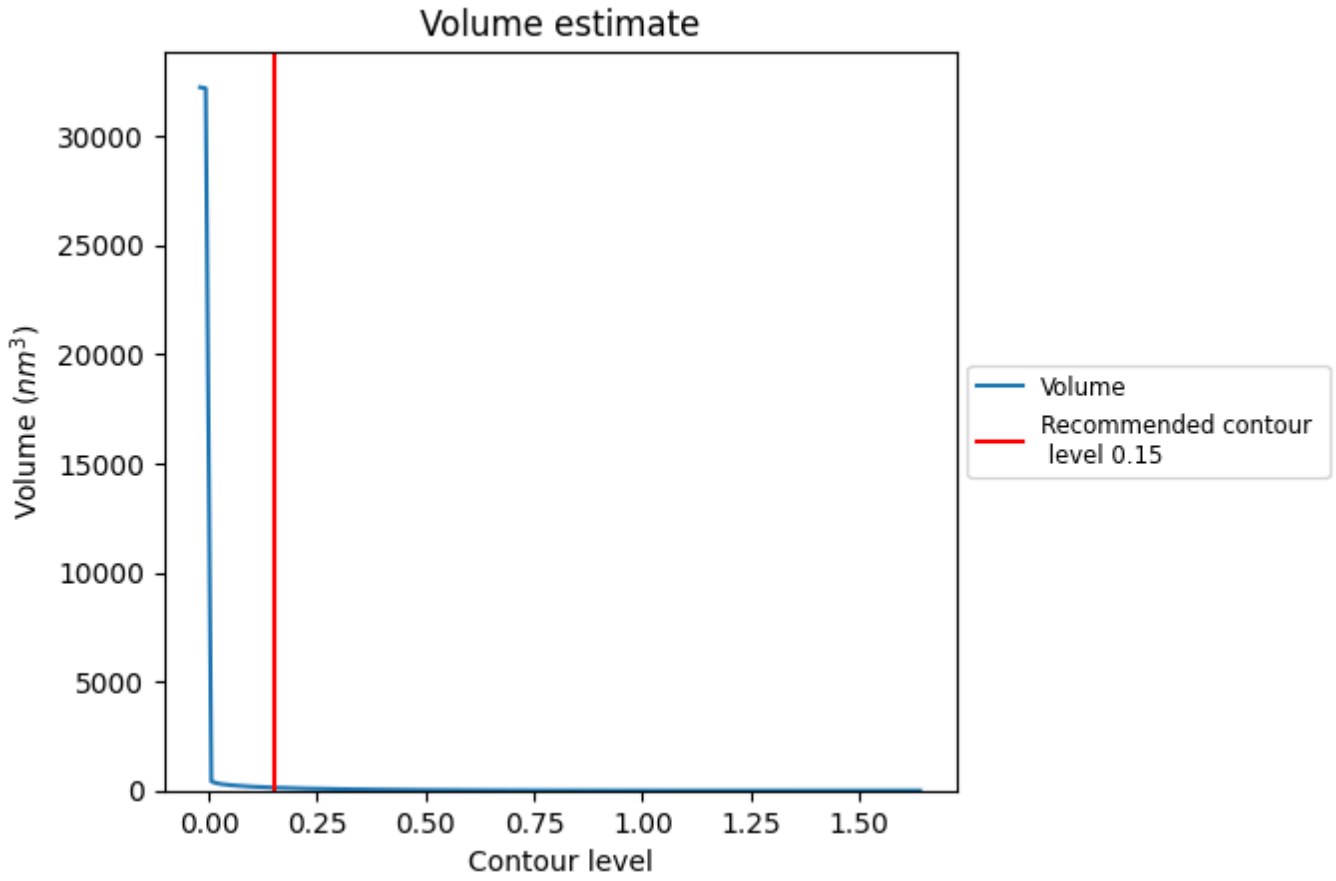
This section contains the results of statistical analysis of the map.

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.

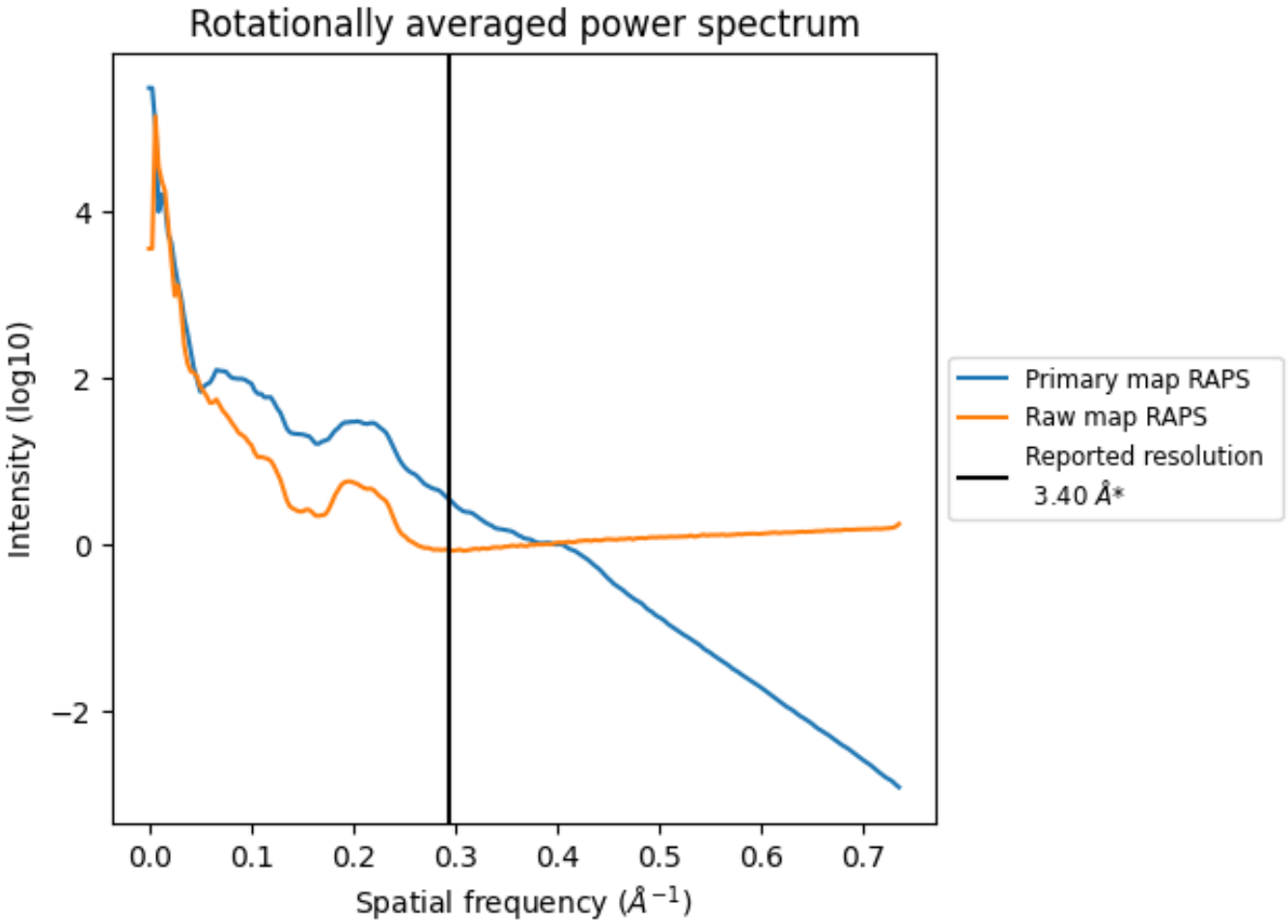
7.2 Volume estimate



The volume at the recommended contour level is 136 nm^3; this corresponds to an approximate mass of 123 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)

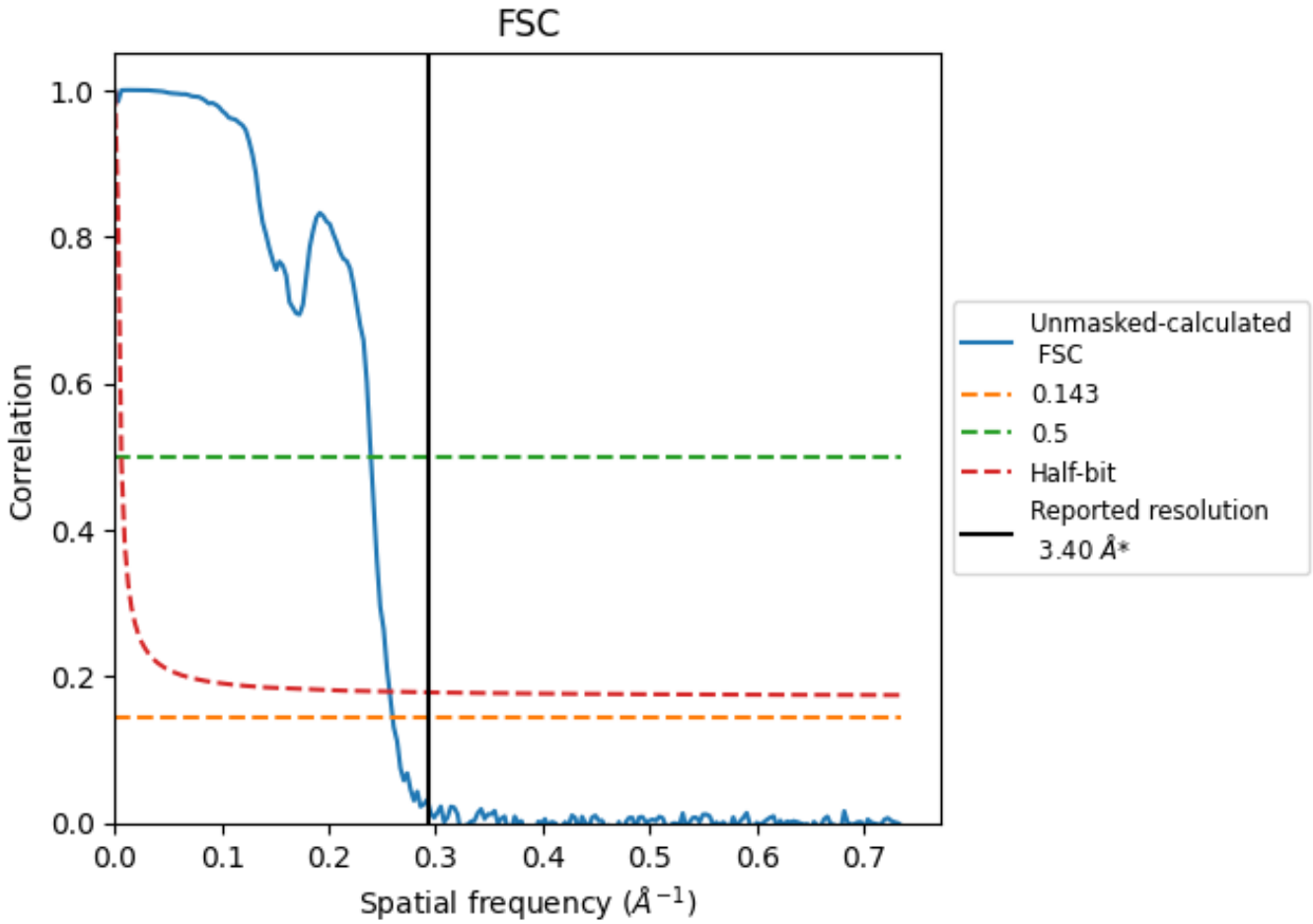


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

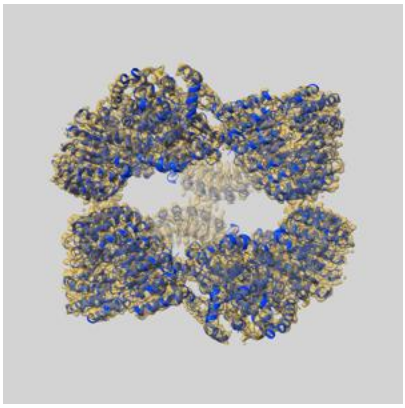
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.85	4.18	3.89

*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 3.85 differs from the reported value 3.4 by more than 10 %

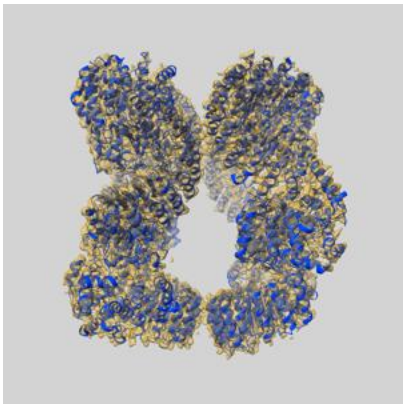
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14713 and PDB model 7ZGU. Per-residue inclusion information can be found in section 3 on page 7.

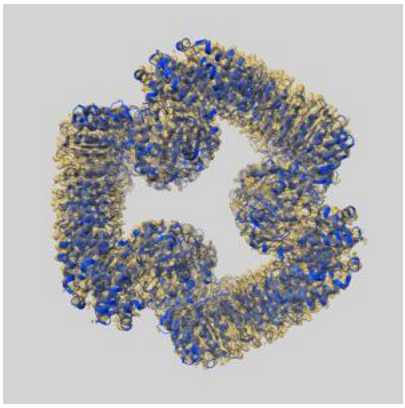
9.1 Map-model overlay



X



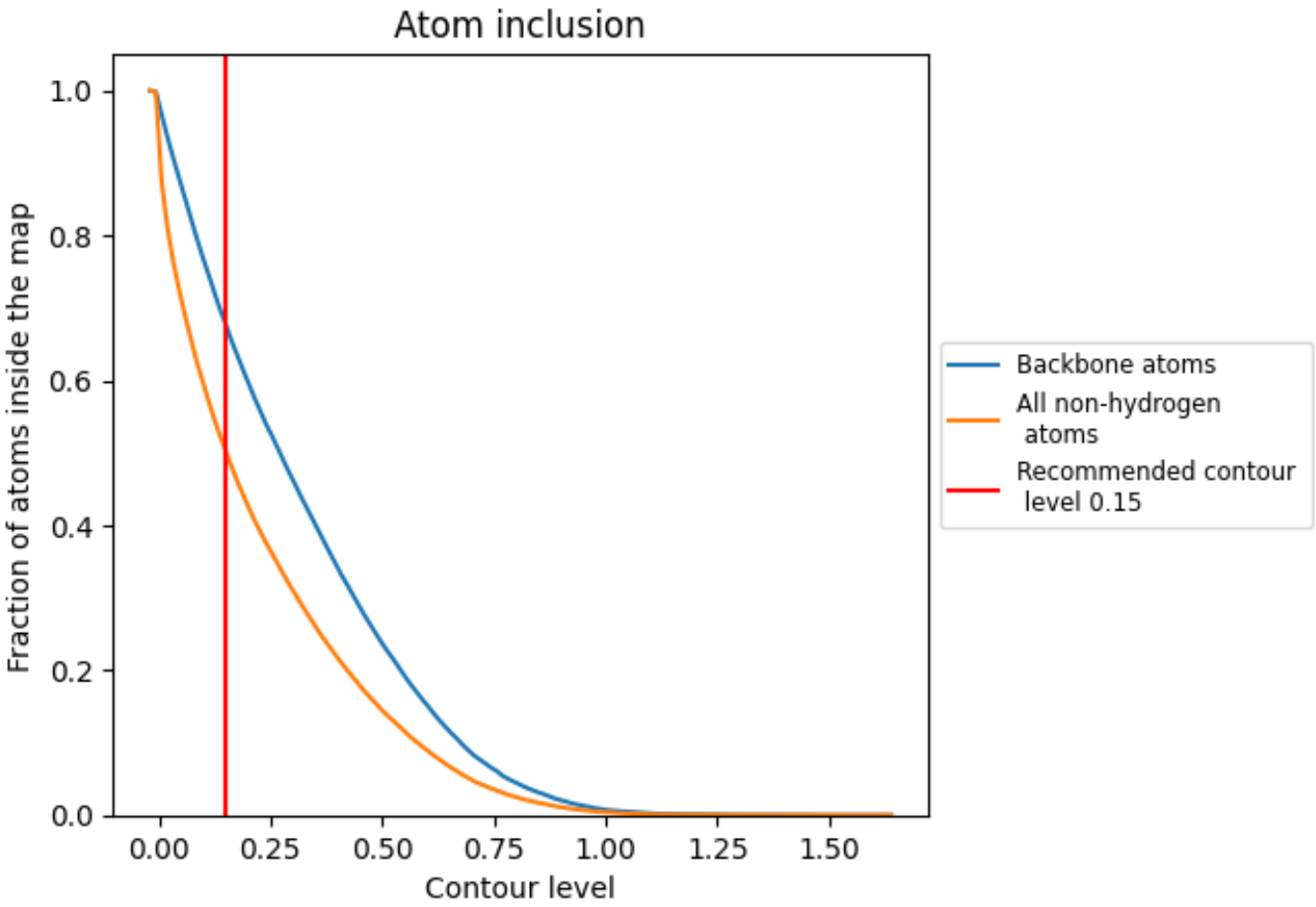
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.