Full wwPDB EM Validation Report ⓘ

May 14, 2024 – 10:11 am BST

PDB ID	:	8Q3R
EMDB ID	:	EMD-18134
Title	:	Cryo-EM structure of the DNA polymerase holoenzyme E9-A20-D4 of vaccinia virus
Authors	:	Burmeister, W.P.; Ballandras-Colas, A.; Boettcher, B.; Grimm, C.
Deposited on	:	2023-08-04
Resolution	:	3.80 Å(reported)
Based on initial models	:	4od8, 8hg1, .

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

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

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

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

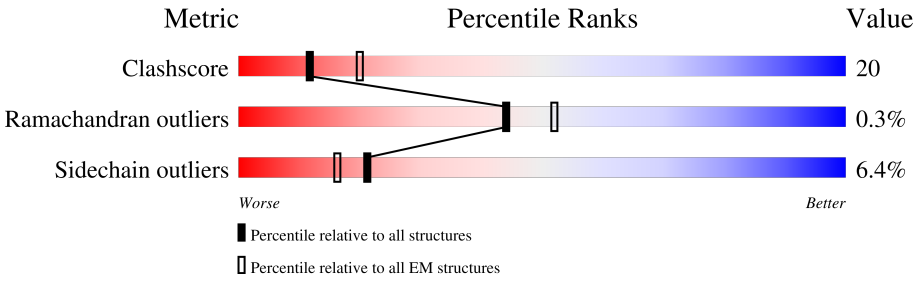
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 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%

Mol	Chain	Length	Quality of chain
1	D	242	55% 34% • 10%
2	A	426	56% 41% ••
3	E	1033	42% 35% • 20%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11921 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 Uracil-DNA glycosylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	D	218	1771	1147	293	325	6	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-23	MET	-	initiating methionine	UNP P20536
D	-22	ALA	-	expression tag	UNP P20536
D	-21	SER	-	expression tag	UNP P20536
D	-20	TRP	-	expression tag	UNP P20536
D	-19	SER	-	expression tag	UNP P20536
D	-18	HIS	-	expression tag	UNP P20536
D	-17	PRO	-	expression tag	UNP P20536
D	-16	GLN	-	expression tag	UNP P20536
D	-15	PHE	-	expression tag	UNP P20536
D	-14	GLU	-	expression tag	UNP P20536
D	-13	LYS	-	expression tag	UNP P20536
D	-12	SER	-	expression tag	UNP P20536
D	-11	GLY	-	expression tag	UNP P20536
D	-10	GLY	-	expression tag	UNP P20536
D	-9	GLY	-	expression tag	UNP P20536
D	-8	GLY	-	expression tag	UNP P20536
D	-7	GLY	-	expression tag	UNP P20536
D	-6	LEU	-	expression tag	UNP P20536
D	-5	VAL	-	expression tag	UNP P20536
D	-4	PRO	-	expression tag	UNP P20536
D	-3	ARG	-	expression tag	UNP P20536
D	-2	GLY	-	expression tag	UNP P20536
D	-1	SER	-	expression tag	UNP P20536
D	0	ALA	-	expression tag	UNP P20536
D	208	ALA	VAL	conflict	UNP P20536

- Molecule 2 is a protein called DNA polymerase processivity factor component OPG148.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	420	Total	C	N	O	S	0	0
			3430	2209	560	651	10		

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	827	Total	C	N	O	S	0	0
			6720	4298	1119	1261	42		

There are 28 discrepancies between the modelled and reference sequences:

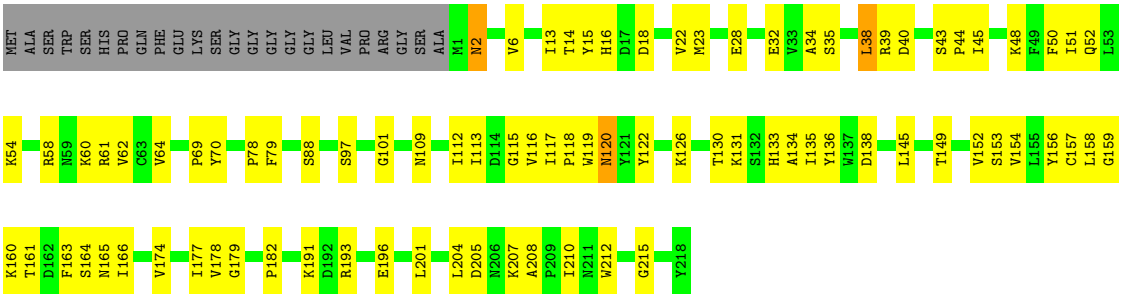
Chain	Residue	Modelled	Actual	Comment	Reference
E	-26	MET	-	initiating methionine	UNP P20509
E	-25	SER	-	expression tag	UNP P20509
E	-24	TYR	-	expression tag	UNP P20509
E	-23	TYR	-	expression tag	UNP P20509
E	-22	HIS	-	expression tag	UNP P20509
E	-21	HIS	-	expression tag	UNP P20509
E	-20	HIS	-	expression tag	UNP P20509
E	-19	HIS	-	expression tag	UNP P20509
E	-18	HIS	-	expression tag	UNP P20509
E	-17	HIS	-	expression tag	UNP P20509
E	-16	ASP	-	expression tag	UNP P20509
E	-15	TYR	-	expression tag	UNP P20509
E	-14	ASP	-	expression tag	UNP P20509
E	-13	ILE	-	expression tag	UNP P20509
E	-12	PRO	-	expression tag	UNP P20509
E	-11	THR	-	expression tag	UNP P20509
E	-10	THR	-	expression tag	UNP P20509
E	-9	GLU	-	expression tag	UNP P20509
E	-8	ASN	-	expression tag	UNP P20509
E	-7	LEU	-	expression tag	UNP P20509
E	-6	TYR	-	expression tag	UNP P20509
E	-5	PHE	-	expression tag	UNP P20509
E	-4	GLN	-	expression tag	UNP P20509
E	-3	GLY	-	expression tag	UNP P20509
E	-2	ALA	-	expression tag	UNP P20509
E	-1	MET	-	expression tag	UNP P20509
E	0	ASP	-	expression tag	UNP P20509
E	1	PRO	-	expression tag	UNP P20509

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. 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. 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.

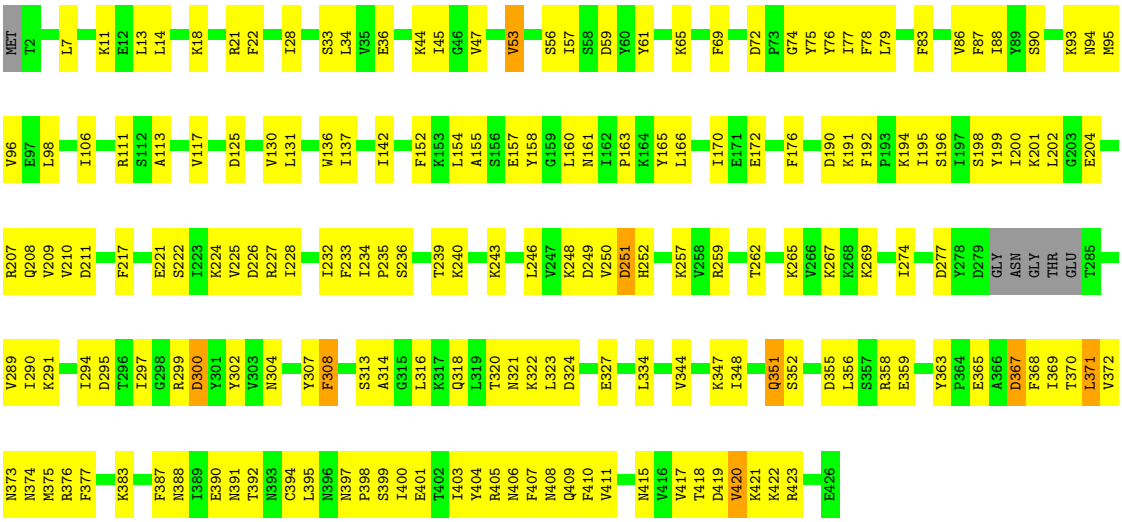
- Molecule 1: Uracil-DNA glycosylase

Chain D:



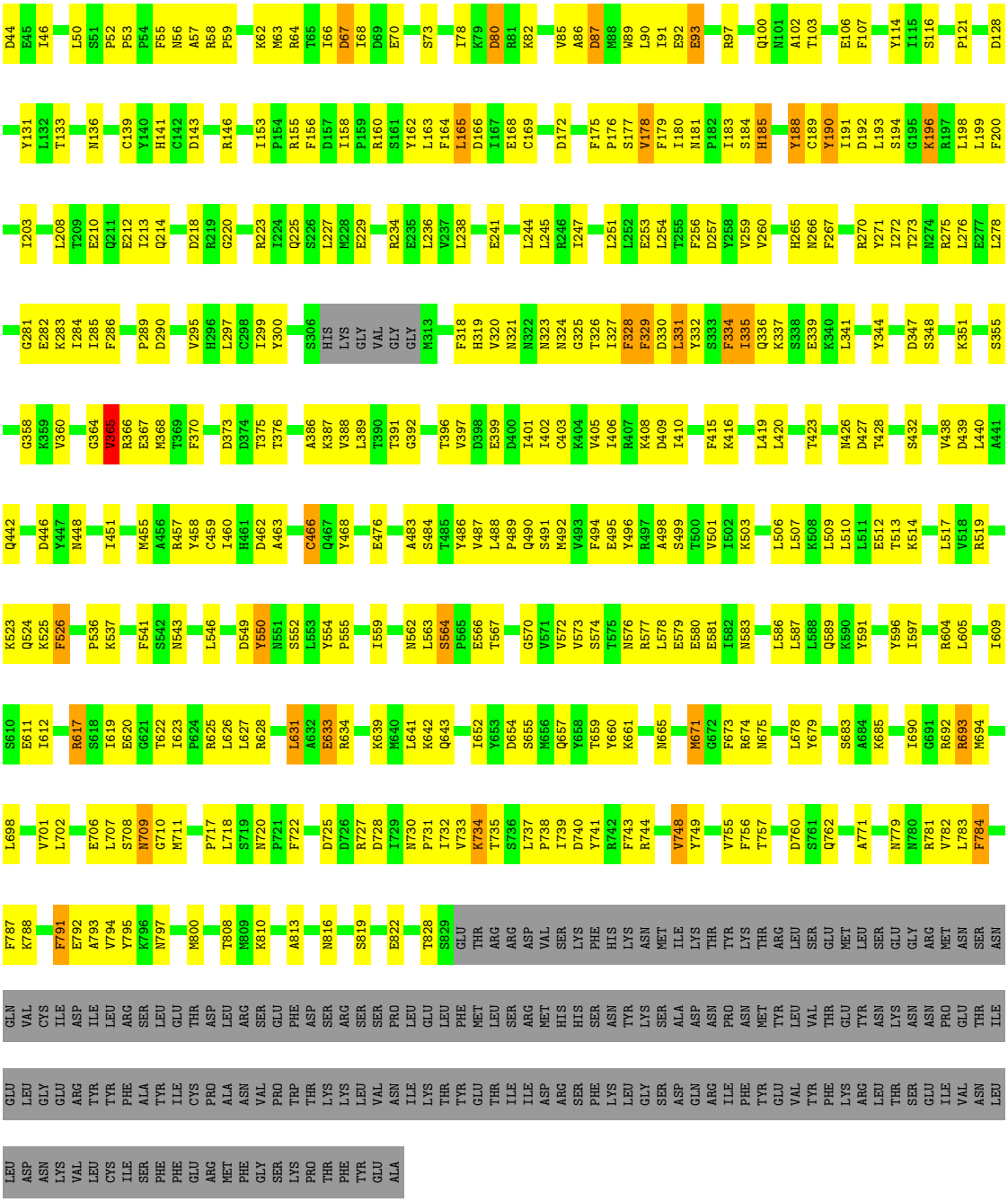
- Molecule 2: DNA polymerase processivity factor component OPG148

Chain A:



- Molecule 3: DNA polymerase

Chain E:


D44 E45 I46 L50 S51 P52 P53 P54 F55 N56 A57 R58 P59 K62 M63 R64 T65 I66 D67 I68 D69 E70 S73 I78 K79 D80 R81 K82 V85 A86 D87 M88 W89 L90 I91 E92 E93 R97 Q100 N101 A102 T103 E106 F107 Y114 I115 S116 P121 D128
Y131 L132 T133 N136 C139 Y140 H141 C142 D143 R146 I153 P154 R155 F156 D157 I158 P159 R160 S161 Y162 L163 F164 L165 D166 I167 E168 C169 D172 F175 P176 S177 V178 F179 I180 N181 P182 I183 S184 H185 Y188 C189 Y190 I191 D192 L193 S194 G195 K196 R197 L198 L199 F200
I203 L208 T209 E210 Q211 E212 I213 Q214 D218 R219 G220 R223 I224 Q225 S226 L227 M228 E229 R234 E235 L236 V237 L238 E241 L244 L245 R246 I247 L251 L252 E253 L254 T255 F256 D257 Y258 V259 V260 H265 N266 F267 R270 Y271 I272 T273 N274 R275 L276 E277 L278
G281 E282 K283 I284 I285 F286 P289 D290 V295 H296 L297 C298 I299 Y300 S306 HIS LYS GLY VAL GLY GLY M313 F318 H319 V320 N321 N322 N323 N324 G325 T326 I327 F328 F329 D330 L331 Y332 S333 F334 I335 Q336 K337 S338 E339 K340 L341 Y344 D347 S348 K351 S355
G358 K359 V360 G364 V366 R366 E367 M368 T369 F370 D373 D374 T375 T376 A386 K387 V388 L389 T390 T391 G392 T396 V397 D398 E399 D400 I401 I402 C403 K404 V405 I406 R407 K408 D409 I410 F415 K416 L419 L420 T423 N426 D427 T428 S432 V438 D439 L440 A441
Q442 D446 Y447 N448 I451 M455 A456 R457 Y458 C459 I460 H461 D462 A463 C466 Q467 Y468 E476 A483 S484 T485 Y486 V487 L488 P489 Q490 S491 M492 V493 F494 E495 Y496 R497 A498 S499 T500 V501 I502 K503 L506 L507 K508 L509 L510 L511 E512 T513 K514 L517 V518 R519
K523 Q524 K525 P526 P536 K537 F541 S542 N543 L546 D549 Y550 N551 S552 L553 Y554 P555 I559 N562 L563 S564 P565 E566 T567 G570 V571 V572 V573 S574 T575 N576 R577 L578 E579 E580 E581 I582 N583 L586 L587 L588 Q589 K590 Y591 Y596 I597 R604 L605 I609
S610 E611 I612 R617 S618 I619 E620 G621 T622 I623 F624 R625 L626 L627 R628 L631 A632 E633 R634 K639 M640 L641 K642 Q643 I652 Y653 D654 S655 M656 Q657 Y658 T659 Y660 K661 N665 M671 G672 F673 R674 N675 L678 Y679 S683 A684 K685 I690 G691 R692 R693 M694
L698 V701 L702 E706 L707 S708 N709 G710 M711 P717 L718 S719 N720 P721 F722 D725 D726 R727 D728 I729 N730 P731 I732 V733 K734 T735 S736 L737 P738 I739 D740 Y741 R742 F743 R744 V748 Y749 V755 F756 T757 D760 S761 Q762 A771 N779 N780 R781 V782 L783 F784
F787 K788 F791 E792 A793 V794 Y795 K796 N797 M800 T808 M809 K810 A813 N816 S819 E822 T828 S829 GLU THR ARG ARG ASP VAL SER LYS PHE HIS LYS ASN MET ILE LYS THR TYR LYS THR ARG LEU SER GLU MET ARG ASP VAL SER GLY ARG MET ASN SER ASN
GLN VAL CYS ILE ASP ILE LEU LEU ARG SER LEU GLU THR ASP LEU ARG SER GLU PHE ASP SER ARG SER SER PRO LEU GLU LEU PHE MET LEU SER ARG MET HIS HIS SER ASN TYR LYS SER ALA ASP ASN PRO ASN MET TYR LEU VAL THR GLU TYR ASN LYS ASN ASN PRO GLU THR ILE
GLU LEU GLY GLU ARG TYR TYR PHE ALA TYR ILE CYS PRO ALA ASN VAL PRO TRP THR LYS LYS LEU VAL ASN ILE LYS THR TYR GLU THR ILE ASP ARG SER PHE LYS LEU GLY SER ASP GLN ARG ILE PHE TYR GLU VAL TYR PHE LYS ARG LEU THR SER GLU ILE VAL ASN LEU
LEU ASP ASN LYS VAL LEU CYS ILE SER PHE PHE GLU ARG MET PHE GLY SER LYS PRO THR PHE TYR GLU ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	104239	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	68	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	42000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	D	0.29	0/1820	0.47	0/2474
2	A	0.27	0/3496	0.47	0/4713
3	E	0.37	0/6864	0.52	0/9278
All	All	0.33	0/12180	0.50	0/16465

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	D	1771	0	1766	57	0
2	A	3430	0	3438	132	0
3	E	6720	0	6687	292	0
All	All	11921	0	11891	469	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 20.

All (469) 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:A:368:PHE:HA	2:A:371:LEU:HD23	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:8:TRP:HB2	3:E:489:PRO:HB3	1.62	0.82
2:A:21:ARG:HB3	2:A:56:SER:H	1.45	0.82
2:A:78:PHE:HB2	2:A:166:LEU:HB2	1.60	0.81
2:A:371:LEU:HB2	2:A:400:ILE:HG23	1.64	0.79
2:A:74:GLY:HA3	2:A:201:LYS:HE2	1.66	0.77
2:A:348:ILE:HD12	2:A:356:LEU:HD21	1.65	0.77
3:E:70:GLU:OE2	3:E:604:ARG:NH1	2.18	0.76
2:A:404:TYR:HA	2:A:407:PHE:HB2	1.67	0.76
3:E:339:GLU:HB3	3:E:341:LEU:HG	1.68	0.75
3:E:67:ASP:HB3	3:E:82:LYS:HB2	1.69	0.75
3:E:365:VAL:HG13	3:E:367:GLU:H	1.52	0.75
3:E:523:LYS:NZ	3:E:674:ARG:O	2.16	0.73
3:E:396:THR:HB	3:E:432:SER:HB2	1.69	0.73
3:E:265:HIS:NE2	3:E:329:PHE:O	2.21	0.73
3:E:562:ASN:ND2	3:E:619:ILE:O	2.22	0.73
2:A:225:VAL:HA	2:A:235:PRO:HA	1.71	0.72
2:A:419:ASP:OD1	2:A:423:ARG:NH2	2.22	0.72
3:E:604:ARG:HG3	3:E:605:LEU:HG	1.72	0.71
3:E:163:LEU:HD23	3:E:259:VAL:HG22	1.73	0.71
3:E:199:LEU:HD22	3:E:460:ILE:HD11	1.73	0.71
1:D:39:ARG:NH1	3:E:278:LEU:O	2.24	0.70
3:E:64:ARG:HA	3:E:85:VAL:HA	1.72	0.70
3:E:164:PHE:HD2	3:E:466:CYS:HB3	1.56	0.70
3:E:116:SER:OG	3:E:146:ARG:NH2	2.24	0.70
3:E:178:VAL:O	3:E:275:ARG:NH1	2.24	0.70
2:A:376:ARG:NH1	3:E:581:GLU:OE2	2.24	0.70
3:E:816:ASN:OD1	3:E:819:SER:OG	2.11	0.69
3:E:20:LEU:HB3	3:E:32:ILE:HG13	1.72	0.69
2:A:370:THR:O	2:A:374:ASN:ND2	2.27	0.68
3:E:164:PHE:HB2	3:E:189:CYS:HB3	1.76	0.68
3:E:160:ARG:NH1	3:E:476:GLU:OE2	2.27	0.68
2:A:392:THR:HA	2:A:395:LEU:HD23	1.76	0.68
2:A:397:ASN:HB3	2:A:400:ILE:HG12	1.76	0.68
2:A:411:VAL:O	2:A:415:ASN:ND2	2.25	0.68
3:E:56:ASN:ND2	3:E:92:GLU:OE1	2.27	0.68
3:E:265:HIS:HD2	3:E:330:ASP:HB2	1.58	0.67
2:A:321:ASN:OD1	2:A:322:LYS:N	2.26	0.67
3:E:718:LEU:O	3:E:727:ARG:NH2	2.26	0.67
3:E:546:LEU:HB2	3:E:757:THR:HB	1.75	0.67
3:E:58:ARG:NH2	3:E:116:SER:OG	2.28	0.67
2:A:45:ILE:HG22	2:A:47:VAL:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:488:LEU:HD11	3:E:501:VAL:HG12	1.77	0.66
3:E:546:LEU:N	3:E:757:THR:O	2.26	0.66
2:A:314:ALA:HA	2:A:318:GLN:HG3	1.78	0.66
3:E:114:TYR:HD2	3:E:487:VAL:HG12	1.61	0.66
2:A:77:ILE:HB	2:A:200:ILE:HG12	1.78	0.65
3:E:728:ASP:OD2	3:E:781:ARG:NH2	2.29	0.65
2:A:65:LYS:HD3	2:A:210:VAL:HG12	1.78	0.65
3:E:169:CYS:HA	3:E:184:SER:H	1.60	0.65
3:E:537:LYS:HD2	3:E:748:VAL:HA	1.78	0.65
1:D:201:LEU:HD23	1:D:204:LEU:HD12	1.79	0.64
3:E:579:GLU:HG2	3:E:583:ASN:HD21	1.61	0.64
2:A:222:SER:OG	2:A:224:LYS:NZ	2.30	0.64
3:E:783:LEU:HD13	3:E:787:PHE:HB3	1.78	0.64
3:E:734:LYS:NZ	3:E:735:THR:O	2.30	0.64
3:E:164:PHE:CD2	3:E:466:CYS:HB3	2.33	0.63
1:D:160:LYS:NZ	1:D:178:VAL:O	2.23	0.63
3:E:552:SER:HB3	3:E:555:PRO:HB2	1.79	0.63
3:E:26:ASN:OD1	3:E:26:ASN:N	2.31	0.63
2:A:376:ARG:N	2:A:388:ASN:O	2.28	0.62
2:A:224:LYS:O	2:A:236:SER:N	2.32	0.62
2:A:294:ILE:HD12	2:A:398:PRO:HB2	1.81	0.62
2:A:249:ASP:OD1	2:A:250:VAL:N	2.32	0.62
1:D:61:ARG:NE	1:D:208:ALA:O	2.31	0.62
3:E:718:LEU:HD22	3:E:782:VAL:HG13	1.82	0.61
2:A:375:MET:HA	2:A:390:GLU:H	1.64	0.61
3:E:389:LEU:HB3	3:E:410:ILE:HD11	1.81	0.61
2:A:195:ILE:O	2:A:269:LYS:NZ	2.33	0.60
2:A:300:ASP:OD1	2:A:300:ASP:N	2.26	0.60
3:E:483:ALA:HB2	3:E:490:GLN:HG3	1.83	0.60
3:E:59:PRO:HA	3:E:89:TRP:HA	1.83	0.60
2:A:211:ASP:OD1	2:A:269:LYS:NZ	2.34	0.60
3:E:9:PHE:HE1	3:E:19:TYR:HB2	1.66	0.60
3:E:324:ASN:OD1	3:E:325:GLY:N	2.34	0.60
2:A:246:LEU:HB2	2:A:274:ILE:HG22	1.83	0.60
1:D:112:ILE:HG13	1:D:215:GLY:HA2	1.84	0.60
3:E:196:LYS:HB3	3:E:198:LEU:HD13	1.83	0.60
3:E:42:VAL:HG12	3:E:102:ALA:HA	1.83	0.59
3:E:203:ILE:HB	3:E:238:LEU:HD22	1.83	0.59
3:E:347:ASP:OD1	3:E:348:SER:N	2.35	0.59
3:E:9:PHE:HE2	3:E:325:GLY:HA2	1.67	0.59
2:A:95:MET:HG3	2:A:106:ILE:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:220:GLY:O	3:E:234:ARG:NH2	2.35	0.59
2:A:208:GLN:N	2:A:208:GLN:OE1	2.34	0.59
3:E:639:LYS:NZ	3:E:643:GLN:OE1	2.34	0.59
3:E:633:GLU:HB3	3:E:660:TYR:CE2	2.38	0.58
1:D:62:VAL:HG22	1:D:154:VAL:HB	1.85	0.58
3:E:80:ASP:N	3:E:80:ASP:OD1	2.37	0.58
3:E:163:LEU:HG	3:E:164:PHE:N	2.18	0.58
2:A:257:LYS:HG2	2:A:289:VAL:HG21	1.86	0.58
3:E:282:GLU:OE1	3:E:282:GLU:N	2.36	0.58
3:E:18:LEU:HB3	3:E:34:PHE:HB2	1.86	0.58
3:E:573:VAL:HG12	3:E:611:GLU:HA	1.86	0.58
1:D:97:SER:O	1:D:101:GLY:N	2.34	0.58
3:E:92:GLU:OE2	3:E:146:ARG:NH2	2.36	0.58
3:E:23:ARG:NH1	3:E:257:ASP:OD2	2.32	0.57
3:E:706:GLU:HA	3:E:744:ARG:HA	1.85	0.57
3:E:725:ASP:OD2	3:E:727:ARG:NE	2.37	0.57
1:D:40:ASP:HB2	1:D:133:HIS:CE1	2.39	0.57
2:A:294:ILE:HG12	2:A:308:PHE:HZ	1.70	0.57
2:A:94:ASN:OD1	2:A:111:ARG:NH1	2.37	0.57
3:E:779:ASN:HB3	3:E:788:LYS:NZ	2.20	0.57
1:D:64:VAL:HG13	1:D:156:TYR:HD2	1.69	0.57
3:E:267:PHE:O	3:E:271:TYR:HB2	2.06	0.56
2:A:373:ASN:HD21	3:E:609:ILE:HD13	1.69	0.56
3:E:270:ARG:HH21	3:E:299:ILE:HG21	1.71	0.56
3:E:509:LEU:HD22	3:E:626:LEU:HB2	1.87	0.56
3:E:720:ASN:HB3	3:E:725:ASP:HB2	1.88	0.56
2:A:313:SER:O	2:A:409:GLN:NE2	2.38	0.56
3:E:327:ILE:O	3:E:329:PHE:N	2.38	0.56
3:E:360:VAL:HG22	3:E:370:PHE:HE2	1.69	0.56
3:E:8:TRP:O	3:E:491:SER:OG	2.23	0.56
3:E:63:MET:HE3	3:E:514:LYS:HA	1.88	0.56
3:E:57:ALA:HA	3:E:91:ILE:HA	1.86	0.56
1:D:51:ILE:HA	1:D:54:LYS:HE2	1.87	0.55
2:A:13:LEU:HD13	2:A:34:LEU:HB2	1.87	0.55
2:A:351:GLN:NE2	2:A:355:ASP:OD2	2.39	0.55
3:E:9:PHE:CE2	3:E:325:GLY:HA2	2.41	0.55
2:A:374:ASN:HB3	2:A:391:ASN:HB3	1.89	0.55
3:E:21:LYS:NZ	3:E:256:PHE:O	2.39	0.55
3:E:358:GLY:O	3:E:428:THR:OG1	2.18	0.55
2:A:417:VAL:O	2:A:421:LYS:HG2	2.06	0.55
3:E:286:PHE:HZ	3:E:297:LEU:HD12	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:492:MET:SD	3:E:496:TYR:OH	2.58	0.55
2:A:377:PHE:CD2	3:E:578:LEU:HD13	2.42	0.55
3:E:318:PHE:O	3:E:319:HIS:ND1	2.39	0.55
2:A:21:ARG:HD2	2:A:56:SER:HB3	1.87	0.55
3:E:265:HIS:HE1	3:E:328:PHE:HB3	1.71	0.55
3:E:284:ILE:HD12	3:E:297:LEU:HD13	1.88	0.55
3:E:566:GLU:OE2	3:E:622:THR:N	2.40	0.55
1:D:113:ILE:HD13	1:D:212:TRP:HA	1.88	0.54
3:E:190:TYR:HD1	3:E:191:ILE:N	2.05	0.54
3:E:56:ASN:O	3:E:92:GLU:N	2.32	0.54
3:E:58:ARG:N	3:E:90:LEU:O	2.34	0.54
3:E:78:ILE:HD13	3:E:570:GLY:HA3	1.89	0.54
3:E:331:LEU:O	3:E:335:ILE:HB	2.07	0.54
3:E:512:GLU:OE2	3:E:625:ARG:NH2	2.41	0.54
2:A:363:TYR:HE2	2:A:410:PHE:HB2	1.72	0.54
3:E:116:SER:HG	3:E:146:ARG:HH21	1.52	0.54
2:A:351:GLN:HB3	2:A:355:ASP:HB2	1.90	0.54
3:E:62:LYS:HA	3:E:87:ASP:HA	1.89	0.54
3:E:633:GLU:HB3	3:E:660:TYR:HE2	1.73	0.54
3:E:59:PRO:HB3	3:E:89:TRP:CE2	2.43	0.54
3:E:52:PRO:O	3:E:97:ARG:NH2	2.41	0.54
3:E:351:LYS:O	3:E:355:SER:OG	2.26	0.54
2:A:190:ASP:O	2:A:194:LYS:NZ	2.40	0.53
3:E:64:ARG:CZ	3:E:66:ILE:HD11	2.38	0.53
3:E:160:ARG:HB2	3:E:162:TYR:CE1	2.43	0.53
3:E:442:GLN:NE2	3:E:446:ASP:OD2	2.41	0.53
3:E:457:ARG:HA	3:E:460:ILE:HG22	1.89	0.53
3:E:525:LYS:HG2	3:E:674:ARG:HH22	1.72	0.53
3:E:562:ASN:OD1	3:E:620:GLU:HA	2.09	0.53
2:A:228:ILE:HD11	2:A:307:TYR:HE1	1.73	0.53
1:D:43:SER:OG	1:D:70:TYR:O	2.26	0.53
2:A:196:SER:OG	2:A:210:VAL:O	2.20	0.53
3:E:68:ILE:HD13	3:E:517:LEU:HB3	1.89	0.53
3:E:203:ILE:HD11	3:E:236:LEU:HD22	1.91	0.53
3:E:265:HIS:CE1	3:E:328:PHE:HB3	2.43	0.53
3:E:330:ASP:OD1	3:E:332:TYR:N	2.42	0.53
2:A:294:ILE:HG12	2:A:308:PHE:CZ	2.43	0.53
3:E:136:ASN:HB2	3:E:139:CYS:HB2	1.91	0.53
3:E:579:GLU:HG2	3:E:583:ASN:ND2	2.24	0.53
2:A:228:ILE:HD11	2:A:307:TYR:CE1	2.43	0.53
3:E:241:GLU:O	3:E:245:LEU:HG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:181:ASN:O	3:E:271:TYR:OH	2.26	0.53
2:A:316:LEU:HG	2:A:334:LEU:HD11	1.91	0.53
3:E:52:PRO:HG2	3:E:97:ARG:NH2	2.24	0.52
2:A:388:ASN:OD1	2:A:388:ASN:N	2.41	0.52
3:E:519:ARG:NH2	3:E:679:TYR:O	2.35	0.52
1:D:35:SER:HA	1:D:38:LEU:HD22	1.92	0.52
2:A:28:ILE:HG13	2:A:53:VAL:HG21	1.90	0.52
3:E:396:THR:N	3:E:432:SER:O	2.28	0.52
3:E:701:VAL:HG12	3:E:702:LEU:HD23	1.92	0.52
3:E:337:LYS:NZ	3:E:494:PHE:O	2.30	0.52
3:E:392:GLY:O	3:E:408:LYS:NZ	2.38	0.52
2:A:368:PHE:HD1	2:A:403:ILE:HG21	1.74	0.52
3:E:329:PHE:HD1	3:E:330:ASP:H	1.57	0.52
3:E:555:PRO:HA	3:E:627:LEU:HD13	1.91	0.52
3:E:707:LEU:HB3	3:E:743:PHE:H	1.75	0.52
2:A:190:ASP:OD1	2:A:191:LYS:N	2.43	0.52
3:E:63:MET:HG2	3:E:514:LYS:HB3	1.92	0.52
3:E:160:ARG:HB2	3:E:162:TYR:CZ	2.45	0.52
1:D:60:LYS:HA	1:D:115:GLY:HA2	1.92	0.52
3:E:18:LEU:O	3:E:34:PHE:N	2.34	0.51
3:E:8:TRP:CD2	3:E:20:LEU:HD13	2.45	0.51
3:E:448:ASN:HD21	3:E:451:ILE:HD12	1.75	0.51
3:E:641:LEU:HD23	3:E:642:LYS:HG3	1.92	0.51
2:A:302:TYR:OH	2:A:304:ASN:ND2	2.44	0.51
3:E:223:ARG:NE	3:E:225:GLN:HE21	2.08	0.51
3:E:8:TRP:CZ3	3:E:18:LEU:HD21	2.46	0.51
1:D:78:PRO:HB2	1:D:118:PRO:HB2	1.93	0.51
1:D:135:ILE:HG22	3:E:179:PHE:HZ	1.75	0.51
2:A:377:PHE:CG	3:E:578:LEU:HD13	2.46	0.51
2:A:294:ILE:HA	2:A:297:ILE:HG12	1.93	0.51
3:E:693:ARG:HG2	3:E:722:PHE:HE1	1.76	0.51
3:E:738:PRO:HB2	3:E:740:ASP:OD1	2.11	0.50
2:A:59:ASP:N	2:A:59:ASP:OD1	2.45	0.50
3:E:254:LEU:O	3:E:256:PHE:N	2.44	0.50
3:E:265:HIS:CD2	3:E:330:ASP:HB2	2.44	0.50
3:E:709:ASN:HB3	3:E:739:ILE:HG23	1.93	0.50
2:A:86:VAL:HG12	2:A:130:VAL:HG22	1.93	0.50
2:A:406:ASN:HB2	2:A:409:GLN:HG3	1.93	0.50
3:E:41:VAL:HA	3:E:89:TRP:O	2.12	0.50
3:E:40:TYR:HB2	3:E:91:ILE:HD11	1.94	0.50
3:E:183:ILE:HD12	3:E:245:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:376:ARG:CZ	3:E:577:ARG:HD3	2.42	0.50
3:E:330:ASP:OD1	3:E:331:LEU:N	2.45	0.50
3:E:25:ARG:HB3	3:E:156:PHE:CE2	2.47	0.49
2:A:251:ASP:N	2:A:251:ASP:OD1	2.44	0.49
3:E:791:PHE:HE2	3:E:813:ALA:HB2	1.77	0.49
2:A:221:GLU:OE1	2:A:221:GLU:N	2.45	0.49
2:A:367:ASP:OD1	2:A:367:ASP:N	2.43	0.49
3:E:139:CYS:SG	3:E:289:PRO:HB2	2.53	0.49
3:E:446:ASP:O	3:E:448:ASN:ND2	2.46	0.49
2:A:88:ILE:HG13	2:A:96:VAL:HG23	1.95	0.49
2:A:259:ARG:O	2:A:262:THR:OG1	2.31	0.49
3:E:373:ASP:N	3:E:376:THR:OG1	2.42	0.49
2:A:83:PHE:CZ	2:A:248:LYS:HG3	2.47	0.49
3:E:405:VAL:HA	3:E:419:LEU:HD23	1.93	0.49
1:D:61:ARG:O	1:D:153:SER:N	2.45	0.49
2:A:318:GLN:HA	2:A:321:ASN:ND2	2.28	0.49
2:A:320:THR:OG1	2:A:327:GLU:OE1	2.31	0.49
2:A:399:SER:O	2:A:403:ILE:HG12	2.12	0.49
3:E:164:PHE:CD2	3:E:260:VAL:HB	2.48	0.49
1:D:157:CYS:HB3	1:D:163:PHE:CG	2.47	0.49
3:E:440:LEU:HD22	3:E:455:MET:HE3	1.94	0.49
2:A:14:LEU:O	2:A:18:LYS:HG2	2.13	0.49
3:E:549:ASP:HB2	3:E:792:GLU:HG2	1.94	0.49
3:E:554:TYR:HB2	3:E:555:PRO:HD3	1.95	0.49
3:E:586:LEU:HA	3:E:589:GLN:NE2	2.28	0.49
3:E:121:PRO:HG2	3:E:483:ALA:O	2.13	0.48
3:E:779:ASN:HB3	3:E:788:LYS:HZ2	1.78	0.48
1:D:62:VAL:O	1:D:116:VAL:HA	2.12	0.48
3:E:8:TRP:HE3	3:E:18:LEU:HD11	1.77	0.48
3:E:397:VAL:HB	3:E:401:ILE:HB	1.95	0.48
1:D:40:ASP:HB3	1:D:126:LYS:HG3	1.95	0.48
1:D:158:LEU:HD23	1:D:182:PRO:HD3	1.95	0.48
2:A:192:PHE:O	2:A:194:LYS:NZ	2.45	0.48
2:A:401:GLU:O	2:A:405:ARG:HG2	2.13	0.48
3:E:574:SER:HB3	3:E:579:GLU:HB3	1.94	0.48
3:E:617:ARG:HH11	3:E:617:ARG:HB2	1.78	0.48
3:E:44:ASP:OD1	3:E:89:TRP:NE1	2.47	0.48
2:A:420:VAL:HG23	2:A:423:ARG:HH22	1.77	0.48
3:E:457:ARG:O	3:E:460:ILE:HG22	2.14	0.48
2:A:226:ASP:N	2:A:234:ILE:O	2.42	0.48
3:E:166:ASP:HB3	3:E:463:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:204:GLU:OE1	2:A:204:GLU:N	2.46	0.48
1:D:130:THR:HG22	1:D:131:LYS:HG3	1.96	0.47
3:E:133:THR:HB	3:E:141:HIS:HB3	1.94	0.47
3:E:524:GLN:HB3	3:E:526:PHE:CZ	2.49	0.47
1:D:13:ILE:HG23	1:D:50:PHE:HB3	1.95	0.47
3:E:373:ASP:OD2	3:E:375:THR:OG1	2.28	0.47
3:E:214:GLN:NE2	3:E:218:ASP:OD2	2.46	0.47
3:E:509:LEU:HD11	3:E:625:ARG:HG2	1.97	0.47
3:E:509:LEU:HD23	3:E:622:THR:HG23	1.96	0.47
3:E:717:PRO:HA	3:E:731:PRO:HB3	1.95	0.47
2:A:408:ASN:HA	2:A:411:VAL:HG22	1.95	0.47
3:E:136:ASN:ND2	3:E:290:ASP:O	2.47	0.47
3:E:760:ASP:OD1	3:E:760:ASP:N	2.47	0.47
2:A:228:ILE:HG13	2:A:232:ILE:HG22	1.97	0.47
3:E:286:PHE:CZ	3:E:297:LEU:HD12	2.49	0.47
1:D:145:LEU:HD12	1:D:145:LEU:HA	1.75	0.47
2:A:406:ASN:HB2	2:A:409:GLN:CG	2.45	0.47
3:E:283:LYS:O	3:E:285:ILE:HG13	2.14	0.47
3:E:509:LEU:O	3:E:513:THR:HG23	2.15	0.47
3:E:591:TYR:HB3	3:E:596:TYR:CG	2.49	0.47
1:D:149:THR:HA	1:D:152:VAL:HG22	1.96	0.47
1:D:174:VAL:HA	2:A:44:LYS:HD2	1.96	0.47
2:A:90:SER:HB3	2:A:93:LYS:HD2	1.96	0.47
2:A:377:PHE:CZ	3:E:578:LEU:HB2	2.49	0.47
3:E:46:ILE:O	3:E:50:LEU:HG	2.14	0.47
3:E:114:TYR:CD2	3:E:487:VAL:HG12	2.47	0.47
3:E:409:ASP:O	3:E:416:LYS:N	2.30	0.47
3:E:543:ASN:HA	3:E:762:GLN:HG2	1.97	0.47
1:D:159:GLY:O	1:D:163:PHE:HD2	1.98	0.47
2:A:347:LYS:HG3	2:A:348:ILE:HD13	1.96	0.47
3:E:0:ASP:HB3	3:E:24:CYS:SG	2.55	0.47
3:E:199:LEU:HD13	3:E:460:ILE:HG12	1.97	0.47
2:A:61:TYR:HA	2:A:207:ARG:O	2.15	0.47
3:E:169:CYS:HA	3:E:184:SER:N	2.29	0.47
3:E:397:VAL:N	3:E:401:ILE:O	2.34	0.47
3:E:634:ARG:NH1	3:E:661:LYS:HD3	2.30	0.47
3:E:163:LEU:HD22	3:E:256:PHE:CE2	2.50	0.46
2:A:227:ARG:HA	2:A:233:PHE:HD1	1.80	0.46
2:A:363:TYR:CE1	2:A:403:ILE:HD12	2.50	0.46
2:A:418:THR:HG22	2:A:422:LYS:HE3	1.98	0.46
3:E:12:HIS:CE1	3:E:321:ASN:HD22	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:730:ASN:HD21	3:E:732:ILE:HB	1.80	0.46
3:E:694:MET:HE1	3:E:784:PHE:CZ	2.51	0.46
3:E:66:ILE:HD13	3:E:566:GLU:HB2	1.97	0.46
3:E:323:ASN:O	3:E:323:ASN:ND2	2.49	0.46
3:E:711:MET:SD	3:E:734:LYS:HE2	2.56	0.46
2:A:407:PHE:O	2:A:411:VAL:HG13	2.15	0.46
3:E:107:PHE:CD2	3:E:503:LYS:HB3	2.51	0.46
3:E:116:SER:HG	3:E:146:ARG:NH2	2.10	0.46
3:E:399:GLU:OE1	3:E:432:SER:OG	2.32	0.46
3:E:579:GLU:O	3:E:583:ASN:ND2	2.36	0.46
3:E:498:ALA:HA	3:E:501:VAL:HG22	1.96	0.46
1:D:16:HIS:CD2	1:D:18:ASP:H	2.34	0.46
1:D:69:PRO:HD3	1:D:122:TYR:O	2.15	0.46
3:E:158:ILE:HD11	3:E:160:ARG:HH21	1.81	0.46
3:E:365:VAL:HG22	3:E:366:ARG:H	1.80	0.46
1:D:2:ASN:HB2	1:D:15:TYR:CE1	2.51	0.46
3:E:106:GLU:O	3:E:503:LYS:NZ	2.28	0.46
3:E:107:PHE:CE2	3:E:507:LEU:HB2	2.51	0.46
1:D:52:GLN:HB3	1:D:119:TRP:CZ3	2.51	0.46
3:E:426:ASN:OD1	3:E:427:ASP:N	2.49	0.46
3:E:744:ARG:H	3:E:760:ASP:CG	2.20	0.46
3:E:163:LEU:HD13	3:E:256:PHE:CE2	2.51	0.45
3:E:36:HIS:CG	3:E:37:TYR:N	2.84	0.45
3:E:368:MET:SD	3:E:423:THR:HA	2.57	0.45
1:D:40:ASP:OD2	1:D:133:HIS:NE2	2.46	0.45
3:E:175:PHE:CG	3:E:176:PRO:HD2	2.51	0.45
3:E:623:ILE:HD13	3:E:671:MET:SD	2.57	0.45
3:E:163:LEU:HD22	3:E:256:PHE:CD2	2.51	0.45
2:A:198:SER:HA	2:A:209:VAL:HG12	1.99	0.45
1:D:163:PHE:HD1	1:D:166:ILE:HG21	1.81	0.45
3:E:406:ILE:HD11	3:E:420:LEU:HB2	1.99	0.45
2:A:234:ILE:HD12	2:A:235:PRO:HD2	1.99	0.45
2:A:383:LYS:HE3	2:A:422:LYS:NZ	2.31	0.45
3:E:192:ASP:OD1	3:E:193:LEU:N	2.47	0.45
3:E:281:GLY:N	3:E:282:GLU:OE1	2.50	0.45
3:E:62:LYS:HG2	3:E:85:VAL:HG12	1.98	0.45
1:D:122:TYR:CZ	1:D:134:ALA:HB1	2.52	0.45
1:D:166:ILE:H	1:D:166:ILE:HG13	1.55	0.45
3:E:225:GLN:N	3:E:229:GLU:OE1	2.48	0.44
3:E:455:MET:HA	3:E:458:TYR:CD2	2.52	0.44
3:E:8:TRP:HZ3	3:E:18:LEU:HD21	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:793:ALA:HB1	3:E:810:LYS:HG3	2.00	0.44
2:A:372:VAL:CG1	3:E:578:LEU:H	2.31	0.44
3:E:8:TRP:CH2	3:E:20:LEU:HD22	2.52	0.44
3:E:106:GLU:H	3:E:106:GLU:CD	2.21	0.44
3:E:121:PRO:HG2	3:E:484:SER:HA	1.99	0.44
3:E:185:HIS:HB3	3:E:203:ILE:HA	2.00	0.44
1:D:2:ASN:HB2	1:D:15:TYR:CZ	2.52	0.44
3:E:673:PHE:HD1	3:E:675:ASN:H	1.66	0.44
1:D:44:PRO:HB2	1:D:48:LYS:HB2	2.00	0.44
1:D:61:ARG:NH2	1:D:210:ILE:HD13	2.33	0.44
2:A:155:ALA:HB1	2:A:160:LEU:HD11	1.99	0.44
3:E:300:TYR:OH	3:E:321:ASN:HB3	2.18	0.44
3:E:623:ILE:HD11	3:E:678:LEU:HB3	2.00	0.44
1:D:161:THR:O	1:D:164:SER:OG	2.28	0.44
3:E:87:ASP:OD1	3:E:87:ASP:N	2.51	0.44
3:E:403:CYS:SG	3:E:419:LEU:HB3	2.58	0.44
2:A:299:ARG:HG3	2:A:405:ARG:NH1	2.32	0.44
2:A:394:CYS:SG	2:A:400:ILE:HG21	2.58	0.44
3:E:155:ARG:NH2	3:E:652:ILE:HG21	2.33	0.44
3:E:546:LEU:HD23	3:E:794:VAL:HG22	1.98	0.44
1:D:88:SER:HA	1:D:182:PRO:HB2	2.00	0.43
1:D:163:PHE:HB3	1:D:166:ILE:HG12	1.99	0.43
3:E:63:MET:HB3	3:E:514:LYS:O	2.18	0.43
3:E:387:LYS:HG2	3:E:468:TYR:CE1	2.53	0.43
3:E:388:VAL:HG12	3:E:388:VAL:O	2.18	0.43
1:D:156:TYR:HA	1:D:177:ILE:O	2.17	0.43
2:A:117:VAL:HG23	2:A:154:LEU:HD23	2.00	0.43
3:E:194:SER:OG	3:E:196:LYS:HB2	2.18	0.43
2:A:154:LEU:HG	2:A:158:TYR:CZ	2.54	0.43
2:A:217:PHE:CE2	2:A:265:LYS:HB3	2.53	0.43
3:E:290:ASP:OD1	3:E:290:ASP:N	2.49	0.43
3:E:506:LEU:O	3:E:510:LEU:HG	2.18	0.43
3:E:733:VAL:HG22	3:E:781:ARG:CZ	2.48	0.43
2:A:290:ILE:O	2:A:294:ILE:HG13	2.19	0.43
3:E:334:PHE:HE2	3:E:494:PHE:CZ	2.37	0.43
3:E:364:GLY:O	3:E:365:VAL:HG12	2.18	0.43
2:A:295:ASP:OD1	2:A:299:ARG:NH1	2.44	0.43
3:E:327:ILE:HG23	3:E:491:SER:HA	2.00	0.43
3:E:795:TYR:CG	3:E:808:THR:HG21	2.54	0.43
2:A:77:ILE:O	2:A:199:TYR:HA	2.19	0.43
3:E:259:VAL:HG23	3:E:326:THR:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:348:ILE:HG23	2:A:356:LEU:HD21	1.99	0.43
1:D:205:ASP:HB3	1:D:207:LYS:HG2	2.01	0.42
2:A:125:ASP:HB3	2:A:142:ILE:HG13	2.01	0.42
2:A:375:MET:HA	2:A:390:GLU:N	2.31	0.42
3:E:388:VAL:HG13	3:E:468:TYR:CD2	2.54	0.42
1:D:28:GLU:O	1:D:32:GLU:HG2	2.18	0.42
1:D:60:LYS:HA	1:D:60:LYS:HD3	1.75	0.42
2:A:226:ASP:HB3	2:A:234:ILE:HG23	1.99	0.42
2:A:252:HIS:NE2	2:A:277:ASP:HB3	2.34	0.42
2:A:358:ARG:NH1	2:A:365:GLU:HG2	2.34	0.42
2:A:418:THR:O	2:A:422:LYS:HG3	2.19	0.42
3:E:15:ASN:HB3	3:E:17:PHE:CE2	2.54	0.42
3:E:536:PRO:HA	3:E:749:TYR:HD2	1.84	0.42
1:D:32:GLU:OE1	3:E:180:ILE:HG13	2.18	0.42
3:E:492:MET:HG2	3:E:495:GLU:OE1	2.19	0.42
3:E:549:ASP:OD1	3:E:550:TYR:N	2.48	0.42
1:D:191:LYS:HB3	1:D:191:LYS:HE2	1.84	0.42
2:A:369:ILE:HG23	3:E:576:ASN:HB3	2.01	0.42
3:E:164:PHE:O	3:E:165:LEU:HB3	2.19	0.42
3:E:208:LEU:HD23	3:E:208:LEU:HA	1.67	0.42
3:E:388:VAL:HG22	3:E:468:TYR:CG	2.54	0.42
3:E:810:LYS:O	3:E:822:GLU:N	2.37	0.42
1:D:18:ASP:OD2	1:D:58:ARG:HG3	2.19	0.42
2:A:323:LEU:HG	2:A:348:ILE:HD11	2.02	0.42
2:A:355:ASP:O	2:A:359:GLU:HG2	2.19	0.42
3:E:299:ILE:HD13	3:E:320:VAL:HG22	2.02	0.42
3:E:589:GLN:HE21	3:E:589:GLN:HB2	1.54	0.42
3:E:690:ILE:O	3:E:694:MET:HG2	2.20	0.42
3:E:749:TYR:O	3:E:756:PHE:N	2.30	0.42
1:D:14:THR:HG22	1:D:54:LYS:HG2	2.02	0.42
2:A:33:SER:HA	2:A:36:GLU:OE1	2.20	0.42
2:A:239:THR:OG1	2:A:243:LYS:N	2.44	0.42
3:E:41:VAL:O	3:E:103:THR:HG22	2.20	0.42
3:E:386:ALA:O	3:E:410:ILE:HD13	2.20	0.42
3:E:409:ASP:N	3:E:416:LYS:O	2.36	0.42
3:E:546:LEU:HD22	3:E:771:ALA:HB2	2.02	0.42
2:A:69:PHE:O	2:A:176:PHE:N	2.52	0.42
3:E:336:GLN:HG2	3:E:344:TYR:CG	2.55	0.42
3:E:396:THR:HG23	3:E:402:ILE:HG12	2.02	0.42
3:E:564:SER:O	3:E:683:SER:OG	2.38	0.42
1:D:45:ILE:HG12	1:D:48:LYS:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:ARG:NE	1:D:196:GLU:OE1	2.49	0.41
2:A:76:TYR:CD2	2:A:170:ILE:HD13	2.55	0.41
2:A:240:LYS:HD3	2:A:240:LYS:HA	1.95	0.41
2:A:376:ARG:HA	2:A:376:ARG:HD3	1.55	0.41
3:E:541:PHE:HE1	3:E:800:MET:HG2	1.84	0.41
3:E:627:LEU:HA	3:E:627:LEU:HD23	1.87	0.41
2:A:152:PHE:HE2	2:A:163:PRO:HG2	1.85	0.41
2:A:154:LEU:HD12	2:A:157:GLU:OE2	2.20	0.41
2:A:176:PHE:CE2	2:A:210:VAL:HG21	2.55	0.41
3:E:31:PHE:O	3:E:139:CYS:HA	2.21	0.41
3:E:188:TYR:N	3:E:188:TYR:CD1	2.88	0.41
3:E:227:LEU:HD13	3:E:247:ILE:HA	2.01	0.41
3:E:410:ILE:HG12	3:E:415:PHE:CB	2.50	0.41
3:E:738:PRO:HD2	3:E:741:TYR:CE1	2.55	0.41
1:D:79:PHE:CZ	1:D:158:LEU:HD13	2.56	0.41
3:E:38:PHE:N	3:E:93:GLU:O	2.43	0.41
3:E:410:ILE:HG12	3:E:415:PHE:HB3	2.02	0.41
3:E:438:VAL:HG21	3:E:458:TYR:CZ	2.55	0.41
3:E:698:LEU:HD12	3:E:698:LEU:HA	1.76	0.41
2:A:131:LEU:HD12	2:A:136:TRP:CH2	2.55	0.41
3:E:183:ILE:HG21	3:E:244:LEU:HD21	2.01	0.41
3:E:604:ARG:HB3	3:E:685:LYS:NZ	2.35	0.41
1:D:52:GLN:HG3	1:D:120:ASN:HD21	1.86	0.41
2:A:75:TYR:HB2	2:A:202:LEU:HD23	2.03	0.41
2:A:137:ILE:HG12	2:A:161:ASN:ND2	2.35	0.41
3:E:7:ASN:OD1	3:E:491:SER:OG	2.37	0.41
3:E:439:ASP:OD1	3:E:442:GLN:N	2.41	0.41
3:E:555:PRO:HA	3:E:627:LEU:CD1	2.50	0.41
3:E:708:SER:O	3:E:710:GLY:N	2.54	0.41
2:A:387:PHE:CE2	2:A:411:VAL:HG11	2.56	0.41
3:E:52:PRO:HA	3:E:53:PRO:HD3	1.95	0.41
1:D:34:ALA:O	1:D:38:LEU:HD13	2.20	0.41
1:D:156:TYR:HE1	1:D:179:GLY:HA3	1.85	0.41
2:A:7:LEU:O	2:A:11:LYS:HG2	2.21	0.41
2:A:79:LEU:HD21	2:A:165:TYR:HB3	2.01	0.41
2:A:392:THR:O	2:A:395:LEU:HB2	2.21	0.41
3:E:208:LEU:HD22	3:E:212:GLU:OE1	2.21	0.41
3:E:128:ASP:HB3	3:E:131:TYR:HB2	2.03	0.41
3:E:631:LEU:HD22	3:E:631:LEU:HA	1.83	0.41
1:D:15:TYR:CZ	1:D:23:MET:HG3	2.55	0.40
2:A:401:GLU:H	2:A:401:GLU:HG2	1.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:20:LEU:HB3	3:E:34:PHE:HE2	1.86	0.40
3:E:266:ASN:HB2	3:E:318:PHE:CD1	2.56	0.40
3:E:577:ARG:O	3:E:580:GLU:HB3	2.21	0.40
3:E:587:LEU:HD12	3:E:612:ILE:HD12	2.02	0.40
3:E:737:LEU:HD23	3:E:737:LEU:HA	1.85	0.40
2:A:113:ALA:HB1	2:A:160:LEU:HD23	2.04	0.40
3:E:55:PHE:N	3:E:93:GLU:OE1	2.35	0.40
3:E:73:SER:O	3:E:572:VAL:HA	2.22	0.40
2:A:87:PHE:HE2	2:A:131:LEU:HB2	1.86	0.40
2:A:320:THR:O	2:A:324:ASP:N	2.55	0.40
2:A:344:VAL:O	2:A:348:ILE:HG12	2.21	0.40
3:E:63:MET:N	3:E:86:ALA:O	2.51	0.40
1:D:109:ASN:ND2	1:D:112:ILE:HG23	2.36	0.40
3:E:210:GLU:HA	3:E:213:ILE:HD12	2.02	0.40
3:E:486:TYR:N	3:E:486:TYR:CD1	2.88	0.40
3:E:499:SER:O	3:E:503:LYS:HE3	2.21	0.40
3:E:559:ILE:HG21	3:E:628:ARG:HB2	2.04	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	D	216/242 (89%)	205 (95%)	11 (5%)	0	100	100
2	A	416/426 (98%)	388 (93%)	26 (6%)	2 (0%)	29	66
3	E	823/1033 (80%)	765 (93%)	56 (7%)	2 (0%)	47	79
All	All	1455/1701 (86%)	1358 (93%)	93 (6%)	4 (0%)	44	74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	365	VAL
2	A	72	ASP
3	E	709	ASN
2	A	53	VAL

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	D	199/215 (93%)	190 (96%)	9 (4%)	27	57
2	A	390/394 (99%)	376 (96%)	14 (4%)	35	63
3	E	755/951 (79%)	692 (92%)	63 (8%)	11	40
All	All	1344/1560 (86%)	1258 (94%)	86 (6%)	21	48

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2	ASN
1	D	6	VAL
1	D	22	VAL
1	D	38	LEU
1	D	117	ILE
1	D	120	ASN
1	D	136	TYR
1	D	138	ASP
1	D	165	ASN
2	A	22	PHE
2	A	57	ILE
2	A	98	LEU
2	A	172	GLU
2	A	251	ASP
2	A	267	LYS
2	A	291	LYS
2	A	300	ASP
2	A	308	PHE
2	A	351	GLN

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Mol	Chain	Res	Type
2	A	352	SER
2	A	367	ASP
2	A	371	LEU
2	A	420	VAL
3	E	6	ILE
3	E	9	PHE
3	E	16	ARG
3	E	26	ASN
3	E	32	ILE
3	E	41	VAL
3	E	67	ASP
3	E	80	ASP
3	E	87	ASP
3	E	93	GLU
3	E	100	GLN
3	E	143	ASP
3	E	153	ILE
3	E	165	LEU
3	E	168	GLU
3	E	172	ASP
3	E	177	SER
3	E	178	VAL
3	E	185	HIS
3	E	188	TYR
3	E	190	TYR
3	E	196	LYS
3	E	200	PHE
3	E	251	LEU
3	E	253	GLU
3	E	272	ILE
3	E	273	THR
3	E	276	LEU
3	E	295	VAL
3	E	328	PHE
3	E	329	PHE
3	E	331	LEU
3	E	334	PHE
3	E	335	ILE
3	E	365	VAL
3	E	391	THR
3	E	459	CYS
3	E	462	ASP

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Mol	Chain	Res	Type
3	E	466	CYS
3	E	526	PHE
3	E	550	TYR
3	E	563	LEU
3	E	564	SER
3	E	567	THR
3	E	597	ILE
3	E	617	ARG
3	E	631	LEU
3	E	633	GLU
3	E	654	ASP
3	E	655	SER
3	E	657	GLN
3	E	659	THR
3	E	665	ASN
3	E	671	MET
3	E	692	ARG
3	E	693	ARG
3	E	734	LYS
3	E	748	VAL
3	E	755	VAL
3	E	784	PHE
3	E	791	PHE
3	E	797	ASN
3	E	828	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	8	HIS
1	D	16	HIS
1	D	120	ASN
1	D	165	ASN
2	A	32	ASN
2	A	48	GLN
2	A	115	ASN
2	A	304	ASN
2	A	318	GLN
2	A	351	GLN
2	A	373	ASN
2	A	374	ASN
2	A	409	GLN

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Mol	Chain	Res	Type
3	E	225	GLN
3	E	323	ASN
3	E	442	GLN
3	E	538	GLN
3	E	583	ASN
3	E	589	GLN
3	E	657	GLN
3	E	780	ASN
3	E	801	GLN

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)

There are no monosaccharides in this entry.

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

This section contains visualisations of the EMDB entry EMD-18134. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

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

9 Map-model fit

This section was not generated.