Full wwPDB EM Validation Report ⓘ

Jun 8, 2025 – 01:36 AM JST

PDB ID	:	9KBD / pdb_00009kbd
EMDB ID	:	EMD-62222
Title	:	Cryo-EM structure of the CUL1-RBX1-SKP1-FBXO3 SCF ubiquition ligase complex
Authors	:	Wei, J.; Xu, C.
Deposited on	:	2024-10-30
Resolution	:	3.70 Å(reported)

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

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

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

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

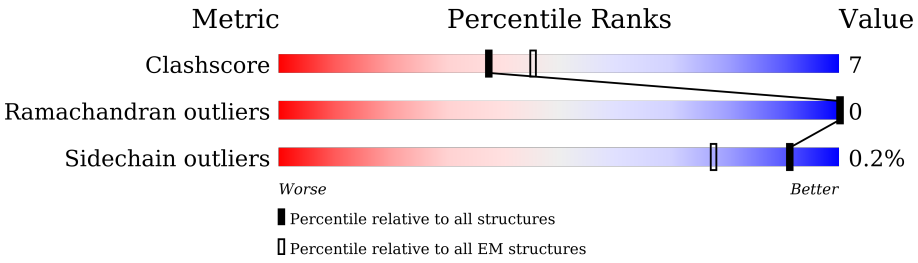
EMDB validation analysis	:	FAILED
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	B	163	78% 20% ..
2	C	436	71% 22% 7%
3	R	108	11% . 85%
4	A	776	80% 15% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10728 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 S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	160	1281	804	207	264	6	0	0

- Molecule 2 is a protein called F-box only protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	405	3277	2101	552	603	21	0	0

- Molecule 3 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	R	16	144	98	25	21	0	0

- Molecule 4 is a protein called Cullin-1.

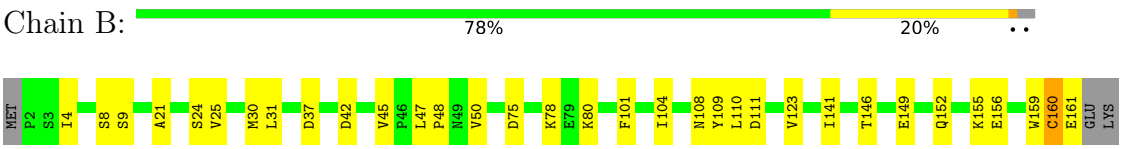
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	737	6026	3821	1029	1147	29	0	0

3 Residue-property plots (i)

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

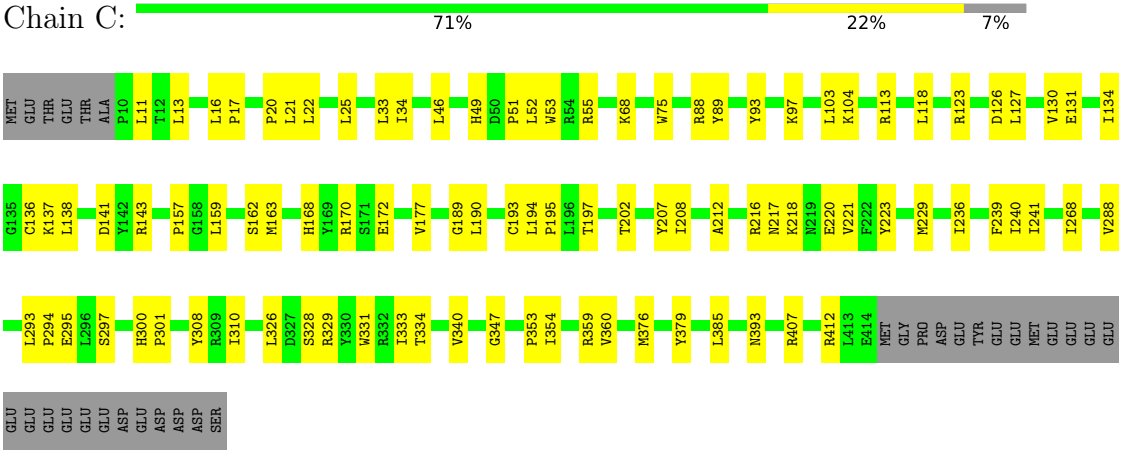
• Molecule 1: S-phase kinase-associated protein 1

Chain B:



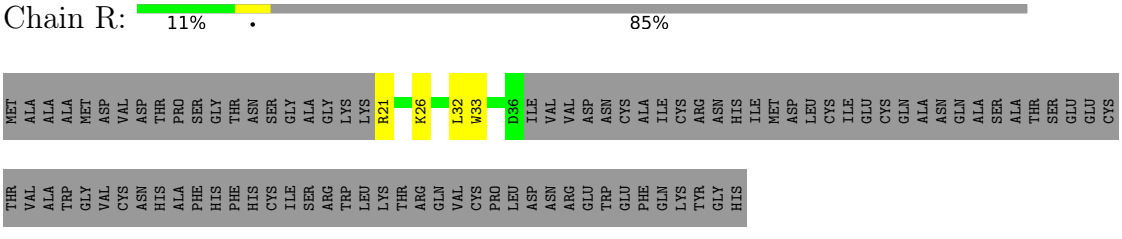
• Molecule 2: F-box only protein 3

Chain C:



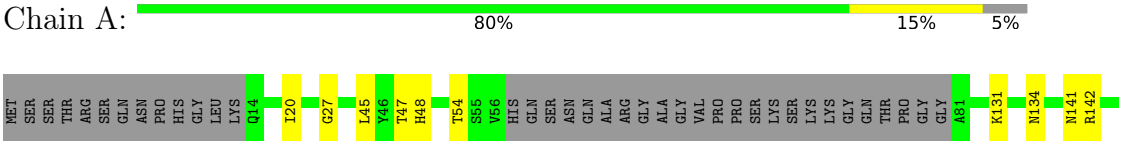
• Molecule 3: E3 ubiquitin-protein ligase RBX1

Chain R:



• Molecule 4: Cullin-1

Chain A:




E158 L162 T180 V183 L184 R191 I196 I201 E233 F236 L237 A238 D239 R242 S248 L252 L269 E270 E271 V275 L279 Q284 H299 I302 F307 L311 M322 L349 I352 C355 A359 Y366 C399 G400
R401 F402 I403 N404 A407 L430 S433 S434 L446 Y455 D460 F465 L474 Q477 K491 K503 Q509 D510 I511 S514 K515 D534 Q538 V539 L540 S541 S542 G543 S544 W545 C551 T552 L555 P556 E560 A571 H574 S575 G576 R577
Y583 K587 N593 Q602 A603 S604 T605 F606 Q607 M608 A609 I610 L611 L612 Q613 Y614 Y620 T621 V622 L625 T626 D627 S628 T629 Q630 D634 I635 L636 A637 L649 V650 L663 L671 Y672 K676 N683 I684 N685 Q696 I703 R707 R722 R745
V746 P747 I757 R764 V765 D766 Y772 S773 Y774 LEU ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	185300	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 ($e^-/Å^2$)	55.62	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k 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	B	0.16	0/1304	0.33	0/1767
2	C	0.13	0/3366	0.32	0/4567
3	R	0.10	0/150	0.26	0/204
4	A	0.16	0/6126	0.35	0/8249
All	All	0.15	0/10946	0.34	0/14787

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	B	1281	0	1251	23	0
2	C	3277	0	3202	61	0
3	R	144	0	137	5	0
4	A	6026	0	6055	81	0
All	All	10728	0	10645	155	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 7.

All (155) 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)
4:A:757:ILE:HD11	4:A:764:ARG:HB2	1.71	0.73
2:C:328:SER:HA	2:C:347:GLY:H	1.54	0.72
4:A:183:VAL:HG23	4:A:201:ILE:HD12	1.72	0.72
1:B:108:ASN:HD22	2:C:20:PRO:HG3	1.55	0.71
2:C:163:MET:HG2	2:C:293:LEU:HD11	1.72	0.70
4:A:745:ARG:HG3	4:A:747:PRO:HD2	1.76	0.67
4:A:622:VAL:HA	4:A:625:LEU:HD12	1.76	0.66
4:A:275:VAL:HG11	4:A:284:GLN:HB2	1.77	0.65
2:C:193:CYS:SG	2:C:216:ARG:NH1	2.71	0.64
4:A:460:ASP:HB2	4:A:703:ILE:HD11	1.81	0.63
2:C:223:TYR:HB2	2:C:239:PHE:HB2	1.81	0.62
4:A:134:ASN:OD1	4:A:141:ASN:ND2	2.33	0.61
2:C:127:LEU:HD23	2:C:143:ARG:HE	1.67	0.60
2:C:88:ARG:NH2	2:C:89:TYR:OH	2.35	0.60
2:C:329:ARG:HE	2:C:331:TRP:HE1	1.50	0.60
4:A:625:LEU:HB3	4:A:636:LEU:HD21	1.84	0.59
1:B:75:ASP:HB2	1:B:78:LYS:HB2	1.84	0.59
2:C:294:PRO:HA	2:C:297:SER:HB3	1.86	0.58
4:A:252:LEU:HD11	4:A:302:ILE:HG21	1.85	0.58
4:A:551:CYS:SG	4:A:552:THR:N	2.77	0.58
2:C:21:LEU:HD23	2:C:46:LEU:HG	1.86	0.58
4:A:400:GLY:O	4:A:404:ASN:ND2	2.36	0.58
1:B:152:GLN:HA	1:B:155:LYS:HE2	1.84	0.58
2:C:333:ILE:HG23	2:C:376:MET:HG2	1.86	0.57
4:A:403:ILE:HD12	4:A:455:TYR:HB2	1.84	0.57
2:C:189:GLY:HA3	2:C:236:ILE:HD12	1.86	0.57
2:C:170:ARG:NE	2:C:295:GLU:OE2	2.38	0.57
2:C:170:ARG:NH2	2:C:202:THR:OG1	2.37	0.57
3:R:32:LEU:HD12	4:A:542:SER:HA	1.86	0.56
2:C:163:MET:N	2:C:170:ARG:O	2.39	0.56
2:C:130:VAL:HG21	2:C:177:VAL:HB	1.87	0.56
4:A:359:ALA:HB1	4:A:366:TYR:HB2	1.87	0.56
4:A:514:SER:OG	4:A:539:VAL:O	2.24	0.55
4:A:650:VAL:HG22	4:A:672:TYR:HB2	1.89	0.55
2:C:359:ARG:NH1	2:C:360:VAL:O	2.40	0.55
4:A:27:GLY:HA3	4:A:45:LEU:HD21	1.90	0.54
4:A:556:PRO:O	4:A:560:GLU:N	2.37	0.54
4:A:764:ARG:HD3	4:A:772:TYR:HB3	1.90	0.54
4:A:446:LEU:HB3	4:A:491:LYS:HZ1	1.72	0.53
2:C:134:ILE:HG13	2:C:136:CYS:H	1.74	0.53
2:C:162:SER:N	2:C:268:ILE:O	2.41	0.53
4:A:509:GLN:NE2	4:A:510:ASP:OD1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:275:VAL:HG21	4:A:284:GLN:HA	1.91	0.52
4:A:556:PRO:HB3	4:A:612:LEU:HD22	1.92	0.52
3:R:21:ARG:O	4:A:593:ASN:ND2	2.42	0.51
1:B:37:ASP:N	1:B:37:ASP:OD1	2.44	0.51
1:B:111:ASP:OD1	4:A:142:ARG:NH2	2.41	0.51
1:B:141:ILE:HD11	2:C:13:LEU:HB3	1.91	0.51
2:C:212:ALA:HB2	2:C:218:LYS:HB2	1.93	0.50
1:B:146:THR:OG1	1:B:149:GLU:OE1	2.30	0.49
2:C:34:ILE:HG13	2:C:53:TRP:HH2	1.77	0.49
4:A:158:GLU:O	4:A:162:LEU:N	2.41	0.49
1:B:48:PRO:HG2	4:A:47:THR:HG21	1.95	0.49
2:C:195:PRO:HA	2:C:207:TYR:HA	1.94	0.49
4:A:239:ASP:OD2	4:A:242:ARG:NH1	2.46	0.49
2:C:308:TYR:OH	2:C:376:MET:SD	2.65	0.48
2:C:68:LYS:HD2	2:C:75:TRP:CE2	2.49	0.48
2:C:288:VAL:HG22	2:C:310:ILE:HG23	1.94	0.48
4:A:514:SER:HB3	4:A:538:GLN:HA	1.95	0.48
4:A:307:PHE:HA	4:A:322:MET:HE1	1.95	0.47
4:A:540:LEU:HD13	4:A:545:TRP:CD2	2.49	0.47
2:C:354:ILE:HG12	2:C:385:LEU:HD11	1.96	0.47
4:A:460:ASP:OD1	4:A:460:ASP:N	2.46	0.47
1:B:30:MET:HE1	1:B:45:VAL:HG11	1.95	0.47
2:C:163:MET:HB3	2:C:170:ARG:HB3	1.96	0.47
4:A:399:CYS:HA	4:A:402:PHE:HB3	1.96	0.47
4:A:606:PHE:O	4:A:610:ILE:HG12	2.14	0.47
2:C:118:LEU:HD21	2:C:159:LEU:HD22	1.96	0.47
2:C:17:PRO:HB3	4:A:54:THR:HB	1.96	0.47
2:C:141:ASP:N	2:C:141:ASP:OD1	2.48	0.47
2:C:300:HIS:CE1	2:C:412:ARG:HH22	2.33	0.47
4:A:433:SER:OG	4:A:434:SER:N	2.48	0.47
2:C:131:GLU:HG2	2:C:138:LEU:HD23	1.96	0.46
4:A:248:SER:HG	4:A:299:HIS:CE1	2.30	0.46
4:A:477:GLN:OE1	4:A:538:GLN:NE2	2.36	0.46
4:A:676:LYS:HA	4:A:676:LYS:HD2	1.76	0.46
1:B:109:TYR:OH	4:A:47:THR:OG1	2.24	0.46
4:A:20:ILE:HD11	4:A:48:HIS:HA	1.96	0.46
2:C:137:LYS:HA	2:C:137:LYS:HD3	1.75	0.46
4:A:465:PHE:HZ	4:A:696:GLN:HG2	1.80	0.45
2:C:138:LEU:HD11	2:C:194:LEU:HD13	1.97	0.45
4:A:540:LEU:HB3	4:A:545:TRP:CD1	2.52	0.45
4:A:722:ARG:O	4:A:722:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:352:ILE:HG22	4:A:407:ALA:HB3	1.97	0.45
2:C:194:LEU:HB3	2:C:208:ILE:HG22	1.98	0.45
4:A:184:LEU:HD21	4:A:236:PHE:HA	1.99	0.45
4:A:583:TYR:HB3	4:A:605:THR:HB	1.99	0.45
1:B:47:LEU:HD13	1:B:110:LEU:HD21	2.00	0.44
2:C:240:ILE:HD11	2:C:407:ARG:HD3	1.99	0.44
4:A:587:LYS:HB3	4:A:685:ASN:HD22	1.83	0.44
4:A:552:THR:OG1	4:A:630:GLN:O	2.29	0.44
1:B:4:ILE:HD12	1:B:31:LEU:HD21	1.98	0.44
2:C:104:LYS:HB3	2:C:104:LYS:HE3	1.76	0.44
3:R:21:ARG:HB3	4:A:593:ASN:HD21	1.83	0.44
3:R:26:LYS:HA	4:A:534:ASP:HB3	1.99	0.44
4:A:571:ALA:O	4:A:575:SER:OG	2.35	0.44
4:A:634:ASP:OD1	4:A:634:ASP:N	2.51	0.44
4:A:614:TYR:HB3	4:A:671:LEU:HD13	2.00	0.44
1:B:101:PHE:HB3	2:C:11:LEU:HD23	2.00	0.44
4:A:515:LYS:HD3	4:A:515:LYS:HA	1.81	0.44
4:A:474:LEU:HD13	4:A:511:ILE:HG13	1.98	0.43
2:C:22:LEU:HD23	2:C:22:LEU:HA	1.89	0.43
2:C:379:TYR:HB2	2:C:393:ASN:HB2	1.99	0.43
4:A:180:THR:HA	4:A:183:VAL:HG12	1.99	0.43
4:A:430:LEU:HD21	4:A:446:LEU:HD21	2.00	0.43
4:A:191:ARG:NH1	4:A:271:GLU:OE2	2.51	0.43
2:C:49:HIS:CD2	2:C:51:PRO:HD2	2.53	0.43
2:C:190:LEU:HA	2:C:216:ARG:HH12	1.83	0.43
2:C:221:VAL:HG12	2:C:241:ILE:HD13	2.01	0.43
2:C:326:LEU:HB3	2:C:353:PRO:HD2	2.00	0.43
4:A:460:ASP:OD2	4:A:707:ARG:NE	2.44	0.43
4:A:766:ASP:N	4:A:766:ASP:OD1	2.50	0.43
2:C:113:ARG:HH21	2:C:157:PRO:HD3	1.82	0.43
1:B:104:ILE:HD11	1:B:123:VAL:HG21	2.00	0.43
1:B:160:CYS:SG	2:C:34:ILE:HD13	2.58	0.43
1:B:78:LYS:O	2:C:55:ARG:NH2	2.51	0.43
2:C:168:HIS:CE1	2:C:202:THR:HG21	2.54	0.42
4:A:503:LYS:HE3	4:A:544:SER:HA	2.02	0.42
1:B:156:GLU:O	1:B:159:TRP:HD1	2.02	0.42
1:B:80:LYS:HG2	2:C:55:ARG:NH2	2.35	0.42
2:C:103:LEU:HD21	2:C:159:LEU:HD11	2.02	0.42
4:A:649:LEU:HA	4:A:672:TYR:HB3	2.01	0.42
2:C:25:LEU:HB3	2:C:33:LEU:HD21	2.02	0.42
4:A:349:LEU:HD23	4:A:349:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:355:CYS:HB3	4:A:359:ALA:HB2	2.02	0.42
4:A:574:HIS:ND1	4:A:577:ARG:HD2	2.35	0.41
2:C:217:ASN:N	2:C:220:GLU:OE2	2.47	0.41
4:A:233:GLU:O	4:A:237:LEU:HB2	2.20	0.41
2:C:13:LEU:HD12	2:C:16:LEU:HD12	2.02	0.41
2:C:123:ARG:NH1	2:C:126:ASP:OD2	2.53	0.41
4:A:311:LEU:HD12	4:A:311:LEU:HA	1.90	0.41
4:A:602:GLN:HG2	4:A:683:ASN:HA	2.03	0.41
4:A:604:SER:O	4:A:608:MET:N	2.46	0.41
1:B:8:SER:OG	1:B:9:SER:N	2.54	0.41
3:R:33:TRP:NE1	4:A:577:ARG:HD3	2.35	0.41
4:A:131:LYS:HD2	4:A:131:LYS:HA	1.84	0.41
1:B:8:SER:OG	1:B:50:VAL:O	2.38	0.41
1:B:42:ASP:OD1	1:B:42:ASP:N	2.54	0.41
4:A:587:LYS:HA	4:A:604:SER:HA	2.03	0.41
1:B:25:VAL:HB	1:B:111:ASP:HB2	2.03	0.41
2:C:33:LEU:HD23	2:C:33:LEU:HA	1.90	0.41
2:C:52:LEU:HD23	2:C:52:LEU:HA	1.85	0.41
4:A:275:VAL:HA	4:A:279:LEU:HB2	2.03	0.41
4:A:511:ILE:HD13	4:A:511:ILE:HA	1.96	0.41
1:B:21:ALA:O	1:B:24:SER:OG	2.39	0.41
2:C:334:THR:HG23	2:C:340:VAL:HG22	2.02	0.41
4:A:627:ASP:O	4:A:630:GLN:NE2	2.54	0.41
4:A:620:TYR:HH	4:A:628:SER:HG	1.63	0.40
2:C:93:TYR:CE1	2:C:97:LYS:HD2	2.56	0.40
2:C:172:GLU:HB2	2:C:197:THR:OG1	2.21	0.40
4:A:196:ILE:HD12	4:A:196:ILE:HA	1.96	0.40
4:A:555:LEU:HD12	4:A:555:LEU:HA	1.93	0.40
4:A:637:ALA:HA	4:A:663:LEU:HD21	2.03	0.40
2:C:229:MET:HG2	2:C:301:PRO:HD3	2.03	0.40
4:A:269:LEU:HD23	4:A:269:LEU:HA	1.94	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	B	158/163 (97%)	152 (96%)	6 (4%)	0	100	100
2	C	403/436 (92%)	378 (94%)	25 (6%)	0	100	100
3	R	14/108 (13%)	14 (100%)	0	0	100	100
4	A	733/776 (94%)	711 (97%)	22 (3%)	0	100	100
All	All	1308/1483 (88%)	1255 (96%)	53 (4%)	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	B	147/150 (98%)	145 (99%)	2 (1%)	62	76
2	C	360/389 (92%)	360 (100%)	0	100	100
3	R	13/90 (14%)	13 (100%)	0	100	100
4	A	668/698 (96%)	668 (100%)	0	100	100
All	All	1188/1327 (90%)	1186 (100%)	2 (0%)	91	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	160	CYS
1	B	161	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	7	GLN
1	B	152	GLN
2	C	185	GLN

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Mol	Chain	Res	Type
4	A	254	GLN
4	A	284	GLN
4	A	304	HIS
4	A	378	ASN
4	A	436	ASN
4	A	548	GLN
4	A	584	GLN
4	A	630	GLN
4	A	694	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 oligosaccharides 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.