



## Full wwPDB EM Validation Report ⓘ

Nov 5, 2024 – 10:16 AM JST

PDB ID : 8IZR  
EMDB ID : EMD-35869  
Title : Multidrug resistance-associated protein 3  
Authors : Yun, C.H.; Gao, H.M.  
Deposited on : 2023-04-07  
Resolution : 3.62 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](mailto: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>.

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

EMDB validation analysis : **FAILED**  
MolProbity : 4.02b-467  
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) : 2.39

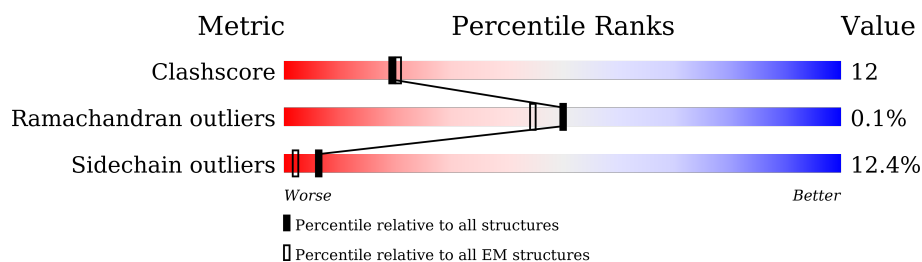
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.62 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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	1589	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11116 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 ATP-binding cassette sub-family C member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1400	Total	C	N	O	S	0	0
			11116	7213	1842	2004	57		

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	PHE	TYR	variant	UNP Q92887
A	1546	LEU	-	expression tag	UNP Q92887
A	1547	GLU	-	expression tag	UNP Q92887
A	1548	GLU	-	expression tag	UNP Q92887
A	1549	ASN	-	expression tag	UNP Q92887
A	1550	LEU	-	expression tag	UNP Q92887
A	1551	TYR	-	expression tag	UNP Q92887
A	1552	PHE	-	expression tag	UNP Q92887
A	1553	GLN	-	expression tag	UNP Q92887
A	1554	GLY	-	expression tag	UNP Q92887
A	1555	SER	-	expression tag	UNP Q92887
A	1556	GLY	-	expression tag	UNP Q92887
A	1557	GLY	-	expression tag	UNP Q92887
A	1558	GLY	-	expression tag	UNP Q92887
A	1559	GLY	-	expression tag	UNP Q92887
A	1560	GLY	-	expression tag	UNP Q92887
A	1561	GLY	-	expression tag	UNP Q92887
A	1562	ASP	-	expression tag	UNP Q92887
A	1563	TYR	-	expression tag	UNP Q92887
A	1564	LYS	-	expression tag	UNP Q92887
A	1565	ASP	-	expression tag	UNP Q92887
A	1566	HIS	-	expression tag	UNP Q92887
A	1567	ASP	-	expression tag	UNP Q92887
A	1568	GLY	-	expression tag	UNP Q92887
A	1569	ASP	-	expression tag	UNP Q92887
A	1570	TYR	-	expression tag	UNP Q92887
A	1571	LYS	-	expression tag	UNP Q92887
A	1572	ASP	-	expression tag	UNP Q92887

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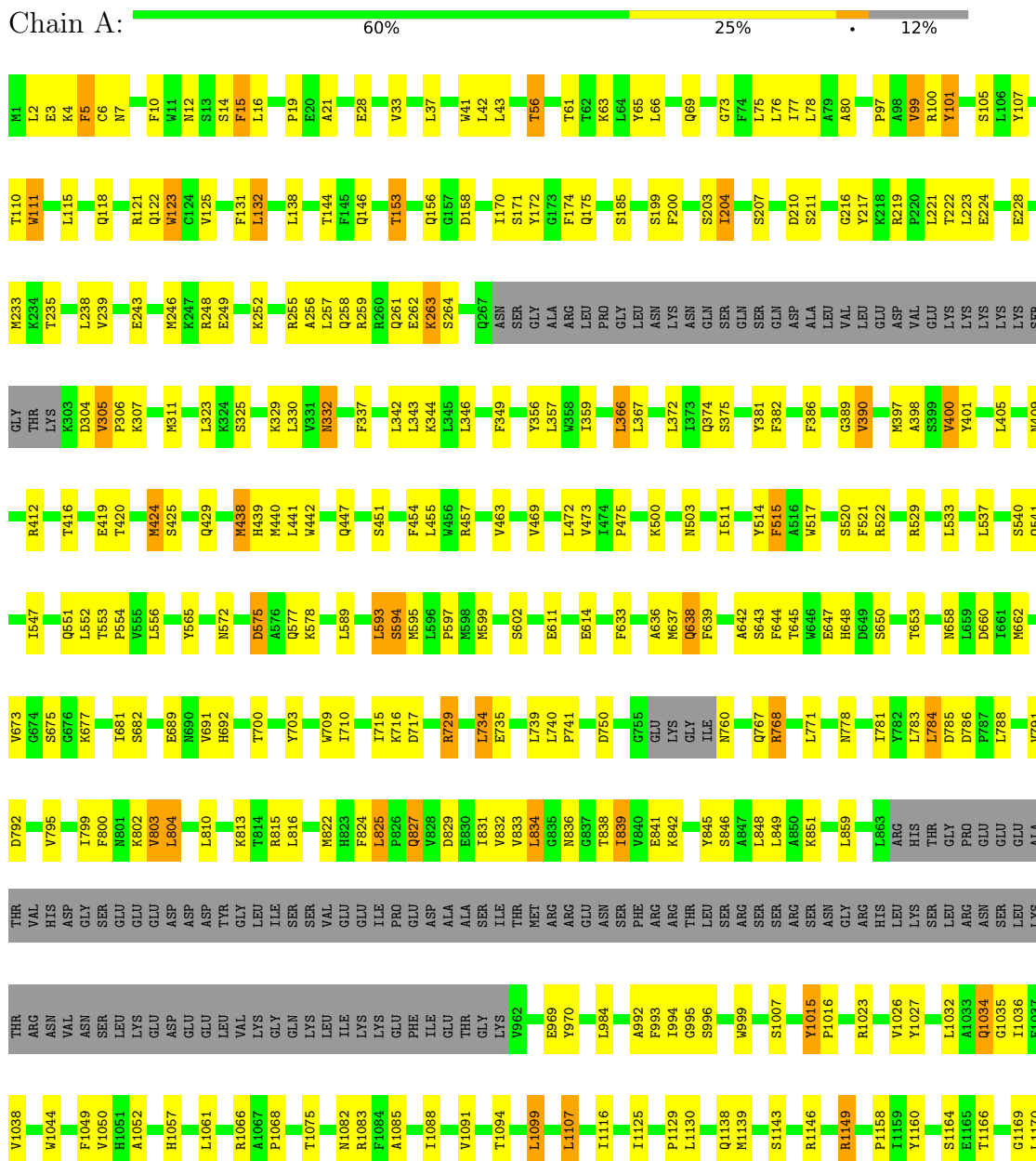
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Chain	Residue	Modelled	Actual	Comment	Reference
A	1573	HIS	-	expression tag	UNP Q92887
A	1574	ASP	-	expression tag	UNP Q92887
A	1575	ILE	-	expression tag	UNP Q92887
A	1576	ASP	-	expression tag	UNP Q92887
A	1577	TYR	-	expression tag	UNP Q92887
A	1578	LYS	-	expression tag	UNP Q92887
A	1579	ASP	-	expression tag	UNP Q92887
A	1580	ASP	-	expression tag	UNP Q92887
A	1581	ASP	-	expression tag	UNP Q92887
A	1582	ASP	-	expression tag	UNP Q92887
A	1583	LYS	-	expression tag	UNP Q92887
A	1584	HIS	-	expression tag	UNP Q92887
A	1585	HIS	-	expression tag	UNP Q92887
A	1586	HIS	-	expression tag	UNP Q92887
A	1587	HIS	-	expression tag	UNP Q92887
A	1588	HIS	-	expression tag	UNP Q92887
A	1589	HIS	-	expression tag	UNP Q92887

### 3 Residue-property plots

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: ATP-binding cassette sub-family C member 2





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101191	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.65	0/11350	0.89	0/15389

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1230	ARG	Sidechain

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11116	0	11376	279	0
All	All	11116	0	11376	279	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 12.



All (279) 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:A:1365:ILE:HG13	1:A:1373:LEU:HD22	1.52	0.90
1:A:1358:ILE:HG23	1:A:1363:VAL:H	1.40	0.86
1:A:78:LEU:CD1	1:A:170:ILE:HG22	2.09	0.82
1:A:1303:ASN:O	1:A:1356:GLY:HA2	1.80	0.82
1:A:97:PRO:HD2	1:A:100:ARG:HD2	1.63	0.80
1:A:1335:ARG:HH21	1:A:1495:LEU:HB2	1.47	0.79
1:A:1305:TYR:HB3	1:A:1320:ILE:HB	1.65	0.79
1:A:1359:ILE:HG13	1:A:1360:ILE:HG13	1.65	0.78
1:A:1357:GLN:HB2	1:A:1364:ASP:HB2	1.68	0.75
1:A:537:LEU:HB2	1:A:1050:VAL:HG21	1.69	0.75
1:A:822:MET:HA	1:A:825:LEU:HG	1.69	0.74
1:A:1138:GLN:HB2	1:A:1256:VAL:HG22	1.68	0.74
1:A:1146:ARG:HA	1:A:1149:ARG:HB2	1.70	0.73
1:A:1333:VAL:HB	1:A:1506:VAL:HG13	1.69	0.73
1:A:999:TRP:HZ2	1:A:1023:ARG:HA	1.54	0.73
1:A:1305:TYR:HA	1:A:1356:GLY:HA3	1.72	0.72
1:A:78:LEU:HD11	1:A:170:ILE:HG22	1.72	0.72
1:A:675:SER:HB2	1:A:836:ASN:H	1.54	0.72
1:A:1308:ARG:HA	1:A:1315:LEU:HA	1.71	0.72
1:A:455:LEU:HB3	1:A:463:VAL:HG11	1.73	0.71
1:A:1335:ARG:NH2	1:A:1495:LEU:H	1.90	0.70
1:A:78:LEU:HD11	1:A:170:ILE:CG2	2.20	0.70
1:A:1334:GLY:HA3	1:A:1340:LYS:HB3	1.74	0.70
1:A:61:THR:HA	1:A:122:GLN:HE22	1.57	0.70
1:A:1335:ARG:CZ	1:A:1493:HIS:O	2.41	0.69
1:A:810:LEU:HB3	1:A:813:LYS:HB2	1.75	0.68
1:A:643:SER:HB2	1:A:691:VAL:HB	1.76	0.68
1:A:1170:LEU:HD21	1:A:1174:ARG:HH22	1.60	0.67
1:A:329:LYS:HB3	1:A:442:TRP:HH2	1.59	0.67
1:A:740:LEU:HB2	1:A:741:PRO:HD3	1.77	0.66
1:A:1508:ASP:HB3	1:A:1513:ILE:HG13	1.77	0.66
1:A:1508:ASP:N	1:A:1513:ILE:HB	2.12	0.65
1:A:257:LEU:HD11	1:A:304:ASP:HB3	1.80	0.64
1:A:1358:ILE:HG23	1:A:1363:VAL:N	2.13	0.63
1:A:28:GLU:HB3	1:A:146:GLN:HG2	1.79	0.63
1:A:256:ALA:HA	1:A:259:ARG:HB2	1.80	0.63
1:A:636:ALA:HB1	1:A:781:ILE:HD11	1.81	0.61
1:A:803:VAL:HG23	1:A:804:LEU:HG	1.80	0.61
1:A:78:LEU:CD1	1:A:170:ILE:CG2	2.77	0.61
1:A:259:ARG:HA	1:A:262:GLU:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:HD13	1:A:170:ILE:HG22	1.80	0.61
1:A:1358:ILE:H	1:A:1364:ASP:H	1.50	0.59
1:A:329:LYS:HB3	1:A:442:TRP:CH2	2.38	0.59
1:A:1309:TYR:HB2	1:A:1316:VAL:HG23	1.84	0.59
1:A:1358:ILE:HG23	1:A:1362:GLY:HA3	1.84	0.59
1:A:996:SER:HB2	1:A:1027:TYR:HE1	1.67	0.58
1:A:970:TYR:HE1	1:A:1091:VAL:HG13	1.68	0.58
1:A:739:LEU:HD21	1:A:768:ARG:HD3	1.85	0.58
1:A:999:TRP:CZ2	1:A:1023:ARG:HA	2.39	0.58
1:A:1099:LEU:HA	1:A:1262:ILE:HD11	1.85	0.57
1:A:1359:ILE:HA	1:A:1364:ASP:O	2.04	0.57
1:A:1358:ILE:H	1:A:1364:ASP:N	2.02	0.57
1:A:800:PHE:CD1	1:A:824:PHE:HB3	2.39	0.57
1:A:647:GLU:HB2	1:A:650:SER:HB3	1.87	0.56
1:A:993:PHE:HA	1:A:1034:GLN:HE21	1.69	0.56
1:A:1358:ILE:C	1:A:1364:ASP:H	2.07	0.56
1:A:397:MET:HG2	1:A:424:MET:HG2	1.86	0.56
1:A:223:LEU:HD21	1:A:1192:THR:HG21	1.86	0.56
1:A:800:PHE:CE2	1:A:827:GLN:HB2	2.41	0.56
1:A:1359:ILE:HA	1:A:1364:ASP:C	2.26	0.56
1:A:332:ASN:HD22	1:A:374:GLN:HG3	1.70	0.56
1:A:675:SER:HB2	1:A:836:ASN:N	2.20	0.56
1:A:56:THR:O	1:A:123:TRP:HD1	1.89	0.55
1:A:43:LEU:HB2	1:A:131:PHE:CE1	2.41	0.55
1:A:1358:ILE:HG13	1:A:1362:GLY:HA3	1.88	0.55
1:A:1469:LEU:HA	1:A:1472:ASP:HB3	1.89	0.55
1:A:1365:ILE:HG21	1:A:1373:LEU:HD13	1.88	0.55
1:A:398:ALA:HB2	1:A:1190:ILE:HD12	1.89	0.55
1:A:1357:GLN:HB2	1:A:1364:ASP:CB	2.37	0.55
1:A:709:TRP:CE2	1:A:1169:GLY:HA3	2.43	0.54
1:A:19:PRO:HB3	1:A:356:TYR:HD1	1.72	0.54
1:A:337:PHE:HB3	1:A:454:PHE:HE2	1.73	0.54
1:A:1411:GLU:HB2	1:A:1416:LYS:HD3	1.90	0.54
1:A:16:LEU:HA	1:A:21:ALA:HB1	1.89	0.53
1:A:644:PHE:HA	1:A:689:GLU:O	2.08	0.53
1:A:455:LEU:CB	1:A:463:VAL:HG11	2.37	0.53
1:A:1407:TRP:HA	1:A:1410:LEU:HD12	1.89	0.53
1:A:1359:ILE:HB	1:A:1367:SER:HB3	1.90	0.53
1:A:153:THR:HG23	1:A:158:ASP:HB3	1.89	0.53
1:A:1066:ARG:NH2	1:A:1282:ALA:O	2.41	0.53
1:A:1088:ILE:HD13	1:A:1272:ILE:HD13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1258:MET:C	1:A:1260:SER:N	2.62	0.53
1:A:1391:LEU:HB2	1:A:1426:LEU:O	2.09	0.52
1:A:1457:ILE:HA	1:A:1487:THR:HB	1.91	0.52
1:A:565:TYR:CZ	1:A:572:ASN:HB3	2.45	0.52
1:A:37:LEU:HD22	1:A:110:THR:HG21	1.90	0.52
1:A:1446:CYS:O	1:A:1449:ARG:HB2	2.10	0.52
1:A:639:PHE:HB2	1:A:658:ASN:HA	1.92	0.52
1:A:520:SER:HB3	1:A:1398:PHE:CZ	2.45	0.52
1:A:2:LEU:HB3	1:A:5:PHE:HB3	1.92	0.51
1:A:1392:ARG:HH21	1:A:1399:ASN:HB3	1.74	0.51
1:A:1306:GLN:HA	1:A:1317:LEU:O	2.11	0.51
1:A:1358:ILE:O	1:A:1364:ASP:N	2.41	0.51
1:A:1472:ASP:HA	1:A:1475:ILE:HD12	1.92	0.51
1:A:594:SER:O	1:A:597:PRO:HD2	2.10	0.51
1:A:832:VAL:HA	1:A:842:LYS:HA	1.93	0.51
1:A:63:LYS:O	1:A:66:LEU:HB3	2.10	0.51
1:A:1358:ILE:CG1	1:A:1362:GLY:HA3	2.41	0.51
1:A:1335:ARG:HH22	1:A:1495:LEU:H	1.58	0.50
1:A:1349:ARG:HE	1:A:1352:GLU:HG2	1.77	0.50
1:A:261:GLN:O	1:A:264:SER:HB3	2.12	0.50
1:A:1275:TYR:HA	1:A:1278:VAL:HG23	1.94	0.50
1:A:647:GLU:HB2	1:A:650:SER:CB	2.42	0.50
1:A:1508:ASP:H	1:A:1513:ILE:HB	1.76	0.50
1:A:799:ILE:HA	1:A:802:LYS:HG2	1.94	0.50
1:A:1116:ILE:HG12	1:A:1241:VAL:HG13	1.93	0.50
1:A:1359:ILE:HG22	1:A:1364:ASP:HB3	1.94	0.50
1:A:144:THR:HG22	1:A:172:TYR:OH	2.12	0.50
1:A:517:TRP:CD1	1:A:1397:PRO:HG3	2.47	0.50
1:A:803:VAL:O	1:A:810:LEU:HB2	2.11	0.49
1:A:305:VAL:HG22	1:A:306:PRO:HD2	1.94	0.49
1:A:633:PHE:CE2	1:A:638:GLN:HB2	2.46	0.49
1:A:1305:TYR:HA	1:A:1356:GLY:CA	2.41	0.49
1:A:252:LYS:HA	1:A:255:ARG:HD2	1.95	0.49
1:A:1333:VAL:HG22	1:A:1498:ILE:HG21	1.95	0.49
1:A:645:THR:HG23	1:A:689:GLU:HB2	1.95	0.48
1:A:999:TRP:CZ2	1:A:1026:VAL:HB	2.47	0.48
1:A:673:VAL:HA	1:A:677:LYS:HD3	1.95	0.48
1:A:1335:ARG:HD3	1:A:1493:HIS:CD2	2.49	0.48
1:A:258:GLN:O	1:A:262:GLU:N	2.42	0.48
1:A:398:ALA:HB2	1:A:1190:ILE:CD1	2.43	0.48
1:A:259:ARG:O	1:A:263:LYS:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1450:ALA:HA	1:A:1453:ARG:HG3	1.96	0.48
1:A:207:SER:O	1:A:210:ASP:HB2	2.14	0.47
1:A:1401:TYR:CE2	1:A:1452:LEU:HB3	2.49	0.47
1:A:511:ILE:HG23	1:A:515:PHE:CE1	2.50	0.47
1:A:111:TRP:HA	1:A:111:TRP:CE3	2.49	0.47
1:A:346:LEU:HD12	1:A:346:LEU:HA	1.81	0.47
1:A:12:ASN:O	1:A:15:PHE:HB2	2.14	0.47
1:A:1107:LEU:HD13	1:A:1107:LEU:HA	1.73	0.47
1:A:28:GLU:OE2	1:A:146:GLN:HA	2.15	0.47
1:A:833:VAL:HB	1:A:841:GLU:HB2	1.96	0.47
1:A:735:GLU:HA	1:A:740:LEU:HD11	1.97	0.47
1:A:788:LEU:HA	1:A:791:VAL:HG23	1.96	0.47
1:A:1289:ARG:H	1:A:1289:ARG:HG2	1.48	0.47
1:A:43:LEU:HB2	1:A:131:PHE:HE1	1.79	0.47
1:A:121:ARG:HA	1:A:121:ARG:HD3	1.74	0.47
1:A:703:TYR:HA	1:A:783:LEU:O	2.14	0.47
1:A:409:ASN:HD21	1:A:412:ARG:HH21	1.64	0.46
1:A:1410:LEU:HD11	1:A:1426:LEU:HD21	1.96	0.46
1:A:69:GLN:HE22	1:A:115:LEU:HA	1.81	0.46
1:A:845:TYR:O	1:A:848:LEU:HB2	2.15	0.46
1:A:1468:ASP:OD2	1:A:1470:GLU:HB3	2.16	0.46
1:A:472:LEU:O	1:A:475:PRO:HD2	2.14	0.46
1:A:729:ARG:HE	1:A:778:ASN:HD21	1.63	0.46
1:A:1201:ILE:HD12	1:A:1201:ILE:HA	1.87	0.46
1:A:1294:TRP:N	1:A:1295:PRO:HD2	2.31	0.46
1:A:993:PHE:HA	1:A:1034:GLN:NE2	2.31	0.46
1:A:1206:TRP:CE2	1:A:1210:ARG:HD3	2.50	0.46
1:A:3:GLU:O	1:A:7:ASN:N	2.48	0.46
1:A:343:LEU:O	1:A:344:LYS:C	2.52	0.46
1:A:1258:MET:C	1:A:1260:SER:H	2.19	0.46
1:A:425:SER:HG	1:A:1160:TYR:HD1	1.64	0.45
1:A:1365:ILE:CG1	1:A:1373:LEU:HD22	2.34	0.45
1:A:1358:ILE:CG2	1:A:1362:GLY:HA3	2.45	0.45
1:A:834:LEU:HA	1:A:839:ILE:HA	1.98	0.45
1:A:1370:LEU:HD23	1:A:1370:LEU:HA	1.82	0.45
1:A:993:PHE:O	1:A:994:ILE:C	2.54	0.45
1:A:995:GLY:O	1:A:996:SER:C	2.55	0.45
1:A:517:TRP:CG	1:A:1397:PRO:HG3	2.52	0.45
1:A:1457:ILE:HA	1:A:1487:THR:O	2.17	0.45
1:A:235:THR:O	1:A:239:VAL:HG23	2.17	0.44
1:A:804:LEU:HA	1:A:815:ARG:HE	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:PHE:O	1:A:204:ILE:HB	2.17	0.44
1:A:441:LEU:HD12	1:A:441:LEU:HA	1.84	0.44
1:A:1274:GLU:O	1:A:1277:LYS:HG2	2.18	0.44
1:A:1426:LEU:HD23	1:A:1426:LEU:HA	1.84	0.44
1:A:349:PHE:CZ	1:A:1230:ARG:HD2	2.52	0.44
1:A:111:TRP:HA	1:A:111:TRP:HE3	1.82	0.44
1:A:1236:ASP:O	1:A:1237:THR:C	2.51	0.44
1:A:522:ARG:HE	1:A:522:ARG:HB3	1.53	0.44
1:A:1068:PRO:HB3	1:A:1281:GLU:HB2	2.00	0.44
1:A:1146:ARG:HA	1:A:1149:ARG:HD3	1.99	0.44
1:A:366:LEU:HD22	1:A:366:LEU:HA	1.84	0.44
1:A:767:GLN:HG2	1:A:791:VAL:HG22	2.00	0.44
1:A:243:GLU:O	1:A:246:MET:HG2	2.18	0.44
1:A:438:MET:HE3	1:A:438:MET:HB3	1.72	0.44
1:A:804:LEU:HA	1:A:815:ARG:NE	2.33	0.44
1:A:1406:ILE:HA	1:A:1452:LEU:HD21	2.00	0.44
1:A:389:GLY:O	1:A:390:VAL:C	2.55	0.43
1:A:405:LEU:HD21	1:A:1166:THR:HG21	2.00	0.43
1:A:575:ASP:N	1:A:575:ASP:OD1	2.51	0.43
1:A:305:VAL:O	1:A:307:LYS:HG2	2.18	0.43
1:A:660:ASP:OD1	1:A:660:ASP:N	2.51	0.43
1:A:675:SER:CB	1:A:836:ASN:H	2.28	0.43
1:A:514:TYR:CZ	1:A:1350:ILE:HD11	2.53	0.43
1:A:553:THR:N	1:A:554:PRO:CD	2.82	0.43
1:A:593:LEU:HD23	1:A:593:LEU:HA	1.79	0.43
1:A:1324:ILE:HD12	1:A:1324:ILE:HA	1.77	0.43
1:A:1316:VAL:HG12	1:A:1317:LEU:HG	2.00	0.43
1:A:1365:ILE:HD13	1:A:1365:ILE:H	1.84	0.43
1:A:1415:LEU:HD22	1:A:1415:LEU:HA	1.79	0.43
1:A:637:MET:O	1:A:660:ASP:HA	2.18	0.43
1:A:842:LYS:H	1:A:851:LYS:NZ	2.16	0.43
1:A:1344:THR:HG22	1:A:1491:ILE:HD12	2.00	0.43
1:A:222:THR:C	1:A:224:GLU:N	2.69	0.43
1:A:636:ALA:HB1	1:A:781:ILE:CD1	2.48	0.43
1:A:1130:LEU:HD23	1:A:1130:LEU:HA	1.82	0.43
1:A:382:PHE:HD2	1:A:1205:ARG:NH1	2.17	0.43
1:A:1015:TYR:O	1:A:1016:PRO:C	2.57	0.43
1:A:41:TRP:HE1	1:A:110:THR:HA	1.83	0.43
1:A:110:THR:O	1:A:111:TRP:C	2.57	0.43
1:A:1035:GLY:O	1:A:1036:ILE:C	2.58	0.43
1:A:1448:GLY:HA2	1:A:1451:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1456:LYS:HD2	1:A:1456:LYS:H	1.84	0.42
1:A:204:ILE:HD12	1:A:204:ILE:HA	1.74	0.42
1:A:469:VAL:HG11	1:A:556:LEU:HD22	2.01	0.42
1:A:734:LEU:HB3	1:A:740:LEU:HD21	2.00	0.42
1:A:1082:ASN:HA	1:A:1085:ALA:HB3	2.00	0.42
1:A:1083:ARG:HG3	1:A:1275:TYR:CE2	2.54	0.42
1:A:1365:ILE:CG2	1:A:1373:LEU:HD13	2.48	0.42
1:A:73:GLY:O	1:A:76:LEU:HB3	2.19	0.42
1:A:132:LEU:HD22	1:A:132:LEU:HA	1.84	0.42
1:A:1328:GLU:HG2	1:A:1329:LYS:N	2.34	0.42
1:A:15:PHE:O	1:A:21:ALA:HB1	2.20	0.42
1:A:69:GLN:HE21	1:A:118:GLN:HB2	1.84	0.42
1:A:529:ARG:HE	1:A:1057:HIS:CG	2.37	0.42
1:A:1445:LEU:HD12	1:A:1445:LEU:HA	1.92	0.42
1:A:715:ILE:HD13	1:A:715:ILE:HA	1.86	0.42
1:A:1258:MET:O	1:A:1260:SER:N	2.52	0.42
1:A:1335:ARG:NH2	1:A:1495:LEU:N	2.62	0.42
1:A:1460:LEU:HB2	1:A:1490:THR:HG23	2.02	0.42
1:A:1479:ILE:H	1:A:1479:ILE:HG13	1.51	0.42
1:A:42:LEU:HD23	1:A:42:LEU:HA	1.84	0.42
1:A:846:SER:O	1:A:849:LEU:HB2	2.19	0.42
1:A:386:PHE:HD2	1:A:1201:ILE:HD11	1.85	0.42
1:A:992:ALA:CB	1:A:1034:GLN:HG3	2.49	0.42
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.91	0.42
1:A:599:MET:HE2	1:A:602:SER:HB2	2.02	0.42
1:A:771:LEU:HD11	1:A:784:LEU:HD22	2.01	0.42
1:A:992:ALA:HB3	1:A:1034:GLN:HG3	2.01	0.42
1:A:1469:LEU:O	1:A:1473:ASN:N	2.50	0.42
1:A:99:VAL:C	1:A:101:TYR:N	2.72	0.42
1:A:330:LEU:HD12	1:A:330:LEU:HA	1.78	0.42
1:A:813:LYS:HA	1:A:813:LYS:HD3	1.74	0.42
1:A:1178:HIS:HB3	1:A:1181:ARG:HH21	1.84	0.42
1:A:1312:GLU:H	1:A:1312:GLU:HG3	1.43	0.42
1:A:3:GLU:HG2	1:A:10:PHE:HB2	2.01	0.42
1:A:28:GLU:HB3	1:A:146:GLN:CG	2.49	0.42
1:A:400:VAL:O	1:A:401:TYR:C	2.56	0.42
1:A:540:SER:O	1:A:541:GLN:C	2.55	0.42
1:A:1301:GLN:HA	1:A:1323:ASP:HA	2.01	0.42
1:A:424:MET:HG2	1:A:424:MET:O	2.20	0.41
1:A:1358:ILE:HG23	1:A:1362:GLY:CA	2.49	0.41
1:A:1479:ILE:HA	1:A:1483:PHE:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:LYS:HA	1:A:503:ASN:ND2	2.35	0.41
1:A:1236:ASP:O	1:A:1239:GLY:N	2.52	0.41
1:A:642:ALA:HA	1:A:692:HIS:O	2.21	0.41
1:A:343:LEU:HD12	1:A:343:LEU:HA	1.92	0.41
1:A:216:GLY:HA2	1:A:221:LEU:HD21	2.02	0.41
1:A:249:GLU:H	1:A:249:GLU:HG2	1.64	0.41
1:A:381:TYR:OH	1:A:439:HIS:HB2	2.21	0.41
1:A:810:LEU:O	1:A:815:ARG:NH1	2.54	0.41
1:A:1310:ARG:HB2	1:A:1313:LEU:HB2	2.01	0.41
1:A:785:ASP:O	1:A:786:ASP:C	2.58	0.41
1:A:1230:ARG:O	1:A:1231:ASP:C	2.58	0.41
1:A:520:SER:HB3	1:A:1398:PHE:CE1	2.55	0.41
1:A:575:ASP:OD1	1:A:578:LYS:HD3	2.21	0.41
1:A:643:SER:CB	1:A:691:VAL:HB	2.48	0.41
1:A:1049:PHE:O	1:A:1052:ALA:HB3	2.21	0.41
1:A:1224:LEU:O	1:A:1227:VAL:N	2.54	0.41
1:A:1359:ILE:HA	1:A:1364:ASP:HB3	2.03	0.41
1:A:1376:LYS:HA	1:A:1376:LYS:HD3	1.83	0.41
1:A:75:LEU:HD21	1:A:174:PHE:HB2	2.02	0.41
1:A:1139:MET:HE3	1:A:1139:MET:HB3	1.91	0.40
1:A:1368:ILE:H	1:A:1368:ILE:HG12	1.81	0.40
1:A:1408:LYS:O	1:A:1412:LEU:HG	2.21	0.40
1:A:65:TYR:O	1:A:69:GLN:HB2	2.21	0.40
1:A:77:ILE:O	1:A:80:ALA:HB3	2.20	0.40
1:A:1125:ILE:O	1:A:1129:PRO:HD2	2.21	0.40
1:A:1358:ILE:N	1:A:1364:ASP:H	2.18	0.40
1:A:1446:CYS:HA	1:A:1449:ARG:HD2	2.02	0.40
1:A:256:ALA:O	1:A:259:ARG:HB2	2.22	0.40
1:A:511:ILE:HD12	1:A:1385:ILE:HB	2.04	0.40
1:A:1252:LEU:HD23	1:A:1252:LEU:HA	1.97	0.40
1:A:199:SER:O	1:A:200:PHE:C	2.60	0.40
1:A:533:LEU:HD23	1:A:533:LEU:HA	1.87	0.40
1:A:1146:ARG:O	1:A:1149:ARG:HB2	2.21	0.40
1:A:1423:GLN:CD	1:A:1423:GLN:H	2.24	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	1392/1589 (88%)	1347 (97%)	43 (3%)	2 (0%)	48	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1015	TYR
1	A	1231	ASP

### 5.3.2 Protein sidechains

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	1241/1408 (88%)	1087 (88%)	154 (12%)	4	20

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	5	PHE
1	A	6	CYS
1	A	14	SER
1	A	15	PHE
1	A	33	VAL
1	A	56	THR
1	A	99	VAL
1	A	101	TYR

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Mol	Chain	Res	Type
1	A	105	SER
1	A	107	TYR
1	A	111	TRP
1	A	123	TRP
1	A	125	VAL
1	A	132	LEU
1	A	138	LEU
1	A	153	THR
1	A	156	GLN
1	A	171	SER
1	A	175	GLN
1	A	185	SER
1	A	203	SER
1	A	204	ILE
1	A	211	SER
1	A	217	TYR
1	A	219	ARG
1	A	228	GLU
1	A	233	MET
1	A	238	LEU
1	A	248	ARG
1	A	263	LYS
1	A	305	VAL
1	A	311	MET
1	A	323	LEU
1	A	325	SER
1	A	332	ASN
1	A	357	LEU
1	A	359	ILE
1	A	366	LEU
1	A	367	LEU
1	A	372	LEU
1	A	375	SER
1	A	390	VAL
1	A	400	VAL
1	A	416	THR
1	A	419	GLU
1	A	420	THR
1	A	424	MET
1	A	429	GLN
1	A	438	MET
1	A	440	MET

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Mol	Chain	Res	Type
1	A	447	GLN
1	A	451	SER
1	A	457	ARG
1	A	473	VAL
1	A	515	PHE
1	A	521	PHE
1	A	547	ILE
1	A	551	GLN
1	A	552	LEU
1	A	575	ASP
1	A	577	GLN
1	A	589	LEU
1	A	593	LEU
1	A	594	SER
1	A	595	MET
1	A	611	GLU
1	A	614	GLU
1	A	638	GLN
1	A	648	HIS
1	A	653	THR
1	A	662	MET
1	A	681	ILE
1	A	682	SER
1	A	700	THR
1	A	710	ILE
1	A	716	LYS
1	A	717	ASP
1	A	729	ARG
1	A	734	LEU
1	A	750	ASP
1	A	760	ASN
1	A	768	ARG
1	A	784	LEU
1	A	792	ASP
1	A	795	VAL
1	A	803	VAL
1	A	804	LEU
1	A	816	LEU
1	A	825	LEU
1	A	827	GLN
1	A	829	ASP
1	A	831	ILE

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Mol	Chain	Res	Type
1	A	834	LEU
1	A	838	THR
1	A	839	ILE
1	A	859	LEU
1	A	969	GLU
1	A	984	LEU
1	A	1007	SER
1	A	1032	LEU
1	A	1034	GLN
1	A	1038	VAL
1	A	1044	TRP
1	A	1061	LEU
1	A	1075	THR
1	A	1094	THR
1	A	1099	LEU
1	A	1107	LEU
1	A	1143	SER
1	A	1149	ARG
1	A	1158	PRO
1	A	1164	SER
1	A	1177	GLU
1	A	1193	ASN
1	A	1210	ARG
1	A	1218	THR
1	A	1222	SER
1	A	1236	ASP
1	A	1242	LEU
1	A	1253	ASN
1	A	1257	ARG
1	A	1259	THR
1	A	1260	SER
1	A	1294	TRP
1	A	1308	ARG
1	A	1312	GLU
1	A	1315	LEU
1	A	1318	ARG
1	A	1323	ASP
1	A	1324	ILE
1	A	1336	THR
1	A	1341	SER
1	A	1344	THR
1	A	1352	GLU

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Mol	Chain	Res	Type
1	A	1358	ILE
1	A	1365	ILE
1	A	1368	ILE
1	A	1379	ILE
1	A	1386	LEU
1	A	1408	LYS
1	A	1414	HIS
1	A	1415	LEU
1	A	1423	GLN
1	A	1438	SER
1	A	1456	LYS
1	A	1458	LEU
1	A	1467	VAL
1	A	1474	LEU
1	A	1479	ILE
1	A	1487	THR
1	A	1496	HIS
1	A	1513	ILE
1	A	1519	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	118	GLN
1	A	122	GLN
1	A	332	ASN
1	A	447	GLN
1	A	503	ASN
1	A	577	GLN
1	A	694	HIS
1	A	711	GLN
1	A	760	ASN
1	A	778	ASN
1	A	794	HIS
1	A	798	HIS
1	A	827	GLN
1	A	997	ASN
1	A	1019	GLN
1	A	1247	ASN

### 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.