



Full wwPDB EM Validation Report ⓘ

Jul 16, 2025 – 12:41 AM JST

PDB ID : 8J5D / pdb_00008j5d
EMDB ID : EMD-35985
Title : Cryo-EM structure of starch degradation complex of BAM1-LSF1-MDH
Authors : Guan, Z.Y.; Liu, J.; Yan, J.J.
Deposited on : 2023-04-21
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ 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) : 2.44

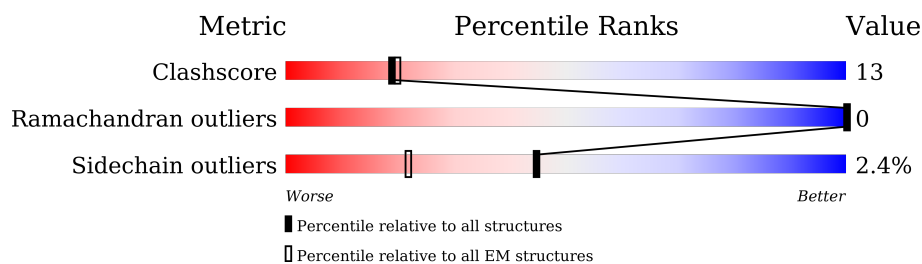
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	499	
2	B	323	
2	C	323	
3	D	529	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9531 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 Beta-amylase 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	422	Total	C	N	O	S	0	0
			3340	2141	563	615	21		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	MET	-	initiating methionine	UNP Q9LIR6
A	78	GLY	-	expression tag	UNP Q9LIR6
A	79	SER	-	expression tag	UNP Q9LIR6
A	80	SER	-	expression tag	UNP Q9LIR6
A	81	HIS	-	expression tag	UNP Q9LIR6
A	82	HIS	-	expression tag	UNP Q9LIR6
A	83	HIS	-	expression tag	UNP Q9LIR6
A	84	HIS	-	expression tag	UNP Q9LIR6
A	85	HIS	-	expression tag	UNP Q9LIR6
A	86	HIS	-	expression tag	UNP Q9LIR6
A	87	SER	-	expression tag	UNP Q9LIR6
A	88	SER	-	expression tag	UNP Q9LIR6
A	89	GLY	-	expression tag	UNP Q9LIR6
A	90	LEU	-	expression tag	UNP Q9LIR6
A	91	VAL	-	expression tag	UNP Q9LIR6
A	92	PRO	-	expression tag	UNP Q9LIR6
A	93	ARG	-	expression tag	UNP Q9LIR6
A	94	GLY	-	expression tag	UNP Q9LIR6
A	95	SER	-	expression tag	UNP Q9LIR6
A	96	HIS	-	expression tag	UNP Q9LIR6
A	97	SER	-	expression tag	UNP Q9LIR6
A	98	ASP	-	expression tag	UNP Q9LIR6
A	99	GLU	-	expression tag	UNP Q9LIR6
A	100	VAL	-	expression tag	UNP Q9LIR6
A	101	ASP	-	expression tag	UNP Q9LIR6
A	102	ALA	-	expression tag	UNP Q9LIR6
A	103	HIS	-	expression tag	UNP Q9LIR6
A	104	MET	-	expression tag	UNP Q9LIR6

- Molecule 2 is a protein called Malate dehydrogenase, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	316	Total	C	N	O	S	0	0
			2356	1498	395	456	7		
2	C	315	Total	C	N	O	S	0	0
			2347	1492	393	455	7		

- Molecule 3 is a protein called Phosphoglucan phosphatase LSF1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	191	Total	C	N	O	S	0	0
			1488	957	248	279	4		

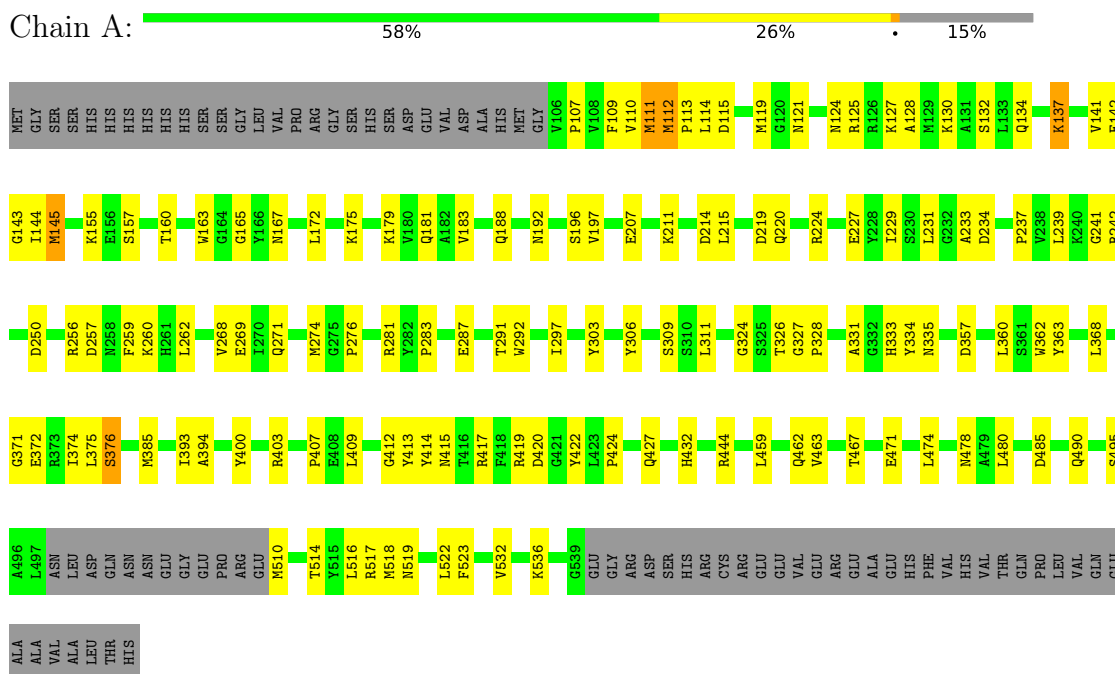
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	592	LEU	-	expression tag	UNP F4J117
D	593	GLU	-	expression tag	UNP F4J117
D	594	HIS	-	expression tag	UNP F4J117
D	595	HIS	-	expression tag	UNP F4J117
D	596	HIS	-	expression tag	UNP F4J117
D	597	HIS	-	expression tag	UNP F4J117
D	598	HIS	-	expression tag	UNP F4J117
D	599	HIS	-	expression tag	UNP F4J117

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: Beta-amylase 1, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	305907	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 ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	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	A	0.16	0/3434	0.40	2/4657 (0.0%)
2	B	0.15	0/2391	0.41	2/3249 (0.1%)
2	C	0.15	0/2382	0.34	0/3238
3	D	0.13	0/1520	0.36	0/2047
All	All	0.15	0/9727	0.38	4/13191 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	207	PRO	N-CD-CG	-5.44	95.04	103.20
1	A	196	SER	CB-CA-C	-5.08	110.70	116.54
2	B	207	PRO	CA-N-CD	-5.01	104.98	112.00
1	A	112	MET	CB-CG-SD	5.00	127.71	112.70

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	3340	0	3224	91	0
2	B	2356	0	2430	58	0
2	C	2347	0	2417	62	0
3	D	1488	0	1493	45	0
All	All	9531	0	9564	241	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 13.

All (241) 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:C:255:ILE:HG22	2:C:264:LEU:HB3	1.54	0.90
1:A:113:PRO:HD3	1:A:518:MET:HB3	1.59	0.84
1:A:372:GLU:OE1	1:A:432:HIS:NE2	2.17	0.77
1:A:183:VAL:HG22	1:A:271:GLN:HB3	1.71	0.71
2:C:331:TYR:HB3	2:C:349:ARG:HD2	1.72	0.70
1:A:130:LYS:HA	1:A:130:LYS:HE2	1.73	0.70
3:D:92:SER:HA	3:D:247:LEU:HA	1.73	0.70
2:C:104:MET:HA	2:C:131:THR:HG21	1.75	0.69
2:C:114:TYR:CE2	2:C:144:LEU:HB2	2.30	0.66
2:B:208:ILE:O	2:B:212:VAL:HG23	1.95	0.66
1:A:360:LEU:HD21	1:A:409:LEU:HD13	1.79	0.65
2:B:103:LYS:NZ	2:B:133:SER:O	2.30	0.65
2:B:343:LEU:HD13	2:B:383:LEU:HD23	1.78	0.65
2:B:281:ILE:O	2:B:285:THR:HG23	1.97	0.65
2:B:232:VAL:O	2:B:236:ASN:ND2	2.30	0.64
3:D:177:TYR:OH	3:D:225:ASN:OD1	2.14	0.64
3:D:82:GLU:O	3:D:107:ASN:ND2	2.29	0.64
2:B:167:THR:HB	2:B:170:ASP:HB2	1.80	0.64
1:A:181:GLN:HG2	1:A:269:GLU:HB3	1.80	0.64
1:A:311:LEU:HG	1:A:324:GLY:HA2	1.79	0.64
2:B:269:LYS:NZ	2:B:364:ASP:OD1	2.30	0.63
2:B:170:ASP:O	2:B:174:ILE:HG12	1.99	0.63
1:A:241:GLY:HA2	3:D:266:PHE:HB2	1.79	0.63
3:D:84:PRO:HB2	3:D:255:VAL:HG13	1.80	0.63
1:A:415:ASN:OD1	1:A:462:GLN:NE2	2.32	0.62
2:C:90:ALA:HB1	2:C:113:LEU:HD23	1.81	0.62
1:A:107:PRO:HB3	1:A:142:GLU:HG2	1.81	0.61
1:A:127:LYS:HD3	1:A:127:LYS:H	1.65	0.61
3:D:77:TYR:OH	3:D:118:ASP:OD2	2.16	0.61
2:B:211:GLU:OE1	2:B:391:VAL:HA	2.01	0.61
1:A:274:MET:HE3	1:A:374:ILE:HB	1.82	0.61
1:A:121:ASN:OD1	1:A:165:GLY:N	2.34	0.60
1:A:281:ARG:HD3	1:A:394:ALA:HB2	1.84	0.60
2:B:323:ALA:HB2	2:B:330:VAL:HG11	1.82	0.60
2:C:341:THR:OG1	2:C:380:LYS:NZ	2.27	0.60
1:A:219:ASP:OD1	1:A:334:TYR:OH	2.20	0.60
1:A:112:MET:SD	1:A:144:ILE:HD11	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ARG:HG3	1:A:417:ARG:HE	1.67	0.59
3:D:91:LEU:HB2	3:D:251:PHE:HE1	1.67	0.59
1:A:467:THR:HG21	1:A:474:LEU:HD13	1.82	0.59
2:C:192:ASN:OD1	2:C:223:LYS:NZ	2.30	0.59
3:D:134:ILE:HG12	3:D:139:ASP:HB2	1.83	0.59
2:B:267:LEU:HD12	2:B:281:ILE:HD13	1.85	0.58
2:B:207:PRO:O	2:B:211:GLU:HG3	2.02	0.58
3:D:181:ARG:HB3	3:D:211:PHE:HB3	1.85	0.58
2:C:174:ILE:O	2:C:178:ILE:HG13	2.03	0.58
3:D:193:SER:OG	3:D:195:ASN:OD1	2.18	0.57
1:A:532:VAL:O	1:A:536:LYS:HD3	2.04	0.57
1:A:419:ARG:HH22	1:A:424:PRO:HG3	1.68	0.57
3:D:198:ALA:HB2	2:C:248:ILE:HG23	1.85	0.57
2:C:103:LYS:NZ	2:C:133:SER:O	2.37	0.57
1:A:119:MET:O	1:A:155:LYS:NZ	2.38	0.57
1:A:274:MET:HE1	1:A:371:GLY:HA2	1.86	0.56
2:B:335:PHE:HD1	2:B:347:ALA:HB2	1.70	0.56
1:A:111:MET:SD	1:A:517:ARG:HG3	2.45	0.56
3:D:270:GLU:OE2	3:D:277:ARG:NH2	2.40	0.55
1:A:110:VAL:HG23	1:A:141:VAL:HG11	1.88	0.55
1:A:420:ASP:OD1	1:A:462:GLN:NE2	2.27	0.55
2:B:336:VAL:HG21	2:B:357:LEU:HD21	1.87	0.55
3:D:213:SER:O	3:D:221:TRP:NE1	2.40	0.55
1:A:242:ARG:NH1	1:A:250:ASP:OD2	2.37	0.54
2:C:372:GLU:O	2:C:376:LEU:HB2	2.07	0.54
2:B:191:PRO:HB3	2:B:218:VAL:HB	1.89	0.54
2:B:143:GLU:OE1	2:B:143:GLU:N	2.41	0.53
2:B:308:SER:OG	2:C:125:ASP:O	2.25	0.53
2:C:171:LEU:O	2:C:175:ASN:ND2	2.30	0.53
2:B:283:GLU:HA	2:B:286:VAL:HG22	1.89	0.53
3:D:135:LYS:N	3:D:139:ASP:OD2	2.41	0.53
2:C:88:LEU:HD13	2:C:182:LEU:HD22	1.89	0.53
2:C:114:TYR:HE2	2:C:144:LEU:HB2	1.70	0.53
2:C:335:PHE:HA	2:C:347:ALA:HA	1.90	0.53
1:A:274:MET:CE	1:A:371:GLY:HA2	2.39	0.52
2:C:315:ARG:O	2:C:318:GLU:HG3	2.09	0.52
1:A:326:THR:OG1	1:A:327:GLY:N	2.43	0.52
2:C:253:PRO:HG2	2:C:266:LEU:HB2	1.92	0.52
1:A:400:TYR:OH	1:A:462:GLN:OE1	2.16	0.52
2:B:309:MET:HE2	2:B:309:MET:HA	1.92	0.52
1:A:109:PHE:HA	1:A:143:GLY:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ASN:ND2	1:A:287:GLU:OE2	2.43	0.52
1:A:112:MET:HE3	1:A:112:MET:HA	1.92	0.52
2:B:166:MET:HE3	2:B:167:THR:H	1.75	0.51
1:A:495:SER:HA	1:A:510:MET:HG2	1.92	0.51
1:A:125:ARG:HG3	1:A:128:ALA:HB3	1.91	0.51
2:C:139:THR:N	2:C:143:GLU:OE1	2.36	0.51
2:C:349:ARG:HG2	2:C:361:ILE:HD12	1.91	0.51
2:B:311:TYR:HE1	3:D:183:SER:HB2	1.75	0.51
2:C:257:GLY:N	2:C:262:THR:OG1	2.44	0.51
2:C:379:LEU:O	2:C:383:LEU:HD13	2.11	0.51
2:B:340:LEU:HD13	2:B:362:GLU:HG2	1.93	0.51
1:A:214:ASP:OD1	1:A:224:ARG:NH2	2.40	0.50
3:D:195:ASN:OD1	3:D:195:ASN:N	2.44	0.50
2:C:222:LYS:HA	2:C:357:LEU:HB2	1.92	0.50
1:A:257:ASP:HA	1:A:260:LYS:HE2	1.93	0.50
2:C:119:VAL:HG12	2:C:137:ASP:HB2	1.92	0.50
1:A:130:LYS:HA	1:A:130:LYS:CE	2.41	0.50
1:A:259:PHE:HD1	1:A:262:LEU:HD12	1.76	0.50
2:B:112:HIS:ND1	2:B:147:CYS:O	2.30	0.49
2:B:255:ILE:HD11	2:B:264:LEU:HD23	1.94	0.49
1:A:132:SER:HA	1:A:523:PHE:CZ	2.47	0.49
3:D:77:TYR:HE1	3:D:157:ARG:HG3	1.77	0.49
1:A:111:MET:O	1:A:518:MET:HB2	2.11	0.49
1:A:130:LYS:HZ2	1:A:172:LEU:CD1	2.24	0.49
1:A:192:ASN:HB3	1:A:287:GLU:HG2	1.94	0.49
2:C:256:GLY:HA3	2:C:379:LEU:HD11	1.93	0.49
1:A:357:ASP:OD1	1:A:414:TYR:OH	2.22	0.49
3:D:137:PHE:HE1	3:D:141:LYS:HD3	1.77	0.49
3:D:187:TRP:CE3	2:C:318:GLU:HG2	2.48	0.49
1:A:112:MET:HE3	1:A:113:PRO:HD2	1.93	0.49
1:A:115:ASP:OD1	1:A:197:VAL:HG11	2.13	0.49
1:A:311:LEU:HB2	1:A:362:TRP:CZ2	2.48	0.49
1:A:393:ILE:HD12	1:A:413:TYR:HE2	1.77	0.49
3:D:91:LEU:HD12	3:D:137:PHE:HB2	1.95	0.48
1:A:188:GLN:HB3	1:A:227:GLU:HA	1.95	0.48
3:D:186:THR:O	3:D:207:GLY:HA2	2.12	0.48
2:C:183:VAL:HA	2:C:186:VAL:HG12	1.94	0.48
1:A:110:VAL:O	1:A:144:ILE:HG13	2.14	0.48
1:A:179:LYS:HD3	1:A:268:VAL:HG21	1.94	0.48
2:B:369:THR:HG22	2:B:370:GLU:H	1.78	0.48
2:C:100:LEU:O	2:C:104:MET:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:GLN:O	1:A:137:LYS:HD3	2.14	0.48
2:B:388:ASP:HA	2:B:391:VAL:HG22	1.96	0.48
2:B:114:TYR:CZ	2:B:144:LEU:HD23	2.49	0.47
2:B:214:LYS:HA	2:B:219:TYR:HB3	1.95	0.47
2:C:267:LEU:HD12	2:C:281:ILE:HG23	1.96	0.47
2:B:103:LYS:HE2	2:B:126:LEU:O	2.14	0.47
3:D:103:LYS:NZ	3:D:259:GLY:O	2.44	0.47
3:D:183:SER:HB3	2:C:104:MET:HB3	1.97	0.47
2:C:89:GLY:N	2:C:114:TYR:O	2.45	0.47
2:C:335:PHE:HD1	2:C:347:ALA:HB2	1.80	0.47
1:A:518:MET:HE3	1:A:519:ASN:H	1.80	0.47
1:A:207:GLU:O	1:A:211:LYS:HG2	2.15	0.46
1:A:471:GLU:HA	1:A:471:GLU:OE1	2.15	0.46
2:C:262:THR:OG1	2:C:383:LEU:HD11	2.16	0.46
2:B:148:LEU:HD22	2:B:186:VAL:HG22	1.98	0.46
1:A:130:LYS:NZ	1:A:172:LEU:HG	2.30	0.46
3:D:109:GLU:HA	3:D:109:GLU:OE1	2.16	0.46
3:D:182:VAL:HG22	2:C:130:ASN:O	2.16	0.46
2:B:236:ASN:O	2:B:240:SER:OG	2.28	0.46
2:C:219:TYR:OH	2:C:337:GLU:OE2	2.29	0.46
2:C:263:ILE:HG21	2:C:288:ILE:HG22	1.98	0.46
2:B:247:LEU:HD11	2:C:130:ASN:HB2	1.97	0.46
1:A:157:SER:HB3	1:A:160:THR:HB	1.98	0.46
1:A:363:TYR:CD2	1:A:412:GLY:HA2	2.51	0.46
3:D:275:LEU:O	3:D:279:LYS:HG3	2.15	0.46
2:B:84:LYS:HG3	2:B:110:THR:HB	1.98	0.45
2:C:221:PRO:HB3	2:C:337:GLU:HG3	1.98	0.45
2:B:374:LYS:HB3	2:B:374:LYS:HE2	1.68	0.45
2:C:318:GLU:OE2	2:C:322:ARG:NH1	2.49	0.45
1:A:124:ASN:O	1:A:125:ARG:HG2	2.16	0.45
1:A:231:LEU:HA	1:A:234:ASP:HB2	1.98	0.45
1:A:292:TRP:HD1	1:A:334:TYR:HB3	1.81	0.45
2:B:184:GLU:HB3	2:B:212:VAL:HG11	1.98	0.45
2:B:311:TYR:CE1	3:D:183:SER:HB2	2.51	0.45
1:A:303:TYR:OH	1:A:326:THR:OG1	2.33	0.45
1:A:309:SER:OG	3:D:78:MET:O	2.32	0.45
2:B:116:ILE:HD12	2:B:117:ALA:N	2.32	0.45
1:A:518:MET:HE1	1:A:522:LEU:HD22	1.98	0.45
2:B:213:LEU:HB3	2:B:219:TYR:HA	1.99	0.45
2:B:235:ALA:O	2:B:239:VAL:HG23	2.17	0.45
2:B:284:LEU:HA	2:B:287:ARG:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:78:MET:HG3	3:D:154:VAL:HG22	1.98	0.45
1:A:516:LEU:HA	1:A:517:ARG:HA	1.79	0.44
1:A:276:PRO:HG2	1:A:283:PRO:HB3	2.00	0.44
1:A:522:LEU:HD23	1:A:522:LEU:O	2.17	0.44
3:D:205:ASN:ND2	2:C:250:VAL:O	2.50	0.44
3:D:274:ALA:HA	3:D:277:ARG:NH1	2.33	0.44
2:B:282:GLN:C	2:B:284:LEU:H	2.25	0.44
2:C:255:ILE:HD12	2:C:347:ALA:O	2.18	0.44
2:C:337:GLU:H	2:C:337:GLU:CD	2.24	0.44
2:B:258:HIS:HA	2:B:263:ILE:HD11	2.00	0.44
2:C:240:SER:OG	2:C:247:LEU:HD13	2.18	0.44
3:D:185:VAL:HA	3:D:208:TYR:O	2.18	0.44
1:A:478:ASN:ND2	1:A:480:LEU:O	2.51	0.43
1:A:220:GLN:OE1	1:A:303:TYR:OH	2.15	0.43
3:D:158:PRO:HB2	3:D:160:SER:O	2.17	0.43
2:C:207:PRO:HG3	2:C:387:ILE:HD13	2.00	0.43
2:B:295:VAL:HG11	2:B:305:ALA:HB2	2.00	0.43
2:B:336:VAL:HG11	2:B:357:LEU:HD11	2.00	0.43
1:A:372:GLU:O	1:A:376:SER:OG	2.31	0.43
2:B:180:LYS:HE2	2:B:180:LYS:HB3	1.81	0.43
2:C:114:TYR:CD1	2:C:114:TYR:C	2.97	0.43
2:C:269:LYS:HE2	2:C:269:LYS:HB3	1.53	0.43
1:A:163:TRP:O	1:A:167:ASN:HB2	2.19	0.42
1:A:333:HIS:CG	1:A:334:TYR:N	2.86	0.42
1:A:422:TYR:CD1	1:A:463:VAL:HG22	2.54	0.42
2:B:251:ASP:OD2	2:B:349:ARG:NH1	2.45	0.42
3:D:96:LYS:HD3	3:D:96:LYS:HA	1.68	0.42
2:C:167:THR:HG22	2:C:169:ASP:H	1.84	0.42
1:A:371:GLY:O	1:A:375:LEU:HB2	2.18	0.42
2:B:98:LEU:HD13	2:B:313:ALA:HB3	2.01	0.42
2:B:201:PRO:O	2:B:205:THR:OG1	2.34	0.42
2:C:94:ILE:HG12	2:C:306:THR:HA	2.01	0.42
2:C:232:VAL:HG21	2:C:333:CYS:HB2	2.01	0.42
1:A:110:VAL:O	1:A:144:ILE:HA	2.20	0.42
2:C:230:LEU:HD22	2:C:309:MET:HG2	2.01	0.42
1:A:155:LYS:HB2	1:A:155:LYS:HE2	1.78	0.42
2:B:190:CYS:SG	2:B:193:ALA:HB2	2.60	0.42
1:A:333:HIS:CD2	1:A:335:ASN:H	2.37	0.42
2:B:276:PHE:HB3	2:B:281:ILE:HG12	2.01	0.42
3:D:137:PHE:CE1	3:D:141:LYS:HD3	2.54	0.42
2:C:337:GLU:HB3	2:C:345:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:ARG:CZ	1:A:490:GLN:HB2	2.49	0.42
2:C:98:LEU:HD13	2:C:313:ALA:HB3	2.01	0.42
2:B:269:LYS:HE2	2:B:269:LYS:HB3	1.67	0.41
3:D:147:LYS:HE2	3:D:147:LYS:HB3	1.85	0.41
1:A:237:PRO:HD3	3:D:115:MET:HE3	2.01	0.41
3:D:205:ASN:HD21	2:C:251:ASP:HB2	1.85	0.41
1:A:256:ARG:HD2	1:A:385:MET:HE1	2.03	0.41
2:B:368:LEU:HB3	2:B:372:GLU:HB2	2.02	0.41
2:B:211:GLU:CD	2:B:391:VAL:HG12	2.46	0.41
3:D:205:ASN:ND2	2:C:251:ASP:HB2	2.35	0.41
2:C:281:ILE:O	2:C:285:THR:OG1	2.29	0.41
1:A:172:LEU:O	1:A:175:LYS:HG2	2.20	0.41
1:A:485:ASP:OD1	1:A:485:ASP:N	2.53	0.41
3:D:120:LEU:HD13	3:D:153:LEU:HD23	2.03	0.41
1:A:134:GLN:HG2	1:A:137:LYS:HZ2	1.85	0.41
1:A:145:MET:HE3	1:A:183:VAL:HG21	2.03	0.41
2:C:103:LYS:HG3	2:C:133:SER:HG	1.86	0.41
1:A:229:ILE:HD13	1:A:239:LEU:HD11	2.02	0.41
1:A:328:PRO:HB2	1:A:331:ALA:HB2	2.03	0.41
2:B:94:ILE:HG13	2:B:306:THR:HG22	2.03	0.41
2:B:231:ASP:OD2	2:B:254:VAL:HG11	2.21	0.41
3:D:196:LEU:HB3	3:D:208:TYR:CE2	2.56	0.41
1:A:241:GLY:N	3:D:267:PRO:HD2	2.36	0.41
2:C:196:HIS:HB3	2:C:227:VAL:HG23	2.02	0.41
2:B:327:ASP:C	2:B:329:ASP:H	2.29	0.40
3:D:104:LYS:NZ	3:D:264:GLY:H	2.19	0.40
3:D:191:LEU:HD22	3:D:220:GLY:HA2	2.02	0.40
2:C:194:PHE:CZ	2:C:356:GLY:HA2	2.55	0.40
2:C:351:LYS:NZ	2:C:358:GLU:OE1	2.44	0.40
2:B:154:VAL:HG23	2:B:193:ALA:HB1	2.03	0.40
1:A:233:ALA:HB2	1:A:306:TYR:CD1	2.57	0.40
1:A:297:ILE:HA	1:A:407:PRO:HG3	2.02	0.40
2:B:329:ASP:OD1	2:B:329:ASP:N	2.52	0.40
1:A:274:MET:HE2	1:A:274:MET:HB3	1.91	0.40
3:D:276:ASP:HA	3:D:279:LYS:NZ	2.37	0.40
2:C:201:PRO:O	2:C:205:THR:HG23	2.21	0.40
2:C:243:LYS:O	2:C:245:LEU:HD12	2.21	0.40
1:A:403:ARG:HG3	1:A:417:ARG:NE	2.36	0.40
1:A:459:LEU:O	1:A:463:VAL:HG23	2.21	0.40
2:C:286:VAL:O	2:C:290:ASN:ND2	2.54	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	418/499 (84%)	404 (97%)	14 (3%)	0	100	100
2	B	314/323 (97%)	294 (94%)	20 (6%)	0	100	100
2	C	313/323 (97%)	300 (96%)	13 (4%)	0	100	100
3	D	187/529 (35%)	172 (92%)	15 (8%)	0	100	100
All	All	1232/1674 (74%)	1170 (95%)	62 (5%)	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	347/413 (84%)	337 (97%)	10 (3%)	37	70
2	B	260/262 (99%)	258 (99%)	2 (1%)	79	90
2	C	259/262 (99%)	252 (97%)	7 (3%)	40	71
3	D	163/456 (36%)	157 (96%)	6 (4%)	29	63
All	All	1029/1393 (74%)	1004 (98%)	25 (2%)	45	74

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	MET
1	A	114	LEU

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Mol	Chain	Res	Type
1	A	137	LYS
1	A	145	MET
1	A	215	LEU
1	A	291	THR
1	A	368	LEU
1	A	376	SER
1	A	427	GLN
1	A	514	THR
2	B	258	HIS
2	B	337	GLU
3	D	91	LEU
3	D	139	ASP
3	D	140	THR
3	D	190	ASN
3	D	244	ILE
3	D	248	VAL
2	C	120	LYS
2	C	133	SER
2	C	199	SER
2	C	255	ILE
2	C	285	THR
2	C	306	THR
2	C	348	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	181	GLN
1	A	448	GLN
2	B	200	ASN
2	B	236	ASN
3	D	205	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 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.