



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 02:38 AM UTC

PDB ID : 7BZY / pdb_00007bzy
EMDB ID : EMD-30263
Title : Hsp21-DXPS
Authors : Lau, W.C.Y.
Deposited on : 2020-04-29
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 : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

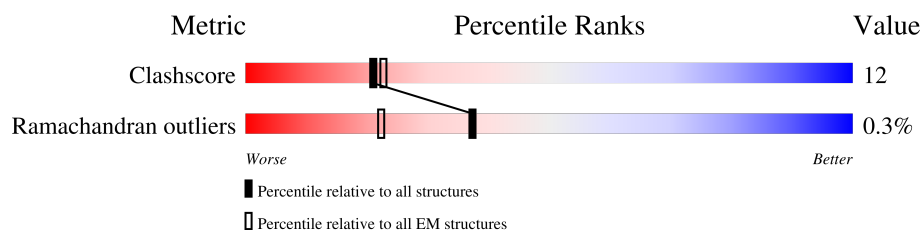
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	229148	23984
Ramachandran outliers	224038	23583

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	11	691	
1	13	691	
2	12	207	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6169 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 1-deoxy-D-xylulose-5-phosphate synthase, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	11	584	Total	C	N	O	0	0
			2857	1691	584	582		
1	13	584	Total	C	N	O	0	0
			2857	1691	584	582		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
11	41	MET	-	expression tag	UNP Q38854
11	42	ALA	-	expression tag	UNP Q38854
11	43	ASP	-	expression tag	UNP Q38854
11	44	LEU	-	expression tag	UNP Q38854
11	45	ASN	-	expression tag	UNP Q38854
11	46	TRP	-	expression tag	UNP Q38854
11	47	ILE	-	expression tag	UNP Q38854
11	48	SER	-	expression tag	UNP Q38854
11	49	ALA	-	expression tag	UNP Q38854
11	50	GLY	-	expression tag	UNP Q38854
11	51	HIS	-	expression tag	UNP Q38854
11	52	ALA	-	expression tag	UNP Q38854
11	53	ILE	-	expression tag	UNP Q38854
11	54	ALA	-	expression tag	UNP Q38854
11	55	ASP	-	expression tag	UNP Q38854
11	56	VAL	-	expression tag	UNP Q38854
11	57	GLY	-	expression tag	UNP Q38854
11	58	THR	-	expression tag	UNP Q38854
11	718	HIS	-	expression tag	UNP Q38854
11	719	HIS	-	expression tag	UNP Q38854
11	720	HIS	-	expression tag	UNP Q38854
11	721	HIS	-	expression tag	UNP Q38854
11	722	HIS	-	expression tag	UNP Q38854
11	723	HIS	-	expression tag	UNP Q38854
11	724	ASP	-	expression tag	UNP Q38854
11	725	TYR	-	expression tag	UNP Q38854

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Chain	Residue	Modelled	Actual	Comment	Reference
11	726	LYS	-	expression tag	UNP Q38854
11	727	ASP	-	expression tag	UNP Q38854
11	728	ASP	-	expression tag	UNP Q38854
11	729	ASP	-	expression tag	UNP Q38854
11	730	ASP	-	expression tag	UNP Q38854
11	731	LYS	-	expression tag	UNP Q38854
13	41	MET	-	expression tag	UNP Q38854
13	42	ALA	-	expression tag	UNP Q38854
13	43	ASP	-	expression tag	UNP Q38854
13	44	LEU	-	expression tag	UNP Q38854
13	45	ASN	-	expression tag	UNP Q38854
13	46	TRP	-	expression tag	UNP Q38854
13	47	ILE	-	expression tag	UNP Q38854
13	48	SER	-	expression tag	UNP Q38854
13	49	ALA	-	expression tag	UNP Q38854
13	50	GLY	-	expression tag	UNP Q38854
13	51	HIS	-	expression tag	UNP Q38854
13	52	ALA	-	expression tag	UNP Q38854
13	53	ILE	-	expression tag	UNP Q38854
13	54	ALA	-	expression tag	UNP Q38854
13	55	ASP	-	expression tag	UNP Q38854
13	56	VAL	-	expression tag	UNP Q38854
13	57	GLY	-	expression tag	UNP Q38854
13	58	THR	-	expression tag	UNP Q38854
13	718	HIS	-	expression tag	UNP Q38854
13	719	HIS	-	expression tag	UNP Q38854
13	720	HIS	-	expression tag	UNP Q38854
13	721	HIS	-	expression tag	UNP Q38854
13	722	HIS	-	expression tag	UNP Q38854
13	723	HIS	-	expression tag	UNP Q38854
13	724	ASP	-	expression tag	UNP Q38854
13	725	TYR	-	expression tag	UNP Q38854
13	726	LYS	-	expression tag	UNP Q38854
13	727	ASP	-	expression tag	UNP Q38854
13	728	ASP	-	expression tag	UNP Q38854
13	729	ASP	-	expression tag	UNP Q38854
13	730	ASP	-	expression tag	UNP Q38854
13	731	LYS	-	expression tag	UNP Q38854

- Molecule 2 is a protein called Heat shock protein 21, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	12	92	Total	C	N	O	0	0
			455	271	92	92		

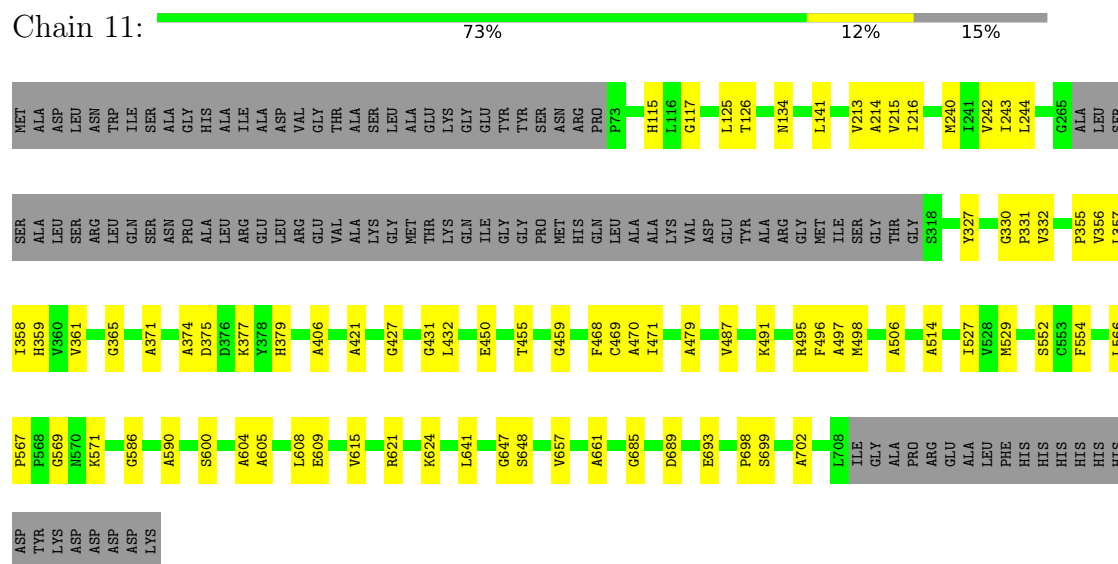
There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
12	21	MET	-	expression tag	UNP P31170
12	22	GLY	-	expression tag	UNP P31170
12	23	SER	-	expression tag	UNP P31170
12	24	SER	-	expression tag	UNP P31170
12	25	HIS	-	expression tag	UNP P31170
12	26	HIS	-	expression tag	UNP P31170
12	27	HIS	-	expression tag	UNP P31170
12	28	HIS	-	expression tag	UNP P31170
12	29	HIS	-	expression tag	UNP P31170
12	30	HIS	-	expression tag	UNP P31170
12	31	SER	-	expression tag	UNP P31170
12	32	GLN	-	expression tag	UNP P31170
12	33	ASP	-	expression tag	UNP P31170
12	34	PRO	-	expression tag	UNP P31170
12	35	ASN	-	expression tag	UNP P31170
12	36	SER	-	expression tag	UNP P31170
12	37	GLU	-	expression tag	UNP P31170
12	38	ASN	-	expression tag	UNP P31170
12	39	LEU	-	expression tag	UNP P31170
12	40	TYR	-	expression tag	UNP P31170
12	41	PHE	-	expression tag	UNP P31170
12	42	GLN	-	expression tag	UNP P31170
12	43	SER	-	expression tag	UNP P31170

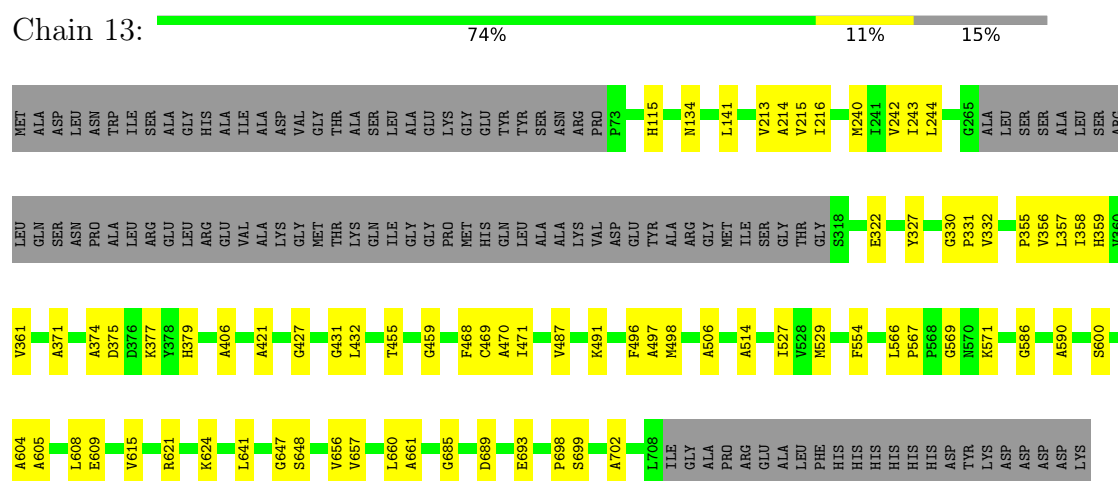
3 Residue-property plots

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: 1-deoxy-D-xylulose-5-phosphate synthase, chloroplastic



- Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase, chloroplastic



- Molecule 2: Heat shock protein 21, chloroplastic



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	162426	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
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	11	0.38	1/2855 (0.0%)	0.69	0/3958
1	13	0.38	1/2855 (0.0%)	0.69	1/3958 (0.0%)
2	12	0.40	0/454	1.05	3/631 (0.5%)
All	All	0.38	2/6164 (0.0%)	0.72	4/8547 (0.0%)

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
2	12	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	11	134	ASN	C-N	-10.36	1.18	1.33
1	13	134	ASN	C-N	-10.35	1.18	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	12	203	LEU	N-CA-C	6.69	117.31	107.88
1	13	322	GLU	N-CA-C	-5.84	105.65	112.89
2	12	216	LYS	CA-C-N	5.53	131.93	121.97
2	12	216	LYS	C-N-CA	5.53	131.93	121.97

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	12	158	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	12	213	PRO	Peptide
2	12	215	THR	Peptide
2	12	216	LYS	Peptide

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	11	2857	0	1363	49	0
1	13	2857	0	1363	44	0
2	12	455	0	188	15	0
All	All	6169	0	2914	108	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 (108) 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)
2:12:163:ILE:O	2:12:186:THR:CB	2.32	0.77
1:13:214:ALA:O	1:13:243:ILE:N	2.18	0.77
1:11:214:ALA:O	1:11:243:ILE:N	2.18	0.75
1:11:327:TYR:O	1:11:357:LEU:N	2.18	0.73
1:13:327:TYR:O	1:13:357:LEU:N	2.18	0.73
1:11:496:PHE:O	1:11:554:PHE:N	2.21	0.73
1:13:470:ALA:HA	1:13:497:ALA:HB3	1.70	0.73
1:13:496:PHE:O	1:13:554:PHE:N	2.21	0.73
1:11:470:ALA:HA	1:11:497:ALA:HB3	1.70	0.72
2:12:158:ASP:O	2:12:160:VAL:N	2.23	0.72
1:13:567:PRO:HA	1:13:571:LYS:H	1.55	0.71
1:11:469:CYS:O	1:11:497:ALA:N	2.23	0.70
1:13:469:CYS:O	1:13:497:ALA:N	2.23	0.70
1:11:567:PRO:HA	1:11:571:LYS:H	1.55	0.70
2:12:164:LYS:HA	2:12:186:THR:H	1.56	0.69
1:11:600:SER:O	1:11:604:ALA:N	2.26	0.69
1:13:605:ALA:O	1:13:609:GLU:N	2.20	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:13:600:SER:O	1:13:604:ALA:N	2.26	0.69
1:11:244:LEU:N	1:11:358:ILE:O	2.27	0.68
1:11:605:ALA:O	1:11:609:GLU:N	2.20	0.67
1:13:375:ASP:O	1:13:379:HIS:N	2.27	0.67
1:13:244:LEU:N	1:13:358:ILE:O	2.27	0.67
1:11:375:ASP:O	1:11:379:HIS:N	2.27	0.67
2:12:199:ILE:HA	2:12:211:THR:O	1.94	0.66
2:12:161:LEU:CB	2:12:188:LEU:O	2.45	0.65
1:13:242:VAL:O	1:13:358:ILE:N	2.30	0.65
1:13:242:VAL:N	1:13:356:VAL:O	2.29	0.65
1:11:242:VAL:N	1:11:356:VAL:O	2.29	0.65
1:11:242:VAL:O	1:11:358:ILE:N	2.30	0.64
1:11:141:LEU:N	1:11:213:VAL:O	2.32	0.63
1:13:141:LEU:N	1:13:213:VAL:O	2.32	0.62
1:13:566:LEU:O	1:13:569:GLY:N	2.33	0.62
1:11:527:ILE:HA	1:11:624:LYS:O	2.00	0.62
2:12:201:ALA:HA	2:12:209:PHE:O	2.00	0.61
1:13:514:ALA:O	1:13:648:SER:N	2.28	0.61
1:11:566:LEU:O	1:11:569:GLY:N	2.33	0.61
1:13:527:ILE:HA	1:13:624:LYS:O	2.00	0.61
1:13:689:ASP:O	1:13:693:GLU:N	2.25	0.61
1:11:689:ASP:O	1:11:693:GLU:N	2.25	0.60
1:13:498:MET:N	1:13:554:PHE:O	2.34	0.60
1:13:455:THR:O	1:13:459:GLY:N	2.25	0.60
2:12:140:MET:O	2:12:209:PHE:HA	2.00	0.60
1:11:455:THR:O	1:11:459:GLY:N	2.25	0.58
1:13:657:VAL:O	1:13:661:ALA:N	2.34	0.58
1:11:141:LEU:O	1:11:215:VAL:N	2.26	0.57
1:11:498:MET:N	1:11:554:PHE:O	2.34	0.57
1:11:657:VAL:O	1:11:661:ALA:N	2.34	0.57
1:11:514:ALA:HB1	1:11:647:GLY:HA2	1.88	0.55
1:13:471:ILE:O	1:13:498:MET:HA	2.07	0.55
1:13:514:ALA:HB1	1:13:647:GLY:HA2	1.88	0.55
1:11:506:ALA:HA	1:11:685:GLY:H	1.73	0.54
1:13:141:LEU:O	1:13:215:VAL:N	2.26	0.53
1:11:514:ALA:O	1:11:648:SER:N	2.28	0.53
1:11:330:GLY:HA3	1:11:359:HIS:O	2.09	0.53
1:13:332:VAL:O	1:13:361:VAL:N	2.35	0.53
1:11:471:ILE:O	1:11:498:MET:HA	2.07	0.52
1:13:506:ALA:HA	1:13:685:GLY:H	1.73	0.52
2:12:170:GLU:O	2:12:179:ARG:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:13:330:GLY:HA3	1:13:359:HIS:O	2.09	0.52
2:12:195:GLU:N	2:12:213:PRO:O	2.44	0.51
1:11:331:PRO:HA	1:11:359:HIS:O	2.12	0.50
1:13:529:MET:HA	1:13:621:ARG:O	2.13	0.49
2:12:200:LYS:O	2:12:210:ILE:HA	2.12	0.49
1:13:331:PRO:HA	1:13:359:HIS:O	2.12	0.49
1:11:529:MET:HA	1:11:621:ARG:O	2.13	0.48
1:11:332:VAL:O	1:11:361:VAL:N	2.35	0.48
1:13:331:PRO:HA	1:13:359:HIS:C	2.38	0.48
1:11:487:VAL:O	1:11:491:LYS:N	2.47	0.48
2:12:159:ASN:O	2:12:190:LEU:N	2.47	0.48
1:13:371:ALA:C	1:13:374:ALA:H	2.22	0.48
1:11:331:PRO:HA	1:11:359:HIS:C	2.38	0.47
1:11:371:ALA:C	1:11:374:ALA:H	2.22	0.47
1:13:487:VAL:O	1:13:491:LYS:N	2.47	0.47
1:11:698:PRO:O	1:11:702:ALA:N	2.38	0.46
2:12:169:LYS:CB	2:12:173:ASP:HA	2.45	0.46
1:11:374:ALA:HB1	1:11:377:LYS:CB	2.47	0.45
1:11:406:ALA:HB2	1:11:432:LEU:HA	1.99	0.45
1:13:374:ALA:HB1	1:13:377:LYS:CB	2.47	0.45
1:13:656:VAL:O	1:13:660:LEU:N	2.42	0.44
1:13:590:ALA:HB3	1:13:641:LEU:HA	1.99	0.44
1:11:590:ALA:HB3	1:11:641:LEU:HA	1.99	0.44
1:13:406:ALA:HB2	1:13:432:LEU:HA	1.98	0.44
1:11:605:ALA:O	1:11:608:LEU:N	2.44	0.44
1:13:605:ALA:C	1:13:608:LEU:H	2.25	0.44
2:12:203:LEU:HA	2:12:207:VAL:O	2.18	0.43
2:12:138:ILE:O	2:12:211:THR:HA	2.19	0.43
1:11:605:ALA:C	1:11:608:LEU:H	2.25	0.42
1:11:240:MET:O	1:11:355:PRO:HA	2.20	0.42
1:13:216:ILE:N	1:13:243:ILE:O	2.30	0.42
1:13:586:GLY:HA3	1:13:615:VAL:C	2.45	0.42
1:13:115:HIS:HA	1:13:379:HIS:O	2.20	0.41
1:11:125:LEU:O	1:11:126:THR:C	2.63	0.41
1:13:240:MET:O	1:13:355:PRO:HA	2.20	0.41
1:11:115:HIS:HA	1:11:379:HIS:O	2.20	0.41
2:12:152:VAL:HA	2:12:164:LYS:O	2.21	0.41
1:13:699:SER:HA	1:13:702:ALA:HB3	2.02	0.41
1:11:117:GLY:HA2	1:11:365:GLY:HA2	2.02	0.41
1:11:586:GLY:HA3	1:11:615:VAL:C	2.45	0.41
1:11:495:ARG:HA	1:11:552:SER:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:11:699:SER:HA	1:11:702:ALA:HB3	2.02	0.41
1:11:427:GLY:O	1:11:431:GLY:N	2.54	0.40
1:11:450:GLU:C	1:11:479:ALA:HB2	2.47	0.40
1:13:421:ALA:HA	1:13:468:PHE:O	2.21	0.40
1:11:216:ILE:N	1:11:243:ILE:O	2.31	0.40
1:13:427:GLY:O	1:13:431:GLY:N	2.54	0.40
1:11:421:ALA:HA	1:11:468:PHE:O	2.21	0.40
1:11:586:GLY:HA3	1:11:615:VAL:O	2.22	0.40
1:13:698:PRO:O	1:13:702:ALA:N	2.38	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	11	580/691 (84%)	498 (86%)	82 (14%)	0	100	100
1	13	580/691 (84%)	498 (86%)	82 (14%)	0	100	100
2	12	90/207 (44%)	62 (69%)	24 (27%)	4 (4%)	2	19
All	All	1250/1589 (79%)	1058 (85%)	188 (15%)	4 (0%)	37	65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	12	159	ASN
2	12	158	ASP
2	12	217	VAL
2	12	218	GLU

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	11	1
1	13	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	11	134:ASN	C	135:THR	N	1.18
1	13	134:ASN	C	135:THR	N	1.18

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30263. 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 ⓘ

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

9 Map-model fit ⓘ

This section was not generated.