



Full wwPDB EM Validation Report ⓘ

Oct 18, 2022 – 09:53 pm BST

PDB ID : 7O14
EMDB ID : EMD-12689
Title : ABC transporter NosDFY, nucleotide-free in lipid nanodisc, R-domain 1
Authors : Mueller, C.; Zhang, L.; Lu, W.; Einsle, O.; Du, J.
Deposited on : 2021-03-28
Resolution : Not provided

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.dev43
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) : 2.31.2

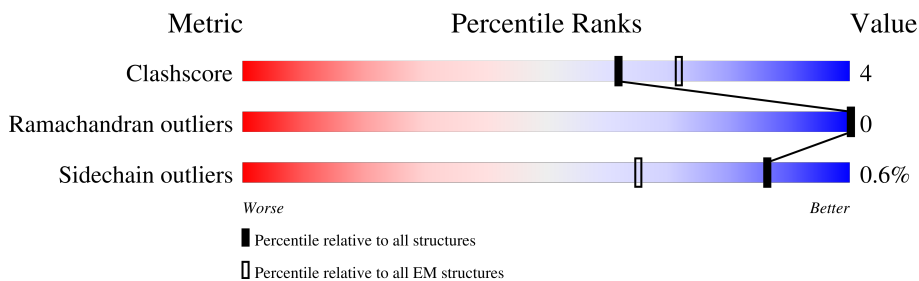
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	B	308	
1	C	308	
2	D	276	
2	E	276	
3	A	436	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11787 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 Probable ABC transporter ATP-binding protein NosF.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	307	Total	C	N	O	S	0	0
			2367	1478	442	441	6		
1	C	307	Total	C	N	O	S	0	0
			2367	1478	442	441	6		

- Molecule 2 is a protein called Probable ABC transporter permease protein NosY.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	267	Total	C	N	O	S	0	0
			2015	1355	319	334	7		
2	E	248	Total	C	N	O	S	0	0
			1896	1284	300	306	6		

- Molecule 3 is a protein called Probable ABC transporter binding protein NosD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	402	Total	C	N	O	S	0	0
			3140	1950	566	613	11		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	A	1	Total	Mg	0
			1	1	

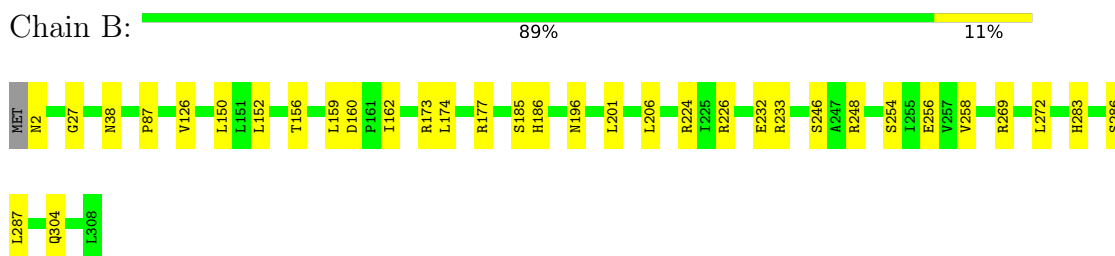
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
5	A	1	Total	O	0
			1	1	

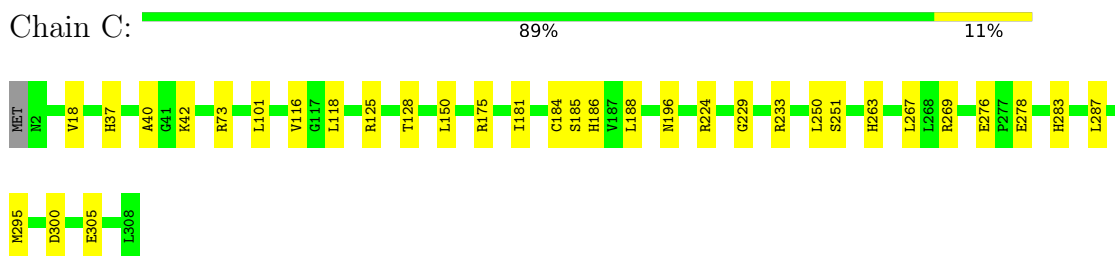
3 Residue-property plots [i](#)

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.

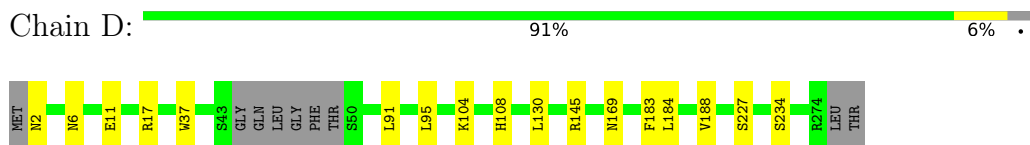
- Molecule 1: Probable ABC transporter ATP-binding protein NosF



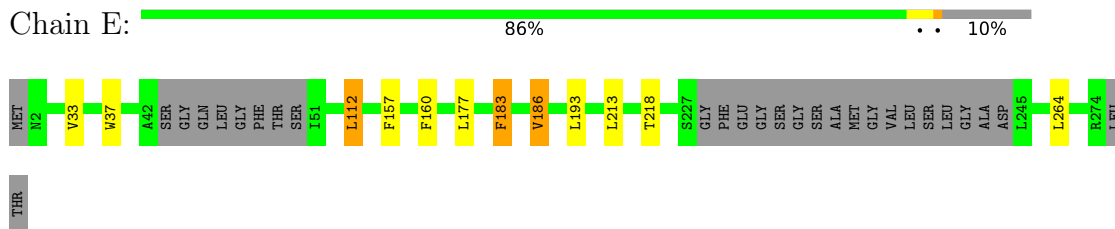
- Molecule 1: Probable ABC transporter ATP-binding protein NosF



- Molecule 2: Probable ABC transporter permease protein NosY

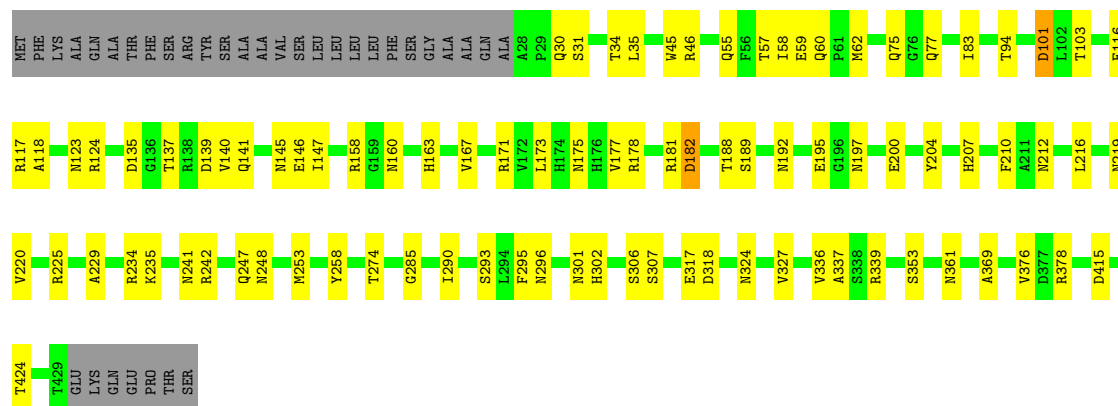


- Molecule 2: Probable ABC transporter permease protein NosY



- Molecule 3: Probable ABC transporter binding protein NosD

Chain A:  72% 20% 8%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	130946	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.43	0/2402	0.69	0/3247
1	C	0.40	0/2402	0.62	0/3247
2	D	0.42	0/2060	0.60	0/2809
2	E	0.41	0/1939	0.69	3/2646 (0.1%)
3	A	0.41	0/3204	0.72	4/4349 (0.1%)
All	All	0.42	0/12007	0.67	7/16298 (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
1	B	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	182	ASP	CB-CG-OD1	8.39	125.86	118.30
3	A	35	LEU	CA-CB-CG	8.28	134.34	115.30
2	E	112	LEU	CA-CB-CG	6.68	130.66	115.30
3	A	216	LEU	CA-CB-CG	5.79	128.61	115.30
2	E	186	VAL	CA-CB-CG1	5.61	119.31	110.90
3	A	101	ASP	CB-CG-OD1	5.36	123.12	118.30
2	E	112	LEU	CB-CG-CD2	5.06	119.60	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	232	GLU	Peptide
1	B	304	GLN	Peptide

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	B	2367	0	2416	20	0
1	C	2367	0	2417	23	0
2	D	2015	0	2136	12	0
2	E	1896	0	2026	6	0
3	A	3140	0	3017	56	0
4	A	1	0	0	0	0
5	A	1	0	0	2	0
All	All	11787	0	12012	106	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 4.

All (106) 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)
3:A:301:ASN:H	3:A:324:ASN:HD22	1.37	0.71
3:A:116:GLU:HG2	3:A:117:ARG:HG3	1.82	0.60
3:A:188:THR:HG22	3:A:210:PHE:HB2	1.87	0.57
3:A:160:ASN:ND2	3:A:182:ASP:OD1	2.38	0.57
1:C:229:GLY:HA3	1:C:278:GLU:HG2	1.87	0.56
3:A:182:ASP:HA	3:A:204:TYR:H	1.70	0.55
1:B:286:SER:OG	1:B:287:LEU:N	2.40	0.55
3:A:327:VAL:HA	3:A:353:SER:HB3	1.89	0.54
1:C:233:ARG:NH1	1:C:251:SER:O	2.41	0.54
3:A:212:ASN:HD22	3:A:234:ARG:H	1.56	0.53
3:A:75:GLN:OE1	3:A:77:GLN:NE2	2.42	0.53
1:B:201:LEU:HB3	1:B:206:LEU:HD12	1.91	0.53
3:A:207:HIS:HA	3:A:229:ALA:HB3	1.91	0.53
3:A:337:ALA:O	3:A:378:ARG:NH2	2.42	0.53
2:D:234:SER:HB2	3:A:369:ALA:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:30:GLN:HG3	3:A:57:THR:HB	1.90	0.53
3:A:146:GLU:OE2	3:A:178:ARG:NH2	2.43	0.52
3:A:361:ASN:ND2	5:A:601:HOH:O	2.42	0.52
1:B:233:ARG:NH1	1:B:254:SER:O	2.42	0.52
1:B:224:ARG:HB2	1:B:283:HIS:HB2	1.92	0.51
1:B:38:ASN:OD1	1:B:186:HIS:NE2	2.43	0.51
2:D:2:ASN:O	2:D:6:ASN:ND2	2.43	0.51
3:A:141:GLN:HG2	3:A:171:ARG:HB2	1.91	0.51
1:C:73:ARG:NH1	2:D:91:LEU:O	2.44	0.51
3:A:317:GLU:OE1	3:A:339:ARG:NH1	2.43	0.51
3:A:318:ASP:OD2	3:A:339:ARG:NH2	2.45	0.50
3:A:197:ASN:OD1	3:A:219:ASN:ND2	2.45	0.50
1:C:125:ARG:HH12	2:D:17:ARG:HH11	1.57	0.50
3:A:192:ASN:N	3:A:192:ASN:OD1	2.44	0.50
1:B:226:ARG:HB2	1:B:283:HIS:HE1	1.75	0.50
3:A:178:ARG:HG2	3:A:200:GLU:HB2	1.94	0.50
1:B:196:ASN:ND2	1:C:250:LEU:O	2.45	0.50
1:C:116:VAL:HG12	1:C:118:LEU:HB2	1.94	0.50
3:A:137:THR:H	3:A:167:VAL:HG12	1.77	0.50
1:B:87:PRO:HA	1:B:126:VAL:HB	1.94	0.49
3:A:75:GLN:HB2	3:A:77:GLN:HE22	1.78	0.49
3:A:135:ASP:N	3:A:135:ASP:OD1	2.46	0.49
3:A:147:ILE:HB	3:A:177:VAL:HG12	1.95	0.49
1:B:150:LEU:HD23	1:B:152:LEU:HD21	1.94	0.49
1:C:42:LYS:HD2	1:C:184:CYS:HB3	1.95	0.49
2:D:145:ARG:NH2	2:D:227:SER:OG	2.43	0.48
3:A:415:ASP:N	3:A:415:ASP:OD1	2.46	0.48
3:A:225:ARG:HA	3:A:247:GLN:HB2	1.95	0.48
3:A:220:VAL:HG12	3:A:242:ARG:HB2	1.94	0.48
1:B:156:THR:HA	1:B:159:LEU:HD12	1.96	0.48
3:A:219:ASN:H	3:A:241:ASN:HD22	1.61	0.48
3:A:123:ASN:OD1	3:A:145:ASN:ND2	2.46	0.48
1:B:174:LEU:HD22	1:B:177:ARG:HH21	1.79	0.48
3:A:189:SER:OG	3:A:192:ASN:ND2	2.47	0.47
3:A:45:TRP:NE1	3:A:62:MET:SD	2.78	0.47
3:A:173:LEU:HG	3:A:195:GLU:HB2	1.96	0.47
3:A:118:ALA:HB3	3:A:140:VAL:HG23	1.96	0.47
1:B:162:ILE:HD11	1:C:295:MET:HG3	1.97	0.47
2:D:11:GLU:OE2	2:D:104:LYS:NZ	2.48	0.47
3:A:160:ASN:OD1	3:A:163:HIS:ND1	2.40	0.46
1:B:248:ARG:HB2	1:B:256:GLU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:TRP:HD1	2:D:130:LEU:HD21	1.81	0.46
1:B:2:ASN:HD22	1:B:27:GLY:HA2	1.80	0.46
1:C:150:LEU:HB2	1:C:181:ILE:HG12	1.97	0.46
1:C:224:ARG:HB2	1:C:283:HIS:HB2	1.97	0.46
1:B:269:ARG:NH1	1:C:276:GLU:OE1	2.49	0.46
3:A:158:ARG:HB2	3:A:181:ARG:HB2	1.96	0.46
1:C:101:LEU:HD22	2:D:95:LEU:HD11	1.98	0.46
3:A:225:ARG:HG2	3:A:274:THR:HA	1.97	0.46
1:C:175:ARG:NH1	1:C:196:ASN:OD1	2.50	0.45
3:A:253:MET:HG3	3:A:290:ILE:HA	1.98	0.45
3:A:101:ASP:OD1	3:A:103:THR:OG1	2.30	0.45
3:A:58:ILE:HD13	3:A:83:ILE:HG12	1.98	0.45
3:A:55:GLN:NE2	3:A:77:GLN:O	2.44	0.45
1:B:185:SER:OG	1:B:186:HIS:N	2.50	0.45
3:A:258:TYR:N	3:A:295:PHE:O	2.48	0.45
3:A:361:ASN:OD1	3:A:361:ASN:N	2.49	0.45
3:A:301:ASN:OD1	3:A:324:ASN:ND2	2.50	0.45
2:E:33:VAL:O	2:E:37:TRP:N	2.50	0.44
1:C:188:LEU:HD23	1:C:287:LEU:HG	1.98	0.44
2:E:193:LEU:HD23	2:E:193:LEU:HA	1.89	0.44
3:A:306:SER:OG	3:A:307:SER:N	2.50	0.44
3:A:361:ASN:CG	5:A:601:HOH:O	2.56	0.44
1:B:246:SER:H	1:B:258:VAL:HG12	1.83	0.44
3:A:94:THR:HG23	3:A:124:ARG:HB2	2.00	0.44
3:A:59:GLU:HG2	3:A:60:GLN:HG2	2.00	0.43
2:D:11:GLU:OE1	2:D:108:HIS:NE2	2.50	0.43
3:A:31:SER:O	3:A:34:THR:OG1	2.36	0.43
1:C:300:ASP:N	1:C:300:ASP:OD1	2.50	0.43
3:A:145:ASN:H	3:A:175:ASN:HD22	1.66	0.43
1:C:125:ARG:HH12	2:D:17:ARG:HD3	1.84	0.43
1:C:125:ARG:HB2	1:C:128:THR:HG23	2.01	0.43
1:B:173:ARG:NH2	1:C:305:GLU:OE2	2.51	0.43
1:C:263:HIS:HB3	1:C:267:LEU:HD23	2.00	0.42
2:E:183:PHE:HD1	2:E:183:PHE:HA	1.74	0.42
3:A:248:ASN:HA	3:A:285:GLY:HA2	2.01	0.42
3:A:293:SER:OG	3:A:296:ASN:ND2	2.52	0.42
1:C:185:SER:OG	1:C:186:HIS:N	2.53	0.42
2:E:157:PHE:HA	2:E:160:PHE:HB2	2.01	0.42
3:A:117:ARG:HG2	3:A:139:ASP:HB2	2.02	0.42
2:E:264:LEU:HD23	2:E:264:LEU:HA	1.87	0.41
3:A:46:ARG:HE	3:A:46:ARG:HB2	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ASP:OD1	1:C:37:HIS:ND1	2.51	0.41
1:B:272:LEU:HD21	1:C:269:ARG:HA	2.01	0.41
3:A:302:HIS:ND1	3:A:424:THR:OG1	2.40	0.41
2:E:177:LEU:HD23	2:E:177:LEU:HA	1.94	0.41
2:D:169:ASN:OD1	2:D:169:ASN:N	2.50	0.40
1:C:18:VAL:HB	1:C:40:ALA:HB1	2.03	0.40
3:A:123:ASN:H	3:A:145:ASN:HD22	1.69	0.40
2:D:184:LEU:HA	2:D:188:VAL:HB	2.02	0.40
3:A:235:LYS:HG2	3:A:258:TYR:HB2	2.03	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	305/308 (99%)	280 (92%)	25 (8%)	0	100	100
1	C	305/308 (99%)	276 (90%)	29 (10%)	0	100	100
2	D	263/276 (95%)	257 (98%)	6 (2%)	0	100	100
2	E	242/276 (88%)	234 (97%)	8 (3%)	0	100	100
3	A	400/436 (92%)	367 (92%)	33 (8%)	0	100	100
All	All	1515/1604 (94%)	1414 (93%)	101 (7%)	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	250/251 (100%)	250 (100%)	0	100	100
1	C	250/251 (100%)	250 (100%)	0	100	100
2	D	205/212 (97%)	204 (100%)	1 (0%)	88	88
2	E	193/212 (91%)	188 (97%)	5 (3%)	46	46
3	A	339/365 (93%)	337 (99%)	2 (1%)	86	86
All	All	1237/1291 (96%)	1229 (99%)	8 (1%)	86	86

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	183	PHE
2	E	112	LEU
2	E	183	PHE
2	E	186	VAL
2	E	213	LEU
2	E	218	THR
3	A	336	VAL
3	A	376	VAL

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

Mol	Chain	Res	Type
1	B	2	ASN
1	B	23	ASN
1	B	207	GLN
1	C	25	ASN
1	C	97	HIS
1	C	270	GLN
2	D	6	ASN
2	D	225	ASN
2	E	225	ASN
3	A	30	GLN
3	A	75	GLN
3	A	77	GLN
3	A	123	ASN
3	A	141	GLN
3	A	145	ASN

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Mol	Chain	Res	Type
3	A	175	ASN
3	A	179	ASN
3	A	190	ASN
3	A	212	ASN
3	A	241	ASN
3	A	301	ASN
3	A	324	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12689. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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 surface views

This section was not generated.

6.5 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.