



Full wwPDB EM Validation Report ⓘ

Apr 12, 2026 – 11:30 AM UTC

PDB ID : 9W3Z / pdb_00009w3z
EMDB ID : EMD-65613
Title : Cryo-EM structure of the 4:4 Lac1-Lip1 complex
Authors : Xie, T.; Gong, X.
Deposited on : 2025-07-30
Resolution : 3.36 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 Phenix2.0
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

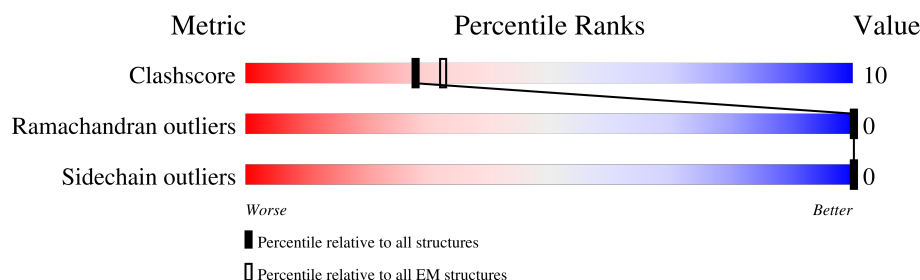
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.36 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
Sidechain outliers	223484	23102

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	428	55% 18% 27%
1	C	428	64% 11% 25%
1	E	428	54% 18% 27%
1	G	428	63% 12% 25%
2	B	150	61% 27% 12%
2	D	150	61% 29% 10%
2	F	150	62% 26% 12%
2	H	150	64% 26% 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29422 atoms, of which 14568 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 Ceramide synthase LAC1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	312	Total	C	H	N	O	S	0	0
			5098	1731	2531	407	416	13		
1	C	321	Total	C	H	N	O	S	0	0
			5323	1802	2650	427	431	13		
1	E	312	Total	C	H	N	O	S	0	0
			5098	1731	2531	407	416	13		
1	G	321	Total	C	H	N	O	S	0	0
			5323	1802	2650	427	431	13		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	LEU	-	expression tag	UNP P28496
A	420	GLU	-	expression tag	UNP P28496
A	421	ASP	-	expression tag	UNP P28496
A	422	TYR	-	expression tag	UNP P28496
A	423	LYS	-	expression tag	UNP P28496
A	424	ASP	-	expression tag	UNP P28496
A	425	ASP	-	expression tag	UNP P28496
A	426	ASP	-	expression tag	UNP P28496
A	427	ASP	-	expression tag	UNP P28496
A	428	LYS	-	expression tag	UNP P28496
C	419	LEU	-	expression tag	UNP P28496
C	420	GLU	-	expression tag	UNP P28496
C	421	ASP	-	expression tag	UNP P28496
C	422	TYR	-	expression tag	UNP P28496
C	423	LYS	-	expression tag	UNP P28496
C	424	ASP	-	expression tag	UNP P28496
C	425	ASP	-	expression tag	UNP P28496
C	426	ASP	-	expression tag	UNP P28496
C	427	ASP	-	expression tag	UNP P28496
C	428	LYS	-	expression tag	UNP P28496
E	419	LEU	-	expression tag	UNP P28496
E	420	GLU	-	expression tag	UNP P28496

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Chain	Residue	Modelled	Actual	Comment	Reference
E	421	ASP	-	expression tag	UNP P28496
E	422	TYR	-	expression tag	UNP P28496
E	423	LYS	-	expression tag	UNP P28496
E	424	ASP	-	expression tag	UNP P28496
E	425	ASP	-	expression tag	UNP P28496
E	426	ASP	-	expression tag	UNP P28496
E	427	ASP	-	expression tag	UNP P28496
E	428	LYS	-	expression tag	UNP P28496
G	419	LEU	-	expression tag	UNP P28496
G	420	GLU	-	expression tag	UNP P28496
G	421	ASP	-	expression tag	UNP P28496
G	422	TYR	-	expression tag	UNP P28496
G	423	LYS	-	expression tag	UNP P28496
G	424	ASP	-	expression tag	UNP P28496
G	425	ASP	-	expression tag	UNP P28496
G	426	ASP	-	expression tag	UNP P28496
G	427	ASP	-	expression tag	UNP P28496
G	428	LYS	-	expression tag	UNP P28496

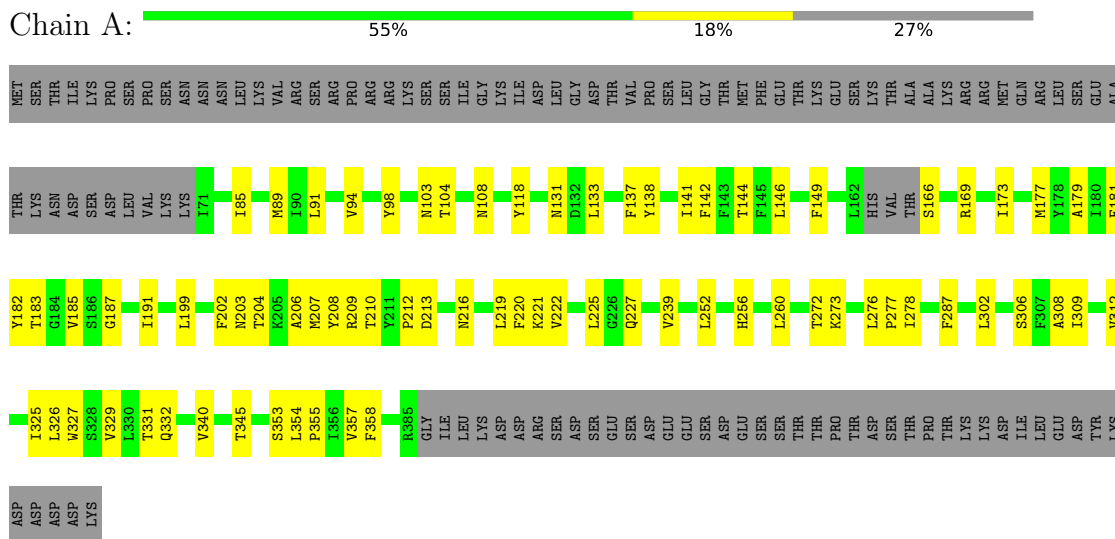
- Molecule 2 is a protein called Ceramide synthase subunit LIP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	132	Total	C	H	N	O	S	0	0
			2120	698	1038	177	201	6		
2	D	135	Total	C	H	N	O	S	0	0
			2170	714	1065	181	204	6		
2	F	132	Total	C	H	N	O	S	0	0
			2120	698	1038	177	201	6		
2	H	135	Total	C	H	N	O	S	0	0
			2170	714	1065	181	204	6		

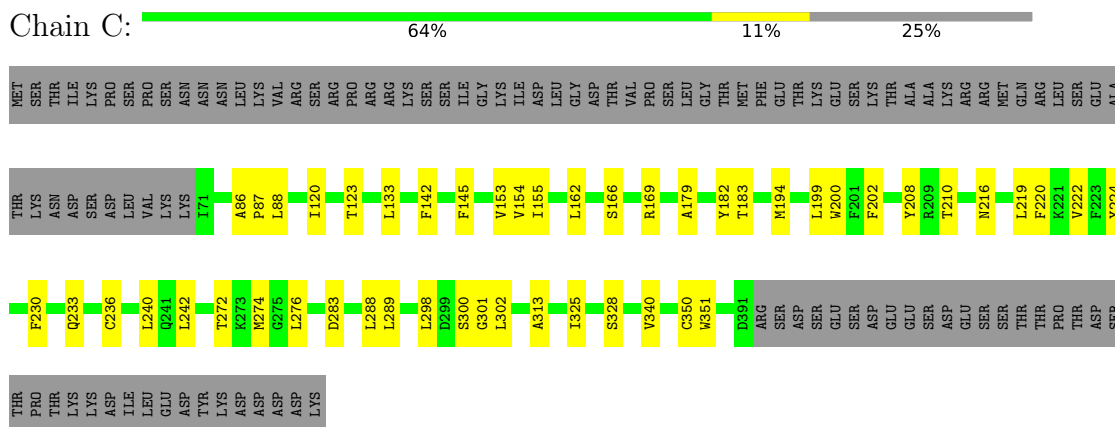
3 Residue-property plots

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.

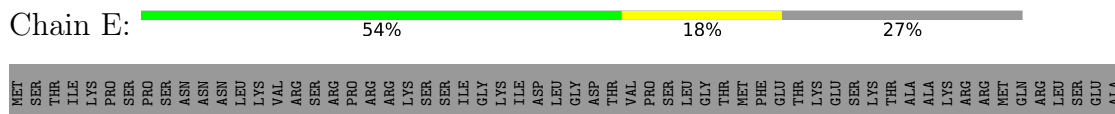
• Molecule 1: Ceramide synthase LAC1

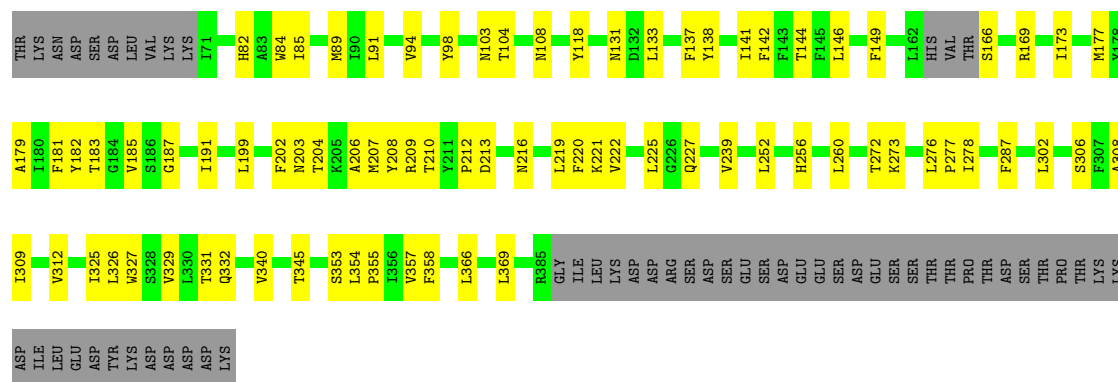


• Molecule 1: Ceramide synthase LAC1



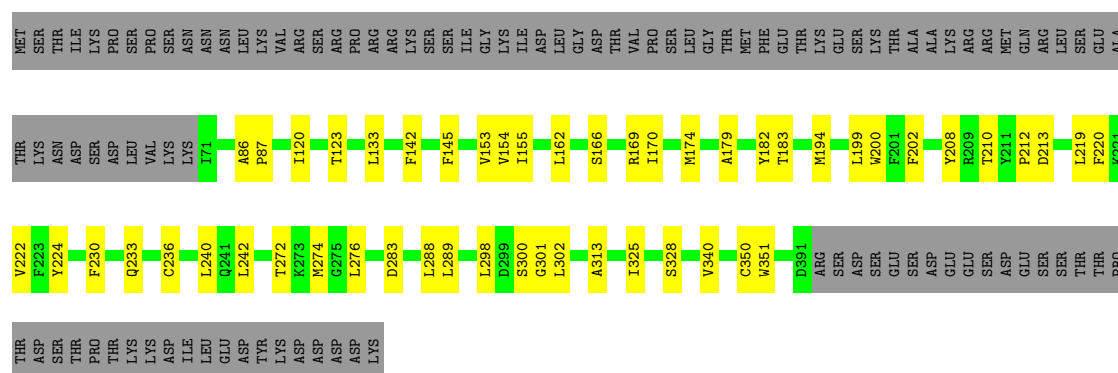
• Molecule 1: Ceramide synthase LAC1





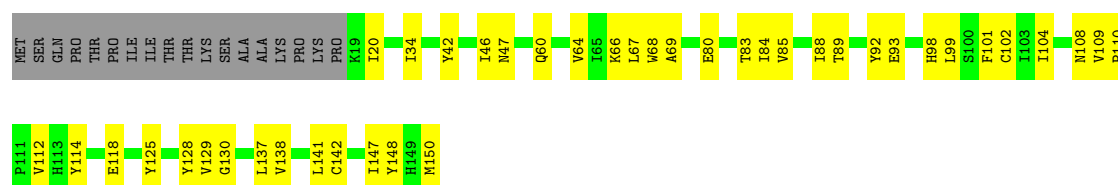
- Molecule 1: Ceramide synthase LAC1

Chain G: 63% 12% 25%



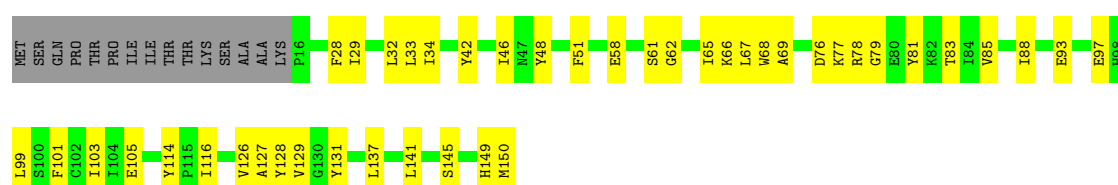
- Molecule 2: Ceramide synthase subunit LIP1

Chain B: 61% 27% 12%



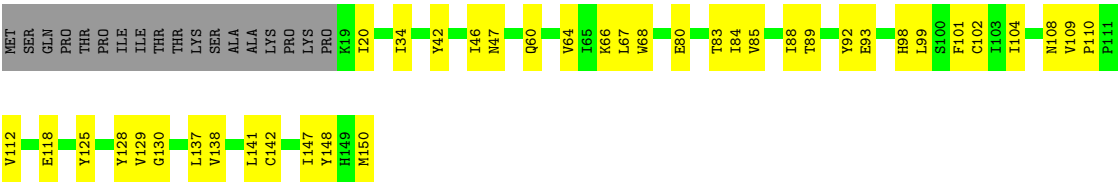
- Molecule 2: Ceramide synthase subunit LIP1

Chain D: 61% 29% 10%

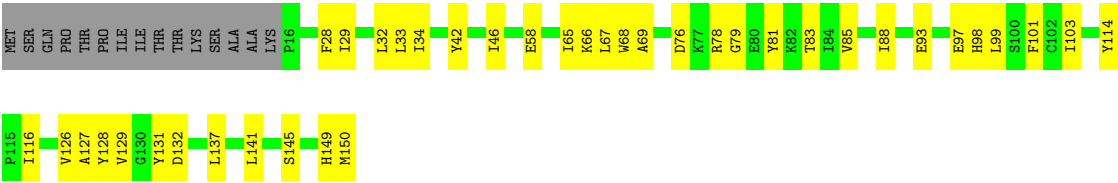


- Molecule 2: Ceramide synthase subunit LIP1

Chain F: 62% 26% 12%



● Molecule 2: Ceramide synthase subunit LIP1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	219798	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	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	0.14	0/2650	0.38	1/3607 (0.0%)
1	C	0.19	0/2762	0.40	0/3758
1	E	0.14	0/2650	0.38	1/3607 (0.0%)
1	G	0.19	0/2762	0.40	0/3758
2	B	0.18	0/1114	0.38	0/1512
2	D	0.18	0/1139	0.35	0/1546
2	F	0.18	0/1114	0.37	0/1512
2	H	0.18	0/1139	0.35	0/1546
All	All	0.17	0/15330	0.38	2/20846 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	VAL	N-CA-C	-5.10	107.86	112.96
1	E	185	VAL	N-CA-C	-5.08	107.88	112.96

There are no chirality outliers.

There are no planarity outliers.

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	2567	2531	2529	49	0
1	C	2673	2650	2649	35	0
1	E	2567	2531	2529	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2673	2650	2649	35	0
2	B	1082	1038	1037	35	0
2	D	1105	1065	1065	29	0
2	F	1082	1038	1037	34	0
2	H	1105	1065	1065	27	0
All	All	14854	14568	14560	283	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 10.

All (283) 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:E:118:TYR:OH	1:E:131:ASN:OD1	1.87	0.92
1:A:118:TYR:OH	1:A:131:ASN:OD1	1.87	0.91
1:G:224:TYR:OH	1:G:272:THR:O	1.90	0.89
1:C:224:TYR:OH	1:C:272:THR:O	1.94	0.86
1:E:137:PHE:CE2	1:E:141:ILE:HD11	2.18	0.79
2:F:64:VAL:HG21	2:F:137:LEU:HD22	1.65	0.78
2:B:64:VAL:HG21	2:B:137:LEU:HD22	1.65	0.78
1:A:146:LEU:HD12	1:A:149:PHE:HE1	1.55	0.72
2:H:88:ILE:HG23	2:H:129:VAL:HG21	1.73	0.71
2:F:60:GLN:OE1	2:F:64:VAL:HG23	1.90	0.71
2:B:60:GLN:OE1	2:B:64:VAL:HG23	1.90	0.71
1:E:146:LEU:HD12	1:E:149:PHE:HE1	1.55	0.71
2:D:88:ILE:HG23	2:D:129:VAL:HG21	1.73	0.70
1:C:86:ALA:HB3	1:C:87:PRO:HD3	1.74	0.70
1:E:216:ASN:OD1	1:E:272:THR:HG21	1.92	0.70
1:A:216:ASN:OD1	1:A:272:THR:HG21	1.92	0.69
2:H:101:PHE:HB3	2:H:129:VAL:HG23	1.74	0.69
2:D:101:PHE:HB3	2:D:129:VAL:HG23	1.74	0.68
1:G:86:ALA:HB3	1:G:87:PRO:HD3	1.74	0.68
1:A:216:ASN:ND2	1:A:272:THR:OG1	2.26	0.68
1:E:216:ASN:ND2	1:E:272:THR:OG1	2.26	0.68
2:B:89:THR:O	2:D:78:ARG:NH2	2.27	0.67
2:F:89:THR:O	2:H:78:ARG:NH2	2.27	0.67
2:D:81:TYR:HE1	2:D:103:ILE:HD13	1.61	0.65
2:B:67:LEU:HB3	2:B:84:ILE:HD12	1.79	0.65
2:H:58:GLU:OE2	2:H:68:TRP:NE1	2.30	0.65
2:F:67:LEU:HB3	2:F:84:ILE:HD12	1.78	0.64
2:D:58:GLU:OE2	2:D:68:TRP:NE1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:81:TYR:HE1	2:H:103:ILE:HD13	1.61	0.64
2:H:69:ALA:O	2:H:114:TYR:OH	2.10	0.64
2:D:69:ALA:O	2:D:114:TYR:OH	2.10	0.63
2:F:125:TYR:OH	2:H:149:HIS:O	2.18	0.62
2:B:125:TYR:OH	2:D:149:HIS:O	2.18	0.61
1:E:210:THR:HG23	1:E:210:THR:O	2.00	0.61
1:E:302:LEU:O	1:E:306:SER:N	2.33	0.60
1:A:210:THR:O	1:A:210:THR:HG23	2.00	0.60
1:G:162:LEU:HD21	1:G:298:LEU:HD13	1.84	0.59
1:A:353:SER:O	1:A:357:VAL:HG23	2.02	0.59
2:F:85:VAL:HG11	2:H:85:VAL:HG11	1.84	0.59
1:C:133:LEU:HD11	2:D:34:ILE:HG21	1.85	0.59
2:B:85:VAL:HG11	2:D:85:VAL:HG11	1.85	0.58
1:E:353:SER:O	1:E:357:VAL:HG23	2.02	0.58
1:G:133:LEU:HD11	2:H:34:ILE:HG21	1.85	0.58
1:A:302:LEU:O	1:A:306:SER:N	2.36	0.58
2:D:103:ILE:O	2:D:145:SER:OG	2.12	0.58
2:F:20:ILE:O	2:F:20:ILE:HG22	2.03	0.58
1:E:187:GLY:O	1:E:191:ILE:HD12	2.04	0.57
1:C:162:LEU:HD21	1:C:298:LEU:HD13	1.85	0.57
1:A:187:GLY:O	1:A:191:ILE:HD12	2.04	0.57
1:A:202:PHE:O	1:A:204:THR:HG23	2.05	0.57
2:D:29:ILE:O	2:D:33:LEU:HD23	2.05	0.56
2:B:20:ILE:HG22	2:B:20:ILE:O	2.03	0.56
1:E:202:PHE:O	1:E:204:THR:HG23	2.05	0.56
2:H:29:ILE:O	2:H:33:LEU:HD23	2.05	0.56
1:E:252:LEU:O	1:E:256:HIS:ND1	2.36	0.55
2:D:99:LEU:HD23	2:D:150:MET:HB2	1.89	0.55
1:E:325:ILE:O	1:E:329:VAL:HG13	2.06	0.55
1:G:220:PHE:HE1	1:G:276:LEU:HD22	1.71	0.55
1:A:256:HIS:O	1:A:260:LEU:HD23	2.06	0.55
1:A:325:ILE:O	1:A:329:VAL:HG13	2.06	0.55
2:B:150:MET:HE2	2:D:78:ARG:HA	1.89	0.55
1:G:210:THR:HG23	1:G:210:THR:O	2.07	0.54
1:C:210:THR:HG23	1:C:210:THR:O	2.08	0.54
1:E:256:HIS:O	1:E:260:LEU:HD23	2.07	0.54
2:D:93:GLU:HG2	2:D:93:GLU:O	2.07	0.54
2:H:65:ILE:HD11	2:H:67:LEU:HD11	1.89	0.54
1:G:302:LEU:HD12	1:G:302:LEU:O	2.08	0.54
1:G:170:ILE:HG22	1:G:174:MET:HE2	1.90	0.54
1:A:239:VAL:HG12	1:A:239:VAL:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:65:ILE:HD11	2:D:67:LEU:HD11	1.89	0.54
1:A:252:LEU:O	1:A:256:HIS:ND1	2.35	0.53
1:E:82:HIS:HD1	1:E:84:TRP:HZ3	1.56	0.53
1:G:208:TYR:HE1	1:G:274:MET:HE2	1.74	0.53
2:F:150:MET:HE2	2:H:78:ARG:HA	1.89	0.53
1:C:302:LEU:HD12	1:C:302:LEU:O	2.08	0.53
1:E:239:VAL:HG12	1:E:239:VAL:O	2.08	0.53
2:H:99:LEU:HD23	2:H:150:MET:HB2	1.89	0.53
2:D:65:ILE:CD1	2:D:67:LEU:HD11	2.38	0.53
2:H:93:GLU:O	2:H:93:GLU:HG2	2.07	0.53
2:B:64:VAL:HG21	2:B:137:LEU:CD2	2.38	0.53
2:H:65:ILE:CD1	2:H:67:LEU:HD11	2.38	0.53
1:C:216:ASN:HD21	1:C:272:THR:HG21	1.74	0.52
1:C:153:VAL:HG12	1:C:153:VAL:O	2.09	0.52
2:D:79:GLY:O	2:D:83:THR:HG22	2.10	0.52
2:H:79:GLY:O	2:H:83:THR:HG22	2.10	0.52
1:A:137:PHE:CE2	1:A:141:ILE:HD11	2.45	0.52
2:B:68:TRP:C	2:B:84:ILE:HD11	2.35	0.52
2:H:126:VAL:HG12	2:H:127:ALA:N	2.25	0.52
2:F:68:TRP:C	2:F:84:ILE:HD11	2.34	0.51
1:G:153:VAL:HG12	1:G:153:VAL:O	2.09	0.51
2:D:126:VAL:HG12	2:D:127:ALA:N	2.25	0.51
2:B:67:LEU:HD22	2:B:88:ILE:HG13	1.93	0.51
2:F:67:LEU:HD22	2:F:88:ILE:HG13	1.92	0.51
1:E:309:ILE:HA	1:E:312:VAL:HG22	1.92	0.51
2:F:64:VAL:HG21	2:F:137:LEU:CD2	2.38	0.51
1:C:220:PHE:HE1	1:C:276:LEU:HD22	1.74	0.51
1:E:203:ASN:OD1	1:E:206:ALA:N	2.42	0.51
1:E:227:GLN:HA	1:E:227:GLN:OE1	2.11	0.51
1:G:142:PHE:O	1:G:145:PHE:HB3	2.11	0.50
1:G:350:CYS:HG	1:G:351:TRP:CD1	2.29	0.50
1:A:227:GLN:HA	1:A:227:GLN:OE1	2.11	0.50
1:C:350:CYS:HG	1:C:351:TRP:CD1	2.30	0.50
2:D:77:LYS:NZ	2:D:105:GLU:OE2	2.28	0.50
1:G:154:VAL:HG23	1:G:155:ILE:N	2.27	0.50
1:A:331:THR:HG23	1:A:332:GLN:N	2.27	0.50
1:A:85:ILE:O	1:A:89:MET:HG3	2.12	0.50
2:B:118:GLU:OE1	2:B:118:GLU:N	2.45	0.50
2:F:92:TYR:HE2	2:F:129:VAL:HG13	1.77	0.50
1:A:309:ILE:HA	1:A:312:VAL:HG22	1.92	0.50
2:B:101:PHE:HB2	2:B:128:TYR:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:331:THR:HG23	1:E:332:GLN:N	2.27	0.49
2:F:101:PHE:HB2	2:F:128:TYR:O	2.12	0.49
2:F:60:GLN:NE2	2:F:66:LYS:HB3	2.27	0.49
2:B:92:TYR:HE2	2:B:129:VAL:HG13	1.77	0.49
1:C:154:VAL:HG23	1:C:155:ILE:N	2.27	0.49
1:G:350:CYS:SG	1:G:351:TRP:N	2.84	0.49
2:F:118:GLU:OE2	2:F:118:GLU:N	2.45	0.49
1:C:350:CYS:SG	1:C:351:TRP:N	2.84	0.49
1:A:219:LEU:HA	1:A:222:VAL:HG12	1.94	0.49
2:B:60:GLN:NE2	2:B:66:LYS:HB3	2.28	0.49
1:C:120:ILE:O	1:C:123:THR:HG22	2.13	0.49
1:C:142:PHE:O	1:C:145:PHE:HB3	2.11	0.49
1:G:240:LEU:O	1:G:240:LEU:HG	2.13	0.49
1:E:179:ALA:HA	1:E:182:TYR:CE1	2.48	0.48
1:E:326:LEU:HD11	1:E:358:PHE:CD2	2.48	0.48
1:G:120:ILE:O	1:G:123:THR:HG22	2.13	0.48
2:F:80:GLU:HA	2:F:83:THR:HG22	1.95	0.48
2:B:64:VAL:HG12	2:B:130:GLY:HA3	1.94	0.48
1:A:179:ALA:HA	1:A:182:TYR:CE1	2.48	0.48
2:D:28:PHE:O	2:D:32:LEU:HD13	2.14	0.48
1:C:240:LEU:HG	1:C:240:LEU:O	2.13	0.48
2:B:80:GLU:HA	2:B:83:THR:HG22	1.95	0.48
1:E:85:ILE:O	1:E:89:MET:HG3	2.13	0.48
2:H:28:PHE:O	2:H:32:LEU:HD13	2.13	0.48
1:E:219:LEU:HA	1:E:222:VAL:HG12	1.95	0.48
2:F:64:VAL:HG12	2:F:130:GLY:HA3	1.94	0.47
2:B:98:HIS:ND1	2:B:150:MET:O	2.48	0.47
1:E:340:VAL:HG23	1:E:340:VAL:O	2.14	0.47
2:F:98:HIS:ND1	2:F:150:MET:O	2.48	0.47
2:B:102:CYS:SG	2:B:104:ILE:HD11	2.54	0.47
2:F:102:CYS:SG	2:F:104:ILE:HD11	2.54	0.47
2:D:58:GLU:O	2:D:66:LYS:N	2.47	0.47
1:A:206:ALA:O	1:A:273:LYS:NZ	2.41	0.47
1:A:340:VAL:HG23	1:A:340:VAL:O	2.14	0.47
1:A:326:LEU:HD11	1:A:358:PHE:CD2	2.49	0.47
1:C:325:ILE:O	1:C:328:SER:OG	2.23	0.46
2:B:137:LEU:HD21	2:B:141:LEU:CD1	2.45	0.46
2:H:103:ILE:O	2:H:145:SER:OG	2.12	0.46
1:A:203:ASN:OD1	1:A:206:ALA:N	2.42	0.46
1:A:278:ILE:HD12	1:A:278:ILE:H	1.80	0.46
2:F:137:LEU:HD21	2:F:141:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:58:GLU:O	2:H:66:LYS:N	2.47	0.46
2:B:108:ASN:C	2:B:109:VAL:HG23	2.41	0.46
1:G:155:ILE:HG22	1:G:174:MET:HG2	1.98	0.46
2:F:108:ASN:C	2:F:109:VAL:HG23	2.41	0.46
1:A:183:THR:HG22	1:A:287:PHE:HB2	1.97	0.46
1:C:179:ALA:HA	1:C:182:TYR:CE1	2.51	0.45
1:C:288:LEU:HD12	1:C:313:ALA:HB3	1.99	0.45
2:H:98:HIS:O	2:H:132:ASP:HB2	2.16	0.45
1:E:183:THR:HG22	1:E:287:PHE:HB2	1.98	0.45
1:E:278:ILE:H	1:E:278:ILE:HD12	1.80	0.45
1:G:179:ALA:HA	1:G:182:TYR:CE1	2.51	0.45
2:F:137:LEU:HD23	2:F:137:LEU:O	2.17	0.45
2:B:112:VAL:O	2:B:112:VAL:HG13	2.16	0.45
1:E:138:TYR:HA	1:E:141:ILE:HD12	1.97	0.45
2:H:137:LEU:O	2:H:141:LEU:HD23	2.16	0.45
1:E:166:SER:N	1:E:169:ARG:HE	2.14	0.45
1:G:220:PHE:CE1	1:G:276:LEU:HD22	2.51	0.45
1:C:236:CYS:O	1:C:240:LEU:HD23	2.17	0.45
2:D:116:ILE:HD12	2:D:116:ILE:H	1.80	0.45
1:E:103:ASN:O	1:E:108:ASN:ND2	2.48	0.45
2:H:116:ILE:HD12	2:H:116:ILE:H	1.80	0.45
2:F:99:LEU:CD2	2:F:150:MET:HB2	2.46	0.45
1:A:166:SER:N	1:A:169:ARG:HE	2.15	0.45
1:A:221:LYS:O	1:A:225:LEU:HD23	2.17	0.45
2:B:137:LEU:HD23	2:B:137:LEU:O	2.17	0.45
1:E:327:TRP:O	1:E:331:THR:HG22	2.17	0.45
1:A:199:LEU:HD13	1:A:207:MET:HG3	1.99	0.45
1:E:331:THR:HG23	1:E:332:GLN:HG2	1.99	0.45
1:G:236:CYS:O	1:G:240:LEU:HD23	2.17	0.45
1:E:206:ALA:O	1:E:273:LYS:NZ	2.41	0.45
2:B:101:PHE:CE2	2:B:148:TYR:HD1	2.35	0.44
2:D:137:LEU:O	2:D:141:LEU:HD23	2.17	0.44
1:A:91:LEU:HD21	1:A:142:PHE:HD1	1.81	0.44
2:B:99:LEU:CD2	2:B:150:MET:HB2	2.46	0.44
1:E:199:LEU:HD13	1:E:207:MET:HG3	1.99	0.44
1:E:221:LYS:O	1:E:225:LEU:HD23	2.17	0.44
1:A:331:THR:HG23	1:A:332:GLN:HG2	1.99	0.44
1:C:300:SER:O	1:C:301:GLY:C	2.61	0.44
1:G:288:LEU:HD12	1:G:313:ALA:HB3	1.99	0.44
1:G:300:SER:O	1:G:301:GLY:C	2.61	0.44
1:A:220:PHE:CE2	1:A:276:LEU:HD22	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ASN:ND2	1:C:272:THR:HG21	2.32	0.44
2:F:112:VAL:HG13	2:F:112:VAL:O	2.16	0.44
1:E:94:VAL:HG11	1:E:138:TYR:CE1	2.53	0.44
1:G:340:VAL:HG23	1:G:340:VAL:O	2.18	0.44
1:A:94:VAL:HG11	1:A:138:TYR:CE1	2.52	0.44
1:C:183:THR:CG2	1:C:283:ASP:O	2.66	0.44
1:A:327:TRP:O	1:A:331:THR:HG22	2.18	0.43
1:E:91:LEU:HD21	1:E:142:PHE:HD1	1.83	0.43
1:E:173:ILE:O	1:E:177:MET:HG2	2.18	0.43
2:F:101:PHE:CE2	2:F:148:TYR:HD1	2.35	0.43
1:A:103:ASN:O	1:A:108:ASN:ND2	2.49	0.43
1:E:212:PRO:O	1:E:213:ASP:C	2.61	0.43
1:A:212:PRO:O	1:A:213:ASP:C	2.61	0.43
1:C:289:LEU:HD12	1:C:289:LEU:O	2.18	0.43
2:D:42:TYR:CZ	2:D:46:ILE:HG21	2.54	0.43
2:F:138:VAL:O	2:F:142:CYS:SG	2.77	0.43
1:E:146:LEU:HD11	1:E:181:PHE:HE2	1.83	0.43
1:G:183:THR:CG2	1:G:283:ASP:O	2.66	0.43
1:G:325:ILE:O	1:G:328:SER:OG	2.24	0.43
2:F:42:TYR:CE1	2:F:46:ILE:HG21	2.53	0.43
1:A:173:ILE:O	1:A:177:MET:HG2	2.18	0.43
2:B:42:TYR:CE1	2:B:46:ILE:HG21	2.53	0.43
1:E:220:PHE:CE2	1:E:276:LEU:HD22	2.53	0.43
1:G:219:LEU:HA	1:G:222:VAL:HG12	2.01	0.43
1:G:289:LEU:O	1:G:289:LEU:HD12	2.19	0.43
1:C:166:SER:OG	1:C:169:ARG:HB2	2.18	0.43
2:B:138:VAL:O	2:B:142:CYS:SG	2.77	0.43
1:G:166:SER:OG	1:G:169:ARG:HB2	2.19	0.43
1:G:199:LEU:O	1:G:200:TRP:C	2.61	0.43
1:C:219:LEU:HA	1:C:222:VAL:HG12	2.00	0.43
2:B:147:ILE:HG22	2:B:148:TYR:N	2.34	0.43
1:C:199:LEU:O	1:C:200:TRP:C	2.61	0.42
1:C:153:VAL:O	1:C:153:VAL:CG1	2.67	0.42
1:C:340:VAL:O	1:C:340:VAL:HG23	2.18	0.42
2:H:42:TYR:CZ	2:H:46:ILE:HG21	2.54	0.42
1:A:91:LEU:HD21	1:A:142:PHE:CD1	2.53	0.42
2:B:69:ALA:O	2:B:114:TYR:OH	2.27	0.42
1:A:345:THR:O	1:A:345:THR:HG22	2.19	0.42
1:G:153:VAL:O	1:G:153:VAL:CG1	2.67	0.42
1:E:345:THR:HG22	1:E:345:THR:O	2.19	0.42
1:C:230:PHE:O	1:C:233:GLN:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:ASP:OD1	2:D:76:ASP:N	2.49	0.42
1:E:208:TYR:O	1:E:209:ARG:C	2.62	0.42
2:F:147:ILE:HG22	2:F:148:TYR:N	2.34	0.42
1:E:91:LEU:HD21	1:E:142:PHE:CD1	2.54	0.42
1:G:212:PRO:O	1:G:213:ASP:C	2.63	0.42
1:C:220:PHE:CE1	1:C:276:LEU:HD22	2.54	0.42
2:D:48:TYR:O	2:D:51:PHE:N	2.43	0.42
1:A:210:THR:O	1:A:210:THR:CG2	2.67	0.41
1:A:308:ALA:O	1:A:312:VAL:HG13	2.20	0.41
2:B:109:VAL:HG12	2:B:110:PRO:O	2.20	0.41
1:C:194:MET:HE2	1:C:202:PHE:H	1.85	0.41
2:F:109:VAL:HG12	2:F:110:PRO:O	2.20	0.41
2:H:101:PHE:HB2	2:H:128:TYR:O	2.20	0.41
2:B:20:ILE:O	2:B:20:ILE:CG2	2.69	0.41
2:B:68:TRP:CA	2:B:84:ILE:HD11	2.51	0.41
2:B:93:GLU:N	2:B:93:GLU:OE2	2.54	0.41
2:F:20:ILE:O	2:F:20:ILE:CG2	2.68	0.41
1:A:203:ASN:C	1:A:204:THR:HG23	2.46	0.41
1:C:208:TYR:HE1	1:C:274:MET:HE2	1.85	0.41
1:G:194:MET:HE2	1:G:202:PHE:H	1.86	0.41
1:A:141:ILE:O	1:A:144:THR:HG22	2.20	0.41
2:D:97:GLU:HB2	2:D:131:TYR:CD1	2.56	0.41
1:E:203:ASN:C	1:E:204:THR:HG23	2.46	0.41
1:G:230:PHE:O	1:G:233:GLN:HG3	2.20	0.41
1:C:240:LEU:O	1:C:242:LEU:HD12	2.21	0.41
1:E:366:LEU:O	1:E:369:LEU:N	2.53	0.41
2:B:47:ASN:OD1	2:B:47:ASN:O	2.38	0.41
2:D:101:PHE:HB2	2:D:128:TYR:O	2.20	0.41
1:G:220:PHE:HE2	1:G:272:THR:OG1	2.04	0.41
2:F:93:GLU:OE2	2:F:93:GLU:N	2.54	0.41
1:A:146:LEU:HD11	1:A:181:PHE:HE2	1.84	0.41
2:D:61:SER:O	2:D:62:GLY:C	2.64	0.41
1:E:141:ILE:O	1:E:144:THR:HG22	2.21	0.41
1:E:308:ALA:O	1:E:312:VAL:HG13	2.20	0.41
1:G:240:LEU:O	1:G:242:LEU:HD12	2.21	0.41
2:F:92:TYR:CE2	2:F:129:VAL:HG13	2.55	0.41
1:A:354:LEU:HB3	1:A:355:PRO:HD3	2.03	0.40
1:C:220:PHE:HE2	1:C:272:THR:OG1	2.04	0.40
1:E:354:LEU:HB3	1:E:355:PRO:HD3	2.03	0.40
1:A:98:TYR:OH	1:A:104:THR:HG23	2.21	0.40
1:A:199:LEU:HD21	1:A:277:PRO:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:47:ASN:OD1	2:F:47:ASN:O	2.38	0.40
2:H:76:ASP:N	2:H:76:ASP:OD1	2.49	0.40
1:A:208:TYR:O	1:A:209:ARG:C	2.62	0.40
1:C:88:LEU:HB2	1:C:145:PHE:CE1	2.56	0.40
1:E:199:LEU:HD21	1:E:277:PRO:CG	2.51	0.40
1:E:98:TYR:OH	1:E:104:THR:HG23	2.21	0.40
1:E:133:LEU:HD11	2:F:34:ILE:HG21	2.04	0.40
2:H:97:GLU:HB2	2:H:131:TYR:CD1	2.55	0.40
1:A:133:LEU:HD11	2:B:34:ILE:HG21	2.04	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	308/428 (72%)	291 (94%)	17 (6%)	0	100	100
1	C	319/428 (74%)	293 (92%)	26 (8%)	0	100	100
1	E	308/428 (72%)	291 (94%)	17 (6%)	0	100	100
1	G	319/428 (74%)	293 (92%)	26 (8%)	0	100	100
2	B	130/150 (87%)	118 (91%)	12 (9%)	0	100	100
2	D	133/150 (89%)	125 (94%)	8 (6%)	0	100	100
2	F	130/150 (87%)	118 (91%)	12 (9%)	0	100	100
2	H	133/150 (89%)	124 (93%)	9 (7%)	0	100	100
All	All	1780/2312 (77%)	1653 (93%)	127 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	266/391 (68%)	266 (100%)	0	100	100
1	C	280/391 (72%)	280 (100%)	0	100	100
1	E	266/391 (68%)	266 (100%)	0	100	100
1	G	280/391 (72%)	280 (100%)	0	100	100
2	B	119/135 (88%)	119 (100%)	0	100	100
2	D	122/135 (90%)	122 (100%)	0	100	100
2	F	119/135 (88%)	119 (100%)	0	100	100
2	H	122/135 (90%)	122 (100%)	0	100	100
All	All	1574/2104 (75%)	1574 (100%)	0	100	100

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

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	216	ASN
1	A	249	HIS
1	A	342	ASN
1	C	216	ASN
1	C	234	GLN
2	B	106	ASN
2	B	113	HIS
2	D	117	HIS
2	D	149	HIS
1	E	216	ASN
1	E	342	ASN
1	G	234	GLN
1	G	322	ASN
1	G	365	GLN
2	F	106	ASN
2	H	117	HIS
2	H	149	HIS

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.