Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Aug 22, 2017 – 07:06 AM EDT

PDB ID	:	5V7V
EMDB ID:	:	EMD-8642
Title	:	Cryo-EM structure of ERAD-associated E3 ubiquitin-protein ligase component HRD3
Authors	:	Mi, W.; Schoebel, S.; Stein, A.; Rapoport, T.A.; Liao, M.
Deposited on	:	unknown
Resolution	:	3.90 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824
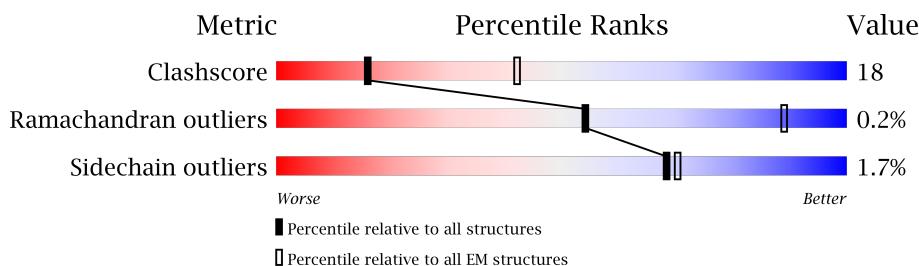
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY
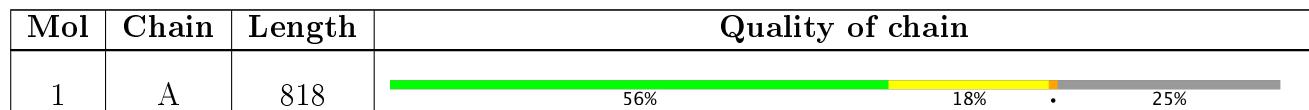
The reported resolution of this entry is 3.90 Å.

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	Percentile Ranks	Value
Clashscore		18
Ramachandran outliers		0.2%
Sidechain outliers		1.7%

Worse *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	818	56% 18% • 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	901	-	-	X	-
2	NAG	A	903	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10035 atoms, of which 4927 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 ERAD-associated E3 ubiquitin-protein ligase component HRD3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	613	9799	3192	4811	845	931	20	0	0

There are 51 discrepancies between the modelled and reference sequences:
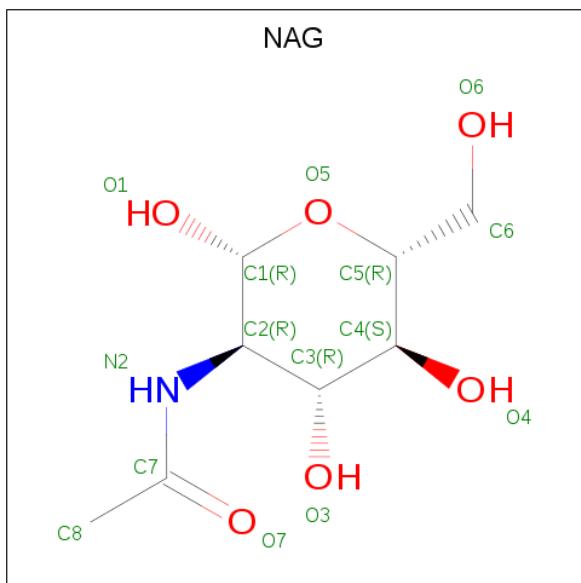
Chain	Residue	Modelled	Actual	Comment	Reference
A	768	GLY	-	expression tag	UNP Q05787
A	769	GLY	-	expression tag	UNP Q05787
A	770	GLY	-	expression tag	UNP Q05787
A	771	GLU	-	expression tag	UNP Q05787
A	772	ASN	-	expression tag	UNP Q05787
A	773	LEU	-	expression tag	UNP Q05787
A	774	TYR	-	expression tag	UNP Q05787
A	775	PHE	-	expression tag	UNP Q05787
A	776	GLN	-	expression tag	UNP Q05787
A	777	SER	-	expression tag	UNP Q05787
A	778	GLY	-	expression tag	UNP Q05787
A	779	GLY	-	expression tag	UNP Q05787
A	780	GLY	-	expression tag	UNP Q05787
A	781	MET	-	expression tag	UNP Q05787
A	782	ASP	-	expression tag	UNP Q05787
A	783	GLU	-	expression tag	UNP Q05787
A	784	LYS	-	expression tag	UNP Q05787
A	785	THR	-	expression tag	UNP Q05787
A	786	THR	-	expression tag	UNP Q05787
A	787	GLY	-	expression tag	UNP Q05787
A	788	TRP	-	expression tag	UNP Q05787
A	789	ARG	-	expression tag	UNP Q05787
A	790	GLY	-	expression tag	UNP Q05787
A	791	GLY	-	expression tag	UNP Q05787
A	792	HIS	-	expression tag	UNP Q05787
A	793	VAL	-	expression tag	UNP Q05787
A	794	VAL	-	expression tag	UNP Q05787
A	795	GLU	-	expression tag	UNP Q05787

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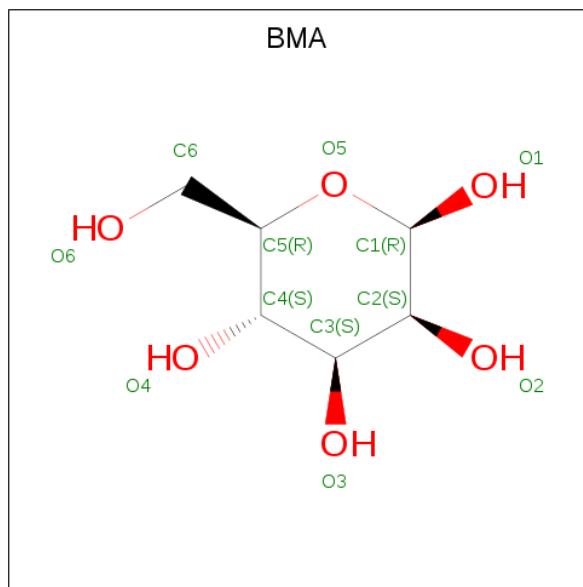
Chain	Residue	Modelled	Actual	Comment	Reference
A	796	GLY	-	expression tag	UNP Q05787
A	797	LEU	-	expression tag	UNP Q05787
A	798	ALA	-	expression tag	UNP Q05787
A	799	GLY	-	expression tag	UNP Q05787
A	800	GLU	-	expression tag	UNP Q05787
A	801	LEU	-	expression tag	UNP Q05787
A	802	GLU	-	expression tag	UNP Q05787
A	803	GLN	-	expression tag	UNP Q05787
A	804	LEU	-	expression tag	UNP Q05787
A	805	ARG	-	expression tag	UNP Q05787
A	806	ALA	-	expression tag	UNP Q05787
A	807	ARG	-	expression tag	UNP Q05787
A	808	LEU	-	expression tag	UNP Q05787
A	809	GLU	-	expression tag	UNP Q05787
A	810	HIS	-	expression tag	UNP Q05787
A	811	HIS	-	expression tag	UNP Q05787
A	812	PRO	-	expression tag	UNP Q05787
A	813	GLN	-	expression tag	UNP Q05787
A	814	GLY	-	expression tag	UNP Q05787
A	815	GLN	-	expression tag	UNP Q05787
A	816	ARG	-	expression tag	UNP Q05787
A	817	GLU	-	expression tag	UNP Q05787
A	818	PRO	-	expression tag	UNP Q05787

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	H	N	O	0
			192	56	94	7	35	
2	A	1	Total	C	H	N	O	0
			192	56	94	7	35	
2	A	1	Total	C	H	N	O	0
			192	56	94	7	35	
2	A	1	Total	C	H	N	O	0
			192	56	94	7	35	
2	A	1	Total	C	H	N	O	0
			192	56	94	7	35	
2	A	1	Total	C	H	N	O	0
			192	56	94	7	35	
2	A	1	Total	C	H	N	O	0
			192	56	94	7	35	

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).
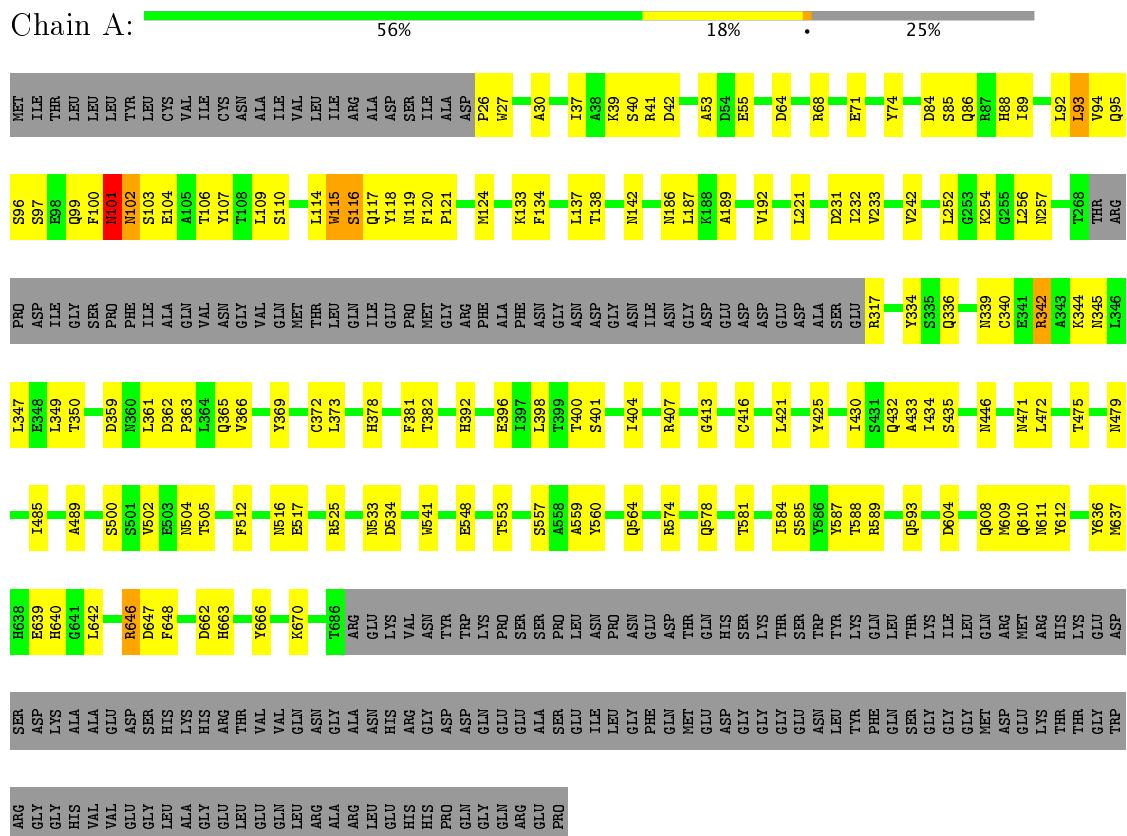
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	H	O	0
			44	12	22	10	
3	A	1	Total	C	H	O	0
			44	12	22	10	

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: ERAD-associated E3 ubiquitin-protein ligase component HRD3

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	204578	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 $(e^-/\text{Å}^2)$	82	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k 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: BMA, NAG

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	#$|Z|$ >2	RMSZ	#$|Z|$ >2
1	A	0.56	2/5116 (0.0%)	0.67	5/6934 (0.1%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	646	ARG	CZ-NH2	7.21	1.42	1.33
1	A	646	ARG	CZ-NH1	6.95	1.42	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	ASN	N-CA-CB	8.83	126.49	110.60
1	A	116	SER	N-CA-CB	8.53	123.29	110.50
1	A	115	TRP	N-CA-C	5.70	126.40	111.00
1	A	116	SER	N-CA-C	-5.61	95.84	111.00
1	A	101	ASN	N-CA-C	5.18	124.98	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	93	LEU	Mainchain

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	4988	4811	4828	175	0
2	A	98	94	87	22	0
3	A	22	22	20	3	0
All	All	5108	4927	4935	182	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 18.

All (182) 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:40:SER:HB2	1:A:117:GLN:NE2	1.23	1.44
1:A:27:TRP:CG	1:A:104:GLU:OE2	1.71	1.38
1:A:40:SER:CB	1:A:117:GLN:HE22	1.37	1.37
1:A:37:ILE:HD11	1:A:118:TYR:CE1	1.59	1.35
1:A:37:ILE:HD11	1:A:118:TYR:CD1	1.69	1.28
1:A:27:TRP:CD2	1:A:104:GLU:OE2	1.90	1.23
1:A:37:ILE:CD1	1:A:118:TYR:CD1	2.22	1.21
2:A:902:NAG:H62	2:A:903:NAG:O7	1.07	1.19
1:A:103:SER:HB2	1:A:137:LEU:CD1	1.75	1.16
1:A:612:TYR:HD2	1:A:642:LEU:HB3	1.14	1.10
1:A:107:TYR:HD2	2:A:905:NAG:O6	1.34	1.08
2:A:902:NAG:C6	2:A:903:NAG:O7	2.01	1.07
1:A:27:TRP:CD1	1:A:104:GLU:OE2	2.09	1.06
1:A:103:SER:HB2	1:A:137:LEU:HD12	1.37	1.02
1:A:103:SER:CB	1:A:137:LEU:CD1	2.38	1.02
1:A:612:TYR:CD2	1:A:642:LEU:HB3	1.94	1.02
1:A:37:ILE:CD1	1:A:118:TYR:HD1	1.65	1.00
1:A:40:SER:HB2	1:A:117:GLN:CD	1.81	1.00
2:A:902:NAG:H62	2:A:903:NAG:C7	1.91	0.99
1:A:106:THR:HA	1:A:109:LEU:CD2	1.93	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:HD13	1:A:118:TYR:HD1	1.24	0.98
1:A:639:GLU:HG2	1:A:646:ARG:NH2	1.81	0.94
1:A:103:SER:CB	1:A:137:LEU:HD13	1.96	0.94
1:A:86:GLN:HG2	1:A:120:PHE:HE1	1.30	0.94
1:A:37:ILE:HD13	1:A:118:TYR:CD1	1.99	0.94
1:A:86:GLN:HG2	1:A:120:PHE:CE1	2.05	0.92
1:A:42:ASP:OD2	1:A:525:ARG:NH1	2.03	0.92
1:A:40:SER:CB	1:A:117:GLN:NE2	2.10	0.90
1:A:37:ILE:HD11	1:A:118:TYR:HE1	1.34	0.88
1:A:106:THR:O	1:A:109:LEU:HD23	1.74	0.87
1:A:102:ASN:ND2	1:A:104:GLU:HG3	1.90	0.86
1:A:639:GLU:O	1:A:646:ARG:CZ	2.25	0.85
1:A:115:TRP:CZ2	1:A:541:TRP:HZ3	1.93	0.85
1:A:639:GLU:HG2	1:A:646:ARG:HH21	1.42	0.82
1:A:339:ASN:O	1:A:342:ARG:NH1	2.14	0.80
1:A:27:TRP:CE2	1:A:104:GLU:OE2	2.35	0.79
1:A:103:SER:HB3	1:A:137:LEU:HD13	1.65	0.78
1:A:612:TYR:HB3	1:A:637:MET:CE	2.14	0.78
1:A:639:GLU:O	1:A:646:ARG:NH1	2.18	0.76
1:A:106:THR:HA	1:A:109:LEU:HD21	1.68	0.76
1:A:612:TYR:HB3	1:A:637:MET:HE1	1.64	0.76
1:A:378:HIS:O	1:A:382:THR:OG1	2.04	0.74
1:A:107:TYR:CD2	2:A:905:NAG:O6	2.17	0.73
1:A:86:GLN:CG	1:A:120:PHE:CE1	2.70	0.73
1:A:475:THR:O	1:A:479:ASN:ND2	2.22	0.73
1:A:106:THR:CA	1:A:109:LEU:CD2	2.68	0.72
1:A:231:ASP:OD2	1:A:425:TYR:OH	2.07	0.72
1:A:26:PRO:HG2	1:A:96:SER:OG	1.89	0.72
1:A:500:SER:OG	1:A:504:ASN:ND2	2.24	0.71
1:A:93:LEU:HD23	1:A:94:VAL:H	1.55	0.70
1:A:560:TYR:O	1:A:564:GLN:NE2	2.25	0.70
1:A:432:GLN:O	1:A:435:SER:OG	2.07	0.69
1:A:102:ASN:ND2	1:A:104:GLU:CG	2.55	0.69
1:A:103:SER:HB3	1:A:137:LEU:CD1	2.21	0.69
1:A:142:ASN:OD1	2:A:905:NAG:N2	2.26	0.69
2:A:901:NAG:O3	2:A:901:NAG:O7	2.11	0.67
1:A:92:LEU:O	1:A:96:SER:N	2.28	0.66
1:A:502:VAL:O	1:A:505:THR:OG1	2.07	0.65
1:A:101:ASN:HB2	2:A:901:NAG:C1	2.26	0.65
1:A:40:SER:HA	1:A:117:GLN:OE1	1.97	0.65
1:A:107:TYR:HE2	2:A:905:NAG:H5	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:TRP:CZ2	1:A:541:TRP:CZ3	2.82	0.64
1:A:85:SER:O	1:A:88:HIS:N	2.32	0.63
1:A:347:LEU:O	1:A:350:THR:OG1	2.07	0.62
1:A:392:HIS:NE2	1:A:396:GLU:OE2	2.33	0.62
1:A:612:TYR:CB	1:A:637:MET:HE1	2.30	0.61
1:A:106:THR:HA	1:A:109:LEU:HD22	1.81	0.61
1:A:612:TYR:CG	1:A:637:MET:HE1	2.36	0.60
1:A:92:LEU:O	1:A:96:SER:HB3	2.01	0.60
1:A:39:LYS:CB	1:A:118:TYR:CD1	2.84	0.60
1:A:86:GLN:NE2	1:A:119:ASN:O	2.34	0.60
1:A:639:GLU:OE1	1:A:640:HIS:HB2	2.02	0.59
1:A:589:ARG:O	1:A:593:GLN:NE2	2.36	0.59
1:A:40:SER:HB3	1:A:117:GLN:HE22	1.56	0.59
1:A:85:SER:O	1:A:89:ILE:HD12	2.02	0.59
1:A:107:TYR:HB2	1:A:134:PHE:CD1	2.38	0.58
1:A:472:LEU:O	1:A:475:THR:OG1	2.13	0.58
1:A:662:ASP:OD1	1:A:663:HIS:N	2.36	0.58
1:A:400:THR:O	1:A:404:ILE:HD12	2.04	0.58
1:A:106:THR:C	1:A:109:LEU:HD23	2.25	0.57
1:A:578:GLN:O	1:A:581:THR:OG1	2.12	0.57
1:A:107:TYR:CE2	2:A:905:NAG:H5	2.40	0.56
1:A:92:LEU:HA	1:A:95:GLN:HB3	1.87	0.56
1:A:40:SER:HB2	1:A:117:GLN:OE1	2.05	0.56
1:A:110:SER:O	1:A:114:LEU:HB2	2.05	0.56
1:A:40:SER:CB	1:A:117:GLN:OE1	2.54	0.55
1:A:114:LEU:O	1:A:114:LEU:HD23	2.07	0.55
1:A:533:ASN:OD1	1:A:534:ASP:N	2.40	0.55
1:A:647:ASP:OD1	1:A:648:PHE:N	2.40	0.55
1:A:666:TYR:O	1:A:670:LYS:NZ	2.40	0.55
1:A:516:ASN:OD1	1:A:517:GLU:N	2.39	0.54
1:A:137:LEU:O	1:A:138:THR:OG1	2.26	0.54
1:A:86:GLN:HG3	1:A:120:PHE:CZ	2.43	0.54
1:A:96:SER:O	1:A:100:PHE:N	2.27	0.54
1:A:102:ASN:CG	1:A:104:GLU:HG3	2.29	0.54
1:A:26:PRO:HB3	1:A:96:SER:CB	2.38	0.53
1:A:553:THR:O	1:A:557:SER:OG	2.16	0.53
1:A:26:PRO:HB3	1:A:96:SER:HB2	1.90	0.53
1:A:40:SER:CB	1:A:117:GLN:CD	2.65	0.53
1:A:40:SER:CA	1:A:117:GLN:OE1	2.56	0.53
1:A:612:TYR:CD2	1:A:642:LEU:CB	2.82	0.53
1:A:359:ASP:H	1:A:361:LEU:HD23	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:903:NAG:O3	3:A:904:BMA:C1	2.57	0.52
1:A:642:LEU:C	1:A:642:LEU:HD13	2.30	0.52
1:A:133:LYS:NZ	2:A:901:NAG:H82	2.26	0.51
1:A:242:VAL:HG11	1:A:334:TYR:HE1	1.74	0.51
1:A:97:SER:O	1:A:100:PHE:O	2.28	0.51
1:A:106:THR:O	1:A:109:LEU:CD2	2.55	0.51
1:A:92:LEU:H	1:A:92:LEU:HD23	1.75	0.51
1:A:430:ILE:O	1:A:434:ILE:HD12	2.10	0.51
1:A:102:ASN:HD21	1:A:104:GLU:CG	2.23	0.50
1:A:252:LEU:O	1:A:257:ASN:ND2	2.28	0.50
1:A:39:LYS:CB	1:A:118:TYR:HA	2.42	0.50
1:A:26:PRO:CB	1:A:96:SER:CB	2.89	0.50
1:A:256:LEU:H	1:A:256:LEU:HD23	1.77	0.50
1:A:26:PRO:CG	1:A:96:SER:OG	2.58	0.50
1:A:559:ALA:HB1	1:A:587:TYR:CE2	2.47	0.50
1:A:504:ASN:OD1	1:A:505:THR:N	2.45	0.49
1:A:340:CYS:O	1:A:344:LYS:N	2.38	0.49
1:A:86:GLN:CG	1:A:120:PHE:CZ	2.96	0.49
1:A:232:ILE:CD1	1:A:233:VAL:HG12	2.43	0.49
1:A:115:TRP:CH2	1:A:541:TRP:HZ3	2.31	0.49
1:A:27:TRP:CE2	1:A:104:GLU:CD	2.86	0.49
1:A:53:ALA:O	1:A:55:GLU:HG3	2.12	0.49
1:A:584:ILE:O	1:A:588:THR:HG23	2.13	0.49
2:A:903:NAG:O3	3:A:904:BMA:H2	2.12	0.49
1:A:92:LEU:O	1:A:96:SER:CB	2.60	0.49
1:A:39:LYS:CB	1:A:118:TYR:HD1	2.27	0.48
1:A:612:TYR:CD2	1:A:637:MET:HE3	2.47	0.48
1:A:93:LEU:CD2	1:A:94:VAL:HG23	2.44	0.48
1:A:84:ASP:OD1	1:A:85:SER:N	2.47	0.48
1:A:133:LYS:NZ	2:A:901:NAG:C8	2.77	0.48
1:A:101:ASN:CB	2:A:901:NAG:C1	2.92	0.48
1:A:133:LYS:HZ2	2:A:901:NAG:H82	1.78	0.48
1:A:639:GLU:O	1:A:646:ARG:NH2	2.46	0.47
1:A:27:TRP:NE1	1:A:104:GLU:OE2	2.44	0.47
1:A:398:LEU:O	1:A:401:SER:OG	2.07	0.47
1:A:101:ASN:HB2	2:A:901:NAG:O5	2.13	0.47
1:A:610:GLN:O	1:A:611:ASN:HB2	2.15	0.47
1:A:585:SER:O	1:A:588:THR:OG1	2.32	0.47
1:A:362:ASP:O	1:A:365:GLN:N	2.43	0.46
1:A:604:ASP:O	1:A:608:GLN:NE2	2.46	0.46
1:A:413:GLY:O	1:A:416:CYS:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LEU:HD21	1:A:94:VAL:HG23	1.98	0.46
1:A:64:ASP:OD1	1:A:574:ARG:N	2.47	0.45
1:A:404:ILE:O	1:A:407:ARG:N	2.47	0.45
1:A:363:PRO:HA	1:A:366:VAL:HG22	1.98	0.45
1:A:74:TYR:CE1	1:A:121:PRO:HG2	2.52	0.45
1:A:345:ASN:O	1:A:349:LEU:HD13	2.16	0.44
1:A:186:ASN:OD1	1:A:187:LEU:N	2.50	0.44
1:A:242:VAL:HG11	1:A:334:TYR:CE1	2.52	0.44
1:A:27:TRP:O	1:A:30:ALA:N	2.49	0.44
1:A:71:GLU:OE2	2:A:903:NAG:O6	2.25	0.44
1:A:381:PHE:CZ	1:A:421:LEU:HD12	2.53	0.44
1:A:107:TYR:HD2	2:A:905:NAG:HO6	0.62	0.43
1:A:232:ILE:HD12	1:A:233:VAL:HG12	2.01	0.43
1:A:124:MET:SD	1:A:124:MET:N	2.92	0.43
1:A:485:ILE:HG21	1:A:512:PHE:HB2	2.01	0.43
1:A:101:ASN:CG	2:A:901:NAG:C1	2.87	0.43
1:A:107:TYR:O	1:A:107:TYR:CD1	2.71	0.42
1:A:192:VAL:HG23	1:A:548:GLU:O	2.18	0.42
1:A:612:TYR:CG	1:A:637:MET:CE	3.02	0.42
1:A:40:SER:CA	1:A:117:GLN:NE2	2.81	0.42
1:A:434:ILE:H	1:A:434:ILE:HD12	1.85	0.42
1:A:106:THR:CA	1:A:109:LEU:HD23	2.49	0.42
1:A:221:LEU:HD13	1:A:516:ASN:ND2	2.35	0.42
1:A:26:PRO:CB	1:A:96:SER:OG	2.68	0.42
1:A:636:TYR:C	1:A:636:TYR:CD1	2.93	0.41
1:A:99:GLN:HA	1:A:99:GLN:HE21	1.85	0.41
1:A:430:ILE:O	1:A:433:ALA:HB3	2.20	0.41
1:A:99:GLN:NE2	1:A:99:GLN:HA	2.35	0.41
1:A:369:TYR:O	1:A:373:LEU:HD23	2.20	0.41
1:A:93:LEU:CG	1:A:94:VAL:N	2.84	0.41
1:A:336:GLN:N	1:A:336:GLN:OE1	2.54	0.41
1:A:93:LEU:CD2	1:A:94:VAL:H	2.29	0.41
2:A:903:NAG:O3	3:A:904:BMA:C2	2.69	0.41
1:A:639:GLU:CG	1:A:646:ARG:NH2	2.68	0.40
1:A:93:LEU:HG	1:A:94:VAL:N	2.36	0.40
1:A:432:GLN:OE1	2:A:908:NAG:H81	2.21	0.40
1:A:485:ILE:O	1:A:489:ALA:N	2.54	0.40
1:A:115:TRP:O	1:A:116:SER:C	2.60	0.40
1:A:189:ALA:O	1:A:192:VAL:HG12	2.22	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	609/818 (74%)	540 (89%)	68 (11%)	1 (0%)	51	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	ASN

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	529/703 (75%)	520 (98%)	9 (2%)	66	86

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	68	ARG
1	A	254	LYS
1	A	317	ARG
1	A	342	ARG
1	A	372	CYS
1	A	446	ASN
1	A	471	ASN
1	A	609	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	102	ASN
1	A	355	GLN
1	A	424	GLN
1	A	479	ASN
1	A	593	GLN
1	A	645	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 carbohydrates in this entry.

5.6   Ligand geometry (i)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	NAG	A	901	-	14,14,15	0.58	0	15,19,21	1.45	2 (13%)
2	NAG	A	902	1,2	14,14,15	0.52	0	15,19,21	0.51	0
2	NAG	A	903	3,2	14,14,15	0.41	0	15,19,21	1.17	2 (13%)
3	BMA	A	904	2	11,11,12	0.41	0	13,15,17	1.14	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	NAG	A	905	1,2	14,14,15	0.48	0	15,19,21	0.50	0
2	NAG	A	906	3,2	14,14,15	0.71	0	15,19,21	1.31	2 (13%)
3	BMA	A	907	2	11,11,12	0.33	0	13,15,17	0.85	1 (7%)
2	NAG	A	908	1	14,14,15	0.29	0	15,19,21	0.64	0
2	NAG	A	909	1	14,14,15	0.41	0	15,19,21	0.87	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	901	-	-	0/6/23/26	0/1/1/1
2	NAG	A	902	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	903	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	904	2	-	0/2/19/22	0/1/1/1
2	NAG	A	905	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	906	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	907	2	-	0/2/19/22	0/1/1/1
2	NAG	A	908	1	-	0/6/23/26	0/1/1/1
2	NAG	A	909	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	904	BMA	C1-O5-C5	-3.33	107.58	112.17
2	A	906	NAG	O7-C7-N2	-2.16	117.77	121.92
2	A	903	NAG	C2-N2-C7	-2.02	120.00	122.94
2	A	903	NAG	C8-C7-N2	2.15	119.99	116.11
3	A	907	BMA	C1-O5-C5	2.25	115.27	112.17
2	A	901	NAG	C1-C2-N2	2.62	114.96	110.49
2	A	909	NAG	C1-O5-C5	2.91	116.17	112.17
2	A	901	NAG	C8-C7-N2	3.15	121.79	116.11
2	A	906	NAG	C8-C7-N2	3.23	121.94	116.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	NAG	8	0
2	A	902	NAG	3	0
2	A	903	NAG	7	0
3	A	904	BMA	3	0
2	A	905	NAG	6	0
2	A	908	NAG	1	0

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.