WORLDWIDE PDB PROTEIN DATA BANK

Preliminary Full wwPDB EM Validation Report ⓘ

Nov 28, 2025 – 12:12 PM JST

Deposition ID : D_1300066582

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the wwPDB Deposition System
during initial deposition but before annotation of the structure.

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:

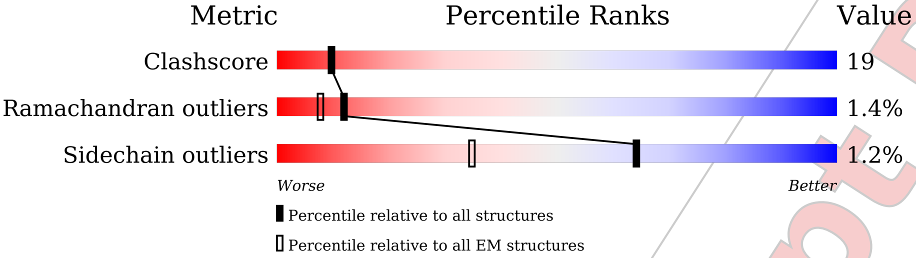
EMDB validation analysis	:	0.0.1.dev129
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

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	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	210	 55% 41% •
2	C	118	 69% 19% 8% •
3	B	111	 83% 17%
4	D	107	 88% 12%
5	E	115	 84% 15% •

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 5167 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	210	1621	1025	268	317	11	0	0

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	118	918	579	149	185	5	0	0

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	111	844	526	143	169	6	0	0

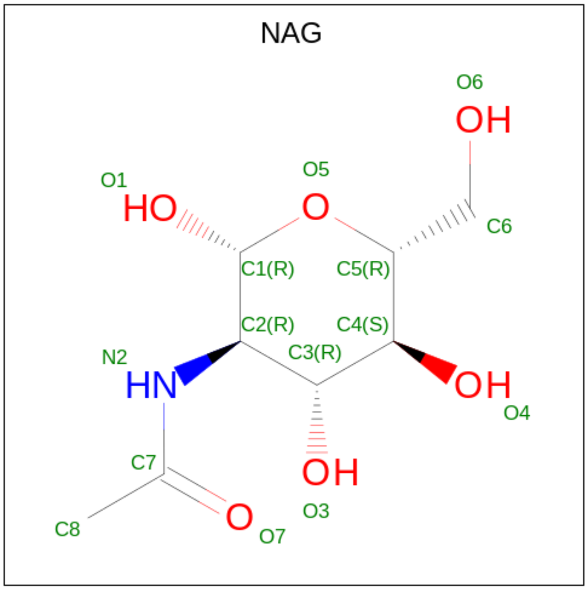
- Molecule 4 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	107	836	527	145	160	4	0	0

- Molecule 5 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	115	892	558	144	186	4	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



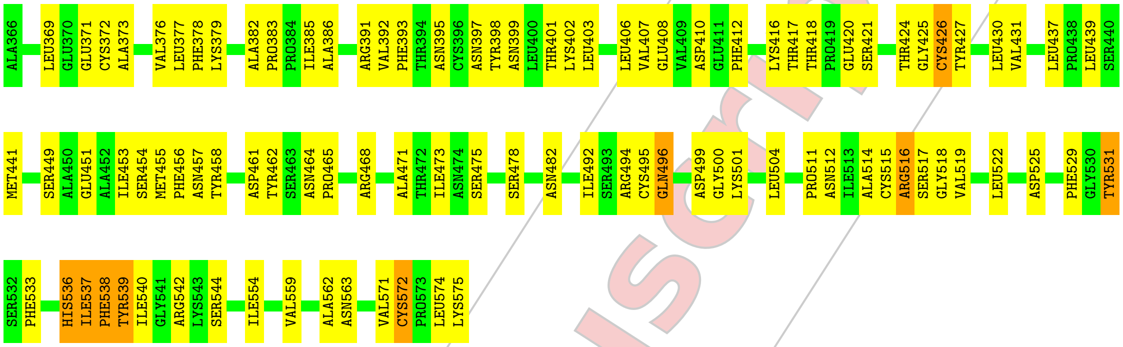
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C N O 14 8 1 5	0
6	A	1	Total C N O 14 8 1 5	0
6	A	1	Total C N O 14 8 1 5	0
6	A	1	Total C N O 14 8 1 5	0

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:

Chain A:



- Molecule 2:

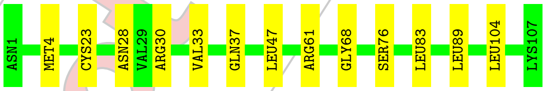
Chain C:

- Molecule 3:

Chain B:

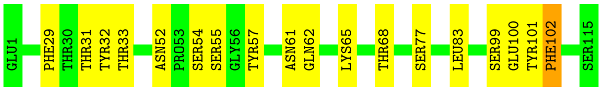
- Molecule 4:

Chain D:



- Molecule 5:

Chain E:


GLU1
PHE29
THR30
THR31
TYR32
THR33
ASN52
PRO53
SER54
SER55
GLY56
TYR57
ASN61
GLN62
LYS65
THR68
SER77
LEU83
SER99
GLU100
TYR101
PHE102
SER115

4 Experimental information (i)

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	Not provided	
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.38	0/1657	0.82	7/2256 (0.3%)
2	C	0.61	0/942	1.21	16/1275 (1.3%)
3	B	0.48	1/863 (0.1%)	0.83	1/1165 (0.1%)
4	D	0.40	0/855	0.78	0/1158
5	E	0.38	0/913	0.76	1/1241 (0.1%)
All	All	0.45	1/5230 (0.0%)	0.89	25/7095 (0.4%)

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
2	C	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	35	SER	CA-CB	-5.94	1.44	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	98	ARG	CB-CA-C	-10.91	90.85	109.72
2	C	100	ASN	N-CA-C	-10.82	99.38	112.59
2	C	99	ASP	CB-CA-C	-9.67	91.48	113.33
1	A	536	HIS	N-CA-CB	-8.61	97.38	110.39
1	A	536	HIS	CA-CB-CG	-8.28	105.52	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	572	CYS	CA-CB-SG	7.67	132.04	114.40
1	A	531	TYR	CB-CA-C	-7.54	101.02	111.95
3	B	30	ASP	CB-CA-C	-7.05	99.80	111.51
2	C	108	TYR	CB-CA-C	-6.77	100.40	110.62
2	C	101	TYR	CB-CA-C	-6.64	97.20	110.42
2	C	99	ASP	N-CA-CB	6.61	119.97	110.45
1	A	426	CYS	CA-CB-SG	6.54	129.44	114.40
2	C	104	TYR	CB-CA-C	6.29	122.37	111.86
1	A	496	GLN	CB-CA-C	-6.17	99.69	109.80
2	C	105	TYR	CA-CB-CG	5.90	124.53	113.90
2	C	100	ASN	CB-CA-C	5.90	120.52	111.02
1	A	539	TYR	CA-C-O	-5.80	113.98	120.54
5	E	61	ASN	N-CA-C	-5.74	101.36	109.96
2	C	108	TYR	CA-C-O	-5.37	114.54	120.33
2	C	98	ARG	CA-C-O	-5.23	114.68	120.38
2	C	102	GLY	N-CA-C	-5.05	101.21	113.18
2	C	65	LYS	CA-C-N	-5.04	115.10	122.46
2	C	65	LYS	C-N-CA	-5.04	115.10	122.46
2	C	59	ASN	CA-C-N	-5.02	116.07	123.00
2	C	59	ASN	C-N-CA	-5.02	116.07	123.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	516	ARG	Sidechain
2	C	98	ARG	Sidechain

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	1621	0	1562	146	0
2	C	918	0	849	51	0
3	B	844	0	805	20	0
4	D	836	0	816	7	0
5	E	892	0	834	54	0

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Mol	**Chain**	**Non-H**	**H(model)**	**H(added)**	**Clashes**	**Symm-Clashes**
6	A	56	0	52	2	0
All	All	5167	0	4918	196	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 19.

All (196) 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:420:GLU:OE2	5:E:100:GLU:CG	1.66	1.42
1:A:424:THR:HG23	5:E:52:ASN:ND2	1.31	1.39
1:A:424:THR:CG2	5:E:52:ASN:HD22	1.38	1.35
1:A:420:GLU:OE2	5:E:100:GLU:HG2	1.09	1.26
1:A:575:LYS:HE3	5:E:57:TYR:HE1	1.00	1.16
1:A:499:ASP:OD2	2:C:52:TYR:CZ	1.98	1.16
1:A:420:GLU:OE2	5:E:100:GLU:CB	1.96	1.13
1:A:575:LYS:HE3	5:E:57:TYR:CE1	1.86	1.10
1:A:424:THR:O	5:E:55:SER:OG	1.73	1.07
1:A:420:GLU:CD	5:E:100:GLU:CG	2.27	1.04
1:A:499:ASP:OD2	2:C:52:TYR:OH	1.76	1.04
1:A:575:LYS:CE	5:E:57:TYR:HE1	1.72	1.03
1:A:512:ASN:HD21	2:C:102:GLY:HA3	1.25	1.01
1:A:424:THR:HG23	5:E:52:ASN:HD22	0.85	0.98
1:A:424:THR:HG23	5:E:52:ASN:CG	1.89	0.95
1:A:575:LYS:CE	5:E:57:TYR:CE1	2.48	0.94
1:A:424:THR:CG2	5:E:52:ASN:HB2	2.00	0.91
2:C:99:ASP:HB2	2:C:101:TYR:H	1.38	0.89
1:A:512:ASN:ND2	2:C:102:GLY:HA3	1.87	0.87
1:A:501:LYS:HD2	2:C:28:THR:HG21	1.56	0.87
1:A:424:THR:OG1	5:E:52:ASN:HB2	1.75	0.86
1:A:424:THR:CG2	5:E:52:ASN:ND2	2.13	0.84
1:A:420:GLU:CD	5:E:100:GLU:HG2	1.95	0.83
2:C:61:ASN:HB2	3:B:99:PRO:HB3	1.61	0.83
1:A:499:ASP:OD2	2:C:52:TYR:CE2	2.31	0.82
1:A:575:LYS:NZ	5:E:57:TYR:CE1	2.47	0.82
1:A:575:LYS:NZ	5:E:57:TYR:CD1	2.47	0.82
1:A:420:GLU:CD	5:E:100:GLU:HB3	2.04	0.81
2:C:103:ASN:HD22	2:C:105:TYR:HE2	1.27	0.80
1:A:533:PHE:CZ	3:B:36:PHE:HZ	2.00	0.79
1:A:420:GLU:CD	5:E:100:GLU:CB	2.55	0.79
1:A:418:THR:HG23	5:E:32:TYR:CE1	2.19	0.78

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:A:464:ASN:HD21	1:A:563:ASN:HA	1.49	0.77
1:A:386:ALA:HA	1:A:457:ASN:HD21	1.51	0.76
1:A:424:THR:HG23	5:E:52:ASN:CB	2.14	0.76
1:A:420:GLU:OE2	5:E:100:GLU:HB3	1.85	0.75
2:C:33:ASN:HB2	2:C:99:ASP:OD1	1.87	0.75
2:C:105:TYR:CE1	2:C:107:ASP:HB3	2.22	0.74
1:A:499:ASP:CG	2:C:52:TYR:CE2	2.66	0.74
1:A:420:GLU:OE2	5:E:100:GLU:N	2.21	0.74
1:A:371:GLU:HA	1:A:397:ASN:HB2	1.70	0.73
1:A:425:GLY:CA	5:E:52:ASN:OD1	2.38	0.71
1:A:425:GLY:HA2	5:E:52:ASN:OD1	1.91	0.70
1:A:424:THR:OG1	5:E:52:ASN:CB	2.40	0.69
2:C:105:TYR:CD1	2:C:107:ASP:HB3	2.27	0.69
1:A:499:ASP:CG	2:C:52:TYR:OH	2.34	0.69
1:A:437:LEU:HD11	1:A:441:MET:HB2	1.75	0.68
3:B:4:MET:CE	3:B:37:MET:HE1	2.24	0.68
1:A:537:ILE:O	1:A:538:PHE:C	2.37	0.67
1:A:424:THR:HG23	5:E:52:ASN:HB2	1.71	0.67
1:A:499:ASP:OD2	2:C:30:THR:O	2.13	0.67
2:C:105:TYR:O	2:C:107:ASP:N	2.29	0.66
1:A:499:ASP:CG	2:C:54:GLY:HA3	2.19	0.66
1:A:501:LYS:HD2	2:C:28:THR:CG2	2.24	0.66
3:B:29:VAL:HA	3:B:96:LYS:HD2	1.78	0.66
2:C:103:ASN:O	2:C:104:TYR:CG	2.49	0.65
1:A:418:THR:HG23	5:E:32:TYR:CD1	2.31	0.65
3:B:31:ASN:HB2	3:B:96:LYS:HE3	1.79	0.65
2:C:62:GLN:O	2:C:63:LYS:C	2.40	0.65
1:A:424:THR:CB	5:E:52:ASN:HB2	2.27	0.64
1:A:449:SER:O	1:A:454:SER:OG	2.16	0.64
1:A:499:ASP:OD1	2:C:52:TYR:HE2	1.81	0.63
2:C:62:GLN:O	2:C:65:LYS:N	2.16	0.63
1:A:473:ILE:N	1:A:554:ILE:O	2.29	0.62
1:A:512:ASN:CG	2:C:102:GLY:HA3	2.24	0.62
1:A:496:GLN:HE21	1:A:500:GLY:HA2	1.63	0.62
1:A:499:ASP:CG	2:C:52:TYR:CZ	2.77	0.62
1:A:398:TYR:HE1	1:A:572:CYS:HA	1.64	0.61
1:A:496:GLN:O	1:A:539:TYR:HB2	1.99	0.61
1:A:499:ASP:OD1	2:C:54:GLY:HA3	2.01	0.61
1:A:418:THR:HG23	5:E:32:TYR:HE1	1.65	0.60
1:A:455:MET:HG2	1:A:456:PHE:HD1	1.66	0.60
1:A:496:GLN:NE2	1:A:500:GLY:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:VAL:HA	1:A:379:LYS:HZ2	1.67	0.60
2:C:2:PHE:HB2	2:C:26:GLY:HA3	1.83	0.59
1:A:425:GLY:CA	5:E:54:SER:HB3	2.33	0.58
4:D:61:ARG:HB2	4:D:76:SER:O	2.03	0.58
1:A:499:ASP:OD1	2:C:52:TYR:CE2	2.56	0.58
2:C:100:ASN:O	2:C:102:GLY:N	2.37	0.57
1:A:525:ASP:OD1	1:A:542:ARG:NH1	2.37	0.57
3:B:4:MET:HE1	3:B:37:MET:HE1	1.84	0.57
1:A:392:VAL:HG13	1:A:431:VAL:HG12	1.87	0.57
1:A:533:PHE:HZ	3:B:36:PHE:HZ	1.50	0.57
1:A:420:GLU:OE2	5:E:100:GLU:CA	2.53	0.56
1:A:494:ARG:O	1:A:540:ILE:HA	2.05	0.56
2:C:100:ASN:O	2:C:101:TYR:C	2.49	0.56
5:E:68:THR:HG22	5:E:83:LEU:HD23	1.88	0.55
1:A:378:PHE:HE2	1:A:406:LEU:HD12	1.73	0.54
1:A:515:CYS:SG	1:A:540:ILE:HG22	2.47	0.54
2:C:105:TYR:CD1	3:B:50:LEU:HD22	2.42	0.54
1:A:369:LEU:O	1:A:397:ASN:ND2	2.40	0.54
1:A:575:LYS:CE	5:E:57:TYR:CD1	2.88	0.54
2:C:2:PHE:CB	2:C:26:GLY:HA3	2.38	0.54
1:A:398:TYR:CE1	1:A:572:CYS:HA	2.42	0.54
1:A:426:CYS:HB3	5:E:55:SER:HB3	1.90	0.54
1:A:525:ASP:CG	1:A:544:SER:HG	2.16	0.53
2:C:35:HIS:HE2	2:C:99:ASP:CG	2.17	0.53
2:C:105:TYR:CD1	3:B:50:LEU:CD2	2.91	0.53
1:A:516:ARG:O	1:A:517:SER:C	2.52	0.53
3:B:58:GLN:HE22	3:B:64:ALA:HA	1.74	0.53
1:A:475:SER:H	6:A:578:NAG:H82	1.74	0.52
4:D:37:GLN:HB2	4:D:47:LEU:HD11	1.92	0.52
4:D:4:MET:HE3	4:D:23:CYS:SG	2.50	0.52
1:A:399:ASN:HB2	1:A:402:LYS:HZ1	1.73	0.52
1:A:533:PHE:CZ	3:B:36:PHE:CZ	2.89	0.52
1:A:424:THR:CB	5:E:52:ASN:HD22	1.97	0.52
4:D:83:LEU:HD12	4:D:104:LEU:O	2.10	0.51
1:A:425:GLY:HA3	5:E:54:SER:HB3	1.93	0.51
1:A:533:PHE:HE1	3:B:32:TYR:HB2	1.75	0.51
1:A:401:THR:HB	6:A:577:NAG:H5	1.92	0.51
1:A:376:VAL:HA	1:A:379:LYS:NZ	2.25	0.51
1:A:417:THR:OG1	1:A:418:THR:N	2.43	0.50
1:A:575:LYS:NZ	5:E:57:TYR:HD1	2.06	0.50
3:B:31:ASN:O	3:B:32:TYR:HB2	2.12	0.50

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:A:512:ASN:OD1	2:C:102:GLY:HA3	2.12	0.49
1:A:496:GLN:HE21	1:A:500:GLY:CA	2.25	0.49
1:A:516:ARG:O	1:A:519:VAL:HG12	2.13	0.49
1:A:536:HIS:HB3	2:C:101:TYR:OH	2.12	0.49
1:A:538:PHE:CZ	2:C:102:GLY:HA2	2.47	0.49
1:A:525:ASP:OD2	1:A:544:SER:OG	2.25	0.49
1:A:403:LEU:O	1:A:407:VAL:HG22	2.12	0.49
2:C:60:TYR:O	2:C:61:ASN:C	2.56	0.49
1:A:424:THR:HG1	5:E:52:ASN:HB2	1.74	0.48
1:A:517:SER:O	1:A:518:GLY:C	2.56	0.48
1:A:455:MET:HG2	1:A:456:PHE:CD1	2.47	0.48
2:C:23:LYS:HE3	2:C:76:SER:O	2.13	0.48
2:C:105:TYR:HE1	2:C:107:ASP:HB3	1.78	0.48
1:A:499:ASP:OD2	2:C:54:GLY:HA3	2.13	0.48
1:A:512:ASN:O	1:A:516:ARG:HG3	2.14	0.48
1:A:522:LEU:HD22	1:A:529:PHE:CE1	2.48	0.48
1:A:531:TYR:O	1:A:531:TYR:CG	2.64	0.47
1:A:372:CYS:HB3	1:A:393:PHE:CE1	2.49	0.47
1:A:408:GLU:OE1	1:A:410:ASP:HB2	2.14	0.47
1:A:385:ILE:HD12	1:A:437:LEU:HD22	1.97	0.47
1:A:512:ASN:HD21	2:C:102:GLY:CA	2.12	0.47
1:A:529:PHE:C	1:A:529:PHE:CD2	2.93	0.47
1:A:439:LEU:HD12	1:A:439:LEU:H	1.80	0.47
1:A:456:PHE:HE2	1:A:495:CYS:H	1.62	0.47
2:C:104:TYR:HB3	3:B:95:SER:OG	2.15	0.46
1:A:418:THR:HG21	5:E:99:SER:HB2	1.97	0.46
1:A:372:CYS:HB3	1:A:393:PHE:HE1	1.80	0.46
2:C:62:GLN:O	2:C:64:PHE:N	2.48	0.46
1:A:420:GLU:CG	5:E:100:GLU:HB3	2.45	0.46
5:E:62:GLN:OE1	5:E:65:LYS:HD3	2.16	0.46
1:A:430:LEU:HD13	1:A:562:ALA:HA	1.97	0.45
2:C:103:ASN:O	2:C:104:TYR:CD2	2.69	0.45
3:B:82:MET:HE1	3:B:108:LEU:HG	1.97	0.45
1:A:529:PHE:C	1:A:529:PHE:HD2	2.24	0.45
1:A:427:TYR:CD2	1:A:562:ALA:HB1	2.51	0.45
1:A:424:THR:CG2	5:E:52:ASN:CB	2.74	0.45
1:A:424:THR:O	5:E:55:SER:CB	2.62	0.45
1:A:496:GLN:HE21	1:A:500:GLY:C	2.25	0.45
1:A:421:SER:OG	5:E:32:TYR:HA	2.17	0.45
1:A:392:VAL:HG22	1:A:431:VAL:HG12	1.99	0.44
1:A:451:GLU:O	1:A:455:MET:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ASN:O	1:A:571:VAL:HG22	2.18	0.44
1:A:397:ASN:CG	1:A:574:LEU:HD21	2.43	0.44
1:A:454:SER:HA	1:A:458:TYR:O	2.17	0.44
1:A:426:CYS:HB2	1:A:572:CYS:HB2	1.08	0.44
1:A:424:THR:OG1	5:E:57:TYR:HB3	2.17	0.44
3:B:4:MET:HE1	3:B:37:MET:CE	2.47	0.44
1:A:478:SER:O	1:A:482:ASN:N	2.51	0.43
1:A:377:LEU:HD12	1:A:403:LEU:HD13	1.99	0.43
1:A:538:PHE:HE2	2:C:101:TYR:CD2	2.35	0.43
1:A:464:ASN:ND2	1:A:563:ASN:OD1	2.52	0.43
1:A:464:ASN:ND2	1:A:563:ASN:HA	2.24	0.43
1:A:533:PHE:CE1	3:B:32:TYR:HB2	2.53	0.43
3:B:41:GLN:HB2	3:B:51:LEU:HD11	2.00	0.43
2:C:26:GLY:O	2:C:27:TYR:HB3	2.19	0.43
1:A:492:ILE:HD13	1:A:515:CYS:HB3	2.01	0.42
5:E:68:THR:HG22	5:E:83:LEU:CD2	2.48	0.42
1:A:372:CYS:SG	1:A:397:ASN:N	2.93	0.42
1:A:461:ASP:OD1	1:A:461:ASP:C	2.62	0.42
2:C:47:TRP:CZ2	2:C:49:GLY:HA2	2.55	0.42
5:E:29:PHE:CD2	5:E:77:SER:HA	2.55	0.42
4:D:28:ASN:ND2	4:D:30:ARG:NH1	2.68	0.42
4:D:33:VAL:HA	4:D:89:LEU:O	2.20	0.42
2:C:4:LEU:HD13	2:C:22:CYS:SG	2.60	0.41
5:E:102:PHE:N	5:E:102:PHE:CD2	2.89	0.41
1:A:391:ARG:HG3	1:A:393:PHE:HE2	1.85	0.41
1:A:417:THR:HA	5:E:31:THR:HG22	2.03	0.41
4:D:28:ASN:OD1	4:D:68:GLY:HA2	2.21	0.41
1:A:453:ILE:HD13	1:A:453:ILE:HA	1.85	0.41
1:A:533:PHE:HE1	3:B:32:TYR:CB	2.33	0.41
1:A:412:PHE:HE1	5:E:101:TYR:OH	2.03	0.41
2:C:105:TYR:HD1	3:B:50:LEU:HD22	1.85	0.41
1:A:461:ASP:OD1	1:A:462:TYR:N	2.54	0.41
1:A:382:ALA:HA	1:A:383:PRO:HD3	1.96	0.40
1:A:424:THR:HG21	5:E:33:THR:HG22	2.01	0.40
1:A:468:ARG:HB2	1:A:559:VAL:HG22	2.02	0.40
1:A:511:PRO:HB2	1:A:516:ARG:HG2	2.03	0.40
1:A:407:VAL:HB	1:A:471:ALA:HB1	2.03	0.40
1:A:373:ALA:O	1:A:376:VAL:N	2.48	0.40
2:C:39:GLN:HB2	2:C:45:LEU:HD23	2.03	0.40
1:A:416:LYS:HB3	1:A:465:PRO:HA	2.02	0.40
2:C:105:TYR:CD1	2:C:105:TYR:O	2.74	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	208/210 (99%)	178 (86%)	27 (13%)	3 (1%)	9	9
2	C	116/118 (98%)	104 (90%)	7 (6%)	5 (4%)	2	2
3	B	109/111 (98%)	102 (94%)	6 (6%)	1 (1%)	14	14
4	D	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
5	E	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
All	All	651/661 (98%)	596 (92%)	46 (7%)	9 (1%)	12	9

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	106	PHE
1	A	504	LEU
2	C	101	TYR
2	C	103	ASN
2	C	102	GLY
1	A	514	ALA
1	A	538	PHE
2	C	26	GLY
3	B	33	GLY

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	182/182 (100%)	181 (100%)	1 (0%)	86	86
2	C	97/97 (100%)	92 (95%)	5 (5%)	19	19
3	B	92/92 (100%)	92 (100%)	0	100	100
4	D	92/92 (100%)	92 (100%)	0	100	100
5	E	97/97 (100%)	96 (99%)	1 (1%)	73	73
All	All	560/560 (100%)	553 (99%)	7 (1%)	64	65

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	537	ILE
2	C	3	GLN
2	C	60	TYR
2	C	61	ASN
2	C	62	GLN
2	C	100	ASN
5	E	102	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	464	ASN
1	A	470	HIS
1	A	569	ASN
2	C	5	GLN
2	C	39	GLN
2	C	43	GLN
2	C	61	ASN
3	B	42	GLN
3	B	58	GLN
4	D	38	GLN
4	D	93	ASN
5	E	39	GLN
5	E	82	GLN

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)

4 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	$\#\|Z\| > 2$
6	NAG	A	577	1	14,14,15	0.29	0	17,19,21	0.37	0
6	NAG	A	579	1	14,14,15	0.25	0	17,19,21	0.38	0
6	NAG	A	576	1	14,14,15	0.46	0	17,19,21	0.92	1 (5%)
6	NAG	A	578	1	14,14,15	0.25	0	17,19,21	0.50	0

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
6	NAG	A	577	1	-	4/6/23/26	0/1/1/1
6	NAG	A	579	1	-	4/6/23/26	0/1/1/1
6	NAG	A	576	1	-	1/6/23/26	0/1/1/1
6	NAG	A	578	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	576	NAG	O5-C1-C2	-2.38	107.52	111.29

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	579	NAG	C4-C5-C6-O6
6	A	579	NAG	O5-C5-C6-O6
6	A	577	NAG	O5-C5-C6-O6
6	A	577	NAG	C4-C5-C6-O6
6	A	577	NAG	C8-C7-N2-C2
6	A	577	NAG	O7-C7-N2-C2
6	A	579	NAG	C8-C7-N2-C2
6	A	579	NAG	O7-C7-N2-C2
6	A	578	NAG	C4-C5-C6-O6
6	A	578	NAG	O5-C5-C6-O6
6	A	576	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	577	NAG	1	0
6	A	578	NAG	1	0

5.7 Other polymers ⓘ

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 D_1300066582. 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 (i)

This section was not generated.