



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 21, 2019 – 04:38 PM EST

PDB ID : 6MMT
EMDB ID: : EMD-9161
Title : Triheteromeric NMDA receptor GluN1/GluN2A/GluN2A* in the '1-Knuckle' conformation, in complex with glycine and glutamate, in the presence of 1 micromolar zinc chloride, and at pH 7.4
Authors : Jalali-Yazdi, F.; Chowdhury, S.; Yoshioka, C.; Gouaux, E.
Deposited on : 2018-10-01
Resolution : 7.46 Å (reported)
Based on PDB ID : 5UOW, 4PE5, 5TQ0, 5I57

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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

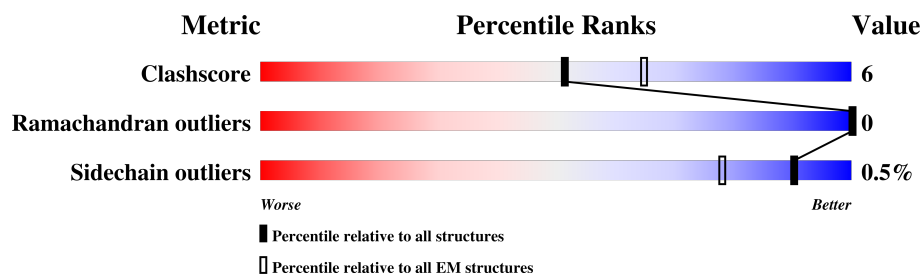
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.46 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	838	75% 18% 7%
1	C	838	77% 16% 6%
2	B	837	77% 15% 8%
3	D	837	77% 15% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25116 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 Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	782	Total	C	N	O	S	0	0
			6189	3951	1065	1138	35		
1	C	786	Total	C	N	O	S	0	0
			6216	3964	1072	1145	35		

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	772	Total	C	N	O	S	0	0
			6099	3935	995	1133	36		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	758	THR	SER	conflict	UNP Q00959

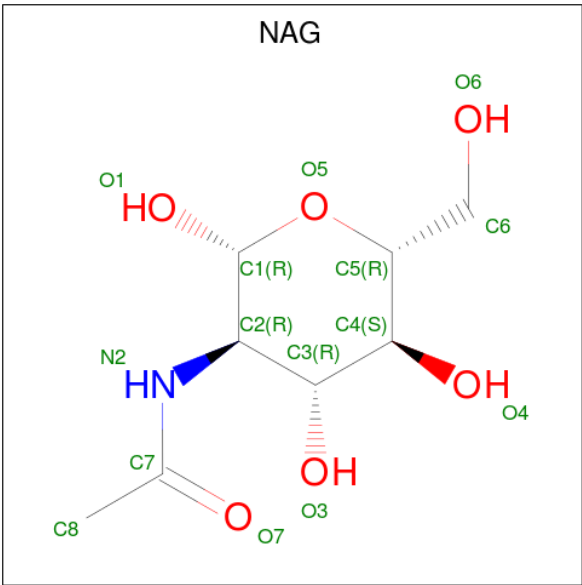
- Molecule 3 is a protein called Glutamate receptor ionotropic, NMDA 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	770	Total	C	N	O	S	0	0
			6094	3933	994	1131	36		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	128	SER	HIS	engineered mutation	UNP Q00959
D	687	GLN	ASN	engineered mutation	UNP Q00959
D	758	THR	SER	conflict	UNP Q00959

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			182	104	13	65	
4	A	1	Total	C	N	O	0
			182	104	13	65	
4	A	1	Total	C	N	O	0
			182	104	13	65	
4	A	1	Total	C	N	O	0
			182	104	13	65	
4	A	1	Total	C	N	O	0
			182	104	13	65	
4	A	1	Total	C	N	O	0
			182	104	13	65	
4	A	1	Total	C	N	O	0
			182	104	13	65	
4	A	1	Total	C	N	O	0
			182	104	13	65	
4	A	1	Total	C	N	O	0
			182	104	13	65	
4	A	1	Total	C	N	O	0
			182	104	13	65	
4	A	1	Total	C	N	O	0
			182	104	13	65	
4	B	1	Total	C	N	O	0
			84	48	6	30	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			84	48	6	30	
4	B	1	Total	C	N	O	0
			84	48	6	30	
4	B	1	Total	C	N	O	0
			84	48	6	30	
4	B	1	Total	C	N	O	0
			84	48	6	30	
4	B	1	Total	C	N	O	0
			84	48	6	30	
4	C	1	Total	C	N	O	0
			182	104	13	65	
4	C	1	Total	C	N	O	0
			182	104	13	65	
4	C	1	Total	C	N	O	0
			182	104	13	65	
4	C	1	Total	C	N	O	0
			182	104	13	65	
4	C	1	Total	C	N	O	0
			182	104	13	65	
4	C	1	Total	C	N	O	0
			182	104	13	65	
4	C	1	Total	C	N	O	0
			182	104	13	65	
4	C	1	Total	C	N	O	0
			182	104	13	65	
4	C	1	Total	C	N	O	0
			182	104	13	65	
4	C	1	Total	C	N	O	0
			182	104	13	65	
4	C	1	Total	C	N	O	0
			182	104	13	65	
4	C	1	Total	C	N	O	0
			182	104	13	65	
4	D	1	Total	C	N	O	0
			70	40	5	25	
4	D	1	Total	C	N	O	0
			70	40	5	25	
4	D	1	Total	C	N	O	0
			70	40	5	25	

Continued on next page...

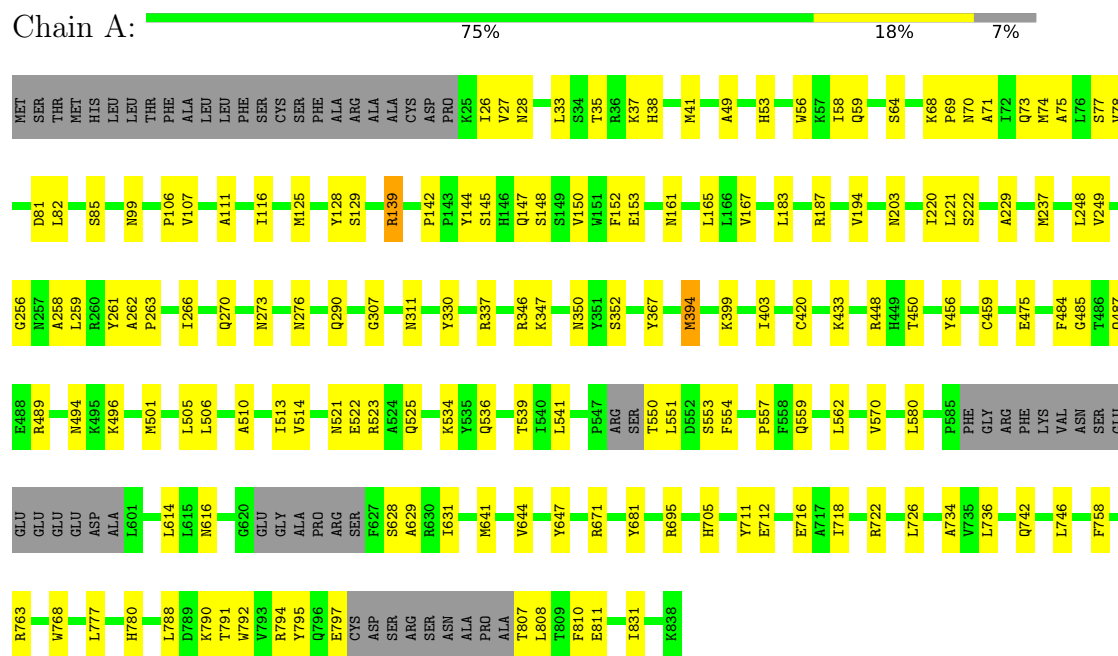
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
4	D	1	Total	C	N	O	0
			70	40	5	25	
4	D	1	Total	C	N	O	0
			70	40	5	25	

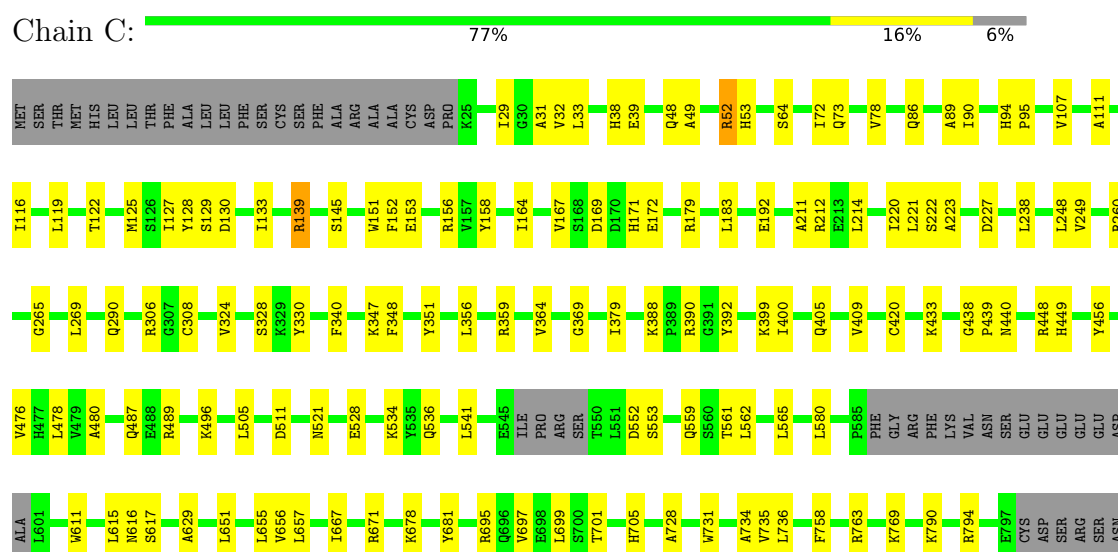
3 Residue-property plots

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: Glutamate receptor ionotropic, NMDA 1



- Molecule 1: Glutamate receptor ionotropic, NMDA 1



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	32232	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 ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 BASE (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: 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	0.27	0/6326	0.49	0/8568
1	C	0.27	0/6354	0.50	2/8606 (0.0%)
2	B	0.27	0/6243	0.47	0/8477
3	D	0.27	0/6237	0.48	0/8464
All	All	0.27	0/25160	0.49	2/34115 (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	C	651	LEU	CA-CB-CG	5.38	127.67	115.30
1	C	562	LEU	CA-CB-CG	5.33	127.57	115.30

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	6189	0	6165	95	0
1	C	6216	0	6187	83	0
2	B	6099	0	6030	77	0
3	D	6094	0	6026	76	0
4	A	182	0	167	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	84	0	78	0	0
4	C	182	0	165	1	0
4	D	70	0	65	1	0
All	All	25116	0	24883	314	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 6.

All (314) 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:B:280:SER:O	2:B:362:VAL:HB	1.80	0.81
3:D:742:ASP:OD2	3:D:746:LYS:N	2.19	0.75
1:C:541:LEU:O	1:C:728:ALA:HA	1.88	0.74
1:A:77:SER:O	1:A:81:ASP:HB2	1.93	0.69
1:A:550:THR:N	1:A:811:GLU:OE2	2.26	0.68
3:D:418:ILE:HB	3:D:457:LYS:O	1.94	0.67
3:D:433:THR:HG22	3:D:457:LYS:HB3	1.76	0.66
2:B:433:THR:HG22	2:B:457:LYS:HB3	1.79	0.65
1:A:273:ASN:HA	1:A:276:ASN:HB2	1.79	0.64
3:D:272:PHE:HB2	3:D:370:ARG:HH12	1.63	0.64
1:A:270:GLN:HB3	1:A:352:SER:HB2	1.80	0.63
1:A:534:LYS:HB3	1:A:758:PHE:HB2	1.81	0.62
1:C:534:LYS:HB3	1:C:758:PHE:HB2	1.80	0.62
2:B:437:ARG:HB2	2:B:451:ASN:HB3	1.82	0.62
2:B:773:ARG:NH1	1:C:528:GLU:OE2	2.34	0.61
1:C:559:GLN:NE2	1:C:561:THR:OG1	2.34	0.61
1:C:212:ARG:NH2	1:C:238:LEU:O	2.34	0.61
1:A:220:ILE:HG12	1:A:248:LEU:HD23	1.83	0.60
2:B:42:HIS:HE1	2:B:75:ASN:HA	1.67	0.60
1:C:790:LYS:HG2	1:C:794:ARG:HE	1.67	0.60
1:C:697:VAL:HG12	3:D:431:ARG:HH22	1.67	0.59
1:C:31:ALA:O	1:C:64:SER:HA	2.03	0.59
1:C:32:VAL:HG12	1:C:94:HIS:HD2	1.66	0.59
1:C:489:ARG:NH1	3:D:193:ASN:O	2.36	0.58
1:C:536:GLN:HE22	1:C:735:VAL:HG23	1.69	0.58
3:D:421:ASP:OD1	3:D:454:LYS:NZ	2.36	0.58
1:C:440:ASN:HD21	1:C:449:HIS:HB2	1.68	0.58
1:A:742:GLN:NE2	1:A:797:GLU:OE2	2.37	0.57
2:B:735:LEU:HD23	2:B:738:LYS:HD3	1.87	0.57
1:A:580:LEU:HD22	1:A:629:ALA:HB2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:535:VAL:HG22	3:D:729:ILE:HG12	1.86	0.57
1:A:394:MET:O	1:A:768:TRP:NE1	2.37	0.56
3:D:466:LYS:HD3	3:D:787:GLU:OE2	2.06	0.56
2:B:513:THR:OG1	2:B:518:ARG:NH1	2.39	0.56
1:A:290:GLN:NE2	1:A:330:TYR:OH	2.39	0.56
3:D:364:ILE:HG22	3:D:374:LYS:HA	1.87	0.56
3:D:275:GLY:H	3:D:366:LEU:HB3	1.71	0.56
2:B:364:ILE:HG22	2:B:374:LYS:HA	1.87	0.56
1:C:405:GLN:H	1:C:409:VAL:HB	1.70	0.56
2:B:157:VAL:HG21	2:B:361:LEU:HG	1.87	0.56
1:C:667:ILE:HD11	1:C:699:LEU:HD11	1.87	0.56
1:A:111:ALA:HB1	1:A:116:ILE:HB	1.88	0.55
1:C:164:ILE:HD13	1:C:211:ALA:HB1	1.87	0.55
1:A:78:VAL:HG21	1:A:107:VAL:HG22	1.88	0.55
1:A:489:ARG:NH2	1:A:494:ASN:OD1	2.40	0.55
1:C:220:ILE:HG12	1:C:248:LEU:HD23	1.88	0.55
1:C:580:LEU:HD22	1:C:629:ALA:HB2	1.88	0.55
1:A:616:ASN:OD1	2:B:615:ASN:ND2	2.39	0.55
2:B:259:SER:HB2	2:B:280:SER:HA	1.88	0.55
2:B:36:ILE:HG12	2:B:97:GLY:HA3	1.89	0.55
1:C:308:CYS:O	3:D:76:ARG:NH1	2.40	0.55
1:A:129:SER:OG	1:A:139:ARG:NH2	2.40	0.54
2:B:535:VAL:HG22	2:B:729:ILE:HG12	1.89	0.54
1:A:718:ILE:O	1:A:722:ARG:HB2	2.06	0.54
1:A:150:VAL:O	1:A:153:GLU:HB2	2.07	0.54
1:A:521:ASN:HB3	1:A:695:ARG:HH12	1.73	0.54
3:D:438:LYS:HB2	3:D:479:LEU:HD12	1.90	0.54
1:A:28:ASN:ND2	1:A:85:SER:O	2.41	0.54
1:A:489:ARG:NH1	2:B:193:ASN:O	2.40	0.54
1:C:400:ILE:HB	1:C:476:VAL:HA	1.89	0.54
3:D:439:PHE:HB3	3:D:481:THR:HG21	1.90	0.54
1:A:56:TRP:HD1	1:A:58:ILE:HB	1.73	0.54
2:B:684:THR:HG22	2:B:729:ILE:HB	1.89	0.54
1:C:399:LYS:H	1:C:511:ASP:HB2	1.74	0.53
3:D:681:ARG:NH2	3:D:723:GLY:O	2.41	0.53
3:D:281:TYR:O	3:D:291:ARG:NH2	2.41	0.53
1:C:153:GLU:OE1	1:C:156:ARG:NH1	2.41	0.53
2:B:565:LEU:HD23	2:B:608:LEU:HD23	1.90	0.53
1:C:39:GLU:OE2	1:C:64:SER:OG	2.21	0.53
2:B:244:ARG:NH1	2:B:397:SER:OG	2.41	0.53
1:C:611:TRP:O	1:C:615:LEU:HB2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:568:VAL:HG11	2:B:608:LEU:HD22	1.91	0.53
1:A:790:LYS:HG2	1:A:794:ARG:HE	1.74	0.53
2:B:128:HIS:NE2	2:B:282:ASP:OD1	2.42	0.53
1:A:26:ILE:HG22	1:A:59:GLN:HB2	1.90	0.53
1:A:553:SER:HA	1:A:557:PRO:HB2	1.91	0.53
1:C:145:SER:HB2	1:C:179:ARG:HG2	1.90	0.53
3:D:513:THR:OG1	3:D:518:ARG:NH1	2.42	0.53
1:C:158:TYR:HD1	1:C:388:LYS:HD3	1.74	0.52
1:A:505:LEU:HA	1:A:510:ALA:HB3	1.91	0.52
1:C:420:CYS:HB3	1:C:433:LYS:HD2	1.90	0.52
1:A:350:ASN:HA	1:A:367:TYR:O	2.10	0.52
3:D:464:LEU:HD13	3:D:509:VAL:HG11	1.91	0.52
1:A:258:ALA:HA	1:A:261:TYR:HB2	1.91	0.52
1:A:399:LYS:HA	1:A:475:GLU:HB3	1.92	0.52
3:D:364:ILE:HD12	3:D:372:TRP:HB3	1.91	0.52
2:B:104:THR:O	2:B:264:ASN:ND2	2.42	0.52
1:C:125:MET:HB2	1:C:128:TYR:HD2	1.74	0.52
1:A:541:LEU:HD11	1:A:746:LEU:HB3	1.92	0.52
2:B:339:VAL:HA	2:B:350:PHE:HB2	1.91	0.52
1:C:221:LEU:HB3	1:C:249:VAL:HG12	1.90	0.52
1:A:487:GLN:HG2	1:A:496:LYS:HB3	1.92	0.51
1:A:505:LEU:HG	1:A:763:ARG:HH21	1.75	0.51
1:A:78:VAL:HG13	1:A:82:LEU:HD12	1.92	0.51
3:D:738:LYS:HG2	3:D:741:ARG:HH11	1.76	0.51
3:D:138:LYS:NZ	3:D:354:GLY:O	2.44	0.51
1:A:142:PRO:HD3	1:A:346:ARG:HB3	1.90	0.51
1:A:807:THR:N	1:A:811:GLU:OE1	2.43	0.51
1:C:439:PRO:HB3	1:C:448:ARG:HH12	1.76	0.51
2:B:421:ASP:OD1	2:B:454:LYS:NZ	2.43	0.51
4:A:904:NAG:N2	4:A:904:NAG:O4	2.43	0.51
2:B:536:MET:SD	2:B:539:ARG:NH1	2.72	0.51
2:B:681:ARG:NH2	2:B:723:GLY:O	2.43	0.51
3:D:375:VAL:HG13	3:D:387:HIS:HD2	1.76	0.51
2:B:39:LEU:HD21	2:B:74:MET:HB2	1.92	0.50
2:B:154:GLN:HE22	2:B:259:SER:H	1.60	0.50
1:A:506:LEU:HA	1:A:763:ARG:HH22	1.75	0.50
3:D:539:ARG:NH2	3:D:744:GLY:O	2.37	0.50
1:A:525:GLN:O	3:D:773:ARG:NH2	2.44	0.50
3:D:681:ARG:HG2	3:D:726:ASP:H	1.77	0.50
2:B:233:LYS:HD2	2:B:263:GLY:HA3	1.93	0.50
3:D:259:SER:HB2	3:D:280:SER:HA	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:ILE:HG13	3:D:626:THR:HG23	1.93	0.50
1:C:678:LYS:NZ	3:D:743:GLU:OE2	2.44	0.50
1:C:49:ALA:O	1:C:53:HIS:ND1	2.45	0.50
1:C:701:THR:OG1	3:D:457:LYS:NZ	2.45	0.50
1:A:144:TYR:O	1:A:147:GLN:HB2	2.11	0.50
1:A:161:ASN:OD1	1:A:187:ARG:NH2	2.44	0.50
1:A:541:LEU:HB2	1:A:736:LEU:HD13	1.94	0.50
2:B:189:THR:O	2:B:193:ASN:ND2	2.42	0.50
2:B:673:PRO:HB2	2:B:679:PRO:HA	1.93	0.50
2:B:487:LYS:N	2:B:494:ASN:OD1	2.44	0.50
1:C:505:LEU:HG	1:C:763:ARG:HH21	1.76	0.50
1:C:192:GLU:OE2	1:C:214:LEU:HB3	2.12	0.49
1:A:33:LEU:HB3	1:A:64:SER:HB2	1.94	0.49
2:B:154:GLN:NE2	2:B:279:VAL:O	2.45	0.49
2:B:813:ASP:HB2	2:B:816:ASN:HB2	1.93	0.49
1:C:260:ARG:O	1:C:359:ARG:NH1	2.42	0.49
1:A:681:TYR:H	1:A:705:HIS:HE1	1.60	0.49
1:C:340:PHE:O	1:C:347:LYS:NZ	2.45	0.49
3:D:546:PRO:HG2	3:D:813:ASP:OD2	2.12	0.49
1:A:38:HIS:HA	1:A:41:MET:HG3	1.94	0.49
2:B:672:ARG:HD2	2:B:673:PRO:HD2	1.93	0.49
3:D:706:THR:O	3:D:709:ASN:ND2	2.45	0.49
2:B:201:GLN:NE2	2:B:221:LYS:O	2.46	0.49
1:C:364:VAL:HB	1:C:379:ILE:HG12	1.94	0.49
1:C:553:SER:O	3:D:811:GLN:NE2	2.45	0.49
1:C:439:PRO:HG2	1:C:480:ALA:HA	1.95	0.49
3:D:461:ILE:HG22	3:D:465:LYS:HE2	1.95	0.49
3:D:735:LEU:HD23	3:D:738:LYS:HD3	1.95	0.49
1:C:731:TRP:HB3	1:C:736:LEU:HD11	1.95	0.48
1:A:229:ALA:HB1	1:A:261:TYR:HD2	1.78	0.48
2:B:170:PHE:HE1	2:B:198:TRP:HB3	1.77	0.48
3:D:346:LYS:HG2	3:D:360:ARG:HH21	1.77	0.48
1:A:541:LEU:HD21	1:A:746:LEU:HD22	1.96	0.48
1:C:671:ARG:NH1	3:D:740:GLY:O	2.46	0.48
3:D:409:VAL:HG13	3:D:496:MET:HG2	1.94	0.48
2:B:600:THR:HA	2:B:603:LYS:HB2	1.95	0.48
2:B:565:LEU:HD22	2:B:605:ILE:HG23	1.96	0.48
1:A:256:GLY:O	1:A:259:LEU:HB3	2.13	0.48
1:A:263:PRO:HG2	1:A:266:ILE:HB	1.96	0.48
1:A:49:ALA:O	1:A:53:HIS:ND1	2.43	0.48
1:A:788:LEU:O	1:A:791:THR:OG1	2.31	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:672:ARG:HD2	3:D:673:PRO:HD2	1.95	0.48
1:A:70:ASN:OD1	1:A:73:GLN:NE2	2.46	0.48
2:B:298:ILE:HG23	2:B:341:VAL:HG21	1.95	0.48
3:D:462:ASP:OD2	3:D:795:TRP:NE1	2.47	0.48
2:B:201:GLN:HE22	2:B:222:ILE:HA	1.78	0.47
1:C:78:VAL:HG11	1:C:107:VAL:HG22	1.96	0.47
1:C:433:LYS:HG2	1:C:456:TYR:HB3	1.95	0.47
1:A:145:SER:O	1:A:148:SER:HB3	2.14	0.47
1:C:487:GLN:HG2	1:C:496:LYS:HB3	1.96	0.47
1:A:152:PHE:HB2	1:A:183:LEU:HD13	1.96	0.47
1:A:485:GLY:O	1:A:523:ARG:NH2	2.48	0.47
1:C:615:LEU:HD23	1:C:617:SER:H	1.79	0.47
1:A:433:LYS:HG2	1:A:456:TYR:HB3	1.95	0.47
1:A:522:GLU:OE2	1:A:695:ARG:NH1	2.47	0.47
1:C:269:LEU:HD12	1:C:351:TYR:HB3	1.96	0.47
1:C:90:ILE:O	1:C:119:LEU:N	2.48	0.47
1:A:71:ALA:HB1	1:A:106:PRO:HG3	1.96	0.47
2:B:672:ARG:HG3	2:B:674:HIS:H	1.79	0.47
1:C:48:GLN:O	1:C:52:ARG:NH1	2.48	0.47
3:D:279:VAL:HG22	3:D:363:VAL:HG22	1.95	0.47
1:C:561:THR:O	1:C:565:LEU:HB2	2.14	0.47
4:C:907:NAG:O6	4:C:908:NAG:O7	2.32	0.47
2:B:539:ARG:HD2	2:B:747:LEU:HA	1.96	0.47
3:D:405:HIS:HB3	3:D:476:ASP:OD2	2.15	0.47
1:A:641:MET:HA	1:A:644:VAL:HG22	1.95	0.47
2:B:105:ASP:OD1	2:B:264:ASN:ND2	2.48	0.47
1:C:33:LEU:HD21	1:C:38:HIS:HB2	1.96	0.47
1:C:681:TYR:H	1:C:705:HIS:HE1	1.62	0.46
3:D:533:ILE:HA	3:D:731:ASP:HA	1.97	0.46
1:A:70:ASN:ND2	2:B:323:GLN:OE1	2.49	0.46
3:D:204:ILE:HG23	3:D:218:GLN:HB3	1.98	0.46
2:B:169:VAL:HA	2:B:199:ASP:HB3	1.98	0.46
1:C:111:ALA:HB1	1:C:116:ILE:HB	1.98	0.46
1:A:554:PHE:O	1:A:647:TYR:OH	2.33	0.46
1:C:169:ASP:HB2	1:C:172:GLU:OE2	2.16	0.46
3:D:244:ARG:HH22	3:D:397:SER:HA	1.80	0.46
3:D:523:ASP:OD2	3:D:767:LYS:HA	2.16	0.46
1:A:536:GLN:HE21	1:A:734:ALA:H	1.63	0.45
3:D:672:ARG:HG3	3:D:674:HIS:H	1.81	0.45
1:A:777:LEU:HA	1:A:780:HIS:HD2	1.81	0.45
2:B:34:LEU:HD11	2:B:313:ILE:HG22	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:ARG:NH1	1:C:392:TYR:O	2.49	0.45
3:D:59:GLN:HE21	3:D:62:GLY:HA2	1.82	0.45
1:A:711:TYR:HE2	1:A:726:LEU:HD11	1.82	0.45
2:B:409:VAL:HG13	2:B:496:MET:HG2	1.98	0.45
1:C:152:PHE:HB2	1:C:183:LEU:HD13	1.98	0.45
3:D:171:SER:OG	3:D:201:GLN:OE1	2.33	0.45
1:A:550:THR:OG1	1:A:551:LEU:N	2.49	0.45
3:D:38:VAL:HB	3:D:71:ALA:HA	1.98	0.45
1:A:148:SER:O	1:A:152:PHE:N	2.47	0.45
1:A:506:LEU:HD23	1:A:763:ARG:HH22	1.82	0.45
1:A:628:SER:HA	1:A:631:ILE:HD12	1.99	0.45
2:B:364:ILE:HD12	2:B:372:TRP:HB3	1.99	0.45
1:A:221:LEU:HB3	1:A:249:VAL:HG12	1.99	0.44
1:A:69:PRO:O	1:A:99:ASN:ND2	2.49	0.44
1:A:712:GLU:N	1:A:716:GLU:OE1	2.49	0.44
2:B:436:CYS:O	2:B:453:LYS:HA	2.18	0.44
1:A:681:TYR:H	1:A:705:HIS:CE1	2.35	0.44
2:B:197:GLY:HA3	2:B:431:ARG:HD3	1.98	0.44
2:B:441:LYS:HA	2:B:449:GLY:HA3	1.98	0.44
1:C:265:GLY:N	1:C:356:LEU:O	2.50	0.44
3:D:436:CYS:O	3:D:453:LYS:HA	2.18	0.44
3:D:731:ASP:OD2	3:D:761:TYR:OH	2.35	0.44
2:B:196:VAL:HG22	2:B:428:THR:HG21	1.99	0.44
1:C:348:PHE:HB3	1:C:369:GLY:HA2	1.99	0.44
1:A:448:ARG:NH2	1:A:450:THR:OG1	2.46	0.44
1:A:539:THR:HG23	1:A:736:LEU:HD12	2.00	0.44
2:B:94:ARG:HB3	2:B:316:ALA:HB3	2.00	0.44
2:B:406:LEU:HD22	2:B:506:VAL:HG11	1.99	0.44
1:A:671:ARG:NH1	2:B:745:CYS:SG	2.91	0.44
2:B:272:PHE:O	2:B:370:ARG:NH1	2.50	0.44
2:B:59:GLN:HE21	2:B:62:GLY:HA2	1.83	0.44
1:C:681:TYR:HB3	1:C:728:ALA:HB3	2.00	0.44
1:C:72:ILE:HD11	3:D:119:GLN:HB3	2.00	0.44
1:C:290:GLN:HB3	1:C:330:TYR:HE1	1.83	0.43
1:C:438:GLY:HA2	1:C:478:LEU:HB2	2.00	0.43
1:C:536:GLN:HE21	1:C:734:ALA:H	1.64	0.43
2:B:730:TYR:HB3	2:B:735:LEU:HD11	2.00	0.43
2:B:117:SER:HB2	2:B:124:ILE:HD12	1.99	0.43
1:C:95:PRO:HD3	1:C:122:THR:HG22	2.00	0.43
1:A:27:VAL:HG23	1:A:58:ILE:HD11	1.99	0.43
2:B:408:ILE:HD12	2:B:475:TYR:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:163:GLN:NE2	3:D:428:THR:OG1	2.45	0.43
1:A:75:ALA:HB2	1:A:106:PRO:HB2	2.00	0.43
1:A:420:CYS:HB3	1:A:433:LYS:HD2	1.99	0.43
2:B:191:VAL:HG13	2:B:198:TRP:HB2	1.99	0.43
1:C:127:ILE:HD13	1:C:171:HIS:HB3	2.01	0.43
1:C:223:ALA:HB1	1:C:227:ASP:HB2	2.00	0.43
3:D:686:PRO:HA	3:D:691:GLU:OE2	2.18	0.43
1:A:501:MET:HB3	1:A:513:ILE:HD13	2.01	0.43
2:B:706:THR:O	2:B:709:ASN:ND2	2.51	0.43
1:C:528:GLU:HB2	1:C:769:LYS:HZ3	1.83	0.43
2:B:413:GLU:O	2:B:417:VAL:N	2.48	0.43
3:D:83:ILE:HG12	3:D:116:ILE:HD11	2.01	0.43
1:A:125:MET:HB2	1:A:128:TYR:HD2	1.84	0.43
1:A:262:ALA:HB1	1:A:266:ILE:HG21	2.00	0.43
2:B:288:LEU:HD12	2:B:291:ARG:HD2	2.01	0.43
2:B:765:LEU:HD21	2:B:775:ILE:HD12	2.00	0.43
1:C:324:VAL:O	1:C:328:SER:OG	2.37	0.43
1:C:505:LEU:O	1:C:763:ARG:NH2	2.51	0.43
3:D:283:ASP:HB2	3:D:362:VAL:HG21	2.00	0.42
2:B:98:LEU:HD23	2:B:124:ILE:HG12	2.01	0.42
2:B:44:HIS:NE2	2:B:266:GLU:OE2	2.52	0.42
2:B:539:ARG:HD2	2:B:748:VAL:H	1.84	0.42
2:B:647:ALA:HB1	1:C:655:LEU:HD11	2.00	0.42
1:C:552:ASP:OD2	1:C:812:ASN:HB3	2.19	0.42
3:D:170:PHE:HE1	3:D:198:TRP:HB3	1.83	0.42
3:D:517:GLU:OE2	3:D:692:ARG:NH2	2.52	0.42
1:A:570:VAL:HG11	1:A:614:LEU:HD22	2.01	0.42
2:B:145:PHE:HZ	2:B:335:HIS:HA	1.84	0.42
1:C:809:THR:HB	1:C:813:MET:HB2	2.02	0.42
1:C:86:GLN:HE21	1:C:306:ARG:HD2	1.85	0.42
3:D:612:VAL:HA	3:D:634:TRP:HE1	1.84	0.42
2:B:733:ALA:HA	2:B:736:ASN:HD22	1.84	0.42
1:C:561:THR:O	1:C:565:LEU:CB	2.67	0.42
1:A:459:CYS:HB3	1:A:514:VAL:HG12	2.01	0.41
1:A:792:TRP:HA	1:A:795:TYR:HB3	2.02	0.41
3:D:154:GLN:NE2	3:D:279:VAL:O	2.53	0.41
3:D:201:GLN:HE22	3:D:222:ILE:HA	1.85	0.41
2:B:480:VAL:HG22	2:B:482:ASN:H	1.85	0.41
1:C:130:ASP:OD2	1:C:133:ILE:HG13	2.20	0.41
1:C:29:ILE:HG23	1:C:89:ALA:HB3	2.03	0.41
1:A:68:LYS:HB2	1:A:74:MET:HG2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:ASP:OD2	2:B:383:LEU:HD23	2.20	0.41
1:C:656:VAL:HG12	1:C:657:LEU:HD12	2.03	0.41
3:D:413:GLU:O	3:D:417:VAL:N	2.50	0.41
1:A:165:LEU:HB3	1:A:194:VAL:HG12	2.01	0.41
1:A:559:GLN:HE22	1:A:562:LEU:HB2	1.85	0.41
1:A:307:GLY:HA2	1:A:311:ASN:HB2	2.02	0.41
3:D:339:VAL:HG11	4:D:902:NAG:H83	2.02	0.41
1:A:403:ILE:HG21	1:A:484:PHE:HE1	1.84	0.41
1:C:167:VAL:HG22	1:C:222:SER:HB3	2.03	0.41
1:A:35:THR:HG22	1:A:37:LYS:H	1.86	0.41
2:B:217:VAL:HG22	3:D:217:VAL:HG22	2.02	0.41
2:B:464:LEU:HB2	2:B:509:VAL:HG11	2.01	0.41
3:D:143:THR:HG22	3:D:335:HIS:HB2	2.02	0.41
1:C:73:GLN:NE2	3:D:320:CYS:O	2.50	0.41
1:A:807:THR:OG1	1:A:808:LEU:N	2.53	0.41
2:B:174:THR:HA	2:B:230:TYR:HB3	2.03	0.41
3:D:201:GLN:NE2	3:D:221:LYS:O	2.53	0.41
3:D:226:VAL:HA	3:D:254:PHE:HB2	2.02	0.41
3:D:54:LEU:HD12	3:D:58:GLU:OE2	2.20	0.41
3:D:89:LEU:HB3	3:D:95:ILE:HD12	2.03	0.41
1:A:810:PHE:HZ	3:D:555:ALA:HB3	1.85	0.40
1:C:763:ARG:O	1:C:769:LYS:NZ	2.50	0.40
3:D:347:ASP:OD2	3:D:358:HIS:HD2	2.04	0.40
3:D:407:SER:HB3	3:D:506:VAL:H	1.86	0.40
1:A:489:ARG:HA	1:A:496:LYS:HA	2.02	0.40
1:C:129:SER:OG	1:C:139:ARG:NH2	2.55	0.40
1:A:167:VAL:HG22	1:A:222:SER:HB3	2.02	0.40
1:A:347:LYS:HB2	1:A:347:LYS:HE2	1.88	0.40
2:B:464:LEU:HD13	2:B:509:VAL:HG21	2.03	0.40
1:C:521:ASN:HB3	1:C:695:ARG:HH22	1.86	0.40
3:D:163:GLN:NE2	3:D:426:THR:O	2.54	0.40
1:C:158:TYR:O	1:C:388:LYS:NZ	2.45	0.40
1:C:151:TRP:HE1	1:C:269:LEU:HD23	1.86	0.40
3:D:169:VAL:HG13	3:D:199:ASP:OD2	2.21	0.40
1:A:33:LEU:HA	1:A:38:HIS:HE1	1.86	0.40
1:A:541:LEU:HD22	1:A:736:LEU:HD22	2.03	0.40
2:B:438:LYS:O	2:B:451:ASN:HA	2.21	0.40
3:D:523:ASP:O	3:D:765:LEU:N	2.51	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	772/838 (92%)	722 (94%)	50 (6%)	0	100	100
1	C	778/838 (93%)	727 (93%)	51 (7%)	0	100	100
2	B	764/837 (91%)	707 (92%)	57 (8%)	0	100	100
3	D	760/837 (91%)	697 (92%)	63 (8%)	0	100	100
All	All	3074/3350 (92%)	2853 (93%)	221 (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	676/722 (94%)	671 (99%)	5 (1%)	85	93
1	C	678/722 (94%)	674 (99%)	4 (1%)	87	93
2	B	676/726 (93%)	675 (100%)	1 (0%)	94	97
3	D	675/726 (93%)	671 (99%)	4 (1%)	87	93
All	All	2705/2896 (93%)	2691 (100%)	14 (0%)	90	95

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	ARG
1	A	203	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	237	MET
1	A	337	ARG
1	A	394	MET
2	B	681	ARG
1	C	52	ARG
1	C	139	ARG
1	C	616	ASN
1	C	813	MET
3	D	75	ASN
3	D	681	ARG
3	D	817	MET
3	D	828	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	67	HIS
1	A	70	ASN
1	A	73	GLN
1	A	94	HIS
1	A	146	HIS
1	A	147	GLN
1	A	290	GLN
1	A	536	GLN
1	A	780	HIS
2	B	42	HIS
2	B	59	GLN
2	B	154	GLN
2	B	696	ASN
2	B	709	ASN
2	B	736	ASN
1	C	67	HIS
1	C	94	HIS
1	C	536	GLN
1	C	559	GLN
1	C	616	ASN
1	C	705	HIS
3	D	154	GLN
3	D	264	ASN
3	D	358	HIS
3	D	387	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	709	ASN
3	D	736	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

37 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	$\# Z > 2$
4	NAG	A	901	1	14,14,15	0.35	0	17,19,21	0.82	1 (5%)
4	NAG	A	902	1	14,14,15	0.41	0	17,19,21	0.73	0
4	NAG	A	903	1	14,14,15	0.38	0	17,19,21	1.42	4 (23%)
4	NAG	A	904	1,4	14,14,15	0.62	0	17,19,21	1.26	1 (5%)
4	NAG	A	905	4	14,14,15	0.38	0	17,19,21	0.79	1 (5%)
4	NAG	A	906	1	14,14,15	0.34	0	17,19,21	0.84	1 (5%)
4	NAG	A	907	1	14,14,15	0.41	0	17,19,21	1.14	1 (5%)
4	NAG	A	908	1,4	14,14,15	0.46	0	17,19,21	2.16	4 (23%)
4	NAG	A	909	4	14,14,15	0.41	0	17,19,21	0.81	0
4	NAG	A	910	1	14,14,15	0.37	0	17,19,21	0.92	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	911	1	14,14,15	0.47	0	17,19,21	0.99	2 (11%)
4	NAG	A	912	1	14,14,15	0.43	0	17,19,21	1.11	1 (5%)
4	NAG	A	913	1	14,14,15	0.38	0	17,19,21	1.12	1 (5%)
4	NAG	B	901	2	14,14,15	0.39	0	17,19,21	0.86	1 (5%)
4	NAG	B	902	2	14,14,15	0.33	0	17,19,21	0.71	0
4	NAG	B	903	2	14,14,15	0.40	0	17,19,21	1.01	1 (5%)
4	NAG	B	904	2	14,14,15	0.36	0	17,19,21	1.63	3 (17%)
4	NAG	B	905	2	14,14,15	0.39	0	17,19,21	1.08	2 (11%)
4	NAG	B	906	2	14,14,15	0.35	0	17,19,21	0.90	1 (5%)
4	NAG	C	901	1	14,14,15	0.33	0	17,19,21	0.82	1 (5%)
4	NAG	C	902	1	14,14,15	0.40	0	17,19,21	0.83	1 (5%)
4	NAG	C	903	1	14,14,15	0.53	0	17,19,21	1.07	2 (11%)
4	NAG	C	904	1	14,14,15	0.39	0	17,19,21	0.86	1 (5%)
4	NAG	C	905	1	14,14,15	0.41	0	17,19,21	1.33	2 (11%)
4	NAG	C	906	1	14,14,15	0.37	0	17,19,21	0.80	1 (5%)
4	NAG	C	907	1,4	14,14,15	0.41	0	17,19,21	2.01	2 (11%)
4	NAG	C	908	4	14,14,15	0.57	0	17,19,21	1.94	3 (17%)
4	NAG	C	909	1	14,14,15	0.59	0	17,19,21	1.84	3 (17%)
4	NAG	C	910	1	14,14,15	0.47	0	17,19,21	0.69	0
4	NAG	C	911	1,4	14,14,15	0.40	0	17,19,21	1.55	3 (17%)
4	NAG	C	912	4	14,14,15	0.41	0	17,19,21	0.80	1 (5%)
4	NAG	C	913	1	14,14,15	0.36	0	17,19,21	0.79	1 (5%)
4	NAG	D	901	3	14,14,15	0.38	0	17,19,21	0.80	1 (5%)
4	NAG	D	902	3	14,14,15	0.35	0	17,19,21	0.90	1 (5%)
4	NAG	D	903	3	14,14,15	0.35	0	17,19,21	0.78	1 (5%)
4	NAG	D	904	3	14,14,15	0.35	0	17,19,21	0.86	1 (5%)
4	NAG	D	905	3	14,14,15	0.42	0	17,19,21	1.32	2 (11%)

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
4	NAG	A	901	1	-	2/6/23/26	0/1/1/1
4	NAG	A	902	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	903	1	-	4/6/23/26	0/1/1/1
4	NAG	A	904	1,4	-	2/6/23/26	0/1/1/1
4	NAG	A	905	4	-	2/6/23/26	0/1/1/1
4	NAG	A	906	1	-	2/6/23/26	0/1/1/1
4	NAG	A	907	1	-	4/6/23/26	0/1/1/1
4	NAG	A	908	1,4	-	4/6/23/26	0/1/1/1
4	NAG	A	909	4	-	3/6/23/26	0/1/1/1
4	NAG	A	910	1	-	2/6/23/26	0/1/1/1
4	NAG	A	911	1	-	3/6/23/26	0/1/1/1
4	NAG	A	912	1	-	3/6/23/26	0/1/1/1
4	NAG	A	913	1	-	3/6/23/26	0/1/1/1
4	NAG	B	901	2	-	4/6/23/26	0/1/1/1
4	NAG	B	902	2	-	0/6/23/26	0/1/1/1
4	NAG	B	903	2	-	4/6/23/26	0/1/1/1
4	NAG	B	904	2	-	3/6/23/26	0/1/1/1
4	NAG	B	905	2	-	3/6/23/26	0/1/1/1
4	NAG	B	906	2	-	3/6/23/26	0/1/1/1
4	NAG	C	901	1	-	2/6/23/26	0/1/1/1
4	NAG	C	902	1	-	3/6/23/26	0/1/1/1
4	NAG	C	903	1	-	4/6/23/26	0/1/1/1
4	NAG	C	904	1	-	0/6/23/26	0/1/1/1
4	NAG	C	905	1	-	3/6/23/26	0/1/1/1
4	NAG	C	906	1	-	3/6/23/26	0/1/1/1
4	NAG	C	907	1,4	-	5/6/23/26	0/1/1/1
4	NAG	C	908	4	-	1/6/23/26	0/1/1/1
4	NAG	C	909	1	-	5/6/23/26	0/1/1/1
4	NAG	C	910	1	-	4/6/23/26	0/1/1/1
4	NAG	C	911	1,4	-	2/6/23/26	0/1/1/1
4	NAG	C	912	4	-	2/6/23/26	0/1/1/1
4	NAG	C	913	1	-	2/6/23/26	0/1/1/1
4	NAG	D	901	3	-	0/6/23/26	0/1/1/1
4	NAG	D	902	3	-	4/6/23/26	0/1/1/1
4	NAG	D	903	3	-	2/6/23/26	0/1/1/1
4	NAG	D	904	3	-	2/6/23/26	0/1/1/1
4	NAG	D	905	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	907	NAG	C1-O5-C5	7.69	122.65	112.20
4	C	908	NAG	C1-O5-C5	6.52	121.06	112.20
4	C	909	NAG	C1-O5-C5	6.28	120.74	112.20
4	B	904	NAG	C1-O5-C5	5.37	119.50	112.20
4	A	908	NAG	C1-O5-C5	4.98	118.97	112.20
4	A	908	NAG	C4-C3-C2	4.90	118.20	111.02
4	A	913	NAG	C1-O5-C5	4.09	117.76	112.20
4	C	911	NAG	O5-C1-C2	-3.83	105.34	111.36
4	D	905	NAG	C1-O5-C5	3.82	117.39	112.20
4	A	908	NAG	C3-C4-C5	3.65	116.80	110.23
4	A	907	NAG	C1-O5-C5	3.64	117.16	112.20
4	B	903	NAG	C1-O5-C5	3.43	116.86	112.20
4	A	904	NAG	C1-O5-C5	3.37	116.78	112.20
4	A	903	NAG	C4-C3-C2	3.33	115.90	111.02
4	C	908	NAG	C4-C3-C2	3.30	115.86	111.02
4	A	912	NAG	C1-O5-C5	3.29	116.67	112.20
4	C	905	NAG	C1-O5-C5	3.21	116.57	112.20
4	A	910	NAG	C1-O5-C5	3.21	116.56	112.20
4	C	911	NAG	C4-C3-C2	3.07	115.51	111.02
4	C	909	NAG	C4-C3-C2	2.98	115.39	111.02
4	C	904	NAG	C1-O5-C5	2.88	116.12	112.20
4	B	906	NAG	C1-O5-C5	2.87	116.10	112.20
4	C	905	NAG	C2-N2-C7	2.76	126.88	122.92
4	D	902	NAG	C1-O5-C5	2.73	115.91	112.20
4	C	901	NAG	C1-O5-C5	2.72	115.90	112.20
4	D	904	NAG	C1-O5-C5	2.69	115.85	112.20
4	A	901	NAG	C1-O5-C5	2.66	115.82	112.20
4	C	903	NAG	C1-C2-N2	2.59	114.92	110.49
4	D	905	NAG	C2-N2-C7	2.57	126.60	122.92
4	A	908	NAG	O5-C1-C2	-2.48	107.47	111.36
4	C	913	NAG	C1-O5-C5	2.47	115.56	112.20
4	A	906	NAG	C1-O5-C5	2.47	115.56	112.20
4	B	905	NAG	C1-O5-C5	2.45	115.54	112.20
4	C	902	NAG	C1-O5-C5	2.44	115.53	112.20
4	A	903	NAG	C2-N2-C7	2.39	126.34	122.92
4	A	905	NAG	C1-O5-C5	2.38	115.44	112.20
4	B	904	NAG	C2-N2-C7	2.36	126.31	122.92
4	D	903	NAG	C1-O5-C5	2.33	115.37	112.20
4	C	903	NAG	C2-N2-C7	2.31	126.23	122.92
4	C	911	NAG	C3-C4-C5	2.26	114.30	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	912	NAG	C1-O5-C5	2.24	115.25	112.20
4	B	905	NAG	C2-N2-C7	2.21	126.08	122.92
4	C	909	NAG	O5-C1-C2	2.19	114.81	111.36
4	B	904	NAG	C1-C2-N2	2.19	114.23	110.49
4	A	903	NAG	C1-O5-C5	2.18	115.17	112.20
4	C	908	NAG	O5-C1-C2	2.16	114.76	111.36
4	A	911	NAG	C4-C3-C2	2.16	114.18	111.02
4	B	901	NAG	O5-C5-C6	2.15	110.55	107.15
4	C	907	NAG	C3-C4-C5	2.13	114.05	110.23
4	A	911	NAG	C2-N2-C7	-2.04	120.00	122.92
4	A	903	NAG	O5-C1-C2	-2.04	108.15	111.36
4	C	906	NAG	C1-O5-C5	2.02	114.95	112.20
4	D	901	NAG	C1-O5-C5	2.02	114.95	112.20

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	905	NAG	C1-C2-N2-C7
4	B	905	NAG	C8-C7-N2-C2
4	B	905	NAG	O7-C7-N2-C2
4	A	910	NAG	C8-C7-N2-C2
4	A	910	NAG	O7-C7-N2-C2
4	C	905	NAG	C1-C2-N2-C7
4	C	905	NAG	C8-C7-N2-C2
4	C	905	NAG	O7-C7-N2-C2
4	A	908	NAG	C8-C7-N2-C2
4	A	908	NAG	O7-C7-N2-C2
4	C	901	NAG	C8-C7-N2-C2
4	C	901	NAG	O7-C7-N2-C2
4	C	906	NAG	C8-C7-N2-C2
4	C	906	NAG	O7-C7-N2-C2
4	C	912	NAG	C8-C7-N2-C2
4	C	912	NAG	O7-C7-N2-C2
4	A	912	NAG	C3-C2-N2-C7
4	A	912	NAG	C8-C7-N2-C2
4	A	912	NAG	O7-C7-N2-C2
4	C	911	NAG	C8-C7-N2-C2
4	C	911	NAG	O7-C7-N2-C2
4	A	907	NAG	C8-C7-N2-C2
4	A	907	NAG	O7-C7-N2-C2
4	C	907	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	907	NAG	O7-C7-N2-C2
4	C	903	NAG	C1-C2-N2-C7
4	C	903	NAG	C8-C7-N2-C2
4	C	903	NAG	O7-C7-N2-C2
4	C	910	NAG	C3-C2-N2-C7
4	C	910	NAG	C8-C7-N2-C2
4	C	910	NAG	O7-C7-N2-C2
4	C	913	NAG	C8-C7-N2-C2
4	C	913	NAG	O7-C7-N2-C2
4	B	901	NAG	C8-C7-N2-C2
4	B	901	NAG	O7-C7-N2-C2
4	C	909	NAG	C3-C2-N2-C7
4	A	913	NAG	C8-C7-N2-C2
4	A	913	NAG	O7-C7-N2-C2
4	D	902	NAG	C8-C7-N2-C2
4	D	902	NAG	O7-C7-N2-C2
4	D	903	NAG	C8-C7-N2-C2
4	D	903	NAG	O7-C7-N2-C2
4	B	904	NAG	C1-C2-N2-C7
4	B	904	NAG	C8-C7-N2-C2
4	B	904	NAG	O7-C7-N2-C2
4	D	905	NAG	C1-C2-N2-C7
4	D	905	NAG	C8-C7-N2-C2
4	D	905	NAG	O7-C7-N2-C2
4	A	903	NAG	C1-C2-N2-C7
4	A	903	NAG	C8-C7-N2-C2
4	A	903	NAG	O7-C7-N2-C2
4	A	904	NAG	C8-C7-N2-C2
4	A	904	NAG	O7-C7-N2-C2
4	A	906	NAG	C8-C7-N2-C2
4	A	906	NAG	O7-C7-N2-C2
4	B	903	NAG	C8-C7-N2-C2
4	B	903	NAG	O7-C7-N2-C2
4	A	911	NAG	C8-C7-N2-C2
4	A	911	NAG	O7-C7-N2-C2
4	C	909	NAG	C8-C7-N2-C2
4	C	909	NAG	O7-C7-N2-C2
4	D	904	NAG	C8-C7-N2-C2
4	D	904	NAG	O7-C7-N2-C2
4	B	906	NAG	C8-C7-N2-C2
4	B	906	NAG	O7-C7-N2-C2
4	A	901	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	901	NAG	O7-C7-N2-C2
4	A	909	NAG	C8-C7-N2-C2
4	A	902	NAG	C8-C7-N2-C2
4	A	905	NAG	C8-C7-N2-C2
4	A	908	NAG	C1-C2-N2-C7
4	D	902	NAG	C1-C2-N2-C7
4	B	903	NAG	C1-C2-N2-C7
4	A	909	NAG	O7-C7-N2-C2
4	A	902	NAG	O7-C7-N2-C2
4	A	905	NAG	O7-C7-N2-C2
4	B	901	NAG	C4-C5-C6-O6
4	C	907	NAG	C1-C2-N2-C7
4	C	902	NAG	C8-C7-N2-C2
4	C	909	NAG	O5-C5-C6-O6
4	C	910	NAG	O5-C5-C6-O6
4	A	913	NAG	O5-C5-C6-O6
4	C	906	NAG	O5-C5-C6-O6
4	C	903	NAG	O5-C5-C6-O6
4	A	911	NAG	O5-C5-C6-O6
4	C	907	NAG	O5-C5-C6-O6
4	A	909	NAG	O5-C5-C6-O6
4	C	902	NAG	O5-C5-C6-O6
4	B	906	NAG	O5-C5-C6-O6
4	B	903	NAG	O5-C5-C6-O6
4	C	908	NAG	O5-C5-C6-O6
4	A	903	NAG	O5-C5-C6-O6
4	A	908	NAG	C3-C2-N2-C7
4	C	907	NAG	C3-C2-N2-C7
4	D	902	NAG	C3-C2-N2-C7
4	B	901	NAG	O5-C5-C6-O6
4	A	907	NAG	C1-C2-N2-C7
4	C	902	NAG	O7-C7-N2-C2
4	C	909	NAG	C1-C2-N2-C7
4	A	907	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	904	NAG	1	0
4	C	907	NAG	1	0
4	C	908	NAG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	902	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.