



Full wwPDB EM Validation Report ⓘ

Apr 26, 2026 – 12:08 AM JST

PDB ID : 9V3S / pdb_00009v3s
EMDB ID : EMD-64755
Title : Nav1.5 in complex with quinidine-azo
Authors : Huang, Z.; Li, Z.; Liu, S.
Deposited on : 2025-05-22
Resolution : 3.00 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**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

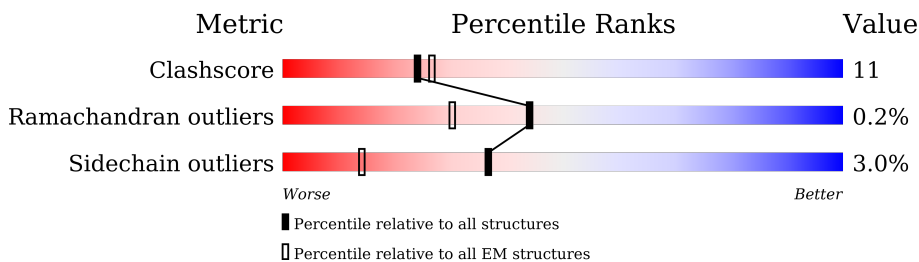
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	1618	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9402 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 Sodium channel protein type 5 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1151	9237	6115	1458	1591	73	0	0

There are 43 discrepancies between the modelled and reference sequences:

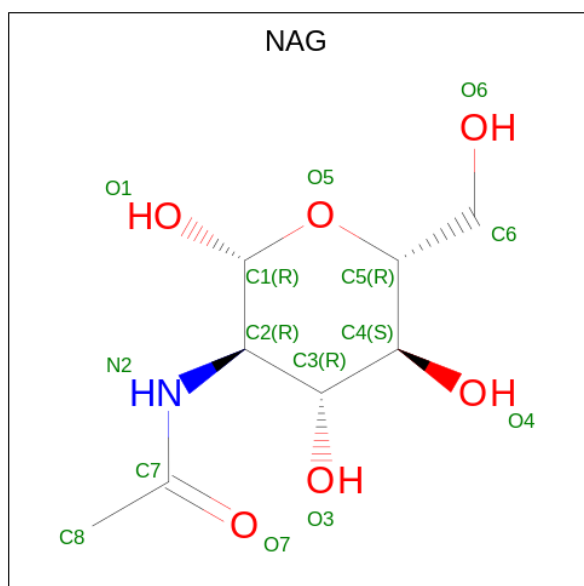
Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	initiating methionine	UNP Q14524
A	-41	ALA	-	expression tag	UNP Q14524
A	-40	SER	-	expression tag	UNP Q14524
A	-39	TRP	-	expression tag	UNP Q14524
A	-38	SER	-	expression tag	UNP Q14524
A	-37	HIS	-	expression tag	UNP Q14524
A	-36	PRO	-	expression tag	UNP Q14524
A	-35	GLN	-	expression tag	UNP Q14524
A	-34	PHE	-	expression tag	UNP Q14524
A	-33	GLU	-	expression tag	UNP Q14524
A	-32	LYS	-	expression tag	UNP Q14524
A	-31	GLY	-	expression tag	UNP Q14524
A	-30	GLY	-	expression tag	UNP Q14524
A	-29	GLY	-	expression tag	UNP Q14524
A	-28	ALA	-	expression tag	UNP Q14524
A	-27	ARG	-	expression tag	UNP Q14524
A	-26	GLY	-	expression tag	UNP Q14524
A	-25	GLY	-	expression tag	UNP Q14524
A	-24	SER	-	expression tag	UNP Q14524
A	-23	GLY	-	expression tag	UNP Q14524
A	-22	GLY	-	expression tag	UNP Q14524
A	-21	GLY	-	expression tag	UNP Q14524
A	-20	SER	-	expression tag	UNP Q14524
A	-19	TRP	-	expression tag	UNP Q14524
A	-18	SER	-	expression tag	UNP Q14524
A	-17	HIS	-	expression tag	UNP Q14524
A	-16	PRO	-	expression tag	UNP Q14524
A	-15	GLN	-	expression tag	UNP Q14524

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	PHE	-	expression tag	UNP Q14524
A	-13	GLU	-	expression tag	UNP Q14524
A	-12	LYS	-	expression tag	UNP Q14524
A	-11	GLY	-	expression tag	UNP Q14524
A	-10	PHE	-	expression tag	UNP Q14524
A	-9	ASP	-	expression tag	UNP Q14524
A	-8	TYR	-	expression tag	UNP Q14524
A	-7	LYS	-	expression tag	UNP Q14524
A	-6	ASP	-	expression tag	UNP Q14524
A	-5	ASP	-	expression tag	UNP Q14524
A	-4	ASP	-	expression tag	UNP Q14524
A	-3	ASP	-	expression tag	UNP Q14524
A	-2	LYS	-	expression tag	UNP Q14524
A	-1	GLY	-	expression tag	UNP Q14524
A	0	THR	-	expression tag	UNP Q14524

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



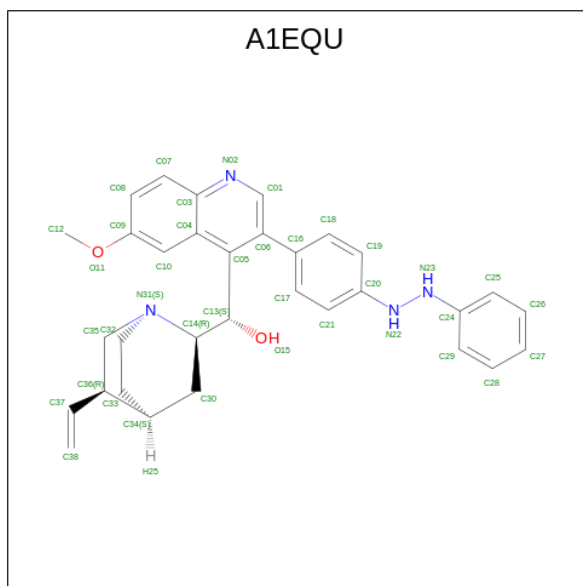
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	

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

- Molecule 3 is ({S})-[(1 {S},2 {R},4 {S},5 {R})-5-ethenyl-1-azabicyclo[2.2.2]octan-2-yl]-[6-methoxy-3-[4-(2-phenylhydrazinyl)phenyl]quinolin-4-yl]methanol (CCD ID: A1EQU) (formula: C₃₂H₃₄N₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			38	32	4	2	

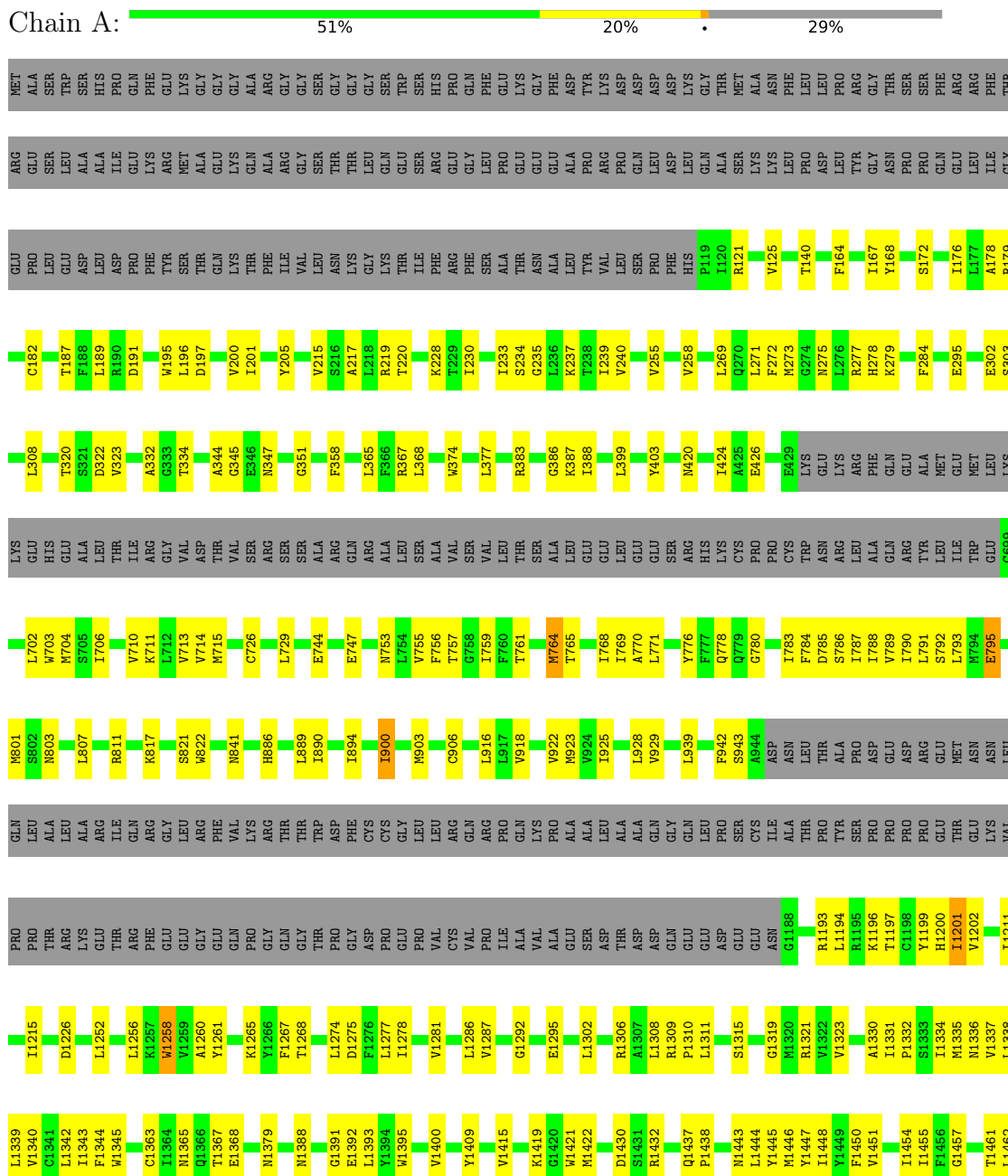
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

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: Sodium channel protein type 5 subunit alpha



ARG	SER	M1651	M1463
ILE	GLU	M1652	L1464
HIS	ASP	S1653	F1465
CYS	ASP	L1654	I1466
MET	PHE	P1655	G1467
ASP	ASP	A1656	V1468
ILE	MET		I1469
LEU	PHE	I1660	I1470
LEU	TYR		D1471
ALA	GLU	F1669	N1472
PHE	ILE		
THR	TRP	I1673	Q1475
LYS	GLU		
ARG	LYS	Y1681	K1478
VAL	PHE		
LEU	ASP	E1685	I1485
GLY	PRO	A1686	F1486
GLU	GLU		M1487
SER	ALA	M1691	T1488
GLY	THR		E1489
GLU	GLN	C1703	E1490
MET	PHE		Q1491
ASP	ILE	I1707	K1492
ALA	GLU		K1493
LEU	TYR	D1714	Y1494
LYS	SER	G1715	
ILE	VAL	L1716	
GLN	LEU		K1499
MET	SER	I1720	K1504
GLU	ASP		
GLU	PHE	T1723	K1508
LYS	ALA	G1724	P1509
PHE	ASP	F1725	
MET	ALA	P1726	R1512
ALA	LEU	Y1727	P1513
ALA	SER	C1728	L1514
ASN	GLU	D1729	N1515
PRO	PRO		
SER	LEU	N1734	Q1518
LYS	ARG		G1519
ILE	ILE	S1738	F1520
SER	ALA		I1521
TYR	LYS	F1752	
GLU	PRO		I1524
PRO	ASN	I1758	V1525
ILE	GLN		
THR	ILE	I1762	Q1528
	SER	V1763	
	LEU		
	ILE	M1766	D1531
	ASN	Y1767	V1532
	MET		I1533
	ASP		I1534
	LEU	I1770	M1535
	PRO		
	MET	E1781	I1538
	VAL	THR	
	SER	GLU	N1541
	GLY	PRO	M1542
	ASP	LEU	V1543
			T1544

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	287376	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI SPIRIT	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, NA, A1EQU

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	0.16	0/9462	0.42	0/12835

There are no bond length outliers.

There are no bond angle outliers.

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	9237	0	9414	204	0
2	A	126	0	117	2	0
3	A	38	0	0	3	0
4	A	1	0	0	0	0
All	All	9402	0	9531	204	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 11.

All (204) 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:1345:TRP:HZ2	3:A:1910:A1EQU:C28	1.86	0.88
1:A:1345:TRP:CZ2	3:A:1910:A1EQU:C28	2.58	0.86
1:A:1337:VAL:HG11	1:A:1468:VAL:HG11	1.62	0.81
1:A:1512:ARG:HD2	1:A:1514:LEU:HD23	1.65	0.79
1:A:714:VAL:HG13	1:A:715:MET:HE3	1.67	0.75
1:A:1388:ASN:HB3	1:A:1393:LEU:HB2	1.70	0.72
1:A:1252:LEU:O	1:A:1256:LEU:HD12	1.90	0.71
1:A:1330:ALA:HA	1:A:1472:ASN:HD21	1.54	0.71
1:A:1601:LEU:HD21	1:A:1628:ALA:HB1	1.73	0.71
1:A:711:LYS:HG2	1:A:770:ALA:HB1	1.72	0.70
1:A:1335:MET:HE3	1:A:1335:MET:HA	1.74	0.69
1:A:1582:LEU:HD12	1:A:1585:TYR:HB2	1.74	0.69
1:A:140:THR:HG21	1:A:167:ILE:HG21	1.74	0.69
1:A:786:SER:O	1:A:790:ILE:HG12	1.94	0.67
1:A:1566:LEU:O	1:A:1570:ILE:HD12	1.94	0.67
1:A:1728:CYS:SG	1:A:1729:ASP:N	2.67	0.67
1:A:1542:MET:O	1:A:1546:MET:HG3	1.95	0.67
1:A:1261:TYR:O	1:A:1265:LYS:NZ	2.29	0.66
1:A:1451:VAL:O	1:A:1455:ILE:HG13	1.96	0.65
1:A:1766:MET:O	1:A:1770:ILE:HG12	1.97	0.65
1:A:179:ARG:HB3	1:A:187:THR:HB	1.79	0.64
1:A:1598:VAL:HG11	1:A:1635:ARG:HD2	1.80	0.64
1:A:711:LYS:HZ3	1:A:771:LEU:HD23	1.62	0.64
1:A:1608:LEU:O	1:A:1612:ILE:HG12	1.98	0.63
1:A:272:PHE:HA	1:A:275:ASN:HD22	1.63	0.62
1:A:1612:ILE:HA	1:A:1615:TYR:HB2	1.80	0.62
1:A:765:THR:O	1:A:769:ILE:HG22	2.00	0.62
1:A:801:MET:HE2	1:A:801:MET:HA	1.81	0.62
1:A:1445:TYR:O	1:A:1448:ILE:HG22	2.00	0.62
1:A:215:VAL:HG13	1:A:217:ALA:H	1.63	0.61
1:A:1450:PHE:O	1:A:1454:ILE:HD12	1.99	0.61
1:A:1444:LEU:O	1:A:1447:TYR:HB2	2.00	0.61
1:A:1432:ARG:NH1	1:A:1437:GLN:O	2.34	0.61
1:A:783:ILE:O	1:A:787:ILE:HG12	2.02	0.59
1:A:1274:LEU:HD21	1:A:1311:LEU:HB3	1.85	0.59
1:A:702:LEU:HD23	1:A:702:LEU:H	1.67	0.59
1:A:271:LEU:HD21	1:A:1627:LEU:HD11	1.85	0.58
1:A:1415:VAL:HA	1:A:1421:TRP:HB3	1.86	0.58
1:A:787:ILE:O	1:A:791:LEU:HG	2.04	0.57
1:A:332:ALA:HB2	1:A:386:GLY:HA2	1.85	0.57
1:A:918:VAL:O	1:A:922:VAL:HG12	2.05	0.57
1:A:1287:VAL:O	1:A:1292:GLY:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1443:ASN:HB3	1:A:1446:MET:HG2	1.86	0.57
1:A:302:GLU:O	1:A:303:SER:OG	2.17	0.57
1:A:795:GLU:HB2	1:A:807:LEU:HG	1.88	0.56
1:A:1197:THR:O	1:A:1201:ILE:HG23	2.06	0.56
1:A:368:LEU:HD21	1:A:377:LEU:HD23	1.88	0.55
1:A:903:MET:HE2	1:A:916:LEU:HD23	1.89	0.55
1:A:1363:CYS:HB2	1:A:1437:GLN:HE22	1.72	0.55
1:A:1457:GLY:O	1:A:1461:THR:HB	2.07	0.55
1:A:1193:ARG:HA	1:A:1196:LYS:HE3	1.88	0.55
1:A:1277:LEU:O	1:A:1281:VAL:HG13	2.07	0.55
1:A:1534:ILE:O	1:A:1538:ILE:HG22	2.07	0.54
1:A:1471:ASP:O	1:A:1475:GLN:HG2	2.07	0.54
1:A:783:ILE:HG13	1:A:784:PHE:N	2.23	0.54
1:A:275:ASN:HA	1:A:278:HIS:CE1	2.43	0.54
1:A:383:ARG:HG3	1:A:1691:MET:HE1	1.90	0.53
1:A:757:THR:O	1:A:761:THR:HG23	2.07	0.53
1:A:1265:LYS:HA	1:A:1268:THR:HG22	1.90	0.53
1:A:1564:ASN:O	1:A:1568:VAL:HG12	2.09	0.53
1:A:788:ILE:HD12	1:A:817:LYS:HE3	1.90	0.53
1:A:1681:TYR:HB3	1:A:1734:ASN:HD21	1.75	0.52
1:A:168:TYR:HD1	1:A:228:LYS:HZ1	1.58	0.52
1:A:1630:ILE:HG23	1:A:1633:ILE:HD12	1.92	0.52
1:A:1651:MET:HA	1:A:1654:LEU:HD12	1.91	0.52
1:A:196:LEU:O	1:A:200:VAL:HG23	2.10	0.52
1:A:125:VAL:HG22	1:A:178:ALA:HB1	1.91	0.51
1:A:1211:ILE:O	1:A:1215:ILE:HG22	2.10	0.51
1:A:1521:ILE:HA	1:A:1524:ILE:HG22	1.92	0.51
1:A:322:ASP:OD2	1:A:323:VAL:N	2.37	0.51
1:A:1345:TRP:CH2	3:A:1910:A1EQU:C28	2.94	0.51
1:A:1607:VAL:O	1:A:1611:ILE:HG13	2.10	0.51
1:A:942:PHE:HZ	1:A:1464:LEU:HA	1.76	0.51
1:A:420:ASN:O	1:A:424:ILE:HG12	2.11	0.51
1:A:1508:LYS:HG2	1:A:1509:PRO:HD2	1.94	0.50
1:A:347:ASN:CB	1:A:351:GLY:HA2	2.42	0.50
1:A:1342:LEU:O	1:A:1409:TYR:OH	2.28	0.50
1:A:189:LEU:HD12	1:A:195:TRP:CD1	2.47	0.50
1:A:121:ARG:O	1:A:125:VAL:HG23	2.12	0.49
1:A:239:ILE:HG13	1:A:841:ASN:HB3	1.94	0.49
1:A:1430:ASP:HB3	1:A:1438:PRO:HB3	1.94	0.49
1:A:1669:PHE:CE1	1:A:1673:ILE:HD11	2.47	0.49
1:A:367:ARG:HG3	1:A:900:ILE:HD12	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1541:ASN:ND2	1:A:1632:ARG:HE	2.11	0.49
1:A:269:LEU:HD21	1:A:1548:GLU:HB2	1.95	0.49
1:A:744:GLU:HA	1:A:747:GLU:HB2	1.94	0.48
1:A:1308:LEU:HD22	1:A:1311:LEU:HD12	1.95	0.48
1:A:358:PHE:CE2	1:A:1546:MET:HE3	2.48	0.48
1:A:1199:TYR:HD2	1:A:1260:ALA:HB1	1.78	0.48
1:A:703:TRP:O	1:A:703:TRP:HD1	1.97	0.48
1:A:308:LEU:HB3	1:A:344:ALA:HB1	1.95	0.48
1:A:726:CYS:SG	1:A:759:ILE:HD13	2.54	0.48
1:A:729:LEU:HB3	1:A:756:PHE:CZ	2.49	0.48
1:A:1201:ILE:HD11	1:A:1256:LEU:HD22	1.96	0.48
1:A:426:GLU:OE2	1:A:426:GLU:N	2.46	0.48
1:A:1315:SER:O	1:A:1321:ARG:NH1	2.47	0.48
1:A:1488:THR:HB	1:A:1491:GLN:HG3	1.96	0.48
1:A:1528:GLN:O	1:A:1532:VAL:HG23	2.14	0.48
1:A:1723:THR:OG1	1:A:1724:GLY:N	2.47	0.48
1:A:755:VAL:O	1:A:759:ILE:HG22	2.13	0.47
1:A:822:TRP:HZ3	1:A:1343:ILE:HD12	1.78	0.47
1:A:939:LEU:O	1:A:943:SER:HB2	2.14	0.47
1:A:1549:THR:O	1:A:1552:GLN:HG2	2.14	0.47
1:A:1763:VAL:O	1:A:1767:TYR:HB2	2.15	0.47
1:A:1487:MET:HE3	1:A:1492:LYS:HG2	1.97	0.47
1:A:1521:ILE:O	1:A:1525:VAL:HG13	2.15	0.47
1:A:284:PHE:HB2	1:A:295:GLU:HB3	1.97	0.47
1:A:1421:TRP:CD1	1:A:1422:MET:HG2	2.50	0.46
1:A:1531:ASP:N	1:A:1531:ASP:OD1	2.49	0.46
1:A:1762:ILE:O	1:A:1766:MET:HB2	2.16	0.46
1:A:273:MET:HE1	1:A:1626:ARG:HH22	1.81	0.46
1:A:1703:CYS:O	1:A:1707:ILE:HD12	2.14	0.46
1:A:1720:ILE:HD12	1:A:1752:PHE:HE2	1.81	0.46
1:A:702:LEU:O	1:A:706:ILE:HG12	2.15	0.46
1:A:1475:GLN:HA	1:A:1478:LYS:HE2	1.98	0.46
1:A:334:THR:O	1:A:334:THR:OG1	2.31	0.46
1:A:1278:ILE:O	1:A:1281:VAL:HG22	2.16	0.46
1:A:164:PHE:O	1:A:168:TYR:HD2	1.99	0.45
1:A:172:SER:O	1:A:176:ILE:HG22	2.16	0.45
1:A:279:LYS:HD2	1:A:344:ALA:O	2.16	0.45
1:A:347:ASN:HB3	1:A:351:GLY:HA2	1.98	0.45
1:A:1379:ASN:O	1:A:1437:GLN:N	2.44	0.45
1:A:1707:ILE:HD11	1:A:1716:LEU:HG	1.98	0.45
1:A:237:LYS:HB2	1:A:237:LYS:HE2	1.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1193:ARG:O	1:A:1196:LYS:HG2	2.17	0.45
1:A:1258:TRP:HE1	1:A:1267:PHE:HE1	1.65	0.45
1:A:1444:LEU:HD12	1:A:1444:LEU:H	1.82	0.45
1:A:1643:ILE:HG22	1:A:1647:LEU:HD23	1.98	0.45
1:A:255:VAL:HA	1:A:258:VAL:HG22	1.99	0.45
1:A:1515:ASN:O	1:A:1519:GLY:N	2.49	0.45
1:A:230:ILE:HD13	1:A:240:VAL:HG21	1.99	0.45
1:A:399:LEU:O	1:A:403:TYR:HB3	2.16	0.45
1:A:792:SER:O	1:A:795:GLU:HG3	2.17	0.45
1:A:1478:LYS:HE2	1:A:1478:LYS:HB3	1.83	0.45
1:A:1586:TYR:CE2	1:A:1592:ASN:HB3	2.52	0.45
1:A:1319:GLY:O	1:A:1323:VAL:HG23	2.17	0.45
1:A:234:SER:OG	1:A:235:GLY:N	2.51	0.44
1:A:1306:ARG:O	1:A:1309:ARG:HG3	2.17	0.44
1:A:368:LEU:HD23	1:A:374:TRP:HB2	1.98	0.44
1:A:1330:ALA:O	1:A:1334:ILE:HG12	2.17	0.44
1:A:1504:LYS:HB2	1:A:1504:LYS:HE3	1.79	0.44
1:A:706:ILE:O	1:A:710:VAL:HG23	2.17	0.44
1:A:1197:THR:HA	1:A:1200:HIS:ND1	2.32	0.44
1:A:1265:LYS:HZ3	1:A:1265:LYS:HB2	1.81	0.44
1:A:1275:ASP:OD1	1:A:1275:ASP:N	2.50	0.44
1:A:1368:GLU:N	1:A:1368:GLU:OE2	2.51	0.44
1:A:1339:LEU:O	1:A:1343:ILE:HG13	2.18	0.44
1:A:1641:LYS:O	1:A:1645:THR:HG23	2.18	0.44
1:A:1472:ASN:OD1	1:A:1472:ASN:C	2.61	0.43
1:A:822:TRP:CZ3	1:A:1343:ILE:HD12	2.52	0.43
1:A:1367:THR:OG1	1:A:1368:GLU:OE2	2.34	0.43
1:A:1518:GLN:H	1:A:1518:GLN:CD	2.21	0.43
1:A:710:VAL:HA	1:A:713:VAL:HG12	1.99	0.43
1:A:1295:GLU:O	1:A:1295:GLU:CD	2.61	0.43
1:A:255:VAL:HG13	1:A:1643:ILE:HD11	2.00	0.43
1:A:778:GLN:C	1:A:780:GLY:H	2.27	0.43
1:A:1544:THR:O	1:A:1547:VAL:HG22	2.18	0.43
1:A:1652:MET:O	1:A:1655:PRO:HD2	2.18	0.43
1:A:1656:ALA:O	1:A:1660:ILE:HD12	2.18	0.43
1:A:1485:ILE:HG22	1:A:1486:PHE:H	1.84	0.43
1:A:1490:GLU:O	1:A:1494:TYR:HD1	2.01	0.43
1:A:1226:ASP:OD1	1:A:1226:ASP:N	2.45	0.43
1:A:1466:ILE:O	1:A:1470:ILE:HG12	2.19	0.43
1:A:1595:ASP:O	1:A:1598:VAL:HG12	2.19	0.43
1:A:1734:ASN:HB2	1:A:1738:SER:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1391:GLY:HA2	2:A:1909:NAG:H5	2.01	0.42
1:A:191:ASP:OD2	1:A:191:ASP:N	2.52	0.42
1:A:367:ARG:NH1	1:A:377:LEU:HB2	2.35	0.42
1:A:890:ILE:O	1:A:894:ILE:HG13	2.19	0.42
1:A:197:ASP:O	1:A:201:ILE:HG23	2.19	0.42
1:A:233:ILE:HG22	1:A:233:ILE:O	2.19	0.42
1:A:388:ILE:HD12	1:A:388:ILE:H	1.84	0.42
1:A:1365:ASN:HA	1:A:1392:GLU:O	2.20	0.42
1:A:1726:PRO:O	1:A:1727:TYR:HB2	2.20	0.42
1:A:1201:ILE:HG13	1:A:1202:VAL:N	2.33	0.42
1:A:822:TRP:HE1	1:A:1336:ASN:ND2	2.17	0.42
1:A:1499:LYS:HB2	1:A:1652:MET:HE1	2.02	0.42
1:A:785:ASP:O	1:A:789:VAL:HG12	2.20	0.42
1:A:1331:ILE:N	1:A:1332:PRO:HD2	2.35	0.42
1:A:1337:VAL:HA	1:A:1340:VAL:HG12	2.01	0.42
1:A:387:LYS:HE2	1:A:1691:MET:HG3	2.02	0.42
1:A:279:LYS:HE2	1:A:345:GLY:HA3	2.01	0.42
1:A:764:MET:O	1:A:768:ILE:HG12	2.19	0.42
1:A:1475:GLN:OE1	1:A:1478:LYS:NZ	2.53	0.42
1:A:789:VAL:O	1:A:793:LEU:HD23	2.18	0.42
1:A:711:LYS:NZ	1:A:771:LEU:HD23	2.34	0.41
1:A:822:TRP:HE1	1:A:1336:ASN:HD21	1.67	0.41
1:A:1685:GLU:HG2	1:A:1686:ALA:H	1.84	0.41
1:A:753:ASN:HD21	1:A:811:ARG:HD2	1.86	0.41
1:A:1647:LEU:HD13	1:A:1647:LEU:HA	1.93	0.41
1:A:1660:ILE:HD12	1:A:1660:ILE:H	1.84	0.41
1:A:925:ILE:O	1:A:929:VAL:HG12	2.19	0.41
1:A:1196:LYS:O	1:A:1200:HIS:CE1	2.74	0.41
1:A:1395:TRP:H	2:A:1909:NAG:H83	1.84	0.41
1:A:1714:ASP:OD1	1:A:1715:GLY:N	2.52	0.41
1:A:275:ASN:HA	1:A:278:HIS:HE1	1.85	0.41
1:A:1596:PHE:C	1:A:1596:PHE:CD2	2.99	0.41
1:A:1622:PHE:CZ	1:A:1626:ARG:HD3	2.56	0.41
1:A:1535:MET:HE3	1:A:1535:MET:HB2	1.87	0.40
1:A:1215:ILE:HD11	1:A:1310:PRO:HA	2.03	0.40
1:A:164:PHE:O	1:A:168:TYR:CD2	2.74	0.40
1:A:803:ASN:HB3	1:A:807:LEU:HD22	2.03	0.40
1:A:886:HIS:HA	1:A:889:LEU:HD12	2.04	0.40
1:A:277:ARG:NH2	1:A:345:GLY:O	2.42	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	1145/1618 (71%)	1079 (94%)	64 (6%)	2 (0%)	43 76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	CYS
1	A	1553	SER

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	1013/1417 (72%)	983 (97%)	30 (3%)	36 69

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	TYR
1	A	219	ARG
1	A	220	THR
1	A	320	THR
1	A	365	LEU
1	A	704	MET
1	A	764	MET
1	A	776	TYR
1	A	795	GLU

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Mol	Chain	Res	Type
1	A	821	SER
1	A	900	ILE
1	A	906	CYS
1	A	923	MET
1	A	928	LEU
1	A	1194	LEU
1	A	1201	ILE
1	A	1258	TRP
1	A	1286	LEU
1	A	1302	LEU
1	A	1338	LEU
1	A	1344	PHE
1	A	1400	VAL
1	A	1419	LYS
1	A	1462	LEU
1	A	1490	GLU
1	A	1544	THR
1	A	1646	LEU
1	A	1647	LEU
1	A	1758	ILE
1	A	1766	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	275	ASN
1	A	278	HIS
1	A	371	GLN
1	A	1383	GLN
1	A	1476	GLN
1	A	1491	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

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	1903	1	14,14,15	0.79	0	17,19,21	1.29	1 (5%)
2	NAG	A	1908	1	14,14,15	0.69	0	17,19,21	0.84	0
2	NAG	A	1902	1	14,14,15	0.76	0	17,19,21	0.76	0
2	NAG	A	1905	1	14,14,15	0.72	0	17,19,21	0.88	1 (5%)
3	A1EQU	A	1910	-	43,43,43	5.70	18 (41%)	59,61,61	2.30	20 (33%)
2	NAG	A	1904	1	14,14,15	0.75	0	17,19,21	0.94	0
2	NAG	A	1906	1	14,14,15	0.74	0	17,19,21	0.86	0
2	NAG	A	1901	1	14,14,15	0.73	0	17,19,21	0.77	0
2	NAG	A	1907	1	14,14,15	0.75	0	17,19,21	0.78	0
2	NAG	A	1909	1	14,14,15	0.74	0	17,19,21	0.85	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
2	NAG	A	1903	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1908	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1902	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1905	1	-	0/6/23/26	0/1/1/1
3	A1EQU	A	1910	-	-	7/21/42/42	0/7/6/6
2	NAG	A	1904	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1906	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1901	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1907	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1909	1	-	0/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1910	A1EQU	C32-N31	-21.63	1.05	1.47
3	A	1910	A1EQU	C35-N31	-16.94	1.20	1.47
3	A	1910	A1EQU	C36-C34	-10.25	1.35	1.54
3	A	1910	A1EQU	C33-C34	-9.71	1.30	1.53
3	A	1910	A1EQU	C30-C34	-8.80	1.32	1.53
3	A	1910	A1EQU	C14-N31	-8.56	1.29	1.48
3	A	1910	A1EQU	C13-C14	7.90	1.63	1.54
3	A	1910	A1EQU	C05-C13	7.74	1.58	1.52
3	A	1910	A1EQU	C06-C16	6.06	1.60	1.49
3	A	1910	A1EQU	N23-N22	-4.45	1.24	1.39
3	A	1910	A1EQU	C33-C32	4.43	1.64	1.52
3	A	1910	A1EQU	C01-N02	3.98	1.38	1.31
3	A	1910	A1EQU	C24-N23	3.77	1.51	1.40
3	A	1910	A1EQU	C35-C36	2.98	1.60	1.55
3	A	1910	A1EQU	C30-C14	2.86	1.59	1.53
3	A	1910	A1EQU	C20-N22	2.72	1.48	1.40
3	A	1910	A1EQU	C36-C37	2.66	1.58	1.50
3	A	1910	A1EQU	O15-C13	-2.50	1.37	1.42

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1910	A1EQU	C30-C14-N31	-6.44	104.27	110.58
3	A	1910	A1EQU	C20-N22-N23	6.40	136.81	118.74
3	A	1910	A1EQU	C24-N23-N22	6.40	136.79	118.74
3	A	1910	A1EQU	C01-C06-C16	-4.92	112.15	119.52
3	A	1910	A1EQU	O15-C13-C14	3.80	117.58	109.69
2	A	1903	NAG	C1-O5-C5	3.58	117.05	112.19
3	A	1910	A1EQU	C06-C05-C13	-3.25	118.08	121.57
3	A	1910	A1EQU	C16-C06-C05	2.98	127.84	123.19
3	A	1910	A1EQU	C26-C25-C24	2.96	123.26	119.72
3	A	1910	A1EQU	C33-C34-C36	-2.83	104.21	108.31
3	A	1910	A1EQU	C13-C05-C04	2.70	124.04	119.69
3	A	1910	A1EQU	C13-C14-N31	2.53	115.80	111.93
3	A	1910	A1EQU	C17-C16-C06	2.52	125.00	120.91
3	A	1910	A1EQU	C18-C16-C06	-2.50	116.85	120.91
3	A	1910	A1EQU	O11-C09-C10	-2.38	117.95	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1910	A1EQU	C32-N31-C35	2.28	110.44	108.19
3	A	1910	A1EQU	C25-C24-N23	2.27	126.58	120.55
2	A	1905	NAG	O5-C1-C2	-2.24	107.75	111.29
3	A	1910	A1EQU	C36-C35-N31	-2.24	109.58	112.41
3	A	1910	A1EQU	C01-N02-C03	2.19	119.55	116.91
3	A	1910	A1EQU	C06-C01-N02	-2.16	121.18	124.52
3	A	1910	A1EQU	C18-C19-C20	2.07	122.69	120.30

There are no chirality outliers.

All (10) torsion outliers are listed below:

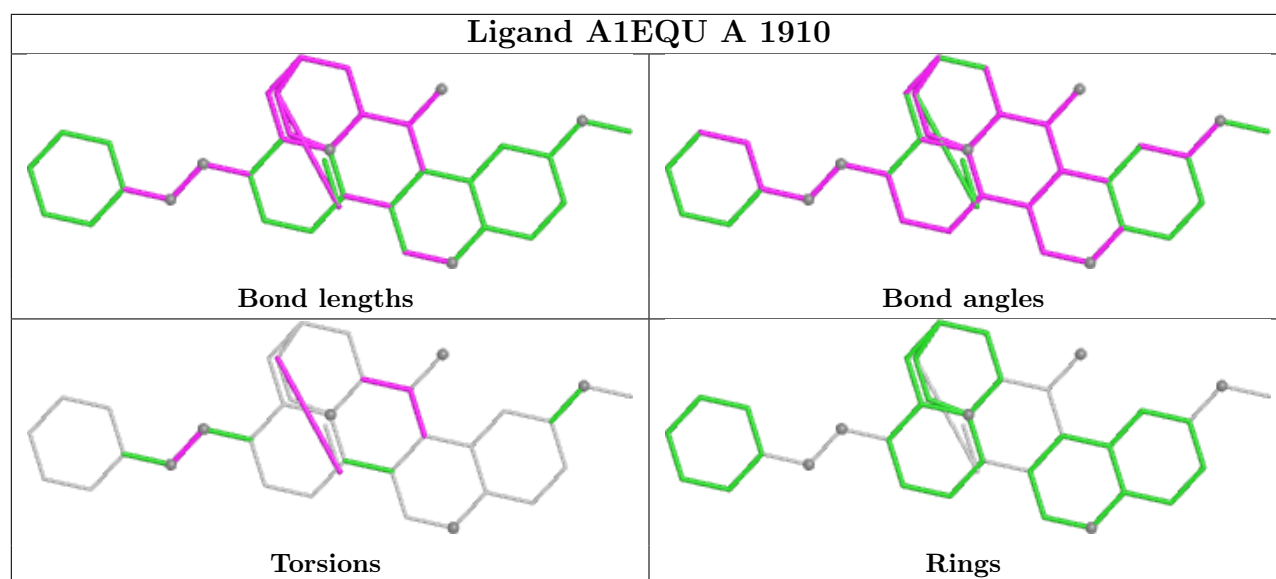
Mol	Chain	Res	Type	Atoms
3	A	1910	A1EQU	C05-C13-C14-C30
3	A	1910	A1EQU	O15-C13-C14-C30
3	A	1910	A1EQU	O15-C13-C14-N31
3	A	1910	A1EQU	C20-N22-N23-C24
2	A	1901	NAG	O5-C5-C6-O6
2	A	1904	NAG	O5-C5-C6-O6
2	A	1902	NAG	O5-C5-C6-O6
3	A	1910	A1EQU	C35-C36-C37-C38
3	A	1910	A1EQU	C04-C05-C13-O15
3	A	1910	A1EQU	C34-C36-C37-C38

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1910	A1EQU	3	0
2	A	1909	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.