



## Full wwPDB EM Validation Report ⓘ

Sep 14, 2025 – 12:16 AM JST

PDB ID : 9KNT / pdb\_00009knt  
EMDB ID : EMD-62461  
Title : ERDRP-0519-bound measles virus L-P complex  
Authors : Wang, Y.R.; Zhang, H.Q.  
Deposited on : 2024-11-19  
Resolution : 3.40 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](mailto: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>.

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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 Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

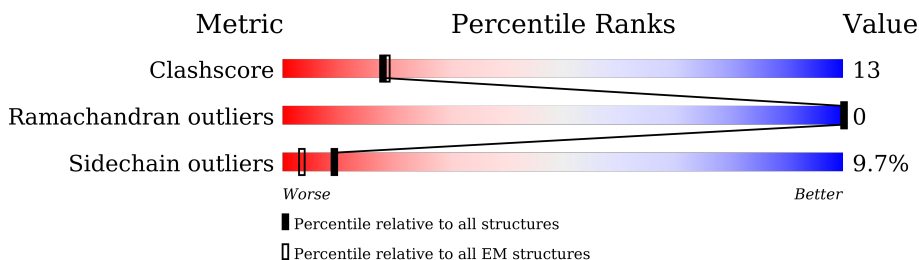
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 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	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  $\geq 3$ , 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	2183	 38% 19% 42%
2	B	507	 94%
2	C	507	 12% 7% 80%
2	D	507	 6% 92%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11580 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1275	Total	C	N	O	S	0	0
			10241	6535	1771	1876	59		

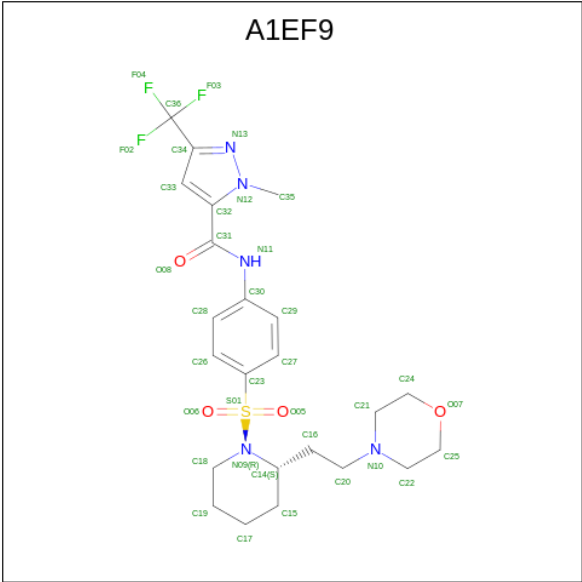
- Molecule 2 is a protein called Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	28	Total	C	N	O	S	0	0
			207	129	37	40	1		
2	D	41	Total	C	N	O	S	0	0
			305	188	53	63	1		
2	C	101	Total	C	N	O	S	0	0
			789	507	139	138	5		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Zn	0
			2	2	

- Molecule 4 is 2-methyl- {N}-[4-[(2 {S})-2-(2-morpholin-4-ylethyl)piperidin-1-yl]sulfonylphenyl]-5-(trifluoromethyl)pyrazole-3-carboxamide (CCD ID: A1EF9) (formula: C<sub>23</sub>H<sub>30</sub>F<sub>3</sub>N<sub>5</sub>O<sub>4</sub>S) (labeled as "Ligand of Interest" by depositor).

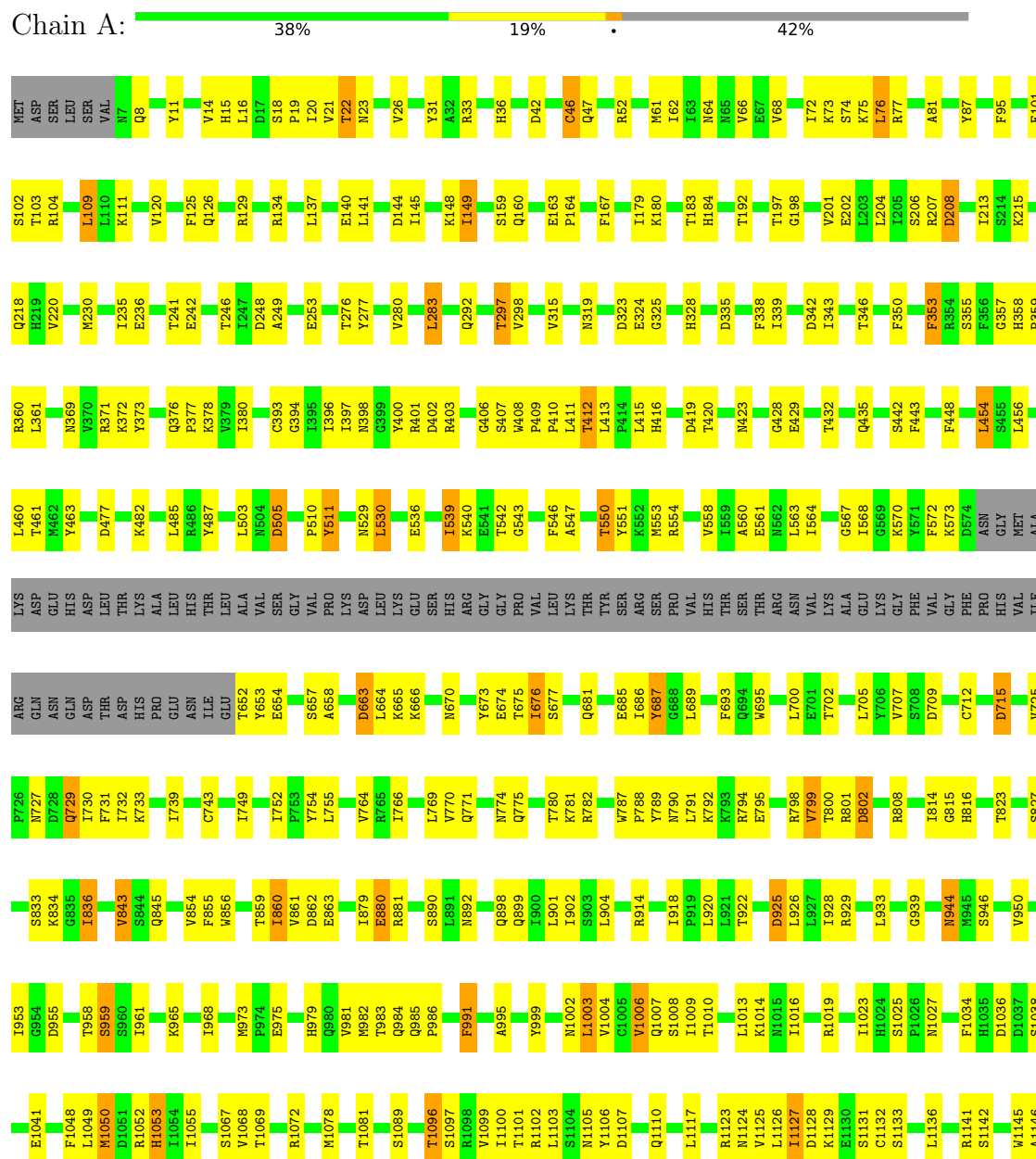


Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	N	O	S	
4	A	1	36	23	3	5	4	1	0

### 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: RNA-directed RNA polymerase L



- Molecule 2: Phosphoprotein

Chain B:  94%

[illegible]







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	111194	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (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: A1EF9, ZN

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	0.17	0/10470	0.37	0/14193
2	B	0.10	0/208	0.27	0/279
2	C	0.14	0/797	0.34	0/1060
2	D	0.15	0/309	0.59	2/421 (0.5%)
All	All	0.16	0/11784	0.38	2/15953 (0.0%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	374	ILE	CA-C-N	5.06	139.15	127.00
2	D	374	ILE	C-N-CA	5.06	139.15	127.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	686	ILE	Peptide

## 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	10241	0	10249	268	0
2	B	207	0	218	6	0
2	C	789	0	865	33	0
2	D	305	0	305	7	0
3	A	2	0	0	0	0
4	A	36	0	0	0	0
All	All	11580	0	11637	305	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 13.

All (305) 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:477:ASP:OD2	1:A:487:TYR:OH	2.02	0.78
1:A:658:ALA:HB3	1:A:800:THR:HG21	1.68	0.75
1:A:52:ARG:NH2	1:A:482:LYS:O	2.20	0.74
1:A:854:VAL:HG12	1:A:855:PHE:H	1.55	0.72
1:A:73:LYS:HA	1:A:76:LEU:HD23	1.72	0.71
1:A:995:ALA:HB2	1:A:1050:MET:HE1	1.72	0.70
1:A:394:GLY:O	1:A:398:ASN:ND2	2.24	0.70
1:A:213:ILE:HG12	1:A:220:VAL:HG13	1.74	0.70
1:A:369:ASN:HD21	1:A:666:LYS:HE2	1.57	0.68
1:A:1132:CYS:SG	1:A:1133:SER:N	2.65	0.68
1:A:1052:ARG:O	1:A:1152:ARG:NH1	2.27	0.68
1:A:652:THR:OG1	1:A:653:TYR:N	2.27	0.68
1:A:999:TYR:O	1:A:1141:ARG:NH2	2.28	0.67
1:A:925:ASP:N	1:A:925:ASP:OD1	2.29	0.66
1:A:1332:ILE:HB	1:A:1335:GLN:HG2	1.77	0.66
1:A:46:CYS:SG	1:A:47:GLN:N	2.70	0.65
1:A:357:GLY:O	1:A:358:HIS:ND1	2.29	0.65
1:A:681:GLN:NE2	1:A:685:GLU:OE2	2.30	0.65
1:A:401:ARG:HG2	1:A:406:GLY:HA2	1.77	0.65
1:A:33:ARG:HH12	1:A:66:VAL:HG22	1.62	0.65
1:A:208:ASP:OD1	1:A:208:ASP:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1166:MET:HG2	1:A:1365:VAL:HG12	1.80	0.64
1:A:456:LEU:HD11	1:A:510:PRO:HB2	1.79	0.63
1:A:795:GLU:OE2	1:A:798:ARG:NE	2.31	0.63
1:A:700:LEU:HD11	1:A:739:ILE:HD11	1.80	0.63
1:A:248:ASP:OD1	1:A:249:ALA:N	2.31	0.63
2:C:476:ASP:OD1	2:C:476:ASP:N	2.30	0.63
1:A:21:VAL:HG12	1:A:23:ASN:H	1.64	0.63
1:A:955:ASP:HB3	1:A:958:THR:HG22	1.80	0.62
1:A:1052:ARG:HD3	1:A:1380:ILE:HD12	1.82	0.62
1:A:343:ILE:O	1:A:346:THR:OG1	2.15	0.62
1:A:315:VAL:O	1:A:319:ASN:ND2	2.26	0.62
1:A:808:ARG:HD3	2:C:442:ILE:HD11	1.80	0.62
1:A:1241:ILE:HB	1:A:1266:ARG:HE	1.65	0.62
1:A:567:GLY:O	1:A:570:LYS:NZ	2.33	0.62
1:A:31:TYR:O	1:A:33:ARG:NH1	2.33	0.61
1:A:454:LEU:HG	2:D:390:LEU:HD21	1.81	0.61
1:A:505:ASP:OD2	1:A:1027:ASN:ND2	2.34	0.61
2:C:455:ASP:OD1	2:C:460:SER:OG	2.18	0.61
1:A:781:LYS:NZ	1:A:782:ARG:O	2.32	0.60
2:C:438:GLN:O	2:C:440:LYS:NZ	2.34	0.60
1:A:530:LEU:HD21	1:A:547:ALA:HB1	1.83	0.60
1:A:961:ILE:HD13	1:A:1136:LEU:HD12	1.82	0.60
1:A:862:ASP:N	1:A:862:ASP:OD1	2.34	0.59
1:A:419:ASP:O	1:A:423:ASN:ND2	2.30	0.59
2:C:497:PHE:HA	2:C:500:MET:HE2	1.83	0.59
1:A:670:ASN:HB3	1:A:816:HIS:HD2	1.67	0.59
1:A:1172:ARG:HB3	1:A:1173:ARG:HE	1.67	0.59
1:A:1105:ASN:O	1:A:1105:ASN:ND2	2.36	0.58
1:A:1237:SER:O	1:A:1240:ARG:HG3	2.03	0.58
1:A:159:SER:OG	1:A:160:GLN:N	2.36	0.58
1:A:1013:LEU:HA	1:A:1016:ILE:HG22	1.85	0.57
1:A:16:LEU:HD22	1:A:230:MET:HB2	1.86	0.57
1:A:1171:ILE:HB	1:A:1360:VAL:HB	1.86	0.57
1:A:1353:ASP:OD1	1:A:1354:THR:N	2.36	0.57
2:D:388:VAL:HG23	2:D:389:GLU:H	1.68	0.57
1:A:946:SER:HA	1:A:1163:LEU:HD12	1.87	0.56
1:A:1252:ASP:HB2	1:A:1255:SER:HB3	1.87	0.56
1:A:1357:SER:OG	1:A:1358:ASN:N	2.38	0.56
1:A:22:THR:HG22	1:A:360:ARG:HB2	1.87	0.56
1:A:790:ASN:OD1	1:A:790:ASN:N	2.39	0.56
1:A:1362:HIS:HB3	1:A:1364:HIS:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:VAL:HG21	1:A:206:SER:HB2	1.88	0.56
2:B:362:THR:O	2:B:366:HIS:ND1	2.38	0.56
1:A:674:GLU:N	1:A:674:GLU:OE1	2.36	0.56
2:B:358:ILE:O	2:B:362:THR:HG23	2.06	0.56
1:A:1003:LEU:HB2	1:A:1006:VAL:HG21	1.88	0.56
1:A:87:TYR:OH	1:A:358:HIS:O	2.18	0.56
1:A:62:ILE:O	1:A:66:VAL:HG23	2.06	0.55
1:A:790:ASN:HB2	1:A:794:ARG:HH21	1.71	0.55
1:A:198:GLY:O	1:A:215:LYS:NZ	2.29	0.55
1:A:401:ARG:NH1	1:A:428:GLY:O	2.41	0.54
2:B:373:ALA:HB2	2:C:397:ILE:HD11	1.89	0.54
1:A:95:PHE:CD1	1:A:235:ILE:HD11	2.42	0.54
1:A:432:THR:H	1:A:435:GLN:HE22	1.54	0.54
1:A:771:GLN:HE21	1:A:833:SER:H	1.56	0.54
1:A:944:ASN:ND2	1:A:959:SER:OG	2.41	0.54
2:C:375:PRO:HD2	2:C:435:LYS:HZ2	1.73	0.54
1:A:353:PHE:CZ	1:A:539:ILE:HG12	2.42	0.54
1:A:1172:ARG:N	1:A:1175:GLU:OE1	2.41	0.54
1:A:1200:ASP:OD1	1:A:1201:ILE:N	2.39	0.54
1:A:855:PHE:O	1:A:899:GLN:NE2	2.41	0.54
1:A:1193:PRO:HA	1:A:1358:ASN:HB3	1.90	0.54
1:A:1236:ARG:HH12	1:A:1277:ILE:HD11	1.72	0.54
1:A:197:THR:HA	1:A:202:GLU:HG2	1.90	0.54
1:A:1241:ILE:HG22	1:A:1266:ARG:HH11	1.73	0.54
1:A:801:ARG:HH11	2:C:444:LYS:HZ1	1.55	0.53
2:C:487:ASP:OD1	2:C:487:ASP:N	2.32	0.53
1:A:248:ASP:OD2	1:A:1349:ARG:NH2	2.41	0.53
1:A:789:TYR:HA	1:A:792:LYS:HD3	1.90	0.53
1:A:859:THR:OG1	1:A:1010:THR:OG1	2.26	0.53
1:A:1097:SER:O	1:A:1101:THR:HG23	2.08	0.53
1:A:242:GLU:O	1:A:246:THR:OG1	2.27	0.53
1:A:1272:GLU:N	1:A:1272:GLU:OE1	2.41	0.53
1:A:836:ILE:HG23	1:A:843:VAL:HG22	1.90	0.53
1:A:965:LYS:NZ	1:A:1129:LYS:O	2.41	0.53
1:A:1067:SER:OG	1:A:1068:VAL:N	2.42	0.53
1:A:1249:TYR:O	1:A:1379:ARG:NH2	2.41	0.53
1:A:754:TYR:CE2	1:A:814:ILE:HG12	2.43	0.53
1:A:134:ARG:NH1	1:A:1164:GLU:O	2.42	0.53
1:A:1036:ASP:OD1	1:A:1036:ASP:N	2.42	0.52
2:C:473:LEU:HD11	2:C:477:ARG:HD2	1.90	0.52
1:A:1176:THR:OG1	1:A:1177:CYS:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LEU:HD13	1:A:511:TYR:CE2	2.44	0.52
2:C:498:HIS:NE2	2:C:502:MET:SD	2.83	0.52
1:A:14:VAL:O	1:A:15:HIS:ND1	2.43	0.52
1:A:416:HIS:CE1	2:D:362:THR:HA	2.44	0.52
1:A:530:LEU:HB3	1:A:705:LEU:HD22	1.92	0.51
1:A:550:THR:HG22	1:A:551:TYR:H	1.76	0.51
1:A:1173:ARG:NH2	1:A:1175:GLU:OE2	2.43	0.51
1:A:944:ASN:OD1	1:A:944:ASN:N	2.37	0.51
1:A:19:PRO:HB3	1:A:536:GLU:HA	1.93	0.51
1:A:323:ASP:OD1	1:A:324:GLU:N	2.43	0.51
1:A:755:LEU:HB3	1:A:766:ILE:HD11	1.93	0.51
1:A:140:GLU:OE1	1:A:141:LEU:N	2.43	0.51
1:A:64:ASN:HD22	1:A:207:ARG:HH21	1.58	0.51
1:A:1072:ARG:HH22	1:A:1389:ARG:HH22	1.58	0.51
1:A:1362:HIS:HB3	1:A:1364:HIS:HE1	1.76	0.51
1:A:167:PHE:HE2	1:A:201:VAL:HG11	1.77	0.51
1:A:298:VAL:HG13	2:C:502:MET:HE3	1.93	0.50
1:A:402:ASP:OD1	1:A:403:ARG:N	2.43	0.50
1:A:1142:SER:O	1:A:1146:ALA:HB2	2.11	0.50
2:C:473:LEU:HD12	2:C:474:GLU:H	1.76	0.50
2:C:496:LYS:O	2:C:500:MET:HG3	2.11	0.50
1:A:1009:ILE:HD11	1:A:1106:TYR:CG	2.46	0.50
1:A:769:LEU:HD21	1:A:771:GLN:HB2	1.94	0.50
1:A:1072:ARG:HH22	1:A:1389:ARG:NH2	2.10	0.50
1:A:1237:SER:O	1:A:1239:VAL:N	2.45	0.50
1:A:1266:ARG:HG3	1:A:1399:TYR:CD2	2.45	0.49
1:A:68:VAL:HG13	1:A:204:LEU:HD21	1.94	0.49
1:A:74:SER:HA	1:A:77:ARG:HH12	1.77	0.49
1:A:880:GLU:OE1	1:A:881:ARG:N	2.45	0.49
1:A:572:PHE:CD2	1:A:749:ILE:HB	2.48	0.49
1:A:802:ASP:OD1	1:A:802:ASP:N	2.46	0.49
1:A:968:ILE:HD11	1:A:975:GLU:HA	1.94	0.49
1:A:1023:ILE:HG13	1:A:1034:PHE:HB3	1.94	0.49
1:A:407:SER:C	1:A:409:PRO:HD3	2.38	0.49
1:A:380:ILE:HG12	2:B:372:ILE:HB	1.94	0.49
1:A:335:ASP:OD1	1:A:339:ILE:HD12	2.12	0.49
1:A:400:TYR:HE2	1:A:409:PRO:HD2	1.77	0.49
1:A:1107:ASP:HA	1:A:1110:GLN:HE22	1.78	0.49
2:D:390:LEU:HD12	2:D:391:ASN:HB3	1.93	0.49
2:C:447:SER:OG	2:C:453:VAL:O	2.28	0.49
2:C:468:ILE:O	2:C:471:SER:OG	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:VAL:HG22	1:A:319:ASN:HD21	1.78	0.49
1:A:1009:ILE:HG23	1:A:1103:LEU:HD12	1.93	0.48
1:A:1368:ASP:N	1:A:1368:ASP:OD1	2.46	0.48
1:A:933:LEU:HB3	1:A:939:GLY:HA3	1.95	0.48
1:A:1007:GLN:N	1:A:1007:GLN:OE1	2.47	0.48
1:A:1400:ASP:OD1	1:A:1400:ASP:N	2.47	0.48
2:D:352:GLN:HA	2:D:355:ARG:NE	2.28	0.48
1:A:982:MET:HE1	1:A:1136:LEU:HD11	1.94	0.48
1:A:276:THR:O	1:A:280:VAL:HG23	2.13	0.48
1:A:1125:VAL:HG23	1:A:1126:LEU:HD12	1.95	0.48
1:A:654:GLU:O	1:A:782:ARG:HA	2.13	0.48
1:A:845:GLN:N	1:A:845:GLN:OE1	2.46	0.48
1:A:1306:ARG:HB2	1:A:1309:ARG:HH12	1.78	0.48
1:A:419:ASP:OD1	1:A:419:ASP:N	2.47	0.48
2:C:477:ARG:O	2:C:481:LEU:HG	2.13	0.48
1:A:991:PHE:HE1	1:A:1050:MET:HG2	1.78	0.48
1:A:529:ASN:OD1	1:A:530:LEU:N	2.45	0.47
1:A:1173:ARG:HB2	1:A:1174:HIS:CD2	2.49	0.47
1:A:1014:LYS:HG3	1:A:1081:THR:HG22	1.95	0.47
1:A:101:GLU:OE1	1:A:104:ARG:NH2	2.47	0.47
1:A:371:ARG:NH2	1:A:731:PHE:O	2.47	0.47
1:A:1173:ARG:CZ	1:A:1174:HIS:H	2.26	0.47
1:A:727:ASN:HB2	1:A:733:LYS:HB2	1.96	0.47
1:A:904:LEU:HD21	1:A:920:LEU:HD13	1.97	0.47
1:A:1166:MET:HE1	1:A:1336:GLY:HA2	1.95	0.47
1:A:1177:CYS:HB2	1:A:1180:CYS:HB3	1.96	0.47
2:C:411:LYS:HD3	2:C:436:GLU:HA	1.95	0.47
2:C:498:HIS:O	2:C:502:MET:HG2	2.15	0.47
1:A:950:VAL:HB	1:A:1335:GLN:HE21	1.79	0.47
1:A:1050:MET:HE2	1:A:1050:MET:HB2	1.60	0.47
1:A:1268:ASN:HD22	1:A:1403:PRO:HD2	1.79	0.47
2:D:388:VAL:HG23	2:D:389:GLU:N	2.30	0.47
1:A:1303:SER:O	1:A:1304:LEU:HD13	2.15	0.47
1:A:81:ALA:HB3	1:A:218:GLN:HE22	1.80	0.47
1:A:929:ARG:HG2	1:A:973:MET:HG2	1.97	0.47
1:A:950:VAL:HB	1:A:1335:GLN:NE2	2.30	0.47
1:A:1006:VAL:N	1:A:1007:GLN:OE1	2.48	0.47
2:C:496:LYS:O	2:C:496:LYS:NZ	2.49	0.46
1:A:11:TYR:HE1	1:A:180:LYS:HE3	1.80	0.46
1:A:61:MET:HG2	1:A:207:ARG:HH22	1.80	0.46
1:A:1053:HIS:CE1	1:A:1380:ILE:HG22	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:859:THR:OG1	1:A:860:ILE:N	2.48	0.46
1:A:163:GLU:HB2	1:A:164:PRO:HD3	1.96	0.46
1:A:1019:ARG:HA	1:A:1019:ARG:HD3	1.62	0.46
1:A:126:GLN:OE1	1:A:129:ARG:NH2	2.49	0.46
1:A:687:TYR:HD1	1:A:687:TYR:HA	1.67	0.46
2:C:495:ALA:O	2:C:499:GLN:HG2	2.16	0.46
2:C:474:GLU:HB3	2:C:476:ASP:OD1	2.16	0.46
1:A:283:LEU:HD13	1:A:338:PHE:HZ	1.80	0.45
1:A:705:LEU:O	1:A:732:ILE:N	2.41	0.45
1:A:1258:GLU:OE1	1:A:1258:GLU:N	2.44	0.45
2:B:371:MET:HB2	2:C:397:ILE:HB	1.98	0.45
1:A:568:ILE:H	1:A:568:ILE:HG13	1.50	0.45
1:A:1245:TYR:OH	1:A:1262:LEU:HB2	2.15	0.45
1:A:253:GLU:OE1	1:A:253:GLU:N	2.40	0.45
1:A:834:LYS:HB3	1:A:834:LYS:HE3	1.78	0.45
1:A:1096:THR:OG1	1:A:1099:VAL:HG23	2.16	0.45
1:A:774:ASN:OD1	1:A:774:ASN:N	2.47	0.45
1:A:1372:ILE:HD12	1:A:1373:PRO:HD2	1.98	0.45
2:C:481:LEU:O	2:C:485:LEU:HB2	2.16	0.45
1:A:33:ARG:NH1	1:A:66:VAL:HG22	2.30	0.45
1:A:982:MET:HB2	1:A:982:MET:HE2	1.61	0.45
1:A:1128:ASP:OD2	1:A:1131:SER:OG	2.33	0.45
1:A:111:LYS:HE3	1:A:111:LYS:HB2	1.67	0.45
1:A:378:LYS:NZ	1:A:815:GLY:O	2.35	0.45
1:A:1009:ILE:HD12	1:A:1103:LEU:HD13	1.99	0.45
1:A:657:SER:HB3	1:A:780:THR:HG22	1.98	0.45
1:A:323:ASP:OD1	1:A:325:GLY:N	2.47	0.45
1:A:1034:PHE:HE1	1:A:1072:ARG:HB3	1.82	0.45
1:A:1124:ASN:OD1	1:A:1127:ILE:N	2.50	0.45
1:A:1358:ASN:N	1:A:1358:ASN:OD1	2.38	0.45
1:A:393:CYS:O	1:A:397:ILE:HG12	2.16	0.44
1:A:854:VAL:HG12	1:A:855:PHE:N	2.30	0.44
1:A:918:ILE:O	1:A:922:THR:HG22	2.17	0.44
2:C:448:SER:OG	2:C:450:VAL:HG12	2.16	0.44
1:A:343:ILE:HD12	1:A:343:ILE:H	1.83	0.44
1:A:687:TYR:HD2	1:A:693:PHE:HE2	1.64	0.44
1:A:372:LYS:HE2	1:A:372:LYS:HB3	1.72	0.44
1:A:673:TYR:HA	1:A:676:ILE:HG22	1.98	0.44
1:A:1048:PHE:CZ	1:A:1386:LEU:HD12	2.53	0.44
1:A:11:TYR:CE2	1:A:861:VAL:HG13	2.52	0.44
1:A:407:SER:C	1:A:408:TRP:HD1	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1038:SER:O	1:A:1041:GLU:HG2	2.18	0.44
1:A:87:TYR:OH	1:A:230:MET:HE1	2.18	0.44
1:A:670:ASN:HB3	1:A:816:HIS:CD2	2.51	0.44
1:A:709:ASP:N	1:A:712:CYS:SG	2.88	0.44
1:A:1337:MET:N	1:A:1337:MET:HE2	2.33	0.44
1:A:1194:SER:O	1:A:1194:SER:OG	2.31	0.43
1:A:1178:VAL:HG13	1:A:1179:ILE:H	1.82	0.43
1:A:1266:ARG:O	1:A:1399:TYR:HB2	2.17	0.43
1:A:42:ASP:OD1	1:A:42:ASP:N	2.35	0.43
1:A:791:LEU:HA	1:A:794:ARG:HD2	2.00	0.43
1:A:1102:ARG:HD3	1:A:1103:LEU:HD22	2.00	0.43
1:A:144:ASP:OD1	1:A:144:ASP:N	2.42	0.43
1:A:764:VAL:HG11	1:A:799:VAL:HG11	2.00	0.43
1:A:754:TYR:CZ	1:A:814:ILE:HG12	2.53	0.43
2:C:394:LEU:HD13	2:C:396:PRO:HD3	2.00	0.43
1:A:8:GLN:OE1	1:A:8:GLN:N	2.47	0.42
1:A:315:VAL:HG22	1:A:319:ASN:ND2	2.34	0.42
1:A:1167:ARG:O	1:A:1363:LEU:HD12	2.19	0.42
1:A:542:THR:OG1	1:A:543:GLY:N	2.52	0.42
1:A:52:ARG:HH21	1:A:485:LEU:H	1.66	0.42
1:A:297:THR:O	1:A:297:THR:OG1	2.36	0.42
1:A:715:ASP:OD1	1:A:729:GLN:NE2	2.53	0.42
1:A:984:GLN:HB3	1:A:1117:LEU:HD13	2.01	0.42
1:A:503:LEU:O	1:A:1025:SER:OG	2.37	0.42
1:A:573:LYS:HA	1:A:573:LYS:HD3	1.83	0.42
1:A:715:ASP:OD1	1:A:715:ASP:N	2.36	0.42
1:A:561:GLU:OE1	1:A:743:CYS:HA	2.19	0.42
1:A:1002:ASN:HB3	1:A:1145:TRP:CZ2	2.54	0.42
1:A:1178:VAL:O	1:A:1181:GLU:HG3	2.19	0.42
2:D:352:GLN:HG2	2:D:353:ILE:H	1.85	0.42
1:A:461:THR:HA	1:A:1078:MET:HE3	2.01	0.42
1:A:554:ARG:O	1:A:558:VAL:HG12	2.20	0.42
1:A:801:ARG:NH1	2:C:444:LYS:HZ1	2.17	0.42
1:A:1253:ASP:OD1	1:A:1253:ASP:N	2.51	0.42
1:A:20:ILE:HD12	1:A:20:ILE:H	1.84	0.42
1:A:400:TYR:CD2	1:A:411:LEU:HD21	2.55	0.42
1:A:572:PHE:CE2	1:A:749:ILE:HB	2.55	0.42
1:A:663:ASP:OD1	1:A:665:LYS:N	2.53	0.42
1:A:1170:LEU:HD23	1:A:1170:LEU:HA	1.84	0.42
1:A:560:ALA:O	1:A:564:ILE:HG22	2.20	0.41
1:A:1343:VAL:HA	1:A:1346:THR:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:371:MET:HE3	2:C:371:MET:HB3	1.79	0.41
1:A:1245:TYR:OH	1:A:1259:ALA:HA	2.21	0.41
1:A:8:GLN:HA	1:A:184:HIS:NE2	2.35	0.41
1:A:788:PRO:HG2	1:A:791:LEU:HB2	2.02	0.41
1:A:148:LYS:H	1:A:148:LYS:HG2	1.68	0.41
2:C:492:ASN:OD1	2:C:492:ASN:N	2.52	0.41
1:A:412:THR:HG23	1:A:448:PHE:CD1	2.56	0.41
1:A:985:GLN:HG2	1:A:986:PRO:HD2	2.03	0.41
1:A:1238:ALA:HA	1:A:1240:ARG:CZ	2.50	0.41
2:C:438:GLN:CD	2:C:439:LEU:H	2.29	0.41
1:A:448:PHE:N	1:A:685:GLU:OE1	2.29	0.41
1:A:664:LEU:HD11	1:A:775:GLN:HB2	2.01	0.41
1:A:860:ILE:H	1:A:860:ILE:HG12	1.74	0.41
1:A:539:ILE:HD12	1:A:540:LYS:HG3	2.03	0.41
1:A:979:HIS:CD2	1:A:1123:ARG:HD3	2.55	0.41
1:A:1002:ASN:HB3	1:A:1145:TRP:CE2	2.56	0.41
1:A:1050:MET:HG3	1:A:1055:ILE:HG23	2.02	0.41
1:A:1339:LEU:O	1:A:1343:VAL:HG12	2.19	0.41
2:C:411:LYS:HE2	2:C:434:LEU:C	2.46	0.41
1:A:277:TYR:CD2	1:A:359:PRO:HB3	2.56	0.41
1:A:353:PHE:HZ	1:A:539:ILE:HG12	1.85	0.41
1:A:109:LEU:HA	1:A:109:LEU:HD22	1.84	0.40
1:A:376:GLN:HA	1:A:377:PRO:HD3	1.94	0.40
1:A:567:GLY:HA3	1:A:687:TYR:OH	2.21	0.40
1:A:1237:SER:OG	1:A:1238:ALA:N	2.51	0.40
2:B:355:ARG:O	2:B:358:ILE:HG13	2.20	0.40
1:A:409:PRO:HB2	1:A:410:PRO:HD3	2.03	0.40
1:A:442:SER:OG	1:A:443:PHE:N	2.53	0.40
1:A:695:TRP:H	1:A:695:TRP:CD1	2.39	0.40
1:A:856:TRP:CE3	1:A:862:ASP:HB2	2.56	0.40
1:A:125:PHE:HB2	1:A:149:ILE:HG21	2.03	0.40
1:A:1333:TYR:O	1:A:1337:MET:HG2	2.22	0.40
2:C:504:ILE:HA	2:C:507:LYS:HD2	2.03	0.40
2:C:505:ILE:HG13	2:C:506:MET:N	2.36	0.40
1:A:342:ASP:O	1:A:346:THR:HG23	2.22	0.40
1:A:408:TRP:N	1:A:409:PRO:HD3	2.35	0.40
1:A:1157:LEU:HB3	1:A:1158:GLU:OE1	2.21	0.40
1:A:120:VAL:HG21	1:A:928:ILE:HD11	2.02	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	1267/2183 (58%)	1183 (93%)	84 (7%)	0	100	100
2	B	26/507 (5%)	25 (96%)	1 (4%)	0	100	100
2	C	95/507 (19%)	87 (92%)	8 (8%)	0	100	100
2	D	39/507 (8%)	33 (85%)	6 (15%)	0	100	100
All	All	1427/3704 (38%)	1328 (93%)	99 (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	1137/1945 (58%)	1022 (90%)	115 (10%)	6	22
2	B	24/416 (6%)	23 (96%)	1 (4%)	25	51
2	C	88/416 (21%)	82 (93%)	6 (7%)	13	38
2	D	36/416 (9%)	33 (92%)	3 (8%)	9	30
All	All	1285/3193 (40%)	1160 (90%)	125 (10%)	9	24

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	SER
1	A	22	THR

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Mol	Chain	Res	Type
1	A	26	VAL
1	A	36	HIS
1	A	46	CYS
1	A	72	ILE
1	A	75	LYS
1	A	76	LEU
1	A	102	SER
1	A	103	THR
1	A	109	LEU
1	A	137	LEU
1	A	145	ILE
1	A	149	ILE
1	A	179	ILE
1	A	183	THR
1	A	192	THR
1	A	208	ASP
1	A	236	GLU
1	A	241	THR
1	A	283	LEU
1	A	292	GLN
1	A	297	THR
1	A	328	HIS
1	A	350	PHE
1	A	353	PHE
1	A	355	SER
1	A	361	LEU
1	A	373	TYR
1	A	396	ILE
1	A	412	THR
1	A	413	LEU
1	A	415	LEU
1	A	420	THR
1	A	429	GLU
1	A	454	LEU
1	A	460	LEU
1	A	463	TYR
1	A	505	ASP
1	A	511	TYR
1	A	530	LEU
1	A	539	ILE
1	A	546	PHE
1	A	550	THR

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Mol	Chain	Res	Type
1	A	553	MET
1	A	563	LEU
1	A	663	ASP
1	A	675	THR
1	A	676	ILE
1	A	677	SER
1	A	687	TYR
1	A	689	LEU
1	A	702	THR
1	A	707	VAL
1	A	715	ASP
1	A	725	VAL
1	A	729	GLN
1	A	730	ILE
1	A	752	ILE
1	A	770	VAL
1	A	787	TRP
1	A	799	VAL
1	A	802	ASP
1	A	823	THR
1	A	827	SER
1	A	836	ILE
1	A	843	VAL
1	A	860	ILE
1	A	863	GLU
1	A	879	ILE
1	A	880	GLU
1	A	890	SER
1	A	892	ASN
1	A	898	GLN
1	A	901	LEU
1	A	902	ILE
1	A	914	ARG
1	A	925	ASP
1	A	926	LEU
1	A	944	ASN
1	A	953	ILE
1	A	959	SER
1	A	981	VAL
1	A	983	THR
1	A	991	PHE
1	A	1003	LEU

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Mol	Chain	Res	Type
1	A	1004	VAL
1	A	1006	VAL
1	A	1008	SER
1	A	1049	LEU
1	A	1050	MET
1	A	1053	HIS
1	A	1069	THR
1	A	1089	SER
1	A	1096	THR
1	A	1100	ILE
1	A	1127	ILE
1	A	1162	VAL
1	A	1163	LEU
1	A	1173	ARG
1	A	1178	VAL
1	A	1179	ILE
1	A	1192	VAL
1	A	1233	ARG
1	A	1235	LEU
1	A	1240	ARG
1	A	1243	THR
1	A	1270	SER
1	A	1313	ILE
1	A	1318	LEU
1	A	1331	PHE
1	A	1350	LEU
1	A	1360	VAL
1	A	1372	ILE
1	A	1391	GLU
2	B	370	ILE
2	D	358	ILE
2	D	370	ILE
2	D	372	ILE
2	C	374	ILE
2	C	397	ILE
2	C	434	LEU
2	C	476	ASP
2	C	487	ASP
2	C	496	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	84	HIS
1	A	91	ASN
1	A	191	HIS
1	A	218	GLN
1	A	313	HIS
1	A	369	ASN
1	A	398	ASN
1	A	425	GLN
1	A	562	ASN
1	A	729	GLN
1	A	771	GLN
1	A	809	GLN
1	A	816	HIS
1	A	817	HIS
1	A	892	ASN
1	A	1024	HIS
1	A	1268	ASN
1	A	1330	ASN
1	A	1335	GLN
2	D	356	GLN
2	D	366	HIS
2	D	382	ASN
2	C	499	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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
4	A1EF9	A	2203	-	38,39,39	4.02	19 (50%)	50,57,57	2.51	12 (24%)

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	A1EF9	A	2203	-	-	4/28/50/50	0/4/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2203	A1EF9	C20-N10	-8.95	1.26	1.47
4	A	2203	A1EF9	C26-C23	8.87	1.52	1.38
4	A	2203	A1EF9	C27-C23	8.70	1.52	1.38
4	A	2203	A1EF9	C29-C30	8.05	1.52	1.39
4	A	2203	A1EF9	C28-C30	8.00	1.52	1.39
4	A	2203	A1EF9	C28-C26	7.72	1.52	1.38
4	A	2203	A1EF9	C29-C27	7.69	1.52	1.38
4	A	2203	A1EF9	S01-N09	5.01	1.71	1.63
4	A	2203	A1EF9	C31-N11	3.49	1.45	1.35
4	A	2203	A1EF9	C23-S01	3.42	1.81	1.76
4	A	2203	A1EF9	C21-N10	-3.00	1.38	1.46
4	A	2203	A1EF9	C17-C15	-2.96	1.45	1.53
4	A	2203	A1EF9	C22-N10	-2.94	1.38	1.46
4	A	2203	A1EF9	O06-S01	2.64	1.46	1.43
4	A	2203	A1EF9	C33-C34	-2.60	1.36	1.39
4	A	2203	A1EF9	O05-S01	2.56	1.46	1.43
4	A	2203	A1EF9	C18-N09	2.55	1.52	1.48
4	A	2203	A1EF9	O08-C31	-2.29	1.18	1.23
4	A	2203	A1EF9	C33-C32	-2.09	1.36	1.39

All (12) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2203	A1EF9	O06-S01-O05	-10.96	101.75	119.52
4	A	2203	A1EF9	C18-N09-C14	-6.22	108.13	116.10
4	A	2203	A1EF9	C36-C34-N13	6.17	126.98	119.72
4	A	2203	A1EF9	C34-N13-N12	4.97	108.10	104.37
4	A	2203	A1EF9	O06-S01-C23	3.17	112.06	108.05
4	A	2203	A1EF9	C16-C14-C15	-3.17	107.75	112.58
4	A	2203	A1EF9	O06-S01-N09	2.87	112.19	106.97
4	A	2203	A1EF9	C33-C34-C36	-2.64	125.11	127.93
4	A	2203	A1EF9	O05-S01-C23	2.58	111.32	108.05
4	A	2203	A1EF9	O05-S01-N09	2.53	111.58	106.97
4	A	2203	A1EF9	C33-C34-N13	-2.42	107.91	111.41
4	A	2203	A1EF9	C19-C18-N09	2.04	113.31	110.31

There are no chirality outliers.

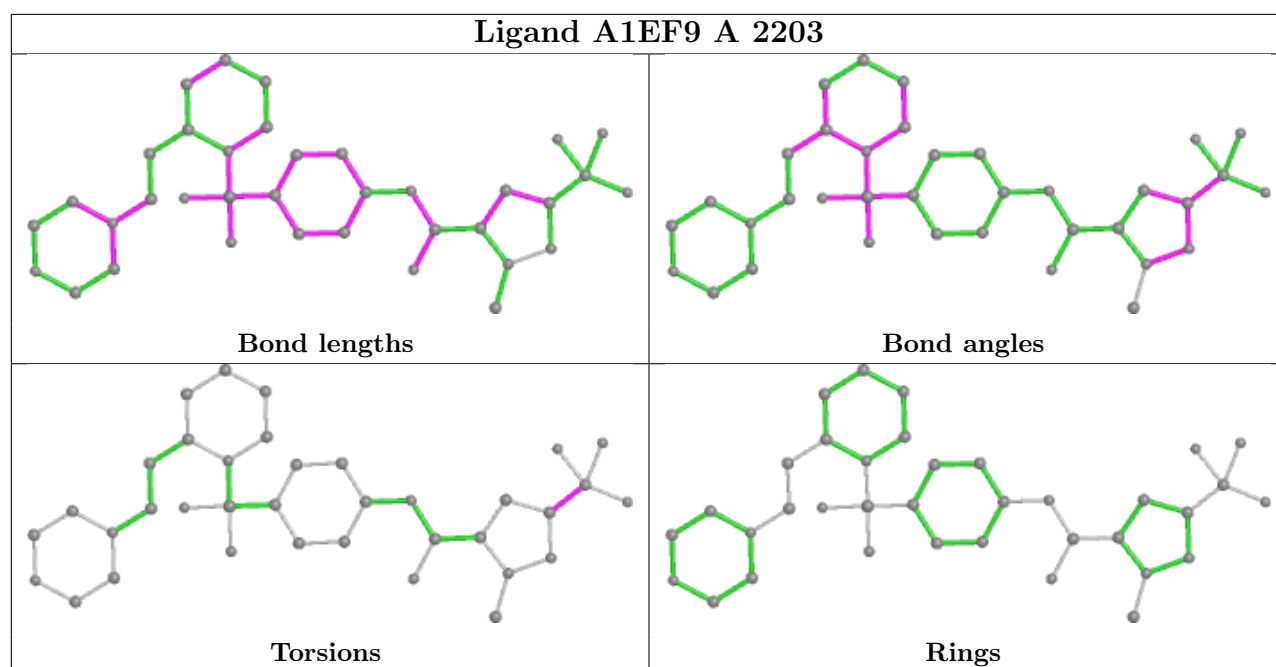
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2203	A1EF9	N13-C34-C36-F04
4	A	2203	A1EF9	N13-C34-C36-F02
4	A	2203	A1EF9	N13-C34-C36-F03
4	A	2203	A1EF9	C33-C34-C36-F02

There are no ring outliers.

No monomer is involved in short contacts.

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.