



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:48 PM BST

PDB ID : 3J9S
EMDB ID: : EMD-6272
Title : Single particle cryo-EM structure of rotavirus VP6 at 2.6 Angstrom resolution
Authors : Grant, T.; Grigorieff, N.
Deposited on : 2015-02-19
Resolution : 2.60 Å(reported)
Based on PDB ID : 1QHD

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

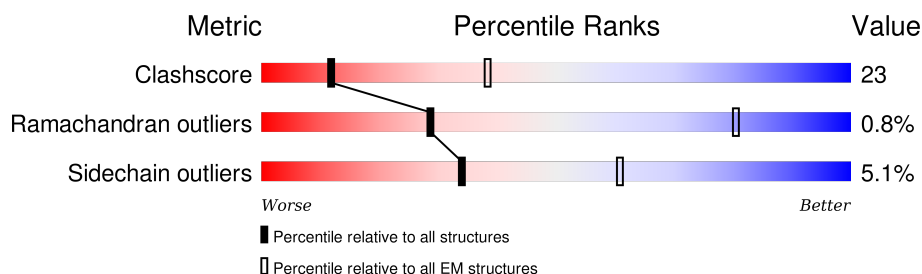
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


The reported resolution of this entry is 2.60 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	398	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3271 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 Intermediate capsid protein VP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	398	Total	C	N	O	S	0	0
			3162	2004	546	597	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ACE	-	ACETYLATION	UNP P04509

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Cl	0
			1	1	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Ca	0
			2	2	

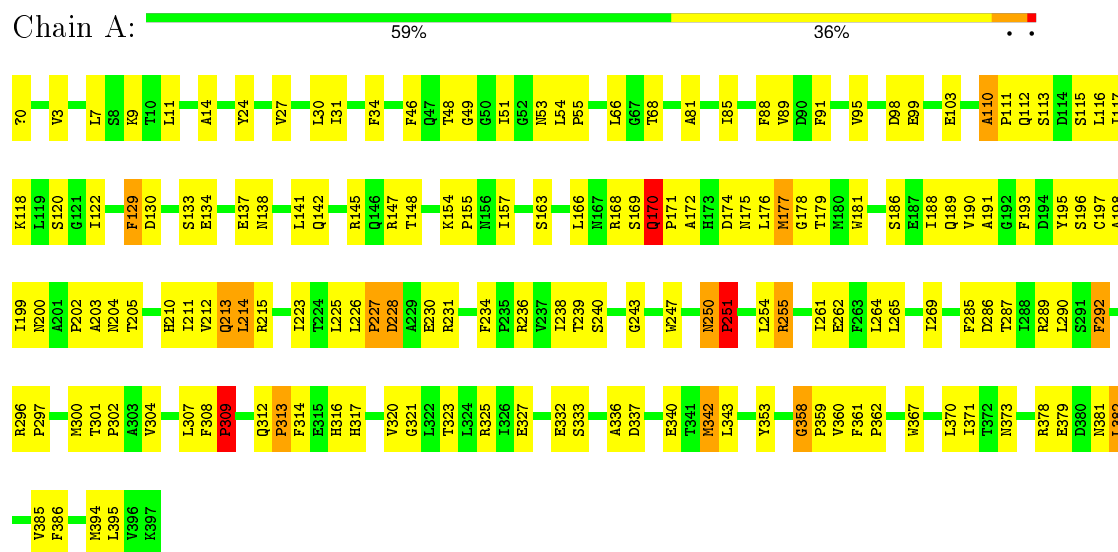
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	105	Total	O	0
			105	105	

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 errors 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: Intermediate capsid protein VP6



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C	Depositor
Number of images	4000	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 (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: ZN, CA, ACE, CL

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	1.00	5/3230 (0.2%)	0.78	10/4396 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	PRO	N-CD	5.79	1.55	1.47
1	A	362	PRO	N-CD	5.24	1.55	1.47
1	A	359	PRO	N-CD	5.21	1.55	1.47
1	A	227	PRO	N-CD	5.18	1.55	1.47
1	A	171	PRO	N-CD	5.08	1.54	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	ASN	C-N-CD	6.42	141.88	128.40
1	A	251	PRO	CA-N-CD	-6.02	103.07	111.50
1	A	308	PHE	C-N-CD	5.97	140.94	128.40
1	A	110	ALA	C-N-CD	5.88	140.74	128.40
1	A	170	GLN	C-N-CD	5.73	140.43	128.40
1	A	309	PRO	CA-N-CD	-5.68	103.55	111.50
1	A	358	GLY	C-N-CD	5.67	140.31	128.40
1	A	226	LEU	C-N-CD	5.66	140.29	128.40
1	A	361	PHE	C-N-CD	5.57	140.10	128.40
1	A	234	PHE	C-N-CD	5.44	139.83	128.40

There are no chirality outliers.

There are no planarity outliers.

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	3162	0	3103	143	0
2	A	1	0	0	0	0
3	A	1	0	0	1	0
4	A	2	0	0	0	0
5	A	105	0	0	4	0
All	All	3271	0	3103	143	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 23.

All (143) 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:261:ILE:CD1	1:A:290:LEU:HD23	1.54	1.35
1:A:261:ILE:HD12	1:A:290:LEU:HD23	1.23	1.17
1:A:111:PRO:HB3	1:A:116:LEU:HD23	1.38	1.05
1:A:103:GLU:HG3	1:A:360:VAL:HG23	1.47	0.93
1:A:199:ILE:HB	1:A:296:ARG:NH1	1.84	0.92
1:A:175:ASN:ND2	1:A:314:PHE:HE2	1.68	0.92
1:A:261:ILE:HD12	1:A:290:LEU:CD2	2.01	0.91
1:A:170:GLN:OE1	1:A:175:ASN:HB3	1.69	0.91
1:A:213:GLN:HG2	5:A:645:HOH:O	1.70	0.90
1:A:163:SER:HB3	1:A:181:TRP:CZ2	2.08	0.88
1:A:103:GLU:HG3	1:A:360:VAL:CG2	2.03	0.88
1:A:262:GLU:OE1	1:A:269:ILE:HG12	1.74	0.87
1:A:138:ASN:OD1	1:A:148:THR:HB	1.75	0.86
1:A:261:ILE:CD1	1:A:290:LEU:CD2	2.49	0.85
1:A:169:SER:HA	1:A:176:LEU:CD2	2.06	0.84
1:A:99:GLU:OE1	1:A:113:SER:HB3	1.78	0.83
1:A:27:VAL:O	1:A:31:ILE:HG12	1.81	0.81
1:A:188:ILE:HD13	1:A:212:VAL:HG21	1.63	0.80
1:A:261:ILE:HD11	1:A:290:LEU:HD23	1.62	0.79
1:A:175:ASN:HD22	1:A:314:PHE:HE2	1.31	0.79
1:A:175:ASN:ND2	1:A:314:PHE:CE2	2.50	0.78
1:A:172:ALA:HB3	1:A:174:ASP:OD1	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:GLN:OE1	1:A:175:ASN:CB	2.32	0.77
1:A:148:THR:O	1:A:332:GLU:HG2	1.85	0.76
1:A:227:PRO:O	1:A:228:ASP:HB2	1.87	0.75
1:A:337:ASP:OD1	1:A:340:GLU:HB2	1.88	0.73
1:A:170:GLN:OE1	1:A:175:ASN:N	2.22	0.72
1:A:307:LEU:HD13	1:A:316:HIS:ND1	2.05	0.72
1:A:169:SER:HA	1:A:176:LEU:HD21	1.71	0.72
1:A:342:MET:CE	1:A:386:PHE:O	2.38	0.72
1:A:103:GLU:OE2	1:A:358:GLY:HA3	1.91	0.70
1:A:46:PHE:CE2	1:A:118:LYS:HD3	2.26	0.69
1:A:166:LEU:HD22	1:A:176:LEU:HD22	1.74	0.69
1:A:170:GLN:OE1	1:A:175:ASN:CA	2.41	0.69
1:A:172:ALA:CB	1:A:174:ASP:OD1	2.41	0.68
1:A:265:LEU:HA	1:A:286:ASP:OD1	1.94	0.67
1:A:168:ARG:O	1:A:176:LEU:HD23	1.94	0.67
1:A:190:VAL:HG21	1:A:210:HIS:HB2	1.78	0.66
1:A:312:GLN:HB3	1:A:313:PRO:HA	1.78	0.65
1:A:178:GLY:O	1:A:193:PHE:CD2	2.49	0.65
1:A:48:THR:HG22	1:A:115:SER:OG	1.96	0.65
1:A:238:ILE:HG22	1:A:239:THR:O	1.96	0.65
1:A:99:GLU:OE1	1:A:113:SER:CB	2.44	0.65
1:A:289:ARG:HG3	1:A:289:ARG:O	1.96	0.65
1:A:157:ILE:HG13	1:A:157:ILE:O	1.97	0.64
1:A:228:ASP:N	1:A:321:GLY:O	2.28	0.64
1:A:113:SER:O	1:A:117:ILE:HG13	1.97	0.64
1:A:178:GLY:O	1:A:193:PHE:CE2	2.52	0.63
1:A:169:SER:HA	1:A:176:LEU:HD23	1.78	0.63
1:A:91:PHE:O	1:A:95:VAL:HG23	1.98	0.63
1:A:9:LYS:HD3	1:A:394:MET:HE1	1.81	0.62
1:A:250:ASN:O	1:A:317:HIS:ND1	2.33	0.61
1:A:133:SER:O	1:A:137:GLU:HG3	2.01	0.61
1:A:154:LYS:HE3	3:A:502:CL:CL	2.38	0.61
1:A:254:LEU:O	1:A:320:VAL:HG12	2.02	0.60
1:A:269:ILE:H	1:A:269:ILE:HD12	1.66	0.60
1:A:170:GLN:NE2	1:A:175:ASN:O	2.35	0.59
1:A:373:ASN:O	1:A:378:ARG:NH1	2.36	0.59
1:A:9:LYS:HD3	1:A:394:MET:CE	2.32	0.59
1:A:81:ALA:O	1:A:85:ILE:HG13	2.03	0.58
1:A:168:ARG:O	1:A:176:LEU:CD2	2.52	0.57
1:A:261:ILE:HD13	1:A:290:LEU:HD23	1.71	0.57
1:A:196:SER:O	1:A:197:CYS:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PRO:O	1:A:228:ASP:CB	2.52	0.57
1:A:3:VAL:HG21	5:A:620:HOH:O	2.06	0.56
1:A:214:LEU:N	1:A:214:LEU:HD23	2.21	0.56
1:A:202:PRO:O	1:A:203:ALA:HB3	2.06	0.56
1:A:262:GLU:OE1	1:A:269:ILE:CG1	2.52	0.55
1:A:24:TYR:OH	1:A:68:THR:HG22	2.07	0.55
1:A:255:ARG:HG3	1:A:255:ARG:NH1	2.22	0.55
1:A:292:PHE:CD1	1:A:292:PHE:N	2.75	0.55
1:A:312:GLN:HG2	1:A:314:PHE:CE2	2.42	0.54
1:A:163:SER:HB3	1:A:181:TRP:CE2	2.42	0.54
1:A:312:GLN:CB	1:A:313:PRO:HA	2.37	0.53
1:A:197:CYS:O	1:A:198:ALA:HB3	2.09	0.53
1:A:122:ILE:HD12	1:A:122:ILE:O	2.09	0.52
1:A:239:THR:CG2	1:A:240:SER:N	2.73	0.52
1:A:239:THR:HG22	1:A:240:SER:N	2.24	0.52
1:A:367:TRP:O	1:A:371:ILE:HG22	2.09	0.52
1:A:14:ALA:HA	1:A:30:LEU:HD21	1.93	0.51
1:A:200:ASN:HB2	5:A:696:HOH:O	2.10	0.51
1:A:177:MET:HA	1:A:193:PHE:O	2.11	0.51
1:A:0:ACE:CH3	1:A:120:SER:HB3	2.41	0.50
1:A:307:LEU:HD13	1:A:316:HIS:CG	2.46	0.50
1:A:231:ARG:HH11	1:A:231:ARG:HG3	1.77	0.50
1:A:51:ILE:O	1:A:51:ILE:HG23	2.11	0.50
1:A:34:PHE:CD2	1:A:66:LEU:HD11	2.47	0.50
1:A:110:ALA:O	1:A:112:GLN:NE2	2.45	0.49
1:A:145:ARG:HG3	1:A:145:ARG:O	2.12	0.49
1:A:211:ILE:HG12	1:A:289:ARG:HB2	1.95	0.49
1:A:301:THR:HB	1:A:302:PRO:CD	2.43	0.49
1:A:301:THR:HB	1:A:302:PRO:HD2	1.94	0.49
1:A:49:GLY:N	1:A:98:ASP:OD2	2.37	0.48
1:A:85:ILE:O	1:A:89:VAL:HG23	2.14	0.48
1:A:360:VAL:HG11	1:A:381:ASN:CG	2.33	0.48
1:A:223:ILE:HG23	1:A:325:ARG:O	2.14	0.48
1:A:24:TYR:OH	1:A:68:THR:CG2	2.62	0.48
1:A:342:MET:HE3	1:A:386:PHE:O	2.14	0.47
1:A:53:ASN:HB2	1:A:353:TYR:O	2.14	0.47
1:A:129:PHE:CD2	1:A:130:ASP:HB2	2.50	0.47
1:A:382:LEU:O	1:A:385:VAL:HG22	2.15	0.47
1:A:175:ASN:HB2	1:A:312:GLN:NE2	2.29	0.47
1:A:46:PHE:CD2	1:A:118:LYS:HD3	2.49	0.47
1:A:103:GLU:HG3	1:A:360:VAL:CB	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PRO:O	1:A:186:SER:HB3	2.15	0.46
1:A:7:LEU:O	1:A:11:LEU:HG	2.14	0.46
1:A:297:PRO:HD2	1:A:300:MET:HE2	1.98	0.46
1:A:177:MET:CG	1:A:177:MET:O	2.64	0.46
1:A:309:PRO:O	1:A:309:PRO:HD2	2.16	0.46
1:A:342:MET:HE1	1:A:386:PHE:O	2.13	0.46
1:A:239:THR:CG2	1:A:240:SER:H	2.28	0.46
1:A:336:ALA:HB2	1:A:343:LEU:HD22	1.97	0.46
1:A:170:GLN:N	1:A:170:GLN:HE21	2.14	0.46
1:A:24:TYR:OH	1:A:68:THR:HB	2.16	0.46
1:A:255:ARG:HH11	1:A:255:ARG:HG3	1.81	0.45
1:A:333:SER:OG	1:A:379:GLU:OE2	2.35	0.45
1:A:264:LEU:O	1:A:286:ASP:OD1	2.35	0.45
1:A:255:ARG:HH11	1:A:255:ARG:CG	2.29	0.45
1:A:176:LEU:O	1:A:195:TYR:CD1	2.70	0.44
1:A:231:ARG:NH1	1:A:231:ARG:HG3	2.32	0.44
1:A:215:ARG:HG3	1:A:371:ILE:O	2.17	0.44
1:A:170:GLN:NE2	1:A:176:LEU:HD23	2.32	0.44
1:A:196:SER:O	1:A:197:CYS:CB	2.66	0.44
1:A:170:GLN:CD	1:A:175:ASN:O	2.56	0.43
1:A:203:ALA:O	1:A:204:ASN:HB2	2.18	0.43
1:A:214:LEU:HD11	1:A:285:PHE:CE2	2.54	0.42
1:A:307:LEU:CD1	1:A:316:HIS:CG	3.02	0.42
1:A:342:MET:H	1:A:342:MET:HG2	1.61	0.42
1:A:11:LEU:HD21	1:A:88:PHE:HB3	2.00	0.42
1:A:382:LEU:HD23	1:A:382:LEU:HA	1.93	0.42
1:A:141:LEU:HB2	1:A:148:THR:HG22	2.02	0.42
1:A:297:PRO:HD2	1:A:300:MET:CE	2.50	0.42
1:A:251:PRO:HA	1:A:317:HIS:O	2.20	0.41
1:A:189:GLN:HG3	1:A:323:THR:HG23	2.01	0.41
1:A:11:LEU:HD12	1:A:395:LEU:HD11	2.00	0.41
1:A:327:GLU:CD	5:A:609:HOH:O	2.59	0.41
1:A:304:VAL:O	1:A:307:LEU:HB2	2.20	0.41
1:A:213:GLN:HG3	1:A:287:THR:HG23	2.02	0.41
1:A:240:SER:O	1:A:243:GLY:N	2.54	0.41
1:A:54:LEU:HA	1:A:55:PRO:HD3	1.89	0.41
1:A:197:CYS:SG	1:A:197:CYS:O	2.78	0.41
1:A:54:LEU:HD12	1:A:55:PRO:HD2	2.03	0.40
1:A:179:THR:HA	1:A:191:ALA:O	2.21	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	396/398 (100%)	388 (98%)	5 (1%)	3 (1%)	24	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	PRO
1	A	228	ASP
1	A	251	PRO

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	350/350 (100%)	332 (95%)	18 (5%)	29	55

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	PHE
1	A	134	GLU
1	A	142	GLN
1	A	147	ARG
1	A	170	GLN
1	A	177	MET
1	A	205	THR
1	A	213	GLN

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Mol	Chain	Res	Type
1	A	214	LEU
1	A	225	LEU
1	A	230	GLU
1	A	236	ARG
1	A	247	TRP
1	A	255	ARG
1	A	292	PHE
1	A	342	MET
1	A	370	LEU
1	A	382	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.