



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 10, 2023 – 11:29 PM EDT

PDB ID : 1AL2
Title : P1/MAHONEY POLIOVIRUS, SINGLE SITE MUTANT V1160I
Authors : Wien, M.W.; Curry, S.; Filman, D.J.; Hogle, J.M.
Deposited on : 1997-06-09
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.2

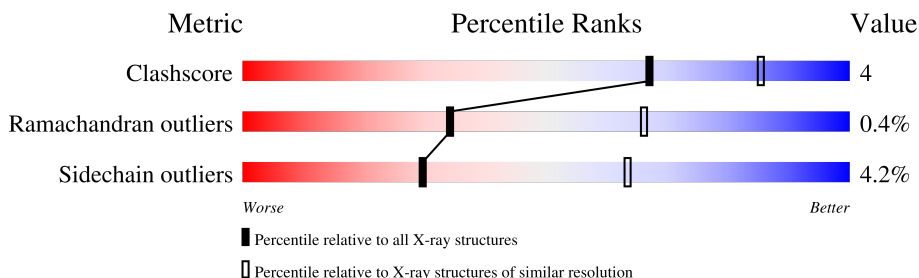
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	5	
2	1	302	
3	2	272	
4	3	238	
5	4	68	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SPH	1	0	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7203 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 P1/MAHONEY POLIOVIRUS.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	0	5	29	15	5	9	0	0	0

- Molecule 2 is a protein called P1/MAHONEY POLIOVIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	1	283	2223	1417	378	423	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	160	ILE	VAL	engineered mutation	UNP P03300

- Molecule 3 is a protein called P1/MAHONEY POLIOVIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	2	268	2085	1317	358	396	14	0	0	0

- Molecule 4 is a protein called P1/MAHONEY POLIOVIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	3	235	1834	1169	299	349	17	0	0	0

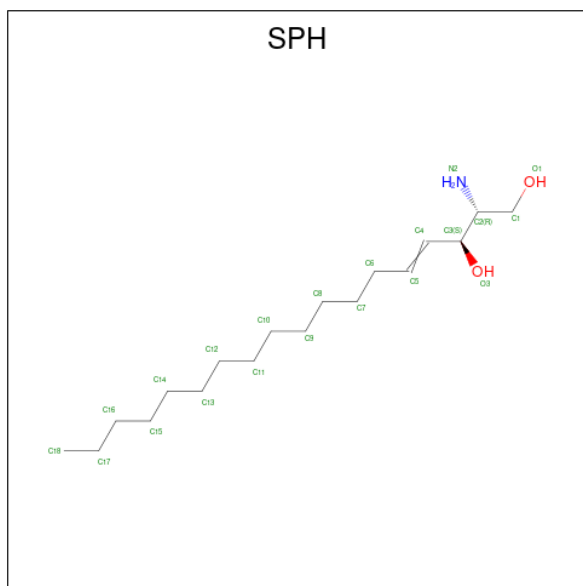
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	123	SER	PHE	conflict	UNP P03300

- Molecule 5 is a protein called P1/MAHONEY POLIOVIRUS.

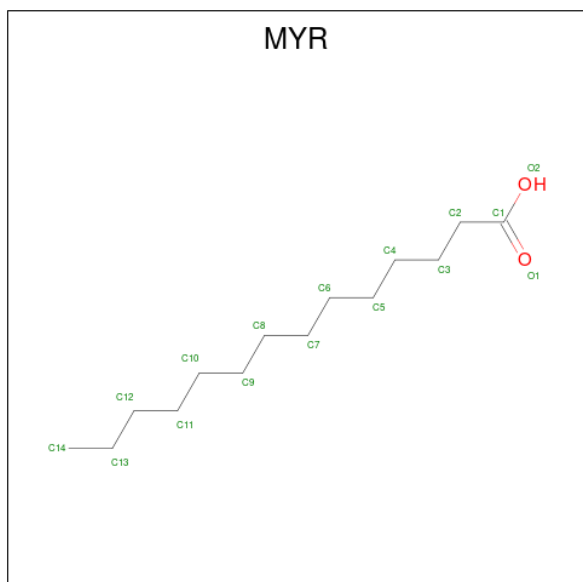
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	4	60	462	286	78	97	1	0	0	0

- Molecule 6 is SPHINGOSINE (three-letter code: SPH) (formula: $C_{18}H_{37}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	1	1	21	18	1	2	0	0

- Molecule 7 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	4	1	Total	C	O	0	0
			15	14	1		

- Molecule 8 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	0	1	Total	O	0	0
			1	1		
8	1	179	Total	O	0	0
			179	179		
8	2	170	Total	O	0	0
			170	170		
8	3	143	Total	O	0	0
			143	143		
8	4	41	Total	O	0	0
			41	41		

3 Residue-property plots [i](#)

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.


Note EDS was not executed.

- Molecule 1: P1/MAHONEY POLIOVIRUS

Chain 0:  80% 20%




- Molecule 2: P1/MAHONEY POLIOVIRUS

Chain 1:  79% 14% 6%




- Molecule 3: P1/MAHONEY POLIOVIRUS

Chain 2:  84% 11% ..



- Molecule 4: P1/MAHONEY POLIOVIRUS

Chain 3:  85% 12% ..



- Molecule 5: P1/MAHONEY POLIOVIRUS

Chain 4:  71% 16% • 12%



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	320.15Å 355.30Å 377.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	11.00 – 2.90	Depositor
% Data completeness (in resolution range)	66.0 (11.00-2.90)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.0	Depositor
R, R_{free}	0.241 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7203	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

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: MYR, SPH

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	0	0.75	0/28	1.42	0/36
2	1	0.80	0/2286	1.44	25/3125 (0.8%)
3	2	0.78	0/2142	1.46	32/2928 (1.1%)
4	3	0.79	0/1881	1.31	14/2562 (0.5%)
5	4	0.76	0/469	1.39	2/632 (0.3%)
All	All	0.79	0/6806	1.41	73/9283 (0.8%)

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	83	ARG	NE-CZ-NH2	-13.06	113.77	120.30
2	1	83	ARG	NE-CZ-NH1	11.41	126.00	120.30
3	2	264	ARG	NE-CZ-NH2	-10.59	115.01	120.30
3	2	227	TRP	CD1-CG-CD2	8.82	113.36	106.30
3	2	80	TRP	CD1-CG-CD2	8.64	113.22	106.30
3	2	78	TRP	CD1-CG-CD2	8.62	113.19	106.30
3	2	79	TRP	CD1-CG-CD2	8.37	113.00	106.30
3	2	79	TRP	CE2-CD2-CG	-8.36	100.61	107.30
2	1	175	TRP	CD1-CG-CD2	8.28	112.92	106.30
3	2	80	TRP	CE2-CD2-CG	-8.18	100.76	107.30
3	2	78	TRP	CE2-CD2-CG	-8.12	100.80	107.30
3	2	38	TRP	CD1-CG-CD2	8.01	112.70	106.30
3	2	264	ARG	NE-CZ-NH1	8.00	124.30	120.30
2	1	108	TRP	CE2-CD2-CG	-8.00	100.90	107.30
2	1	269	TRP	CD1-CG-CD2	7.96	112.67	106.30
2	1	175	TRP	CE2-CD2-CG	-7.88	101.00	107.30
2	1	170	TRP	CE2-CD2-CG	-7.84	101.02	107.30
2	1	108	TRP	CD1-CG-CD2	7.79	112.53	106.30
2	1	170	TRP	CD1-CG-CD2	7.78	112.53	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	227	TRP	CE2-CD2-CG	-7.72	101.12	107.30
4	3	110	TRP	CD1-CG-CD2	7.71	112.47	106.30
2	1	112	TYR	CB-CG-CD2	-7.55	116.47	121.00
5	4	34	ARG	NE-CZ-NH1	7.53	124.07	120.30
4	3	145	ARG	NE-CZ-NH2	-7.51	116.55	120.30
4	3	156	TRP	CD1-CG-CD2	7.48	112.29	106.30
4	3	156	TRP	CE2-CD2-CG	-7.29	101.47	107.30
4	3	110	TRP	CE2-CD2-CG	-7.29	101.47	107.30
2	1	269	TRP	CE2-CD2-CG	-7.19	101.55	107.30
3	2	100	TYR	CB-CG-CD2	-7.08	116.75	121.00
3	2	71	TRP	CE2-CD2-CG	-7.02	101.68	107.30
3	2	38	TRP	CE2-CD2-CG	-6.94	101.75	107.30
3	2	103	ARG	NE-CZ-NH1	6.90	123.75	120.30
2	1	70	ARG	NE-CZ-NH2	-6.83	116.89	120.30
4	3	170	TRP	CE2-CD2-CG	-6.73	101.91	107.30
4	3	170	TRP	CD1-CG-CD2	6.73	111.68	106.30
4	3	71	ARG	NE-CZ-NH1	6.68	123.64	120.30
3	2	71	TRP	CD1-CG-CD2	6.65	111.62	106.30
4	3	223	ARG	NE-CZ-NH2	-6.59	117.00	120.30
2	1	64	ARG	NE-CZ-NH1	6.33	123.46	120.30
2	1	175	TRP	CG-CD2-CE3	6.20	139.48	133.90
3	2	37	ARG	NE-CZ-NH2	-6.14	117.23	120.30
3	2	98	TYR	CB-CG-CD1	-6.01	117.40	121.00
2	1	275	ARG	NE-CZ-NH1	5.96	123.28	120.30
4	3	160	LEU	CB-CG-CD1	-5.93	100.91	111.00
2	1	269	TRP	CB-CG-CD1	-5.78	119.48	127.00
5	4	61	LEU	CA-CB-CG	5.78	128.59	115.30
2	1	108	TRP	CG-CD2-CE3	5.75	139.07	133.90
3	2	168	THR	CA-CB-CG2	5.74	120.44	112.40
3	2	79	TRP	CB-CG-CD1	-5.55	119.78	127.00
4	3	85	LEU	CA-CB-CG	5.50	127.96	115.30
3	2	172	ARG	NE-CZ-NH1	5.44	123.02	120.30
3	2	201	ARG	NE-CZ-NH1	5.43	123.02	120.30
3	2	227	TRP	CG-CD1-NE1	-5.43	104.67	110.10
2	1	83	ARG	CA-CB-CG	5.37	125.22	113.40
3	2	222	VAL	CG1-CB-CG2	-5.37	102.32	110.90
3	2	78	TRP	CG-CD2-CE3	5.34	138.71	133.90
3	2	79	TRP	CG-CD2-CE3	5.33	138.70	133.90
4	3	156	TRP	CG-CD2-CE3	5.30	138.67	133.90
2	1	264	LYS	CB-CA-C	-5.26	99.88	110.40
4	3	65	MET	CG-SD-CE	-5.25	91.81	100.20
2	1	264	LYS	CA-CB-CG	5.23	124.91	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	175	TRP	CB-CG-CD1	-5.23	120.20	127.00
4	3	145	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	1	83	ARG	CG-CD-NE	-5.20	100.88	111.80
3	2	76	ARG	NE-CZ-NH2	-5.19	117.70	120.30
3	2	270	ARG	NE-CZ-NH2	-5.18	117.71	120.30
2	1	264	LYS	CB-CG-CD	-5.16	98.19	111.60
2	1	220	GLN	CA-CB-CG	5.12	124.68	113.40
3	2	78	TRP	CG-CD1-NE1	-5.12	104.98	110.10
3	2	78	TRP	CB-CG-CD1	-5.08	120.40	127.00
3	2	62	ARG	NE-CZ-NH1	5.04	122.82	120.30
3	2	103	ARG	NE-CZ-NH2	-5.02	117.79	120.30
2	1	120	ARG	NE-CZ-NH2	-5.01	117.80	120.30

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	0	29	0	24	0	0
2	1	2223	0	2175	27	0
3	2	2085	0	2000	16	0
4	3	1834	0	1816	15	0
5	4	462	0	446	6	0
6	1	21	0	37	9	0
7	4	15	0	27	0	0
8	0	1	0	0	0	0
8	1	179	0	0	2	0
8	2	170	0	0	1	0
8	3	143	0	0	1	0
8	4	41	0	0	0	0
All	All	7203	0	6525	52	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 4.

All (52) 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)
2:1:177:THR:HG22	2:1:180:ASN:HB2	1.68	0.74
2:1:158:MET:SD	2:1:177:THR:HG23	2.28	0.73
3:2:5:GLU:HG2	3:2:9:TYR:HD2	1.56	0.69
3:2:5:GLU:HG3	3:2:7:CYS:H	1.63	0.63
3:2:37:ARG:HG3	4:3:37:PRO:HB3	1.83	0.61
4:3:167:VAL:O	4:3:169:PRO:HD3	2.01	0.61
5:4:55:GLU:HG2	5:4:61:LEU:HD23	1.84	0.60
2:1:274:PRO:HG2	4:3:102:GLU:HG3	1.85	0.58
2:1:273:PRO:HB3	3:2:189:ASN:HB2	1.86	0.57
2:1:294:LEU:HD13	4:3:67:MET:SD	2.46	0.56
3:2:5:GLU:HG2	3:2:9:TYR:CD2	2.40	0.56
2:1:177:THR:HG21	2:1:182:SER:OG	2.04	0.56
5:4:57:ILE:HD11	5:4:61:LEU:HB3	1.87	0.55
3:2:213:VAL:HG22	4:3:37:PRO:HG2	1.89	0.54
2:1:144:GLU:HG2	8:1:443:HOH:O	2.07	0.54
2:1:159:TYR:HB2	6:1:0:SPH:H162	1.90	0.53
2:1:237:PHE:CG	6:1:0:SPH:H91	2.45	0.52
2:1:42:PRO:HA	5:4:63:LYS:O	2.09	0.51
3:2:187:LEU:HD13	3:2:232:LEU:HD22	1.92	0.51
3:2:116:LYS:HE3	4:3:124:MET:SD	2.51	0.51
2:1:216:PRO:HB2	3:2:270:ARG:HB3	1.92	0.50
2:1:57:PRO:HB3	4:3:169:PRO:HB3	1.93	0.49
5:4:10:VAL:HG21	5:4:25:ILE:HD12	1.94	0.49
2:1:191:PRO:HG2	4:3:13:TYR:HB2	1.93	0.49
2:1:89:ILE:HG12	2:1:258:ARG:HG2	1.95	0.48
2:1:158:MET:SD	2:1:177:THR:CG2	3.00	0.48
2:1:273:PRO:HB3	3:2:189:ASN:CB	2.44	0.48
3:2:103:ARG:HD2	3:2:217:SER:O	2.14	0.48
2:1:159:TYR:CZ	6:1:0:SPH:H122	2.49	0.47
4:3:55:PHE:HE2	4:3:212:GLY:HA3	1.79	0.46
2:1:237:PHE:CE2	6:1:0:SPH:H71	2.51	0.46
3:2:5:GLU:HB3	3:2:9:TYR:HB2	1.96	0.46
2:1:115:THR:HA	4:3:233:GLN:HE22	1.81	0.46
8:3:324:HOH:O	5:4:46:PHE:HB2	2.17	0.45
2:1:237:PHE:CD2	6:1:0:SPH:H71	2.52	0.45
3:2:187:LEU:HD22	4:3:65:MET:CE	2.48	0.44
4:3:87:LEU:HD11	4:3:114:LEU:HD12	1.99	0.43
6:1:0:SPH:H4	8:1:400:HOH:O	2.18	0.43
3:2:60:ALA:O	3:2:255:PRO:HG2	2.20	0.42
2:1:237:PHE:HZ	6:1:0:SPH:H3	1.83	0.42
4:3:64:THR:O	4:3:67:MET:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:144:GLU:HG3	2:1:146:ASN:HB2	2.02	0.42
2:1:280:TYR:HB3	2:1:285:ASP:O	2.20	0.41
4:3:10:SER:O	4:3:11:ASN:HB2	2.21	0.41
2:1:218:LYS:HD2	8:2:412:HOH:O	2.20	0.41
2:1:110:ILE:HD13	6:1:0:SPH:H131	2.03	0.41
5:4:49:ASP:HA	5:4:50:PRO:HD3	1.98	0.41
4:3:54:PRO:HD2	4:3:94:ARG:O	2.21	0.41
3:2:48:ASN:HB3	3:2:49:PRO:HD3	2.03	0.40
2:1:96:ALA:HA	2:1:249:ASN:O	2.22	0.40
2:1:237:PHE:CZ	6:1:0:SPH:H3	2.56	0.40
3:2:13:VAL:HA	3:2:25:THR: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 X-ray entries followed by that with respect to entries of similar resolution.

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	0	3/5 (60%)	3 (100%)	0	0	100	100
2	1	281/302 (93%)	266 (95%)	14 (5%)	1 (0%)	34	66
3	2	266/272 (98%)	250 (94%)	15 (6%)	1 (0%)	34	66
4	3	233/238 (98%)	221 (95%)	12 (5%)	0	100	100
5	4	56/68 (82%)	52 (93%)	3 (5%)	1 (2%)	8	29
All	All	839/885 (95%)	792 (94%)	44 (5%)	3 (0%)	34	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	48	ASN
5	4	60	VAL
2	1	270	CYS

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 X-ray entries followed by that with respect to entries of similar resolution.

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	0	4/4 (100%)	3 (75%)	1 (25%)	0	2
2	1	245/261 (94%)	235 (96%)	10 (4%)	30	64
3	2	228/232 (98%)	218 (96%)	10 (4%)	28	61
4	3	210/212 (99%)	202 (96%)	8 (4%)	33	67
5	4	52/57 (91%)	50 (96%)	2 (4%)	33	67
All	All	739/766 (96%)	708 (96%)	31 (4%)	30	63

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	10	THR
2	1	145	THR
2	1	147	ASN
2	1	177	THR
2	1	216	PRO
2	1	220	GLN
2	1	224	LEU
2	1	233	SER
2	1	236	ASP
2	1	282	PRO
2	1	293	PRO
3	2	49	PRO
3	2	52	GLN
3	2	66	LEU
3	2	74	GLU
3	2	168	THR
3	2	169	SER
3	2	187	LEU
3	2	238	ASN
3	2	241	SER
3	2	264	ARG
4	3	33	PRO
4	3	71	ARG

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Mol	Chain	Res	Type
4	3	85	LEU
4	3	89	PRO
4	3	146	LYS
4	3	208	MET
4	3	218	ASN
4	3	224	LEU
5	4	56	PRO
5	4	61	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
4	3	218	ASN
5	4	13	HIS
5	4	31	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SPH	1	0	-	19,20,20	0.81	1 (5%)	18,21,21	2.40	4 (22%)
7	MYR	4	1	5	14,14,15	0.34	0	13,13,15	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
6	SPH	1	0	-	-	6/21/21/21	-
7	MYR	4	1	5	-	6/11/12/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1	0	SPH	C1-C2	3.04	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1	0	SPH	O3-C3-C2	-6.82	96.49	107.31
6	1	0	SPH	O1-C1-C2	4.62	121.14	111.43
6	1	0	SPH	O3-C3-C4	-4.12	99.82	110.85
6	1	0	SPH	C1-C2-C3	-3.41	105.69	113.03

There are no chirality outliers.

All (12) torsion outliers are listed below:

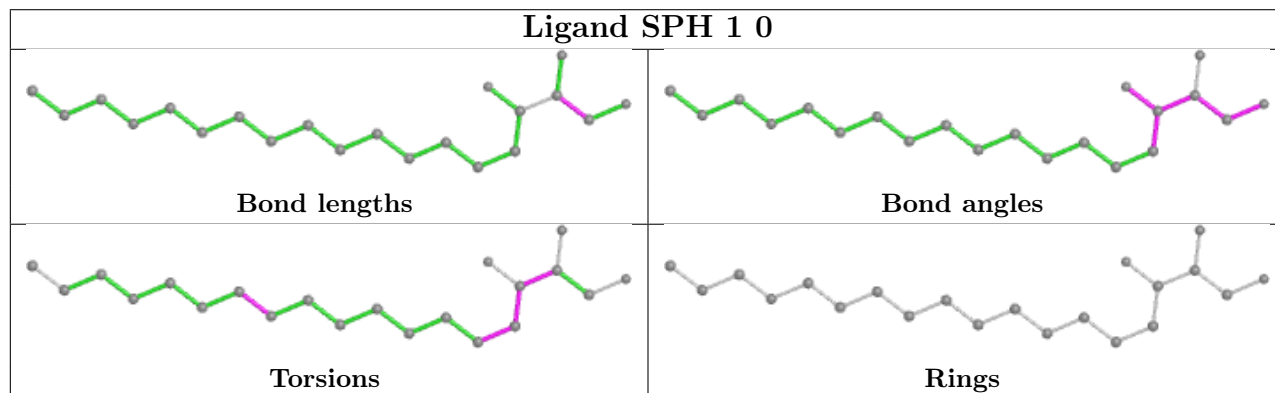
Mol	Chain	Res	Type	Atoms
6	1	0	SPH	C1-C2-C3-O3
6	1	0	SPH	N2-C2-C3-O3
6	1	0	SPH	C2-C3-C4-C5
6	1	0	SPH	O3-C3-C4-C5
6	1	0	SPH	C3-C4-C5-C6
7	4	1	MYR	C6-C7-C8-C9
7	4	1	MYR	C5-C6-C7-C8
7	4	1	MYR	C11-C12-C13-C14
6	1	0	SPH	C10-C11-C12-C13
7	4	1	MYR	C10-C11-C12-C13
7	4	1	MYR	C7-C8-C9-C10
7	4	1	MYR	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	1	0	SPH	9	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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.