Full wwPDB X-ray Structure Validation Report (i)

Apr 10, 2023 – 06:15 PM EDT

PDB ID	:	1AR8
Title	:	P1/MAHONEY POLIOVIRUS, MUTANT P1095S
Authors	:	Wien, M.W.; Curry, S.; Filman, D.J.; Hogle, J.M.
Deposited on	:	1997-08-11
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 (i) 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 (1)) were used in the production of this report:

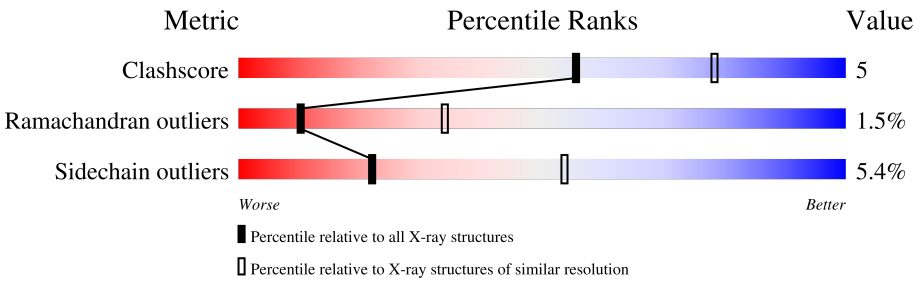
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	8	25% 75%
2	1	302	76% 16% •• 6%
3	2	272	79% 16% • •
4	3	238	85% 12% ••
5	4	68	66% 18% • 12%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7184 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	8	43	24	8	11	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	2221	1414	378	424	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	95	SER	PRO	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

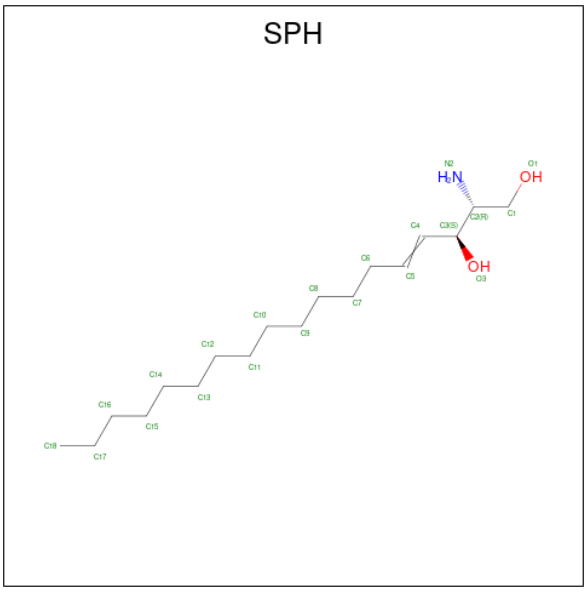
There is a discrepancy between the modelled and reference sequences:

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

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

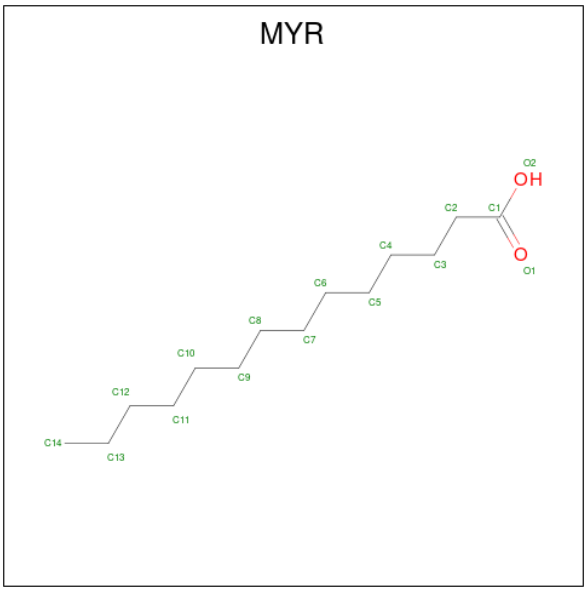
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	4	60	462	286	78	97	1	0	0	0

- 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
			Total	C	O		
7	4	1	15	14	1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	0	1	1	1	0	0
			Total	O		
8	1	184	184	184	0	0
			Total	O		
8	2	143	143	143	0	0
			Total	O		
8	3	135	135	135	0	0
			Total	O		
8	4	40	40	40	0	0

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: 25% 75%

A3 A4 A5 A6 S7 S8 S9 T10

• Molecule 2: P1/MAHONEY POLIOVIRUS

Chain 1: 76% 16% •• 6%

GLY LEU GLY GLN MET LEU GLU SER MET ILE ASP ASN THR VAL ARG GLU THR VAL GLY A20 R24 L27 P28 E40 E48 R64 R83 I89 N94 S95 A96 S97 T98 T99 D102 V107 W108 K109 V116 R129 T145 N146 N147 G148 H149 M158

Y159 W170 W175 Q176 T177 N180 P181 S182 P191 V196 S206 K218 D219 Q220 S221 A222 D226 S233 L234 N235 D236 F237 G238 I239 H248 K252 R258 K264 W269 P273 K287 L294 S295 T296 Y302

• Molecule 3: P1/MAHONEY POLIOVIRUS

Chain 2: 79% 16% • •

SER PRO ASN ILE E5 A6 C7 G8 Y9 S10 D11 R12 V13 Q26 N30 A34 R37 W38 S45 N48 P49 Q52 A60 F63 W71 T72 K73 W78 W79 W80 A114 P128 N137 T138 T139 T143 Q146 P150 G151 E152 T158

N165 N166 Q167 T168 R173 Y179 L187 G188 N189 I197 P211 Y212 V213 W227 F239 A240 S241 E242 S243 L251 A254 P255 R264 R270 L271 Q272

• Molecule 4: P1/MAHONEY POLIOVIRUS

Chain 3: 85% 12% ••

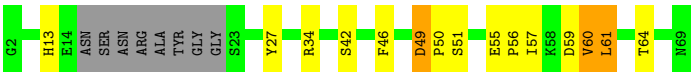
G1 Y13 P33 P37 F55 D56 L57 T64 M65 E66 M67 R71 L85 S86 L87 W110 M124 K143 K146 M149 L150 W156 S163 V167 V168 P169 W170 Y189 I190 R206 E207 M208 G212 N218 L224 L225 R226 Q233 K234

A235 LEU ALA GLN

• Molecule 5: P1/MAHONEY POLIOVIRUS

Chain 4:

66%
18%
•
12%


G2
H13
E14
ASN
SER
ASN
ARG
ALA
TYR
GLY
GLY
S23
Y27
R34
S42
F46
D49
P50
S51
E55
P56
I57
K58
D59
V60
L61
T64
N69

4 Data and refinement statistics (i)

Xtriage (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	323.04Å 358.22Å 380.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	11.00 – 2.90	Depositor
% Data completeness (in resolution range)	34.0 (11.00-2.90)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.0	Depositor
R, R_{free}	0.270 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7184	wwPDB-VP
Average B, all atoms (Å^2)	15.0	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	0.47	0/41	1.53	0/53
2	1	0.81	0/2283	1.36	23/3120 (0.7%)
3	2	0.84	1/2142 (0.0%)	1.43	20/2928 (0.7%)
4	3	0.80	0/1881	1.28	12/2562 (0.5%)
5	4	0.75	0/469	1.37	3/632 (0.5%)
All	All	0.81	1/6816 (0.0%)	1.36	58/9295 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	7	CYS	CB-SG	5.03	1.90	1.82

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	2	5	GLU	OE1-CD-OE2	-10.42	110.79	123.30
2	1	175	TRP	CD1-CG-CD2	8.51	113.11	106.30
3	2	78	TRP	CD1-CG-CD2	8.48	113.08	106.30
2	1	170	TRP	CD1-CG-CD2	8.39	113.01	106.30
4	3	110	TRP	CD1-CG-CD2	8.31	112.95	106.30
3	2	80	TRP	CD1-CG-CD2	8.12	112.80	106.30
3	2	71	TRP	CE2-CD2-CG	-8.09	100.83	107.30
2	1	175	TRP	CE2-CD2-CG	-8.02	100.89	107.30
3	2	38	TRP	CD1-CG-CD2	8.00	112.70	106.30
4	3	170	TRP	CE2-CD2-CG	-8.00	100.90	107.30
3	2	227	TRP	CD1-CG-CD2	7.92	112.63	106.30
3	2	80	TRP	CE2-CD2-CG	-7.90	100.98	107.30
3	2	227	TRP	CE2-CD2-CG	-7.80	101.06	107.30
4	3	170	TRP	CD1-CG-CD2	7.80	112.54	106.30
4	3	110	TRP	CE2-CD2-CG	-7.77	101.08	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	269	TRP	CD1-CG-CD2	7.68	112.45	106.30
3	2	78	TRP	CE2-CD2-CG	-7.62	101.20	107.30
4	3	156	TRP	CE2-CD2-CG	-7.57	101.24	107.30
3	2	79	TRP	CD1-CG-CD2	7.56	112.35	106.30
5	4	34	ARG	NE-CZ-NH1	7.50	124.05	120.30
3	2	71	TRP	CD1-CG-CD2	7.41	112.23	106.30
3	2	79	TRP	CE2-CD2-CG	-7.38	101.39	107.30
2	1	269	TRP	CE2-CD2-CG	-7.34	101.43	107.30
2	1	108	TRP	CE2-CD2-CG	-7.22	101.52	107.30
2	1	108	TRP	CD1-CG-CD2	7.19	112.05	106.30
3	2	38	TRP	CE2-CD2-CG	-7.13	101.60	107.30
4	3	156	TRP	CD1-CG-CD2	6.97	111.88	106.30
2	1	170	TRP	CE2-CD2-CG	-6.97	101.73	107.30
2	1	129	ARG	NE-CZ-NH1	6.67	123.64	120.30
2	1	129	ARG	NE-CZ-NH2	-6.57	117.02	120.30
3	2	270	ARG	NE-CZ-NH1	6.16	123.38	120.30
2	1	175	TRP	CG-CD2-CE3	6.02	139.32	133.90
2	1	24	ARG	NE-CZ-NH2	-6.00	117.30	120.30
3	2	264	ARG	NE-CZ-NH1	5.87	123.24	120.30
5	4	34	ARG	NE-CZ-NH2	-5.79	117.41	120.30
3	2	5	GLU	CG-CD-OE1	5.75	129.79	118.30
3	2	78	TRP	CG-CD1-NE1	-5.67	104.43	110.10
5	4	27	TYR	CB-CG-CD2	-5.67	117.60	121.00
3	2	227	TRP	CG-CD2-CE3	5.57	138.91	133.90
4	3	170	TRP	CG-CD2-CE3	5.55	138.89	133.90
2	1	147	ASN	OD1-CG-ND2	-5.52	109.21	121.90
2	1	170	TRP	CG-CD1-NE1	-5.50	104.60	110.10
2	1	146	ASN	N-CA-CB	-5.46	100.77	110.60
3	2	71	TRP	CG-CD2-CE3	5.38	138.75	133.90
2	1	83	ARG	NE-CZ-NH1	5.36	122.98	120.30
4	3	226	ARG	NE-CZ-NH1	5.34	122.97	120.30
2	1	175	TRP	CB-CG-CD1	-5.33	120.07	127.00
3	2	168	THR	CA-CB-CG2	5.28	119.79	112.40
4	3	206	ARG	NE-CZ-NH2	-5.28	117.66	120.30
4	3	110	TRP	CG-CD1-NE1	-5.23	104.87	110.10
2	1	226	ASP	N-CA-C	5.17	124.95	111.00
2	1	64	ARG	NE-CZ-NH1	5.12	122.86	120.30
4	3	110	TRP	CG-CD2-CE3	5.08	138.47	133.90
2	1	147	ASN	CB-CG-ND2	5.07	128.87	116.70
2	1	196	VAL	CG1-CB-CG2	-5.03	102.85	110.90
4	3	65	MET	CG-SD-CE	-5.01	92.18	100.20
2	1	108	TRP	CG-CD2-CE3	5.01	138.41	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	264	LYS	CA-CB-CG	5.01	124.42	113.40

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	0	43	0	39	2	0
2	1	2221	0	2171	30	0
3	2	2085	0	2000	26	0
4	3	1834	0	1816	17	0
5	4	462	0	446	7	0
6	1	21	0	37	4	0
7	4	15	0	27	1	0
8	0	1	0	0	0	0
8	1	184	0	0	4	0
8	2	143	0	0	2	0
8	3	135	0	0	2	0
8	4	40	0	0	0	0
All	All	7184	0	6536	68	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 5.

All (68) 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)
2:1:158:MET:SD	2:1:177:THR:HG23	2.16	0.84
3:2:5:GLU:OE2	3:2:7:CYS:HB3	1.78	0.83
4:3:124:MET:HG3	8:3:277:HOH:O	1.81	0.80
1:0:6:ALA:CA	1:0:7:SER:N	2.48	0.77
2:1:177:THR:HG22	2:1:180:ASN:HB2	1.69	0.73
2:1:40:GLU:HB3	5:4:64:THR:HB	1.71	0.73
3:2:5:GLU:HG2	3:2:9:TYR:HD2	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:287:LYS:HA	3:2:137:ASN:HD21	1.55	0.70
2:1:218:LYS:HD2	8:2:405:HOH:O	1.93	0.68
2:1:107:VAL:HG13	2:1:239:ILE:HD13	1.75	0.67
2:1:109:LYS:HA	2:1:239:ILE:HG22	1.78	0.65
2:1:236:ASP:HB3	2:1:237:PHE:CD2	2.32	0.64
3:2:5:GLU:OE2	3:2:7:CYS:CB	2.46	0.63
2:1:218:LYS:HA	3:2:270:ARG:HB2	1.80	0.63
3:2:187:LEU:HD22	4:3:65:MET:CE	2.29	0.61
3:2:143:THR:HG23	3:2:173:ARG:HA	1.80	0.61
3:2:213:VAL:HG22	4:3:37:PRO:HG2	1.86	0.58
2:1:177:THR:HG21	2:1:182:SER:OG	2.04	0.57
5:4:57:ILE:HD11	5:4:61:LEU:HB3	1.87	0.57
6:1:0:SPH:H4	8:1:448:HOH:O	2.04	0.56
3:2:179:TYR:HA	4:3:65:MET:CE	2.36	0.56
2:1:159:TYR:HB2	6:1:0:SPH:H162	1.87	0.55
3:2:146:GLN:NE2	3:2:270:ARG:HD2	2.22	0.55
2:1:48:GLU:HA	3:2:197:ILE:HB	1.89	0.55
2:1:287:LYS:HA	3:2:137:ASN:ND2	2.21	0.54
2:1:89:ILE:HG12	2:1:258:ARG:HG2	1.90	0.53
3:2:48:ASN:HB3	3:2:49:PRO:HD3	1.92	0.52
2:1:191:PRO:HG2	4:3:13:TYR:HB2	1.92	0.52
2:1:222:ALA:HA	8:1:336:HOH:O	2.09	0.51
8:3:317:HOH:O	5:4:46:PHE:HB2	2.10	0.51
4:3:167:VAL:O	4:3:169:PRO:HD3	2.11	0.50
2:1:96:ALA:HB2	2:1:248:HIS:CD2	2.47	0.50
2:1:27:LEU:HB3	2:1:28:PRO:HD2	1.94	0.50
2:1:149:HIS:CE1	8:1:303:HOH:O	2.64	0.49
3:2:30:ASN:HD21	5:4:59:ASP:HB2	1.76	0.49
4:3:55:PHE:HE2	4:3:212:GLY:HA3	1.78	0.49
4:3:64:THR:O	4:3:67:MET:HG2	2.14	0.48
2:1:302:TYR:CE1	4:3:189:TYR:HB3	2.49	0.47
3:2:60:ALA:O	3:2:255:PRO:HG2	2.15	0.47
3:2:73:LYS:HE2	3:2:243:SER:O	2.15	0.47
4:3:87:LEU:HD13	4:3:190:ILE:HD11	1.97	0.47
2:1:206:SER:O	6:1:0:SPH:H11	2.14	0.47
5:4:13:HIS:H	5:4:13:HIS:CD2	2.32	0.47
2:1:273:PRO:HB3	3:2:189:ASN:HB2	1.97	0.46
4:3:149:MET:CE	4:3:150:LEU:HG	2.46	0.46
2:1:294:LEU:HD12	4:3:67:MET:SD	2.56	0.46
2:1:94:ASN:ND2	2:1:248:HIS:HA	2.31	0.46
3:2:5:GLU:CD	3:2:7:CYS:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:34:ALA:HB3	3:2:211:PRO:HD2	1.99	0.45
2:1:296:THR:HA	4:3:57:LEU:O	2.17	0.44
5:4:49:ASP:HA	5:4:50:PRO:HD3	1.88	0.44
3:2:63:PHE:CD1	3:2:254:ALA:HB2	2.53	0.43
3:2:37:ARG:HG3	4:3:37:PRO:HB3	2.00	0.43
2:1:96:ALA:O	2:1:98:THR:HG23	2.19	0.43
3:2:138:THR:HG23	8:2:395:HOH:O	2.19	0.42
4:3:71:ARG:CZ	4:3:71:ARG:HB2	2.49	0.42
5:4:55:GLU:N	5:4:56:PRO:HD3	2.34	0.42
2:1:237:PHE:CD2	6:1:0:SPH:H71	2.55	0.42
4:3:143:LYS:HA	4:3:143:LYS:HD3	1.75	0.42
3:2:146:GLN:HE21	3:2:270:ARG:HD2	1.85	0.41
3:2:13:VAL:HG22	3:2:26:GLN:HA	2.03	0.41
2:1:96:ALA:HB2	2:1:248:HIS:NE2	2.35	0.41
2:1:102:ASP:N	8:1:456:HOH:O	2.51	0.41
2:1:116:VAL:CG2	4:3:233:GLN:HB2	2.50	0.41
3:2:37:ARG:O	3:2:211:PRO:HG3	2.20	0.41
1:0:3:ALA:O	1:0:6:ALA:N	2.53	0.41
7:4:1:MYR:H71	7:4:1:MYR:H101	1.80	0.40
3:2:239:PHE:O	3:2:241:SER:N	2.54	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	4/8 (50%)	3 (75%)	0	1 (25%)	0 0
2	1	281/302 (93%)	256 (91%)	21 (8%)	4 (1%)	11 36
3	2	266/272 (98%)	246 (92%)	15 (6%)	5 (2%)	8 28
4	3	233/238 (98%)	222 (95%)	10 (4%)	1 (0%)	34 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	4	56/68 (82%)	51 (91%)	3 (5%)	2 (4%)	3 14
All	All	840/888 (95%)	778 (93%)	49 (6%)	13 (2%)	10 34

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	99	THR
3	2	166	ASN
1	0	4	ALA
2	1	147	ASN
2	1	234	LEU
3	2	240	ALA
5	4	60	VAL
2	1	146	ASN
3	2	48	ASN
4	3	234	LYS
3	2	7	CYS
3	2	114	ALA
5	4	51	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 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%)	2 (50%)	2 (50%)	0 0
2	1	245/261 (94%)	235 (96%)	10 (4%)	30 64
3	2	228/232 (98%)	213 (93%)	15 (7%)	16 44
4	3	210/212 (99%)	201 (96%)	9 (4%)	29 62
5	4	52/57 (91%)	48 (92%)	4 (8%)	13 35
All	All	739/766 (96%)	699 (95%)	40 (5%)	22 54

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	9	SER
1	0	10	THR
2	1	129	ARG
2	1	145	THR
2	1	146	ASN
2	1	147	ASN
2	1	177	THR
2	1	220	GLN
2	1	221	SER
2	1	233	SER
2	1	252	LYS
2	1	264	LYS
3	2	10	SER
3	2	11	ASP
3	2	45	SER
3	2	52	GLN
3	2	73	LYS
3	2	128	PRO
3	2	139	THR
3	2	150	PRO
3	2	152	GLU
3	2	158	THR
3	2	165	ASN
3	2	168	THR
3	2	241	SER
3	2	251	LEU
3	2	264	ARG
4	3	33	PRO
4	3	71	ARG
4	3	85	LEU
4	3	146	LYS
4	3	149	MET
4	3	163	SER
4	3	208	MET
4	3	218	ASN
4	3	224	LEU
5	4	42	SER
5	4	49	ASP
5	4	60	VAL
5	4	61	LEU

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

Mol	Chain	Res	Type
2	1	69	HIS
3	2	48	ASN
3	2	165	ASN
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	$\#\|Z\| > 2$
7	MYR	4	1	5	14,14,15	0.46	0	13,13,15	0.90	0
6	SPH	1	0	-	19,20,20	0.42	0	18,21,21	2.08	4 (22%)

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
7	MYR	4	1	5	-	4/11/12/13	-
6	SPH	1	0	-	-	4/21/21/21	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	1	0	SPH	O3-C3-C2	-4.91	99.53	107.31
6	1	0	SPH	O3-C3-C4	-4.66	98.39	110.85
6	1	0	SPH	C1-C2-C3	-3.40	105.70	113.03
6	1	0	SPH	O1-C1-C2	3.40	118.58	111.43

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	C10-C11-C12-C13
6	1	0	SPH	C11-C10-C9-C8
7	4	1	MYR	C5-C6-C7-C8
7	4	1	MYR	C7-C8-C9-C10

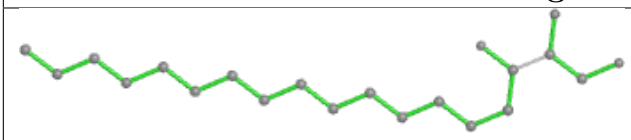
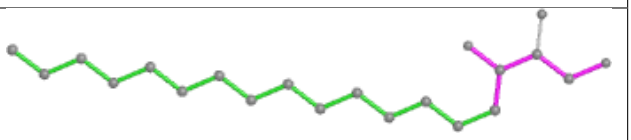
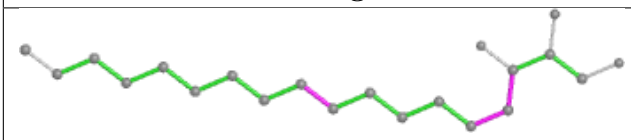
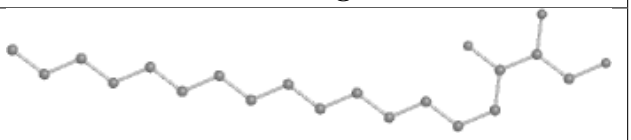
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	4	1	MYR	1	0
6	1	0	SPH	4	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 then 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.

Ligand SPH 1 0	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.