Full wwPDB X-ray Structure Validation Report (i)

Apr 10, 2023 – 11:42 PM EDT

PDB ID	:	1POV
Title	:	ROLE AND MECHANISM OF THE MATURATION CLEAVAGE OF VP0 IN POLIOVIRUS ASSEMBLY: STRUCTURE OF THE EMPTY CAPSID ASSEMBLY INTERMEDIATE AT 2.9 ANGSTROMS RESOLUTION
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Deposited on	:	1995-08-10
Resolution	:	2.80 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:

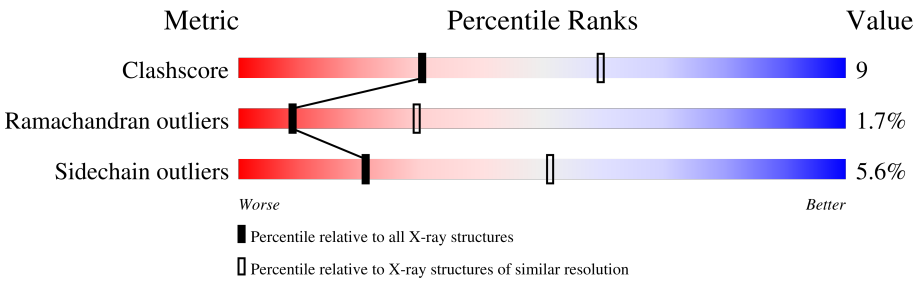
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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	340	63% 20% • • 12%
2	1	302	61% 14% • • 22%
3	3	238	77% 21% •

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
5	SPH	1	0	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6281 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 POLIOVIRUS NATIVE EMPTY CAPSID (TYPE 1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	0	300	2312	1460	401	436	15	0	0	0

- Molecule 2 is a protein called POLIOVIRUS NATIVE EMPTY CAPSID (TYPE 1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	1	235	1874	1204	315	350	5	0	0	0

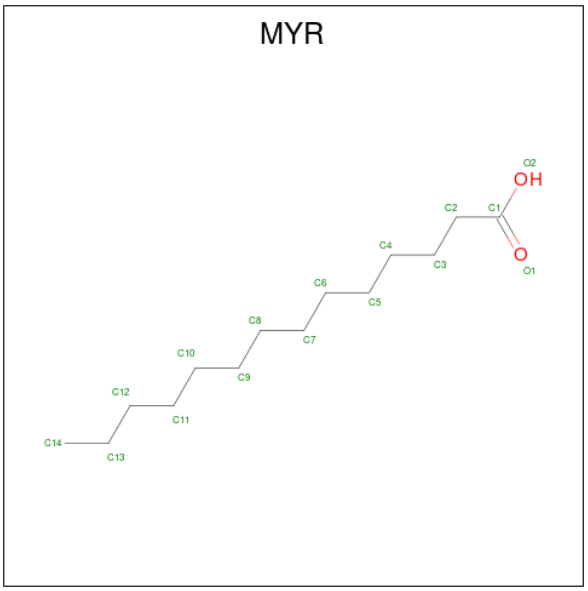
- Molecule 3 is a protein called POLIOVIRUS NATIVE EMPTY CAPSID (TYPE 1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	3	238	1849	1177	302	353	17	0	0	0

There is a discrepancy between the modelled and reference sequences:

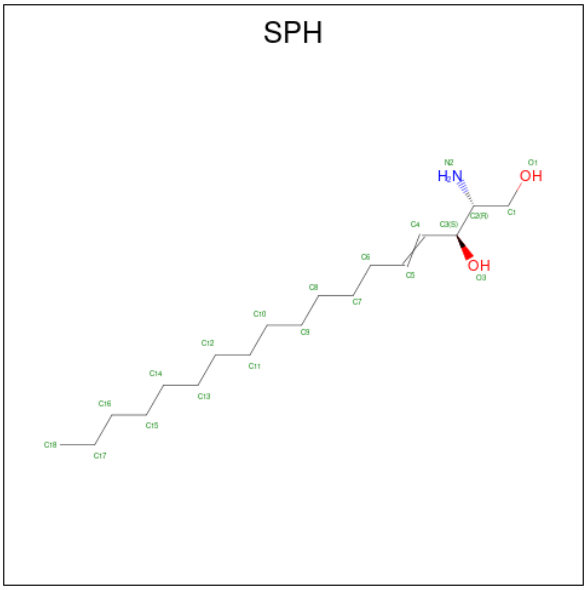
Chain	Residue	Modelled	Actual	Comment	Reference
3	123	SER	PHE	conflict	UNP P03300

- Molecule 4 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



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

- Molecule 5 is SPHINGOSINE (three-letter code: SPH) (formula: $C_{18}H_{37}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	1	1	21	18	1	2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	0	73	73	73	0	0
			Total	O		
6	1	75	75	75	0	0
			Total	O		
6	3	62	62	62	0	0

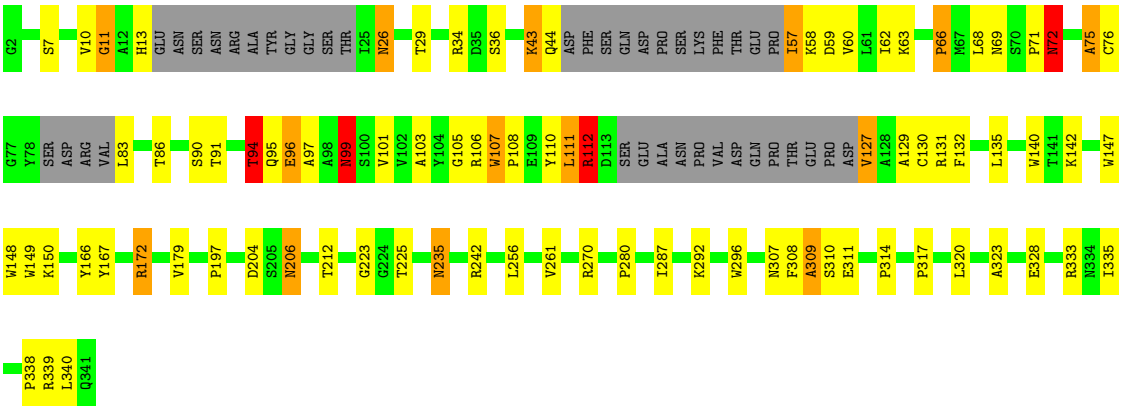
3 Residue-property plots (i)

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.

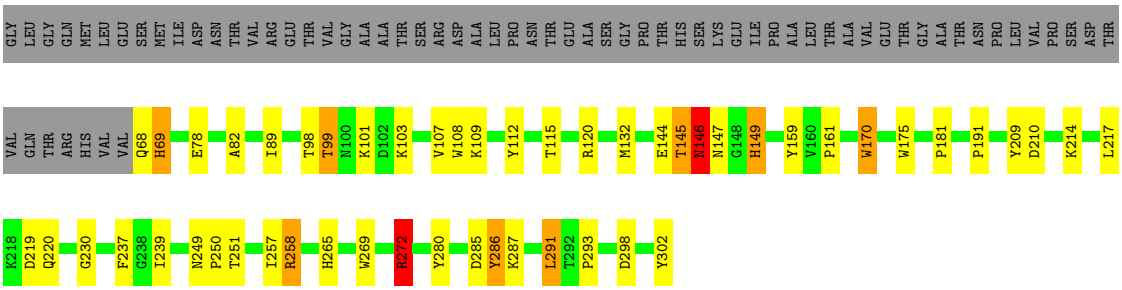
• Molecule 1: POLIOVIRUS NATIVE EMPTY CAPSID (TYPE 1)

Chain 0:



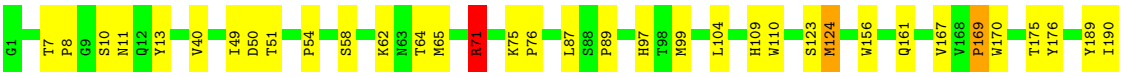
• Molecule 2: POLIOVIRUS NATIVE EMPTY CAPSID (TYPE 1)

Chain 1:



• Molecule 3: POLIOVIRUS NATIVE EMPTY CAPSID (TYPE 1)

Chain 3:



R197
P201
L202
S203
T204
P205
M208
D209
S215
A216
C217
N218
R223
L224
L225
R226
H230
I231
E232
Q233
K234
A235
L236
A237
Q238

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	322.90Å 358.00Å 380.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.281 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6281	wwPDB-VP
Average B, all atoms (Å^2)	18.0	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	0.91	0/2367	1.47	24/3225 (0.7%)
2	1	0.87	0/1930	1.41	14/2634 (0.5%)
3	3	0.92	0/1896	1.36	14/2584 (0.5%)
All	All	0.90	0/6193	1.42	52/8443 (0.6%)

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	272	ARG	NE-CZ-NH1	9.98	125.29	120.30
3	3	223	ARG	NE-CZ-NH1	8.79	124.70	120.30
2	1	170	TRP	CD1-CG-CD2	7.90	112.62	106.30
1	0	296	TRP	CD1-CG-CD2	7.77	112.52	106.30
2	1	258	ARG	NE-CZ-NH2	7.57	124.08	120.30
1	0	149	TRP	CD1-CG-CD2	7.46	112.27	106.30
3	3	110	TRP	CD1-CG-CD2	7.46	112.27	106.30
1	0	148	TRP	CD1-CG-CD2	7.26	112.11	106.30
1	0	147	TRP	CD1-CG-CD2	7.23	112.09	106.30
1	0	130	CYS	CA-CB-SG	-7.06	101.30	114.00
2	1	269	TRP	CD1-CG-CD2	7.03	111.92	106.30
2	1	175	TRP	CD1-CG-CD2	6.98	111.88	106.30
3	3	223	ARG	CA-CB-CG	6.80	128.36	113.40
1	0	107	TRP	CD1-CG-CD2	6.77	111.72	106.30
1	0	131	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	0	148	TRP	CE2-CD2-CG	-6.42	102.16	107.30
3	3	170	TRP	CD1-CG-CD2	6.33	111.36	106.30
1	0	296	TRP	CE2-CD2-CG	-6.32	102.25	107.30
2	1	170	TRP	CE2-CD2-CG	-6.30	102.26	107.30
2	1	175	TRP	CE2-CD2-CG	-6.21	102.33	107.30
3	3	156	TRP	CD1-CG-CD2	6.12	111.19	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	226	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	1	108	TRP	CD1-CG-CD2	5.97	111.08	106.30
1	0	149	TRP	CE2-CD2-CG	-5.94	102.55	107.30
2	1	108	TRP	CE2-CD2-CG	-5.82	102.64	107.30
2	1	146	ASN	N-CA-C	5.81	126.70	111.00
3	3	170	TRP	CE2-CD2-CG	-5.81	102.65	107.30
1	0	140	TRP	CD1-CG-CD2	5.79	110.94	106.30
2	1	269	TRP	CE2-CD2-CG	-5.79	102.67	107.30
1	0	140	TRP	CE2-CD2-CG	-5.75	102.70	107.30
3	3	110	TRP	CE2-CD2-CG	-5.74	102.71	107.30
3	3	110	TRP	CG-CD1-NE1	-5.65	104.45	110.10
3	3	197	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	0	72	ASN	CB-CA-C	-5.59	99.23	110.40
2	1	120	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	0	94	THR	N-CA-C	5.50	125.86	111.00
3	3	156	TRP	CE2-CD2-CG	-5.48	102.92	107.30
1	0	112	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	0	99	ASN	CA-CB-CG	-5.28	101.80	113.40
3	3	124	MET	CG-SD-CE	5.26	108.62	100.20
1	0	112	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	0	107	TRP	CE2-CD2-CG	-5.23	103.12	107.30
1	0	147	TRP	CE2-CD2-CG	-5.19	103.15	107.30
1	0	127	VAL	CG1-CB-CG2	-5.16	102.64	110.90
3	3	223	ARG	NH1-CZ-NH2	-5.15	113.73	119.40
2	1	146	ASN	CB-CA-C	-5.13	100.15	110.40
1	0	296	TRP	CG-CD1-NE1	-5.10	105.00	110.10
1	0	147	TRP	CG-CD1-NE1	-5.06	105.04	110.10
1	0	204	ASP	CB-CG-OD1	5.05	122.84	118.30
1	0	235	ASN	OD1-CG-ND2	-5.04	110.31	121.90
3	3	71	ARG	NE-CZ-NH1	5.03	122.81	120.30
2	1	170	TRP	CG-CD1-NE1	-5.02	105.08	110.10

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	2312	0	2230	56	0
2	1	1874	0	1822	37	0
3	3	1849	0	1820	33	0
4	0	15	0	27	0	0
5	1	21	0	36	6	0
6	0	73	0	0	3	0
6	1	75	0	0	1	0
6	3	62	0	0	2	0
All	All	6281	0	5935	112	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 9.

All (112) 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)
1:0:95:GLN:HG3	1:0:96:GLU:N	1.83	0.94
1:0:256:LEU:HD22	3:3:65:MET:SD	2.17	0.85
2:1:217:LEU:H	2:1:220:GLN:NE2	1.74	0.84
2:1:109:LYS:HA	2:1:239:ILE:HG22	1.63	0.79
2:1:217:LEU:H	2:1:220:GLN:HE21	1.30	0.79
1:0:292:LYS:HE2	2:1:214:LYS:HA	1.63	0.79
3:3:232:GLU:HG2	6:3:272:HOH:O	1.89	0.72
1:0:127:VAL:HG12	1:0:129:ALA:H	1.56	0.71
3:3:175:THR:HG22	3:3:176:TYR:CD1	2.27	0.69
2:1:191:PRO:HG2	3:3:13:TYR:HB2	1.75	0.69
1:0:212:THR:HG23	1:0:242:ARG:HA	1.74	0.69
2:1:68:GLN:O	2:1:69:HIS:HB2	1.92	0.69
3:3:167:VAL:O	3:3:169:PRO:HD3	1.93	0.67
3:3:124:MET:HG3	6:3:275:HOH:O	1.95	0.66
1:0:311:GLU:HG3	6:0:405:HOH:O	1.97	0.64
1:0:112:ARG:NE	1:0:112:ARG:HA	2.14	0.63
2:1:132:MET:CE	5:1:0:SPH:H101	2.27	0.63
3:3:109:HIS:ND1	3:3:223:ARG:NH1	2.47	0.62
1:0:112:ARG:HA	1:0:112:ARG:HE	1.64	0.62
2:1:115:THR:HA	3:3:233:GLN:HE22	1.64	0.61
1:0:63:LYS:HE3	1:0:69:ASN:ND2	2.15	0.60
1:0:106:ARG:O	1:0:280:PRO:HG3	2.03	0.58
1:0:206:ASN:HD21	2:1:287:LYS:HA	1.68	0.58
2:1:217:LEU:N	2:1:220:GLN:HE21	1.98	0.58
3:3:50:ASP:HA	3:3:215:SER:HB3	1.87	0.57
3:3:201:PRO:O	3:3:204:THR:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:7:SER:HA	1:0:26:ASN:HB3	1.87	0.57
1:0:90:SER:HB2	1:0:132:PHE:HB2	1.87	0.57
1:0:150:LYS:HE3	2:1:210:ASP:OD2	2.05	0.57
3:3:202:LEU:O	3:3:204:THR:HG22	2.05	0.56
2:1:132:MET:HE2	5:1:0:SPH:H101	1.87	0.56
1:0:83:LEU:HB2	1:0:94:THR:O	2.07	0.55
1:0:112:ARG:HE	1:0:112:ARG:CA	2.20	0.55
2:1:217:LEU:O	2:1:220:GLN:HG2	2.07	0.55
1:0:167:TYR:CE2	1:0:335:ILE:HD12	2.42	0.54
1:0:142:LYS:HE3	1:0:314:PRO:HD2	1.88	0.54
1:0:111:LEU:C	1:0:112:ARG:HE	2.11	0.54
2:1:249:ASN:CG	2:1:250:PRO:HD2	2.29	0.53
1:0:197:PRO:O	2:1:272:ARG:NH2	2.42	0.52
1:0:111:LEU:HB2	1:0:172:ARG:HD3	1.90	0.52
2:1:132:MET:HE1	5:1:0:SPH:H101	1.90	0.52
3:3:75:LYS:HB2	3:3:76:PRO:HD2	1.91	0.52
1:0:72:ASN:H	1:0:75:ALA:HB3	1.74	0.51
1:0:95:GLN:HG3	1:0:96:GLU:H	1.73	0.51
1:0:71:PRO:O	1:0:101:VAL:HA	2.11	0.51
1:0:60:VAL:HA	3:3:218:ASN:OD1	2.10	0.51
1:0:107:TRP:CG	1:0:108:PRO:HD2	2.45	0.50
1:0:103:ALA:HB3	1:0:280:PRO:HD2	1.94	0.49
2:1:146:ASN:O	2:1:147:ASN:HB3	2.12	0.49
1:0:110:TYR:O	1:0:112:ARG:N	2.46	0.49
2:1:103:LYS:HD3	2:1:170:TRP:CG	2.47	0.49
1:0:107:TRP:CD1	1:0:108:PRO:HD2	2.47	0.49
2:1:99:THR:HG22	2:1:101:LYS:N	2.28	0.49
1:0:57:ILE:HG12	1:0:58:LYS:H	1.77	0.49
3:3:231:ILE:HG13	3:3:232:GLU:N	2.28	0.48
2:1:98:THR:OG1	2:1:99:THR:N	2.47	0.48
1:0:59:ASP:HB3	1:0:62:ILE:HD12	1.95	0.48
1:0:34:ARG:O	1:0:34:ARG:HG2	2.13	0.48
2:1:103:LYS:HD3	2:1:170:TRP:CD2	2.49	0.47
3:3:233:GLN:HB3	3:3:236:LEU:CB	2.44	0.47
2:1:159:TYR:O	2:1:161:PRO:HD3	2.14	0.47
2:1:280:TYR:HB3	2:1:285:ASP:O	2.14	0.47
1:0:71:PRO:HG2	1:0:105:GLY:HA2	1.96	0.47
3:3:232:GLU:HG3	3:3:234:LYS:H	1.79	0.47
1:0:179:VAL:HG22	1:0:320:LEU:CD2	2.45	0.47
1:0:308:PHE:O	1:0:310:SER:N	2.48	0.46
1:0:86:THR:OG1	1:0:91:THR:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:51:THR:HG21	3:3:99:MET:HB2	1.97	0.46
1:0:132:PHE:CD1	1:0:323:ALA:HB2	2.51	0.46
2:1:112:TYR:HD2	5:1:0:SPH:H5	1.80	0.46
1:0:112:ARG:NH2	1:0:328:GLU:OE1	2.49	0.46
1:0:223:GLY:HA3	6:0:364:HOH:O	2.17	0.46
3:3:7:THR:HB	3:3:8:PRO:HD2	1.98	0.45
1:0:112:ARG:NE	1:0:112:ARG:CA	2.78	0.45
1:0:270:ARG:NH1	3:3:123:SER:O	2.50	0.45
1:0:83:LEU:O	1:0:94:THR:N	2.51	0.44
2:1:145:THR:O	2:1:147:ASN:N	2.51	0.44
2:1:107:VAL:HG13	2:1:239:ILE:HD13	1.99	0.44
1:0:66:PRO:O	1:0:69:ASN:N	2.48	0.44
1:0:261:VAL:HA	3:3:49:ILE:HG21	2.00	0.44
3:3:97:HIS:CE1	3:3:230:HIS:ND1	2.86	0.44
2:1:302:TYR:CE1	3:3:189:TYR:HB3	2.54	0.43
1:0:13:HIS:N	1:0:13:HIS:ND1	2.65	0.43
1:0:309:ALA:HA	3:3:205:PRO:HD3	2.00	0.43
2:1:144:GLU:HB2	2:1:146:ASN:ND2	2.34	0.42
1:0:10:VAL:HG12	1:0:11:GLY:O	2.20	0.42
1:0:338:PRO:HB2	1:0:340:LEU:HG	2.00	0.42
1:0:311:GLU:HB3	6:0:346:HOH:O	2.19	0.42
2:1:149:HIS:CD2	6:1:307:HOH:O	2.73	0.42
3:3:89:PRO:HB2	3:3:104:LEU:CD1	2.50	0.42
2:1:89:ILE:HG12	2:1:258:ARG:HG2	2.02	0.42
2:1:237:PHE:CZ	5:1:0:SPH:H4	2.55	0.41
3:3:89:PRO:HB2	3:3:104:LEU:HD12	2.01	0.41
1:0:172:ARG:HB3	1:0:287:ILE:HG13	2.01	0.41
3:3:71:ARG:NH1	3:3:209:ASP:OD1	2.49	0.41
3:3:233:GLN:O	3:3:236:LEU:N	2.53	0.41
1:0:68:LEU:HD11	3:3:40:VAL:HG22	2.02	0.41
2:1:209:TYR:O	2:1:230:GLY:HA2	2.20	0.41
2:1:257:ILE:HD12	2:1:257:ILE:N	2.36	0.41
3:3:97:HIS:CE1	3:3:230:HIS:CE1	3.08	0.41
1:0:60:VAL:HB	3:3:217:CYS:HB3	2.02	0.41
2:1:144:GLU:HB2	2:1:146:ASN:HD22	1.86	0.41
1:0:103:ALA:HB3	1:0:280:PRO:CD	2.50	0.41
3:3:87:LEU:HD13	3:3:190:ILE:HD11	2.03	0.41
3:3:10:SER:O	3:3:11:ASN:HB2	2.21	0.40
3:3:62:LYS:O	3:3:64:THR:HG23	2.21	0.40
1:0:97:ALA:C	1:0:99:ASN:N	2.73	0.40
1:0:43:LYS:HD3	1:0:43:LYS:HA	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:78:GLU:OE2	2:1:265:HIS:N	2.54	0.40
2:1:286:TYR:HB2	2:1:291:LEU:HD11	2.03	0.40
1:0:166:TYR:CE1	1:0:338:PRO:HG3	2.57	0.40
2:1:112:TYR:CD2	5:1:0:SPH:H5	2.56	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	290/340 (85%)	258 (89%)	26 (9%)	6 (2%)	7 23
2	1	233/302 (77%)	213 (91%)	15 (6%)	5 (2%)	7 23
3	3	236/238 (99%)	218 (92%)	16 (7%)	2 (1%)	19 49
All	All	759/880 (86%)	689 (91%)	57 (8%)	13 (2%)	9 29

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	111	LEU
1	0	309	ALA
2	1	146	ASN
3	3	234	LYS
3	3	235	ALA
1	0	11	GLY
1	0	43	LYS
2	1	99	THR
1	0	75	ALA
2	1	82	ALA
2	1	219	ASP
1	0	66	PRO
2	1	69	HIS

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	250/289 (86%)	230 (92%)	20 (8%)	12	34
2	1	205/261 (78%)	196 (96%)	9 (4%)	28	61
3	3	210/212 (99%)	202 (96%)	8 (4%)	33	67
All	All	665/762 (87%)	628 (94%)	37 (6%)	21	51

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	26	ASN
1	0	29	THR
1	0	36	SER
1	0	44	GLN
1	0	57	ILE
1	0	72	ASN
1	0	76	CYS
1	0	94	THR
1	0	96	GLU
1	0	99	ASN
1	0	112	ARG
1	0	135	LEU
1	0	172	ARG
1	0	206	ASN
1	0	225	THR
1	0	235	ASN
1	0	307	ASN
1	0	317	PRO
1	0	333	ARG
1	0	339	ARG
2	1	145	THR
2	1	149	HIS
2	1	181	PRO
2	1	251	THR
2	1	272	ARG
2	1	286	TYR

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Mol	Chain	Res	Type
2	1	291	LEU
2	1	293	PRO
2	1	298	ASP
3	3	54	PRO
3	3	58	SER
3	3	71	ARG
3	3	161	GLN
3	3	169	PRO
3	3	204	THR
3	3	208	MET
3	3	224	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	69	ASN
1	0	235	ASN
1	0	330	ASN
2	1	100	ASN
2	1	146	ASN
2	1	220	GLN
3	3	233	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 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	$\#\|Z\| > 2$
4	MYR	0	1	1	14,14,15	0.52	0	13,13,15	0.90	0
5	SPH	1	0	-	19,20,20	0.86	1 (5%)	18,21,21	3.61	6 (33%)

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	MYR	0	1	1	-	5/11/12/13	-
5	SPH	1	0	-	2/2/2/4	8/21/21/21	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	0	SPH	O3-C3	2.98	1.49	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	1	0	SPH	O3-C3-C2	-10.21	91.11	107.31
5	1	0	SPH	O1-C1-C2	9.22	130.80	111.43
5	1	0	SPH	O3-C3-C4	-4.06	99.99	110.85
5	1	0	SPH	C3-C4-C5	-3.29	117.45	124.79
5	1	0	SPH	C6-C5-C4	-3.13	111.41	125.39
5	1	0	SPH	C1-C2-C3	2.16	117.67	113.03

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	1	0	SPH	C3
5	1	0	SPH	C2

All (13) torsion outliers are listed below:

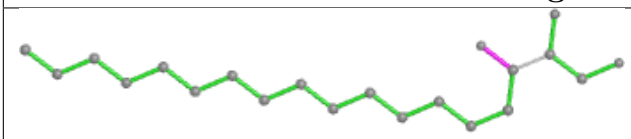
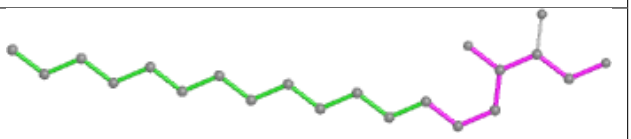
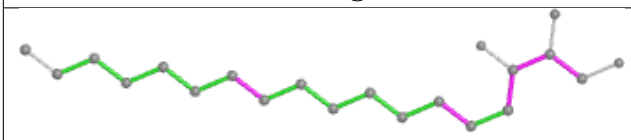
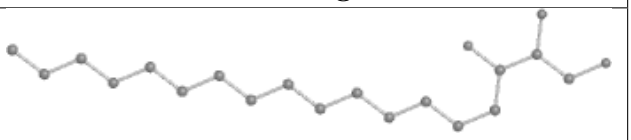
Mol	Chain	Res	Type	Atoms
5	1	0	SPH	O1-C1-C2-N2
5	1	0	SPH	O1-C1-C2-C3
5	1	0	SPH	N2-C2-C3-O3
5	1	0	SPH	N2-C2-C3-C4
5	1	0	SPH	C2-C3-C4-C5
5	1	0	SPH	O3-C3-C4-C5
4	0	1	MYR	C4-C5-C6-C7
4	0	1	MYR	C9-C10-C11-C12
4	0	1	MYR	C3-C4-C5-C6
5	1	0	SPH	C4-C5-C6-C7
4	0	1	MYR	C6-C7-C8-C9
4	0	1	MYR	C11-C12-C13-C14
5	1	0	SPH	C10-C11-C12-C13

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	0	SPH	6	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.