Full wwPDB X-ray Structure Validation Report (i)

Feb 4, 2024 – 06:37 AM EST

PDB ID	:	1OOP
Title	:	The Crystal Structure of Swine Vesicular Disease Virus
Authors	:	Fry, E.E.; Knowles, N.J.; Newman, J.W.I.; Wilsden, G.; Rao, Z.; King, A.M.Q.; Stuart, D.I.
Deposited on	:	2003-03-04
Resolution	:	3.00 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:

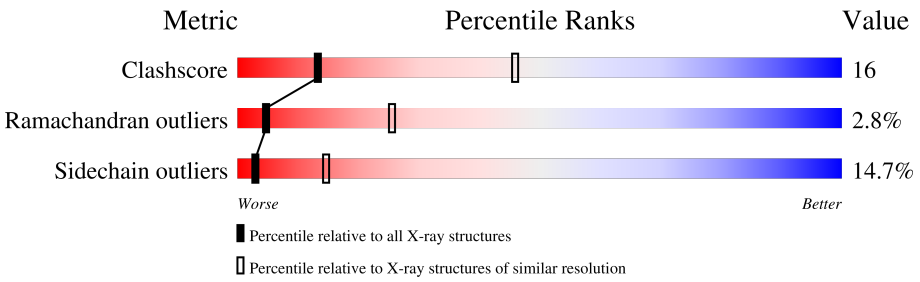
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 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	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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	A	283	55% 31% 9% • •
2	B	261	66% 21% 8% • •
3	C	238	65% 26% 8% •
4	D	69	59% 20% • • 16%

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	A	284	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6399 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 Coat protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	271	2140	1349	373	407	11	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	80	GLU	LYS	conflict	UNP P13900
A	182	VAL	ILE	conflict	UNP P13900

- Molecule 2 is a protein called Coat protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	252	1942	1227	328	369	18	0	0	0

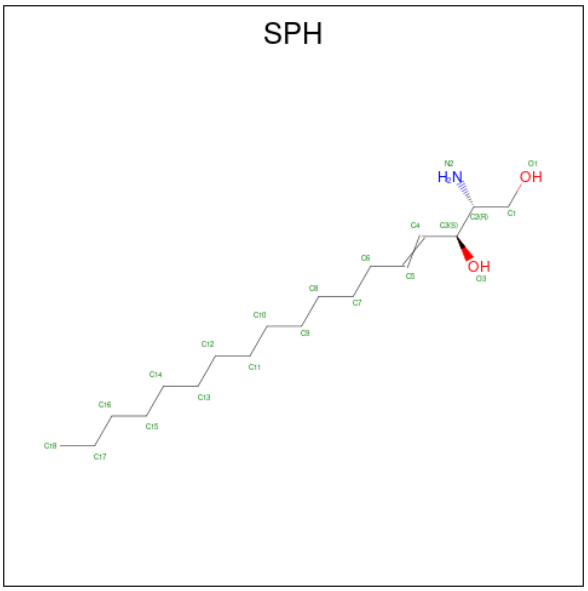
- Molecule 3 is a protein called Coat protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	238	1829	1168	293	352	16	0	0	0

- Molecule 4 is a protein called Coat protein VP4.

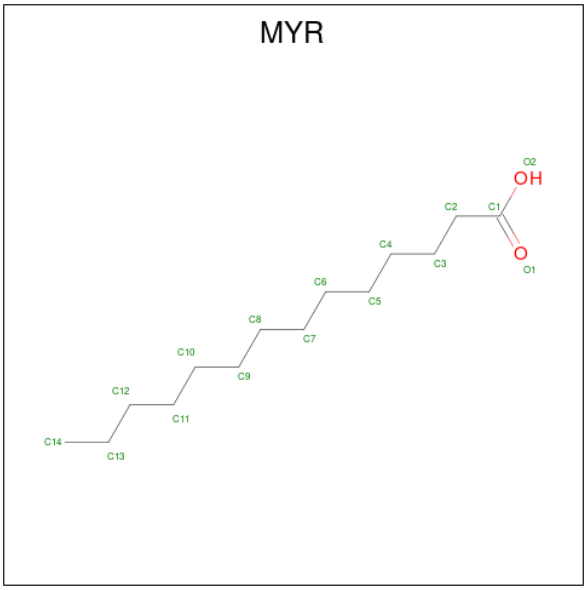
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	58	452	279	79	92	2	0	0	0

- 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	A	1	21	18	1	2	0	0

- Molecule 6 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



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

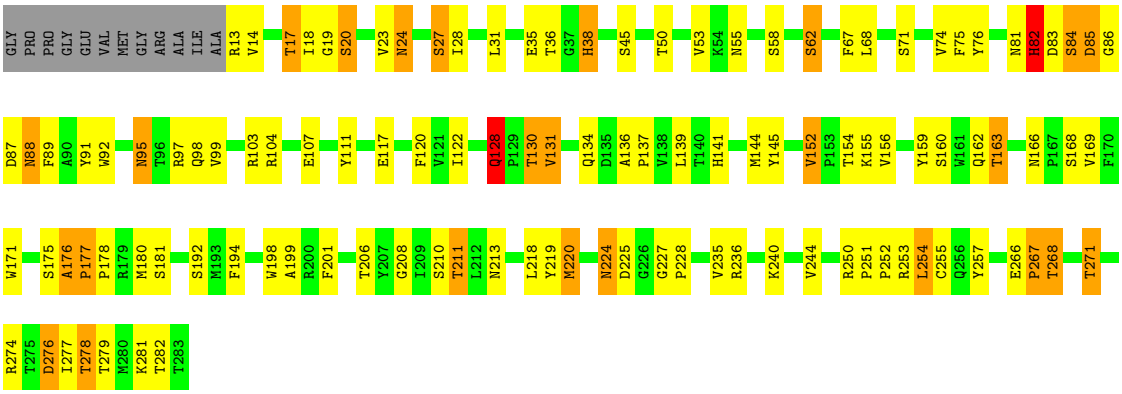
3 Residue-property plots (i)

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.

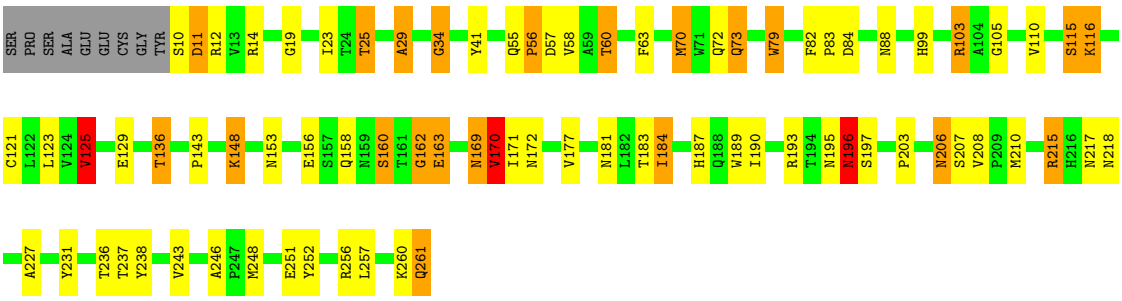
• Molecule 1: Coat protein VP1

Chain A: 55% 31% 9% • •



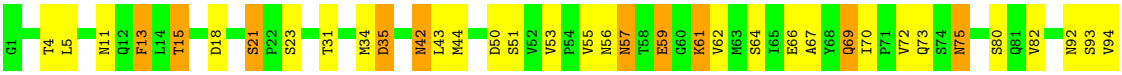
• Molecule 2: Coat protein VP2

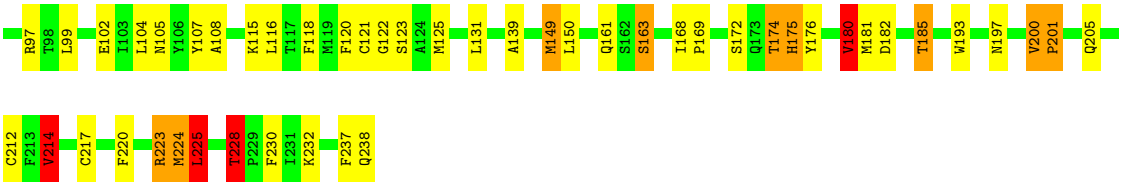
Chain B: 66% 21% 8% • •



• Molecule 3: Coat protein VP3

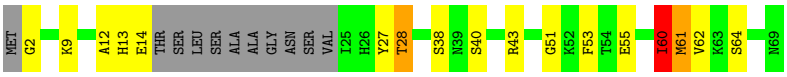
Chain C: 65% 26% 8% •





• Molecule 4: Coat protein VP4

Chain D:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	354.10Å 371.70Å 318.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.00)	Depositor
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.245 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6399	wwPDB-VP
Average B, all atoms (Å^2)	14.0	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: SPH, MYR

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	0.74	0/2201	1.00	6/3003 (0.2%)
2	B	0.82	0/1992	1.02	8/2719 (0.3%)
3	C	0.81	2/1878 (0.1%)	0.96	5/2564 (0.2%)
4	D	0.65	0/460	0.98	1/619 (0.2%)
All	All	0.78	2/6531 (0.0%)	1.00	20/8905 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	121	CYS	CB-SG	-6.13	1.71	1.82
3	C	180	VAL	CB-CG2	5.05	1.63	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	86	GLY	N-CA-C	-9.75	88.72	113.10
1	A	84	SER	N-CA-C	9.64	137.03	111.00
2	B	170	VAL	CB-CA-C	-7.15	97.82	111.40
3	C	214	VAL	CB-CA-C	-7.12	97.86	111.40
1	A	130	THR	N-CA-C	7.06	130.06	111.00
1	A	85	ASP	N-CA-C	6.53	128.63	111.00
1	A	128	GLN	N-CA-C	6.45	128.42	111.00
2	B	125	VAL	CB-CA-C	-6.02	99.96	111.40
2	B	115	SER	N-CA-C	6.01	127.24	111.00
3	C	174	THR	N-CA-C	5.67	126.30	111.00
4	D	12	ALA	N-CA-C	5.62	126.18	111.00
2	B	56	PRO	C-N-CA	-5.48	108.00	121.70
2	B	56	PRO	N-CA-C	-5.39	98.08	112.10
2	B	227	ALA	N-CA-C	-5.35	96.57	111.00
3	C	139	ALA	N-CA-C	-5.34	96.57	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	27	SER	N-CA-C	-5.30	96.70	111.00
3	C	225	LEU	CA-CB-CG	5.28	127.44	115.30
2	B	29	ALA	N-CA-C	-5.26	96.81	111.00
2	B	162	GLY	N-CA-C	-5.11	100.33	113.10
3	C	228	THR	CB-CA-C	-5.05	97.97	111.60

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	A	2140	0	2061	90	0
2	B	1942	0	1875	70	0
3	C	1829	0	1770	69	0
4	D	452	0	429	11	0
5	A	21	0	36	5	0
6	D	15	0	27	4	0
All	All	6399	0	6198	204	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 16.

All (204) 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)
3:C:42:ASN:HD22	3:C:44:MET:H	1.14	0.94
2:B:183:THR:HG21	3:C:50:ASP:O	1.70	0.92
1:A:163:THR:HG21	1:A:168:SER:OG	1.71	0.91
1:A:274:ARG:HE	3:C:57:ASN:HD21	1.20	0.90
3:C:57:ASN:HD22	3:C:57:ASN:H	1.19	0.90
1:A:180:MET:HE1	5:A:284:SPH:H172	1.55	0.89
1:A:31:LEU:HB3	3:C:161:GLN:HG3	1.55	0.88
1:A:36:THR:HG22	2:B:29:ALA:HB1	1.57	0.85
2:B:260:LYS:O	2:B:261:GLN:HB2	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:THR:HG21	3:C:93:SER:O	1.77	0.84
3:C:34:MET:O	3:C:35:ASP:HB2	1.79	0.80
3:C:107:TYR:CE2	3:C:225:LEU:HD13	2.17	0.80
3:C:53:VAL:HG22	3:C:214:VAL:HG22	1.64	0.79
1:A:88:ASN:HB3	1:A:156:VAL:HG13	1.65	0.78
1:A:144:MET:SD	1:A:163:THR:HG23	2.23	0.78
2:B:156:GLU:OE1	2:B:160:SER:HB3	1.83	0.76
1:A:180:MET:CE	5:A:284:SPH:H172	2.17	0.74
3:C:75:ASN:H	3:C:197:ASN:HD21	1.36	0.72
1:A:274:ARG:HE	3:C:57:ASN:ND2	1.87	0.72
3:C:53:VAL:CG2	3:C:214:VAL:HG22	2.19	0.72
1:A:255:CYS:SG	1:A:268:THR:HG23	2.30	0.71
2:B:256:ARG:HG3	2:B:256:ARG:HH11	1.55	0.71
1:A:208:GLY:O	1:A:211:THR:HG23	1.91	0.71
2:B:136:THR:HG21	2:B:163:GLU:HA	1.72	0.70
2:B:206:ASN:HD22	2:B:207:SER:H	1.38	0.70
1:A:274:ARG:NE	3:C:57:ASN:HD21	1.88	0.70
2:B:82:PHE:O	2:B:217:ASN:O	2.09	0.70
4:D:2:GLY:N	6:D:70:MYR:C1	2.56	0.69
3:C:55:VAL:HG21	3:C:70:ILE:HD11	1.76	0.67
3:C:116:LEU:HD23	3:C:214:VAL:HG13	1.77	0.66
1:A:268:THR:H	2:B:172:ASN:HD21	1.41	0.66
1:A:92:TRP:HE1	1:A:98:GLN:NE2	1.94	0.66
2:B:70:MET:HE1	2:B:238:TYR:HA	1.78	0.66
1:A:120:PHE:HB2	1:A:178:PRO:HG2	1.77	0.65
3:C:174:THR:O	3:C:175:HIS:HB2	1.97	0.65
2:B:206:ASN:ND2	2:B:207:SER:H	1.94	0.65
2:B:257:LEU:H	2:B:257:LEU:HD23	1.63	0.64
1:A:97:ARG:HA	1:A:103:ARG:HD2	1.78	0.64
1:A:159:TYR:O	1:A:162:GLN:HG2	1.97	0.64
3:C:61:LYS:HG2	3:C:66:GLU:HB3	1.80	0.63
3:C:105:ASN:HB3	3:C:228:THR:HG22	1.78	0.63
2:B:217:ASN:O	2:B:218:ASN:HB2	1.99	0.63
1:A:152:VAL:HG22	1:A:219:TYR:CZ	2.34	0.62
2:B:136:THR:HG22	2:B:162:GLY:O	1.99	0.62
1:A:266:GLU:O	1:A:268:THR:HG22	1.99	0.62
2:B:123:LEU:HG	2:B:125:VAL:HG22	1.82	0.61
1:A:17:THR:HG23	1:A:53:VAL:HB	1.81	0.61
1:A:175:SER:O	1:A:176:ALA:HB3	2.00	0.61
1:A:180:MET:HE1	5:A:284:SPH:C17	2.29	0.61
4:D:2:GLY:N	6:D:70:MYR:O1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ASN:ND2	1:A:97:ARG:H	1.98	0.60
2:B:183:THR:CG2	3:C:50:ASP:O	2.45	0.60
2:B:70:MET:HE1	2:B:238:TYR:CA	2.32	0.59
1:A:38:HIS:CD2	4:D:55:GLU:HG2	2.36	0.59
1:A:251:PRO:HD3	2:B:184:ILE:HD11	1.85	0.59
3:C:42:ASN:ND2	3:C:44:MET:H	1.93	0.59
3:C:108:ALA:HB3	3:C:224:MET:HB3	1.84	0.59
2:B:172:ASN:HA	2:B:177:VAL:O	2.03	0.58
3:C:131:LEU:C	3:C:131:LEU:HD23	2.24	0.58
3:C:116:LEU:CD2	3:C:214:VAL:HG13	2.34	0.58
2:B:136:THR:CG2	2:B:162:GLY:O	2.52	0.58
1:A:277:ILE:HD12	3:C:82:VAL:O	2.04	0.57
1:A:68:LEU:HD12	1:A:244:VAL:HG11	1.86	0.57
1:A:199:ALA:HB2	1:A:211:THR:HB	1.86	0.56
2:B:34:GLY:HA3	2:B:203:PRO:HD3	1.87	0.56
1:A:19:GLY:HA2	1:A:50:THR:HG22	1.86	0.56
1:A:163:THR:HG22	1:A:166:ASN:HB2	1.87	0.56
3:C:66:GLU:HA	3:C:69:GLN:HG3	1.86	0.56
3:C:200:VAL:HG22	3:C:201:PRO:HD2	1.87	0.56
1:A:71:SER:HB2	3:C:15:THR:HG22	1.86	0.56
3:C:57:ASN:HD22	3:C:57:ASN:N	1.97	0.55
1:A:35:GLU:HB3	2:B:195:ASN:HD21	1.72	0.55
1:A:128:GLN:O	1:A:128:GLN:NE2	2.39	0.55
3:C:18:ASP:OD2	4:D:43:ARG:HD2	2.07	0.55
2:B:56:PRO:HG2	2:B:60:THR:HG21	1.89	0.54
3:C:57:ASN:H	3:C:57:ASN:ND2	1.98	0.54
2:B:103:ARG:HD2	2:B:210:MET:HG2	1.90	0.54
1:A:130:THR:O	1:A:131:VAL:HB	2.08	0.54
3:C:115:LYS:HG3	3:C:217:CYS:SG	2.47	0.54
1:A:81:ASN:O	1:A:82:HIS:HB2	2.06	0.53
1:A:255:CYS:SG	1:A:268:THR:CG2	2.96	0.53
2:B:25:THR:HG21	2:B:197:SER:OG	2.08	0.53
1:A:194:PHE:CE1	1:A:250:ARG:HD2	2.44	0.53
1:A:198:TRP:O	2:B:215:ARG:HG3	2.09	0.53
3:C:174:THR:O	3:C:175:HIS:CB	2.57	0.53
4:D:60:ILE:O	4:D:61:MET:HB2	2.10	0.52
4:D:27:TYR:O	4:D:28:THR:CB	2.57	0.52
2:B:110:VAL:HG22	2:B:243:VAL:HG22	1.90	0.52
2:B:148:LYS:H	2:B:153:ASN:HD21	1.57	0.52
3:C:149:MET:CE	3:C:150:LEU:HD23	2.39	0.52
3:C:42:ASN:HD22	3:C:44:MET:N	1.96	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:GLY:HA2	2:B:58:VAL:CG2	2.39	0.52
2:B:169:ASN:HD22	2:B:169:ASN:C	2.12	0.52
1:A:89:PHE:HE1	1:A:155:LYS:HA	1.74	0.52
4:D:2:GLY:N	6:D:70:MYR:H21	2.25	0.52
1:A:103:ARG:O	1:A:107:GLU:HG3	2.10	0.51
1:A:144:MET:SD	1:A:163:THR:CG2	2.96	0.51
1:A:176:ALA:HB2	3:C:11:ASN:HB3	1.92	0.51
1:A:20:SER:OG	1:A:50:THR:HB	2.09	0.51
1:A:177:PRO:HG2	3:C:13:PHE:HB2	1.93	0.51
1:A:254:LEU:HB2	2:B:177:VAL:HA	1.92	0.51
1:A:27:SER:HB2	4:D:64:SER:HB2	1.92	0.51
2:B:23:ILE:HD12	2:B:63:PHE:CZ	2.47	0.50
1:A:23:VAL:HG12	1:A:24:ASN:N	2.27	0.50
1:A:35:GLU:HA	2:B:189:TRP:HB2	1.93	0.50
1:A:257:TYR:HB2	3:C:237:PHE:CZ	2.47	0.50
1:A:201:PHE:CD2	2:B:215:ARG:HD2	2.47	0.49
2:B:115:SER:O	2:B:116:LYS:HB2	2.11	0.49
3:C:56:ASN:O	3:C:67:ALA:HA	2.13	0.49
3:C:180:VAL:HG12	3:C:180:VAL:O	2.13	0.49
2:B:99:HIS:CG	2:B:252:TYR:HB3	2.48	0.49
2:B:206:ASN:HD22	2:B:207:SER:N	2.06	0.48
2:B:206:ASN:ND2	2:B:207:SER:N	2.61	0.48
3:C:92:ASN:ND2	3:C:94:VAL:H	2.10	0.48
3:C:149:MET:HE2	3:C:150:LEU:HD23	1.94	0.48
1:A:18:ILE:O	1:A:50:THR:HG21	2.14	0.48
1:A:152:VAL:HG22	1:A:219:TYR:CE1	2.48	0.48
1:A:62:SER:HB2	3:C:42:ASN:ND2	2.29	0.47
3:C:44:MET:HE2	3:C:220:PHE:HD1	1.79	0.47
1:A:128:GLN:O	1:A:130:THR:N	2.47	0.47
2:B:63:PHE:CD1	2:B:246:ALA:HB2	2.48	0.47
3:C:116:LEU:HD12	3:C:168:ILE:HD11	1.97	0.47
1:A:139:LEU:HA	1:A:224:ASN:HD21	1.77	0.47
2:B:55:GLN:C	2:B:56:PRO:O	2.50	0.47
1:A:208:GLY:O	1:A:211:THR:CG2	2.61	0.47
2:B:125:VAL:HG13	2:B:187:HIS:HB3	1.96	0.47
2:B:196:ASN:OD1	2:B:196:ASN:C	2.53	0.47
3:C:42:ASN:ND2	3:C:44:MET:HG2	2.29	0.47
3:C:120:PHE:CE2	3:C:122:GLY:HA3	2.50	0.47
3:C:228:THR:HB	3:C:230:PHE:H	1.79	0.47
2:B:19:GLY:HA2	2:B:58:VAL:HG22	1.96	0.46
3:C:125:MET:HE3	3:C:125:MET:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:ASN:HD22	2:B:170:VAL:N	2.13	0.46
2:B:73:GLN:H	2:B:73:GLN:HG2	1.41	0.46
2:B:121:CYS:HA	2:B:190:ILE:O	2.15	0.46
1:A:141:HIS:N	1:A:141:HIS:CD2	2.84	0.46
3:C:97:ARG:NH1	3:C:102:GLU:OE2	2.49	0.46
1:A:76:TYR:HA	1:A:235:VAL:O	2.15	0.45
2:B:193:ARG:HH11	2:B:193:ARG:HG3	1.81	0.45
2:B:231:TYR:CE1	2:B:237:THR:HG22	2.52	0.45
3:C:118:PHE:O	3:C:163:SER:HA	2.15	0.45
1:A:163:THR:HG21	1:A:168:SER:HG	1.76	0.45
2:B:256:ARG:HG3	2:B:256:ARG:NH1	2.28	0.45
1:A:13:ARG:CG	1:A:14:VAL:N	2.80	0.45
1:A:92:TRP:HE1	1:A:98:GLN:HE22	1.62	0.45
1:A:267:PRO:HA	2:B:172:ASN:ND2	2.32	0.45
2:B:257:LEU:H	2:B:257:LEU:CD2	2.28	0.44
2:B:10:SER:O	2:B:11:ASP:HB2	2.17	0.44
1:A:181:SER:O	3:C:23:SER:HA	2.16	0.44
2:B:41:TYR:HD1	2:B:251:GLU:CG	2.31	0.44
1:A:91:TYR:CD2	1:A:91:TYR:C	2.91	0.44
1:A:176:ALA:HA	1:A:177:PRO:HD3	1.66	0.44
1:A:104:ARG:NH1	1:A:253:ARG:O	2.50	0.44
2:B:115:SER:O	2:B:116:LYS:CB	2.65	0.44
2:B:256:ARG:HH11	2:B:256:ARG:CG	2.26	0.44
3:C:64:SER:C	3:C:66:GLU:N	2.70	0.44
4:D:2:GLY:N	6:D:70:MYR:C2	2.81	0.44
1:A:35:GLU:HB3	2:B:195:ASN:ND2	2.32	0.44
1:A:97:ARG:CA	1:A:103:ARG:HD2	2.46	0.44
1:A:145:TYR:O	1:A:166:ASN:HB3	2.18	0.43
1:A:276:ASP:C	1:A:278:THR:H	2.22	0.43
2:B:193:ARG:HG3	2:B:193:ARG:NH1	2.33	0.43
3:C:21:SER:O	4:D:38:SER:HB3	2.18	0.43
3:C:176:TYR:CZ	3:C:223:ARG:HD3	2.53	0.43
1:A:82:HIS:HD2	1:A:227:GLY:O	2.02	0.43
1:A:180:MET:HE1	5:A:284:SPH:C18	2.47	0.43
1:A:13:ARG:HA	1:A:58:SER:HA	2.01	0.43
1:A:251:PRO:HA	1:A:252:PRO:HD3	1.89	0.43
2:B:181:ASN:C	2:B:183:THR:H	2.22	0.42
1:A:62:SER:CB	3:C:42:ASN:HD21	2.32	0.42
2:B:260:LYS:HE3	2:B:260:LYS:HB2	1.74	0.42
3:C:53:VAL:HG22	3:C:214:VAL:CG2	2.42	0.42
1:A:117:GLU:HB3	1:A:240:LYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:208:VAL:HG23	2:B:210:MET:O	2.20	0.42
3:C:42:ASN:HD21	3:C:44:MET:HG2	1.84	0.42
2:B:257:LEU:HD23	2:B:257:LEU:N	2.32	0.42
1:A:122:ILE:HB	1:A:171:TRP:CZ3	2.55	0.41
1:A:220:MET:SD	1:A:220:MET:N	2.93	0.41
1:A:74:VAL:O	1:A:75:PHE:HB2	2.19	0.41
2:B:83:PRO:O	2:B:84:ASP:C	2.59	0.41
2:B:256:ARG:NH1	2:B:257:LEU:O	2.51	0.41
3:C:44:MET:CE	3:C:220:PHE:HD1	2.33	0.41
3:C:182:ASP:HB3	3:C:185:THR:HB	2.02	0.41
1:A:67:PHE:CG	3:C:43:LEU:HD11	2.55	0.41
3:C:168:ILE:HA	3:C:169:PRO:HD2	1.86	0.41
1:A:180:MET:CE	5:A:284:SPH:C17	2.91	0.41
1:A:111:TYR:CD1	2:B:207:SER:HB3	2.55	0.41
3:C:18:ASP:OD1	4:D:40:SER:HB2	2.21	0.41
3:C:75:ASN:N	3:C:197:ASN:HD21	2.11	0.41
1:A:136:ALA:HA	1:A:137:PRO:HD3	1.89	0.41
2:B:79:TRP:CD1	2:B:79:TRP:C	2.94	0.41
2:B:105:GLY:O	2:B:248:MET:N	2.51	0.41
1:A:251:PRO:CD	2:B:184:ILE:HD11	2.50	0.41
3:C:105:ASN:HB3	3:C:228:THR:CG2	2.47	0.41
2:B:136:THR:CG2	2:B:163:GLU:HA	2.45	0.40
2:B:193:ARG:NH1	3:C:123:SER:O	2.54	0.40
3:C:5:LEU:HD23	3:C:5:LEU:O	2.22	0.40
3:C:149:MET:O	3:C:149:MET:HG2	2.21	0.40
1:A:13:ARG:HG3	1:A:14:VAL:N	2.36	0.40
1:A:175:SER:O	1:A:176:ALA:CB	2.63	0.40
3:C:193:TRP:CD1	3:C:193:TRP:N	2.89	0.40
1:A:31:LEU:HD13	3:C:161:GLN:HG3	2.04	0.40
1:A:255:CYS:SG	2:B:172:ASN:ND2	2.95	0.40
1:A:255:CYS:HA	1:A:268:THR:HG21	2.03	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	A	269/283 (95%)	242 (90%)	17 (6%)	10 (4%)	3	19
2	B	250/261 (96%)	222 (89%)	23 (9%)	5 (2%)	7	34
3	C	236/238 (99%)	219 (93%)	13 (6%)	4 (2%)	9	39
4	D	54/69 (78%)	45 (83%)	5 (9%)	4 (7%)	1	5
All	All	809/851 (95%)	728 (90%)	58 (7%)	23 (3%)	5	25

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	A	87	ASP
2	B	11	ASP
3	C	35	ASP
3	C	59	GLU
4	D	28	THR
4	D	60	ILE
1	A	83	ASP
1	A	85	ASP
1	A	131	VAL
2	B	12	ARG
2	B	34	GLY
2	B	116	LYS
3	C	175	HIS
2	B	196	ASN
4	D	61	MET
1	A	176	ALA
3	C	224	MET
1	A	24	ASN
1	A	213	ASN
1	A	228	PRO
1	A	177	PRO
4	D	51	GLY

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	A	238/245 (97%)	201 (84%)	37 (16%)	2 13
2	B	213/220 (97%)	186 (87%)	27 (13%)	4 19
3	C	206/206 (100%)	172 (84%)	34 (16%)	2 11
4	D	49/57 (86%)	43 (88%)	6 (12%)	5 21
All	All	706/728 (97%)	602 (85%)	104 (15%)	3 15

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	20	SER
1	A	28	ILE
1	A	38	HIS
1	A	45	SER
1	A	55	ASN
1	A	62	SER
1	A	82	HIS
1	A	84	SER
1	A	88	ASN
1	A	95	ASN
1	A	99	VAL
1	A	128	GLN
1	A	134	GLN
1	A	152	VAL
1	A	154	THR
1	A	160	SER
1	A	163	THR
1	A	169	VAL
1	A	192	SER
1	A	206	THR
1	A	210	SER
1	A	211	THR
1	A	218	LEU
1	A	220	MET
1	A	224	ASN
1	A	225	ASP
1	A	236	ARG
1	A	254	LEU
1	A	267	PRO

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Mol	Chain	Res	Type
1	A	268	THR
1	A	271	THR
1	A	276	ASP
1	A	278	THR
1	A	279	THR
1	A	281	LYS
1	A	282	THR
2	B	14	ARG
2	B	25	THR
2	B	57	ASP
2	B	60	THR
2	B	70	MET
2	B	72	GLN
2	B	73	GLN
2	B	79	TRP
2	B	88	ASN
2	B	103	ARG
2	B	125	VAL
2	B	129	GLU
2	B	136	THR
2	B	143	PRO
2	B	148	LYS
2	B	158	GLN
2	B	160	SER
2	B	163	GLU
2	B	169	ASN
2	B	170	VAL
2	B	171	ILE
2	B	184	ILE
2	B	196	ASN
2	B	206	ASN
2	B	215	ARG
2	B	236	THR
2	B	261	GLN
3	C	4	THR
3	C	13	PHE
3	C	15	THR
3	C	21	SER
3	C	31	THR
3	C	42	ASN
3	C	51	SER
3	C	57	ASN

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Mol	Chain	Res	Type
3	C	59	GLU
3	C	61	LYS
3	C	62	VAL
3	C	69	GLN
3	C	72	VAL
3	C	73	GLN
3	C	75	ASN
3	C	80	SER
3	C	99	LEU
3	C	104	LEU
3	C	149	MET
3	C	163	SER
3	C	172	SER
3	C	180	VAL
3	C	181	MET
3	C	185	THR
3	C	200	VAL
3	C	201	PRO
3	C	205	GLN
3	C	212	CYS
3	C	214	VAL
3	C	223	ARG
3	C	225	LEU
3	C	228	THR
3	C	232	LYS
3	C	238	GLN
4	D	9	LYS
4	D	13	HIS
4	D	14	GLU
4	D	53	PHE
4	D	60	ILE
4	D	62	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	82	HIS
1	A	88	ASN
1	A	95	ASN
1	A	98	GLN
1	A	128	GLN

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Mol	Chain	Res	Type
1	A	256	GLN
2	B	73	GLN
2	B	169	ASN
2	B	172	ASN
2	B	188	GLN
2	B	195	ASN
2	B	206	ASN
3	C	12	GLN
3	C	42	ASN
3	C	57	ASN
3	C	69	GLN
3	C	92	ASN
3	C	197	ASN
4	D	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	MYR	D	70	-	14,14,15	0.65	0	13,13,15	0.78	1 (7%)
5	SPH	A	284	-	19,20,20	1.21	3 (15%)	18,21,21	1.75	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
6	MYR	D	70	-	-	5/11/12/13	-
5	SPH	A	284	-	1/1/2/4	9/21/21/21	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	284	SPH	C1-C2	3.06	1.57	1.52
5	A	284	SPH	O1-C1	-2.69	1.31	1.42
5	A	284	SPH	C3-C4	2.60	1.54	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	284	SPH	C1-C2-C3	4.07	121.78	113.03
5	A	284	SPH	O3-C3-C4	-3.78	100.73	110.85
5	A	284	SPH	O3-C3-C2	-2.57	103.25	107.31
5	A	284	SPH	C9-C8-C7	-2.36	102.42	114.42
6	D	70	MYR	O1-C1-C2	-2.18	112.55	126.89

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	284	SPH	C3

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	284	SPH	O1-C1-C2-N2
5	A	284	SPH	O1-C1-C2-C3
5	A	284	SPH	C1-C2-C3-O3
5	A	284	SPH	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
5	A	284	SPH	O3-C3-C4-C5
5	A	284	SPH	C10-C11-C12-C13
6	D	70	MYR	C6-C7-C8-C9
6	D	70	MYR	C5-C6-C7-C8
5	A	284	SPH	N2-C2-C3-C4
6	D	70	MYR	C10-C11-C12-C13
6	D	70	MYR	C1-C2-C3-C4
6	D	70	MYR	C11-C12-C13-C14
5	A	284	SPH	C4-C5-C6-C7
5	A	284	SPH	C6-C7-C8-C9

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	70	MYR	4	0
5	A	284	SPH	5	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.

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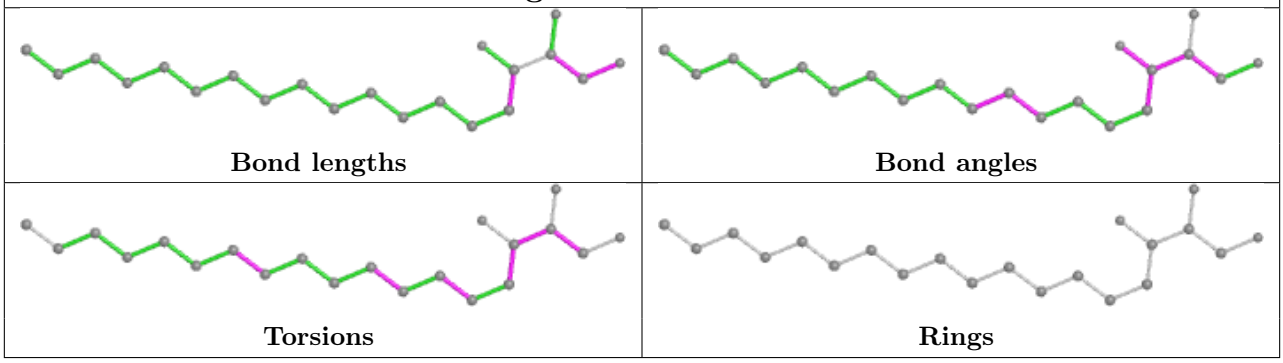

5.7 Other polymers (i)

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.