Full wwPDB X-ray Structure Validation Report (i)

May 23, 2020 – 05:40 am BST

PDB ID	:	6FLA
Title	:	3H5 Fab bound to EDIII of DenV 2 Xtal form 1
Authors	:	Flanagan, A.; Renner, M.; Grimes, J.M.
Deposited on	:	2018-01-25
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
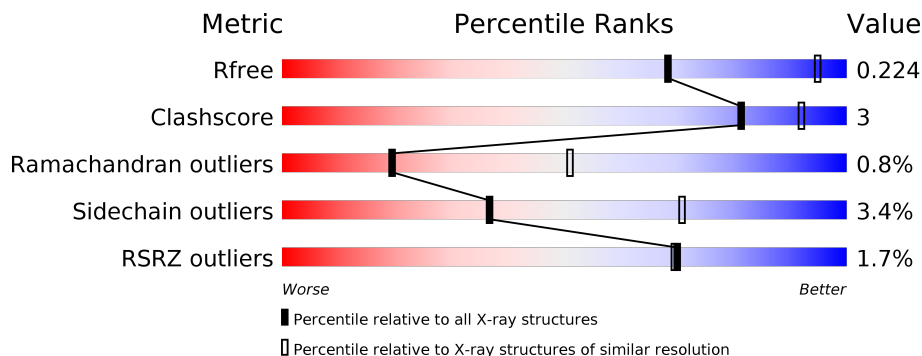with specific help available everywhere you see the (i) symbol.

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	Percentile Ranks	Value
Rfree		0.224
Clashscore		3
Ramachandran outliers		0.8%
Sidechain outliers		3.4%
RSRZ outliers		1.7%

Worse *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 on 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	227	% 88% 5% 7%
1	H	227	% 88% 7% ··
2	B	218	92% 7% ·
2	L	218	91% 7% ·
3	G	98	7% 88% 8% ··
4	I	101	4% 81% 14% ··

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	GOL	H	301	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8142 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 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total 1601	C 1013	N 266	O 315	S 7	0	0	0
1	H	217	Total 1632	C 1030	N 272	O 323	S 7	0	0	0

- Molecule 2 is a protein called Light Chain of 3H5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total 1671	C 1039	N 287	O 338	S 7	0	0	0
2	L	216	Total 1671	C 1039	N 287	O 338	S 7	0	0	0

- Molecule 3 is a protein called Domain III of Dengue virus 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	98	Total 776	C 500	N 127	O 144	S 5	0	0	0

- Molecule 4 is a protein called Domain III of Dengue virus 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	99	Total 777	C 500	N 128	O 145	S 4	0	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Cl 1	0	0
5	L	1	Total 1	Cl 1	0	0

• Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
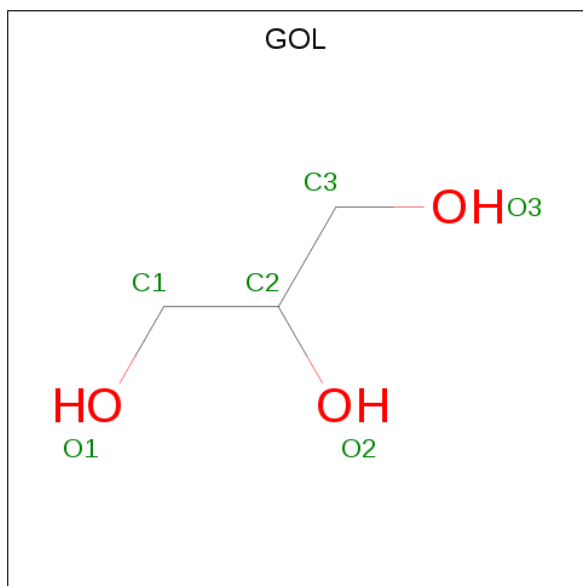
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total C O			0	0
			6	3	3		
6	L	1	Total C O			0	0
			6	3	3		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
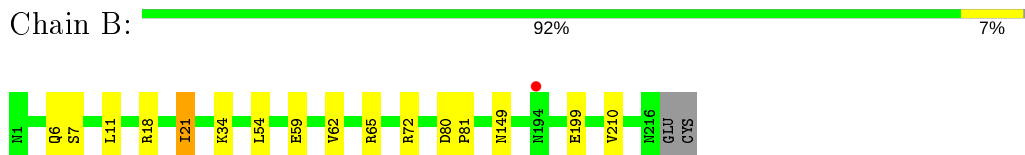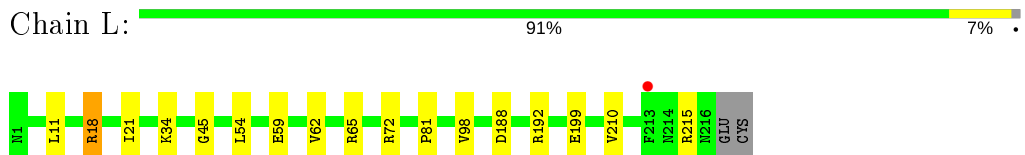
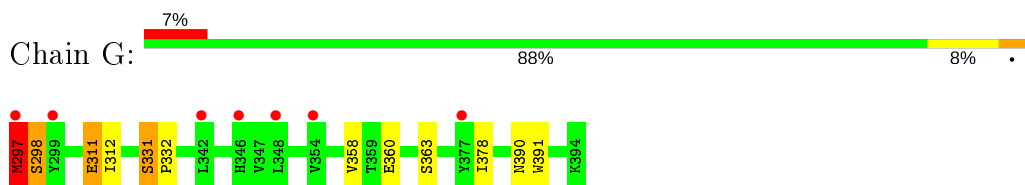- Molecule 1: Heavy chain
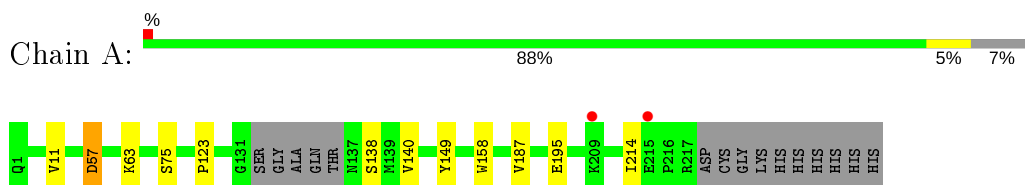
- Molecule 1: Heavy chain
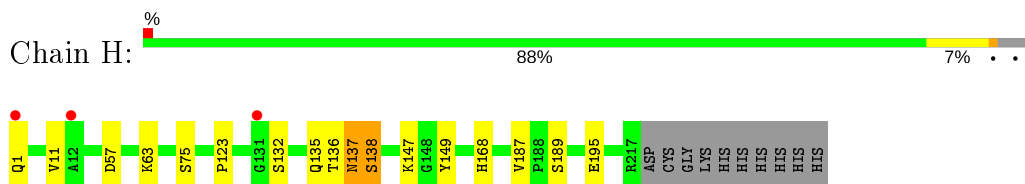
- Molecule 2: Light Chain of 3H5
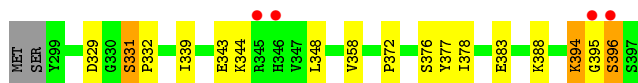

- Molecule 2: Light Chain of 3H5

- Molecule 3: Domain III of Dengue virus 2

- Molecule 4: Domain III of Dengue virus 2

Chain I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	40.84Å 263.87Å 272.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.59 – 2.90 39.59 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.59-2.90) 99.3 (39.59-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.86 (at 2.90Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.203 , 0.221 0.209 , 0.224	Depositor DCC
R_{free} test set	1689 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	66.7	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 53.8	EDS
L-test for twinning[2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8142	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.48	0/1644	0.72	0/2245
1	H	0.51	0/1676	0.76	0/2290
2	B	0.50	0/1708	0.72	0/2319
2	L	0.54	0/1708	0.77	2/2319 (0.1%)
3	G	0.55	0/793	0.83	1/1070 (0.1%)
4	I	0.57	0/794	0.82	0/1073
All	All	0.52	0/8323	0.76	3/11316 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	215	ARG	C-N-CA	8.35	142.57	121.70
2	L	215	ARG	CA-C-N	5.53	129.36	117.20
3	G	297	MET	C-N-CA	5.49	135.42	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1601	0	1554	3	0
1	H	1632	0	1583	6	0

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1671	0	1608	6	0
2	L	1671	0	1608	8	0
3	G	776	0	789	11	0
4	I	777	0	788	11	0
5	B	1	0	0	0	0
5	L	1	0	0	0	0
6	H	6	0	8	1	0
6	L	6	0	8	1	0
All	All	8142	0	7946	42	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 3.

All (42) 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:G:297:MET:HA	3:G:298:SER:HB2	1.49	0.92
1:H:135:GLN:O	1:H:138:SER:HB2	1.70	0.91
4:I:331:SER:HB3	4:I:332:PRO:HD3	1.72	0.71
2:L:65:ARG:HD2	2:L:81:PRO:O	1.90	0.70
2:B:65:ARG:HD2	2:B:81:PRO:O	1.92	0.69
3:G:331:SER:HB3	3:G:332:PRO:HD3	1.76	0.65
1:H:168:HIS:HA	6:H:301:GOL:H12	1.81	0.61
3:G:297:MET:HA	3:G:298:SER:CB	2.28	0.59
4:I:348:LEU:HB3	4:I:372:PRO:HG3	1.88	0.56
2:L:199:GLU:HG2	2:L:210:VAL:HG22	1.87	0.56
2:L:34:LYS:HG2	2:L:54:LEU:HD13	1.87	0.55
3:G:312:ILE:CD1	3:G:378:ILE:HD13	2.37	0.55
1:A:123:PRO:HB3	1:A:149:TYR:HB3	1.90	0.54
2:B:199:GLU:HG2	2:B:210:VAL:HG22	1.91	0.52
1:H:123:PRO:HB3	1:H:149:TYR:HB3	1.93	0.50
4:I:339:ILE:HG12	4:I:378:ILE:HD12	1.94	0.50
4:I:395:GLY:O	4:I:396:SER:HB2	2.12	0.49
2:L:45:GLY:H	6:L:302:GOL:H2	1.77	0.48
3:G:311:GLU:OE1	1:H:147:LYS:NZ	2.45	0.47
3:G:378:ILE:HD11	3:G:391:TRP:HB2	1.99	0.45
4:I:344:LYS:HE3	4:I:377:TYR:HE2	1.82	0.45
4:I:332:PRO:HA	4:I:358:VAL:O	2.17	0.45
3:G:312:ILE:HD13	3:G:378:ILE:HD13	1.99	0.44
2:L:18:ARG:HG3	2:L:18:ARG:O	2.16	0.44
4:I:377:TYR:OH	4:I:388:LYS:HD3	2.18	0.44

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:312:ILE:HD11	3:G:378:ILE:HD13	1.99	0.44
4:I:394:LYS:HD3	4:I:395:GLY:H	1.82	0.44
4:I:331:SER:HB3	4:I:332:PRO:CD	2.45	0.44
3:G:332:PRO:HA	3:G:358:VAL:O	2.18	0.43
1:H:136:THR:HG22	1:H:137:ASN:OD1	2.19	0.43
2:B:6:GLN:HE21	2:B:21:ILE:CD1	2.32	0.43
3:G:360:GLU:HB2	3:G:363:SER:HB3	2.01	0.42
1:A:57:ASP:HA	2:L:192:ARG:NH2	2.33	0.42
2:B:18:ARG:HG3	2:B:80:ASP:HB2	2.01	0.42
1:H:138:SER:HB3	1:H:189:SER:OG	2.19	0.42
4:I:383:GLU:HG3	2:L:98:VAL:HG23	2.01	0.42
2:B:59:GLU:HB2	2:B:62:VAL:HG13	2.01	0.42
2:B:34:LYS:HG2	2:B:54:LEU:HD13	2.00	0.42
3:G:378:ILE:HD11	3:G:391:TRP:CB	2.50	0.41
4:I:348:LEU:CB	4:I:372:PRO:HG3	2.50	0.41
2:L:59:GLU:HB2	2:L:62:VAL:HG13	2.03	0.41
1:A:158:TRP:HZ3	1:A:214:ILE:HD12	1.86	0.41

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	208/227 (92%)	203 (98%)	4 (2%)	1 (0%)	29	61
1	H	215/227 (95%)	210 (98%)	4 (2%)	1 (0%)	29	61
2	B	214/218 (98%)	210 (98%)	3 (1%)	1 (0%)	29	61
2	L	214/218 (98%)	210 (98%)	3 (1%)	1 (0%)	29	61
3	G	96/98 (98%)	90 (94%)	4 (4%)	2 (2%)	7	26
4	I	97/101 (96%)	91 (94%)	4 (4%)	2 (2%)	7	26
All	All	1044/1089 (96%)	1014 (97%)	22 (2%)	8 (1%)	19	51

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	331	SER
4	I	331	SER
3	G	298	SER
4	I	396	SER
1	H	132	SER
2	B	72	ARG
2	L	72	ARG
1	A	138	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	A	177/189 (94%)	170 (96%)	7 (4%)	31	65
1	H	180/189 (95%)	171 (95%)	9 (5%)	24	57
2	B	191/193 (99%)	187 (98%)	4 (2%)	53	81
2	L	191/193 (99%)	187 (98%)	4 (2%)	53	81
3	G	88/88 (100%)	85 (97%)	3 (3%)	37	71
4	I	88/90 (98%)	84 (96%)	4 (4%)	27	61
All	All	915/942 (97%)	884 (97%)	31 (3%)	37	71

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

Mol	Chain	Res	Type
1	A	11	VAL
1	A	57	ASP
1	A	63	LYS
1	A	75	SER
1	A	140	VAL
1	A	187	VAL
1	A	195	GLU
2	B	7	SER
2	B	11	LEU

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Mol	Chain	Res	Type
2	B	21	ILE
2	B	149	ASN
3	G	297	MET
3	G	311	GLU
3	G	390	ASN
1	H	1	GLN
1	H	11	VAL
1	H	57	ASP
1	H	63	LYS
1	H	75	SER
1	H	137	ASN
1	H	138	SER
1	H	187	VAL
1	H	195	GLU
4	I	329	ASP
4	I	343	GLU
4	I	376	SER
4	I	394	LYS
2	L	11	LEU
2	L	18	ARG
2	L	21	ILE
2	L	188	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	G	390	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	GOL	H	301	-	5,5,5	1.68	2 (40%)	5,5,5	1.94	1 (20%)
6	GOL	L	302	-	5,5,5	0.96	0	5,5,5	0.83	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	GOL	H	301	-	-	4/4/4/4	-
6	GOL	L	302	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	301	GOL	O1-C1	2.70	1.53	1.42
6	H	301	GOL	C1-C2	2.38	1.61	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	301	GOL	O1-C1-C2	3.13	125.20	110.20

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	301	GOL	O1-C1-C2-C3
6	H	301	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	H	301	GOL	O2-C2-C3-O3
6	L	302	GOL	C1-C2-C3-O3
6	H	301	GOL	O1-C1-C2-O2
6	L	302	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	301	GOL	1	0
6	L	302	GOL	1	0

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)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	212/227 (93%)	0.08	2 (0%)	84 84	46, 68, 93, 116	0
1	H	217/227 (95%)	0.04	3 (1%)	75 75	34, 61, 89, 101	0
2	B	216/218 (99%)	-0.10	1 (0%)	91 91	45, 64, 87, 100	0
2	L	216/218 (99%)	-0.08	1 (0%)	91 91	34, 57, 83, 95	0
3	G	98/98 (100%)	0.47	7 (7%)	16 12	46, 80, 116, 129	0
4	I	99/101 (98%)	0.32	4 (4%)	38 33	50, 75, 101, 117	0
All	All	1058/1089 (97%)	0.06	18 (1%)	70 69	34, 65, 97, 129	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	131	GLY	3.3
4	I	345	ARG	3.0
3	G	342	LEU	2.7
4	I	346	HIS	2.7
3	G	297	MET	2.6
4	I	396	SER	2.6
2	L	213	PHE	2.5
2	B	194	ASN	2.4
3	G	346	HIS	2.4
1	H	1	GLN	2.4
3	G	348	LEU	2.3
3	G	354	VAL	2.3
1	A	209	LYS	2.3
1	H	12	ALA	2.2
3	G	299	TYR	2.1
1	A	215	GLU	2.1
4	I	395	GLY	2.1
3	G	377	TYR	2.0

Full wwPDB X-ray Structure Validation Report

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	L	302	6/6	0.84	0.26	69,70,71,73	0
6	GOL	H	301	6/6	0.86	0.26	57,59,59,60	0
5	CL	L	301	1/1	0.95	0.10	52,52,52,52	0
5	CL	B	301	1/1	0.98	0.11	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.