Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:49 pm BST

PDB ID	:	3G5V
Title	:	Antibodies Specifically Targeting a Locally Misfolded Region of Tumor Associated EGFR
Authors	:	Garrett, T.P.J.; Burgess, A.W.; Huyton, T.; Xu, Y.
Deposited on	:	2009-02-05
Resolution	:	2.00 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 ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

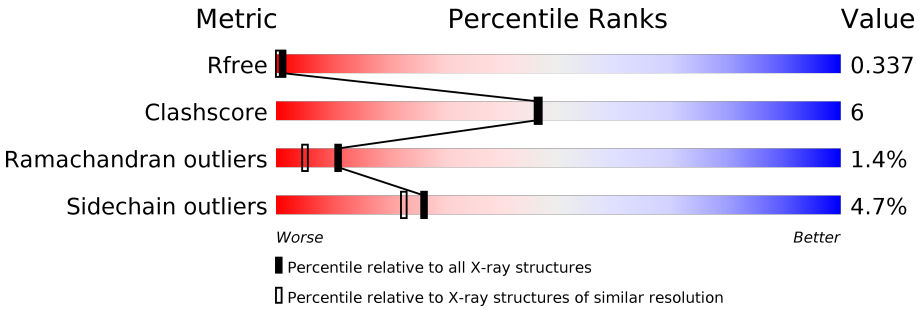
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.00 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))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 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%

Mol	Chain	Length	Quality of chain
1	A	212	85% 13% ·
2	B	213	71% 17% 5% 6%
3	C	16	94% 6%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3516 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 806 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	212	1643	1022	271	343	7	15	1	0

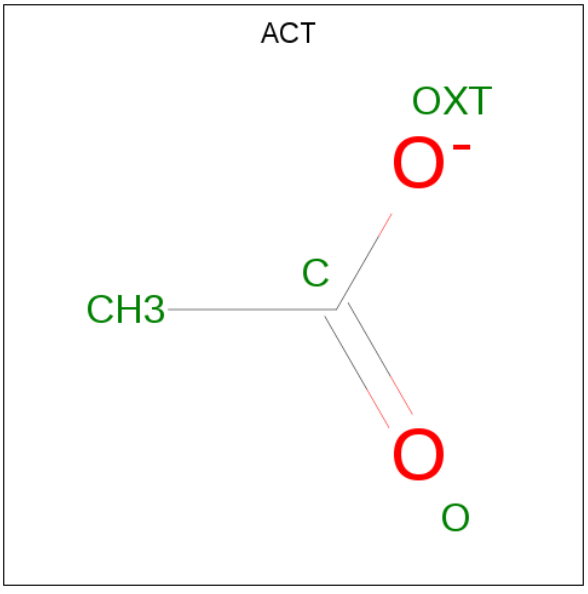
- Molecule 2 is a protein called 808 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	200	1529	971	246	306	6	23	2	0

- Molecule 3 is a protein called Epidermal Growth Factor Receptor peptide.

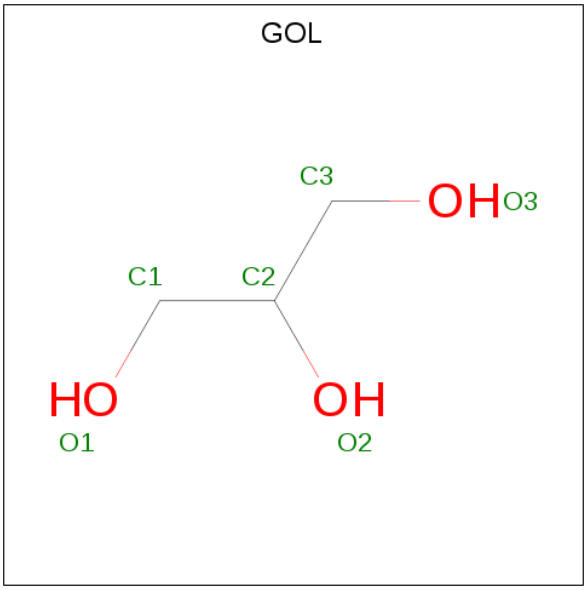
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	16	122	70	20	29	3	0	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



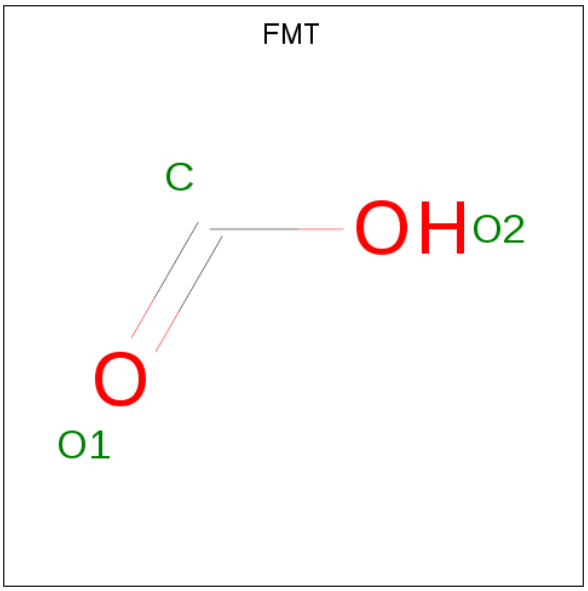
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 3 1 2	0	0
6	B	1	Total C O 3 1 2	0	0
6	C	1	Total C O 3 1 2	0	0

- Molecule 7 is water.

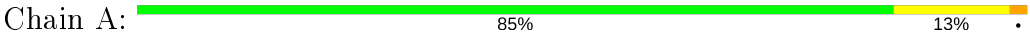
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	112	Total O 112 112	0	0
7	B	82	Total O 82 82	0	0
7	C	5	Total O 5 5	0	0

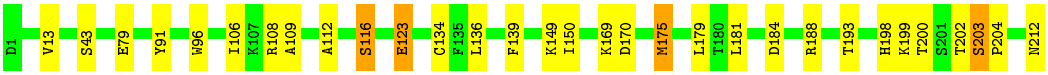
3 Residue-property plots (i)

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. 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.

- Molecule 1: 806 light chain

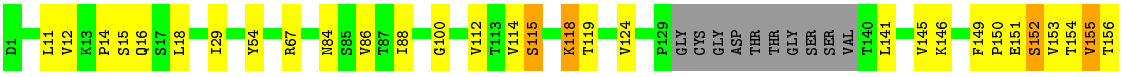
Chain A:

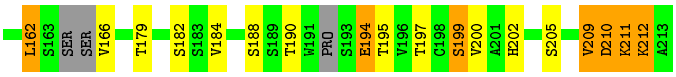




- Molecule 2: 808 heavy chain

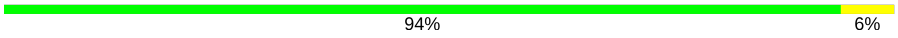
Chain B:





- Molecule 3: Epidermal Growth Factor Receptor peptide

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	35.92Å 83.16Å 72.21Å 90.00° 92.43° 90.00°	Depositor
Resolution (Å)	41.58 – 2.00 41.58 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.6 (41.58-2.00) 96.6 (41.58-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 2.00Å)	Xtriage
Refinement program	PHENIX, REFMAC 5.2.0019	Depositor
R, R_{free}	0.226 , 0.279 0.302 , 0.337	Depositor DCC
R_{free} test set	1389 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	3516	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% 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, FMT, ACT

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	0.55	2/1684 (0.1%)	0.73	9/2284 (0.4%)
2	B	0.68	4/1573 (0.3%)	0.95	10/2152 (0.5%)
3	C	0.44	0/122	0.65	0/159
All	All	0.61	6/3379 (0.2%)	0.84	19/4595 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	1	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	SER	CA-CB	-12.80	1.33	1.52
2	B	199	SER	CA-CB	-11.97	1.34	1.52
2	B	210	ASP	CA-CB	-11.65	1.28	1.53
2	B	194	GLU	CB-CG	-9.46	1.34	1.52
2	B	162	LEU	CA-CB	-8.65	1.33	1.53
1	A	106	ILE	CG1-CD1	-7.73	0.97	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	118	LYS	CB-CA-C	18.11	146.62	110.40
2	B	199	SER	CB-CA-C	12.63	134.10	110.10
2	B	118	LYS	N-CA-CB	-11.12	90.59	110.60
2	B	162	LEU	CB-CA-C	10.82	130.75	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	210	ASP	CA-CB-CG	-10.78	89.69	113.40
1	A	170	ASP	N-CA-CB	10.39	129.31	110.60
1	A	203	SER	CB-CA-C	9.77	128.66	110.10
2	B	210	ASP	N-CA-CB	9.49	127.69	110.60
1	A	106	ILE	CB-CG1-CD1	9.46	140.40	113.90
2	B	209	VAL	CA-CB-CG2	8.80	124.10	110.90
1	A	169	LYS	CB-CA-C	-8.01	94.37	110.40
1	A	202	THR	CB-CA-C	7.12	130.83	111.60
2	B	209	VAL	CB-CA-C	6.82	124.36	111.40
1	A	202	THR	N-CA-CB	-6.51	97.93	110.30
1	A	202	THR	CA-CB-OG1	-6.12	96.14	109.00
2	B	197	THR	CA-CB-CG2	-5.73	104.38	112.40
1	A	170	ASP	CB-CA-C	-5.67	99.05	110.40
2	B	199	SER	N-CA-CB	-5.42	102.36	110.50
1	A	169	LYS	CA-CB-CG	-5.14	102.10	113.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	210	ASP	CA

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	1643	0	1551	13	0
2	B	1529	0	1490	27	0
3	C	122	0	102	0	0
4	A	8	0	6	0	0
5	B	6	0	8	0	0
6	B	6	0	2	0	0
6	C	3	0	1	0	0
7	A	112	0	0	1	0
7	B	82	0	0	1	0
7	C	5	0	0	0	0
All	All	3516	0	3160	40	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 6.

All (40) 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:B:211:LYS:HA	2:B:212:LYS:HB3	1.05	1.03
2:B:211:LYS:CA	2:B:212:LYS:HB3	1.93	0.99
2:B:211:LYS:HA	2:B:212:LYS:CB	1.95	0.93
2:B:155:VAL:HG12	2:B:200:VAL:HG22	1.59	0.85
2:B:210:ASP:O	2:B:211:LYS:HB2	1.82	0.80
2:B:18:LEU:HD13	2:B:112:VAL:HG11	1.66	0.75
2:B:202:HIS:ND1	2:B:205:SER:HB2	2.09	0.68
2:B:166:VAL:HG22	2:B:184:VAL:HG23	1.88	0.55
2:B:211:LYS:CA	2:B:212:LYS:CB	2.71	0.55
1:A:136:LEU:HB2	1:A:175:MET:HG3	1.89	0.55
2:B:210:ASP:O	2:B:211:LYS:CB	2.54	0.54
2:B:115:SER:HG	2:B:149:PHE:HZ	1.56	0.54
2:B:18:LEU:CD1	2:B:112:VAL:HG11	2.37	0.51
2:B:155:VAL:HG21	2:B:182:SER:HB2	1.94	0.50
2:B:14:PRO:O	2:B:15:SER:HB3	2.12	0.49
1:A:198:HIS:HD2	1:A:199:LYS:H	1.62	0.48
1:A:150:ILE:HD11	1:A:179:LEU:HD21	1.94	0.48
2:B:146:LYS:HG2	2:B:179:THR:HG23	1.97	0.47
2:B:67:ARG:HG2	2:B:84:ASN:O	2.14	0.47
1:A:112:ALA:HA	1:A:200:THR:HG21	1.97	0.46
1:A:203:SER:HA	1:A:204:PRO:HD3	1.86	0.45
1:A:116:SER:O	1:A:134:CYS:HA	2.17	0.45
2:B:151:GLU:HA	2:B:151:GLU:OE1	2.17	0.43
1:A:184:ASP:O	1:A:188:ARG:HG3	2.19	0.43
2:B:16:GLN:O	2:B:86:VAL:HG22	2.18	0.43
1:A:43:SER:HA	7:A:317:HOH:O	2.19	0.43
2:B:202:HIS:CE1	2:B:205:SER:HB2	2.53	0.42
1:A:139:PHE:HB2	1:A:198:HIS:CE1	2.55	0.42
2:B:29:ILE:O	2:B:54:TYR:HA	2.18	0.42
2:B:88:ILE:HG13	7:B:214:HOH:O	2.20	0.42
2:B:12:VAL:O	2:B:114:VAL:HA	2.19	0.42
2:B:151:GLU:O	2:B:152:SER:HB2	2.19	0.42
1:A:108:ARG:NH1	1:A:109:ALA:O	2.51	0.42
2:B:190:THR:HA	2:B:194:GLU:H	1.86	0.41
2:B:124:VAL:HG22	2:B:145:VAL:HG22	2.03	0.41
2:B:153:VAL:HG12	2:B:202:HIS:HB2	2.03	0.41
1:A:123:GLU:H	1:A:123:GLU:HG2	1.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:TYR:HA	1:A:96:TRP:CD1	2.56	0.40
2:B:11:LEU:HB2	2:B:150:PRO:HG3	2.03	0.40
1:A:149:LYS:HB2	1:A:193:THR:HB	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	211/212 (100%)	203 (96%)	8 (4%)	0	100 100
2	B	194/213 (91%)	176 (91%)	12 (6%)	6 (3%)	4 1
3	C	14/16 (88%)	13 (93%)	1 (7%)	0	100 100
All	All	419/441 (95%)	392 (94%)	21 (5%)	6 (1%)	11 5

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	152	SER
2	B	211	LYS
2	B	212	LYS
2	B	188	SER
2	B	209	VAL
2	B	100	GLY

5.3.2 Protein sidechains

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	190/189 (100%)	183 (96%)	7 (4%)	34 32
2	B	179/187 (96%)	169 (94%)	10 (6%)	21 17
3	C	13/13 (100%)	12 (92%)	1 (8%)	13 8
All	All	382/389 (98%)	364 (95%)	18 (5%)	26 22

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	79	GLU
1	A	116	SER
1	A	123	GLU
1	A	175	MET
1	A	181	LEU
1	A	212	ASN
2	B	115	SER
2	B	118	LYS
2	B	119	THR
2	B	141	LEU
2	B	154	THR
2	B	155	VAL
2	B	156	THR
2	B	162	LEU
2	B	195	THR
2	B	199	SER
3	C	294	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	HIS
2	B	44	ASN

5.3.3 RNA

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)

6 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	FMT	B	700	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	C	702	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	B	500	-	5,5,5	0.33	0	5,5,5	0.46	0
6	FMT	B	701	-	0,2,2	0.00	-	0,1,1	0.00	-
4	ACT	A	600	-	1,3,3	1.39	0	0,3,3	0.00	-
4	ACT	A	400	-	1,3,3	1.39	0	0,3,3	0.00	-

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
5	GOL	B	500	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	500	GOL	O1-C1-C2-C3
5	B	500	GOL	O2-C2-C3-O3
5	B	500	GOL	O1-C1-C2-O2
5	B	500	GOL	C1-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.