



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 19, 2020 – 08:07 pm BST

PDB ID : 4KTY  
Title : Fibrin-stabilizing factor with a bound ligand  
Authors : Stieler, M.; Heine, A.; Klebe, G.  
Deposited on : 2013-05-21  
Resolution : 1.98 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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

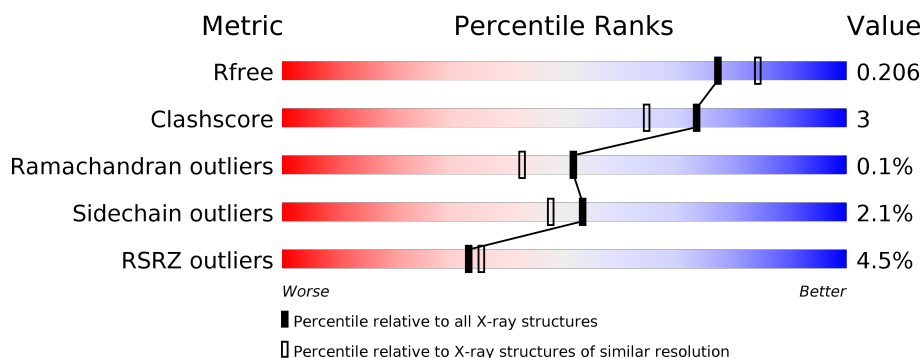
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	738	<div> <div>3%</div> <div>86%</div> <div>8% • 6%</div> </div>
1	B	738	<div> <div>5%</div> <div>86%</div> <div>8% • 5%</div> </div>
2	C	9	<div> <div>11%</div> <div>78%</div> <div>22%</div> </div>
2	D	9	<div> <div>67%</div> <div>33%</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12087 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 Coagulation factor XIII A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	695	Total	C	N	O	S	0	12	0
			5458	3476	919	1037	26			
1	B	698	Total	C	N	O	S	0	10	0
			5496	3501	925	1043	27			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	EXPRESSION TAG	UNP P00488
A	-5	HIS	-	EXPRESSION TAG	UNP P00488
A	-4	HIS	-	EXPRESSION TAG	UNP P00488
A	-3	HIS	-	EXPRESSION TAG	UNP P00488
A	-2	HIS	-	EXPRESSION TAG	UNP P00488
A	-1	HIS	-	EXPRESSION TAG	UNP P00488
A	0	HIS	-	EXPRESSION TAG	UNP P00488
A	649	ILE	THR	ENGINEERED MUTATION	UNP P00488
A	651	GLU	GLN	ENGINEERED MUTATION	UNP P00488
B	-6	MET	-	EXPRESSION TAG	UNP P00488
B	-5	HIS	-	EXPRESSION TAG	UNP P00488
B	-4	HIS	-	EXPRESSION TAG	UNP P00488
B	-3	HIS	-	EXPRESSION TAG	UNP P00488
B	-2	HIS	-	EXPRESSION TAG	UNP P00488
B	-1	HIS	-	EXPRESSION TAG	UNP P00488
B	0	HIS	-	EXPRESSION TAG	UNP P00488
B	649	ILE	THR	ENGINEERED MUTATION	UNP P00488
B	651	GLU	GLN	ENGINEERED MUTATION	UNP P00488

- Molecule 2 is a protein called Peptide-like ligand.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	0	0	0
			74	51	9	14			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	9	Total	C	N	O	0	0	0
			74	51	9	14			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Ca	0	0
			3	3		
3	A	3	Total	Ca	0	0
			3	3		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

*Continued on next page...*

Continued from previous page...

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

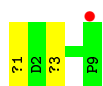


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	435	Total	O	0	0
			435	435		
6	B	474	Total	O	0	0
			474	474		
6	C	4	Total	O	0	0
			4	4		
6	D	7	Total	O	0	0
			7	7		





- Molecule 2: Peptide-like ligand

Chain D:  67% 33%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.76Å 80.51Å 102.84Å 88.14° 76.70° 82.01°	Depositor
Resolution (Å)	20.80 – 1.98 48.27 – 1.98	Depositor EDS
% Data completeness (in resolution range)	96.9 (20.80-1.98) 96.8 (48.27-1.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 1.98Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.169 , 0.206 0.170 , 0.206	Depositor DCC
$R_{free}$ test set	5985 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.7	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 55.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,-h+l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12087	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.20 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8237e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 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: ABA, GOL, CA, 1TX, NLE, SO4, DAS, ACY

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	0.47	0/5619	0.58	0/7657
1	B	0.49	0/5656	0.59	2/7705 (0.0%)
2	C	0.64	0/40	0.97	0/55
2	D	0.62	0/40	1.11	0/55
All	All	0.48	0/11355	0.59	2/15472 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	491	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	491	ARG	NE-CZ-NH1	5.20	122.90	120.30

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	5458	0	5163	36	0
1	B	5496	0	5220	32	0
2	C	74	0	70	2	0
2	D	74	0	70	5	0
3	A	3	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	0	0
4	A	36	0	48	5	0
4	B	18	0	24	0	0
5	B	5	0	0	0	0
6	A	435	0	0	3	0
6	B	474	0	0	3	0
6	C	4	0	0	1	0
6	D	7	0	0	1	0
All	All	12087	0	10595	71	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.

The worst 5 of 71 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:A:565:LYS:HD2	1:A:599:LEU:HD11	1.74	0.70
1:A:637:ARG:NH2	1:A:692:GLU:OE2	2.29	0.66
1:B:43[A]:GLU:OE2	6:B:1374:HOH:O	2.13	0.65
1:B:651:GLU:OE1	1:B:690:GLN:NE2	2.30	0.65
1:B:549:ILE:HB	1:B:575:VAL:HG12	1.80	0.64

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	701/738 (95%)	683 (97%)	17 (2%)	1 (0%)	51	42
1	B	702/738 (95%)	682 (97%)	19 (3%)	1 (0%)	51	42
2	C	3/9 (33%)	3 (100%)	0	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	3/9 (33%)	3 (100%)	0	0	100	100
All	All	1409/1494 (94%)	1371 (97%)	36 (3%)	2 (0%)	51	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	669	GLY
1	B	669	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	578/651 (89%)	563 (97%)	15 (3%)	46	37
1	B	587/651 (90%)	576 (98%)	11 (2%)	57	50
2	C	4/4 (100%)	4 (100%)	0	100	100
2	D	4/4 (100%)	4 (100%)	0	100	100
All	All	1173/1310 (90%)	1147 (98%)	26 (2%)	53	46

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	524	VAL
1	A	617	ASP
1	B	668	ASP
1	A	577	LEU
1	A	599	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	724	GLN
1	B	690	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	459	HIS
1	A	450	HIS
1	B	421	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues 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
2	1TX	C	3	1,2	10,11,12	1.26	1 (10%)	7,12,14	1.39	1 (14%)
2	NLE	C	5	2	6,7,8	0.55	0	2,7,9	0.32	0
2	ABA	D	4	2	4,5,6	0.70	0	1,5,7	0.10	0
2	1TX	D	3	1,2	10,11,12	1.32	1 (10%)	7,12,14	1.45	1 (14%)
2	ABA	C	4	2	4,5,6	0.61	0	1,5,7	0.25	0
2	NLE	D	5	2	6,7,8	0.48	0	2,7,9	0.62	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
2	1TX	C	3	1,2	-	1/10/11/13	-
2	NLE	C	5	2	-	3/5/6/8	-
2	ABA	D	4	2	-	0/3/4/6	-
2	1TX	D	3	1,2	-	1/10/11/13	-
2	ABA	C	4	2	-	1/3/4/6	-
2	NLE	D	5	2	-	0/5/6/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	1TX	O14-C25	3.70	1.44	1.33
2	C	3	1TX	O14-C25	3.61	1.44	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	1TX	C22-C23-C24	-2.37	104.67	113.19
2	D	3	1TX	C22-C23-C24	-2.35	104.72	113.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	5	NLE	N-CA-CB-CG
2	C	5	NLE	C-CA-CB-CG
2	C	3	1TX	C22-C23-C24-C25
2	D	3	1TX	C22-C23-C24-C25
2	C	5	NLE	CA-CB-CG-CD

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	1TX	1	0
2	D	3	1TX	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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	$\# Z  > 2$
4	GOL	B	804	-	5,5,5	0.25	0	5,5,5	0.51	0
4	GOL	A	805	-	5,5,5	0.44	0	5,5,5	0.44	0
4	GOL	A	808	-	5,5,5	0.38	0	5,5,5	0.29	0
4	GOL	A	806	-	5,5,5	0.33	0	5,5,5	0.61	0
4	GOL	B	806	-	5,5,5	0.28	0	5,5,5	0.83	0
4	GOL	A	809	-	5,5,5	0.34	0	5,5,5	0.27	0
4	GOL	B	805	-	5,5,5	0.40	0	5,5,5	0.45	0
5	SO4	B	807	-	4,4,4	0.13	0	6,6,6	0.29	0
4	GOL	A	807	-	5,5,5	0.34	0	5,5,5	0.40	0
4	GOL	A	804	-	5,5,5	0.57	0	5,5,5	0.62	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
4	GOL	B	804	-	-	2/4/4/4	-
4	GOL	A	805	-	-	2/4/4/4	-
4	GOL	A	808	-	-	1/4/4/4	-
4	GOL	A	806	-	-	1/4/4/4	-
4	GOL	B	806	-	-	0/4/4/4	-
4	GOL	A	809	-	-	4/4/4/4	-
4	GOL	B	805	-	-	2/4/4/4	-
4	GOL	A	807	-	-	2/4/4/4	-
4	GOL	A	804	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	804	GOL	O1-C1-C2-C3
4	A	805	GOL	C1-C2-C3-O3
4	A	809	GOL	O1-C1-C2-O2
4	A	809	GOL	C1-C2-C3-O3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	B	805	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	805	GOL	1	0
4	A	806	GOL	3	0
4	A	807	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	695/738 (94%)	0.03	23 (3%) 46 49	11, 25, 54, 80	0
1	B	698/738 (94%)	0.10	39 (5%) 24 26	11, 26, 53, 86	0
2	C	4/9 (44%)	0.79	1 (25%) 0 0	34, 40, 40, 47	0
2	D	4/9 (44%)	0.93	0 100 100	36, 40, 46, 51	0
All	All	1401/1494 (93%)	0.07	63 (4%) 33 35	11, 25, 54, 86	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	729	PRO	6.8
1	B	358	GLY	6.6
1	B	730	SER	6.2
1	A	358	GLY	5.3
1	A	444	ALA	5.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	ABA	C	4	6/7	0.95	0.10	26,29,32,35	0
2	DAS	D	2	8/9	0.95	0.12	31,36,40,46	0
2	DAS	C	2	8/9	0.96	0.10	25,29,39,40	0
2	NLE	D	5	8/9	0.96	0.12	32,34,37,39	0
2	1TX	D	3	12/13	0.96	0.10	29,30,32,34	0
2	NLE	C	5	8/9	0.97	0.10	30,33,35,36	0
2	ABA	D	4	6/7	0.97	0.10	32,32,37,41	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	1TX	C	3	12/13	0.97	0.10	21,24,32,37	0

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	GOL	A	809	6/6	0.81	0.27	52,54,56,58	0
4	GOL	A	808	6/6	0.86	0.20	27,32,33,34	6
4	GOL	B	806	6/6	0.88	0.14	38,44,45,45	0
4	GOL	A	806	6/6	0.90	0.14	33,37,40,41	6
4	GOL	A	805	6/6	0.94	0.17	33,34,37,37	0
4	GOL	A	807	6/6	0.94	0.17	16,22,24,26	6
4	GOL	B	805	6/6	0.95	0.13	31,34,35,36	0
4	GOL	B	804	6/6	0.95	0.14	23,26,27,27	0
5	SO4	B	807	5/5	0.96	0.14	32,34,36,38	5
4	GOL	A	804	6/6	0.96	0.13	18,27,27,27	0
3	CA	B	802	1/1	0.97	0.04	26,26,26,26	0
3	CA	A	803	1/1	0.98	0.04	20,20,20,20	0
3	CA	B	803	1/1	0.99	0.04	22,22,22,22	0
3	CA	B	801	1/1	0.99	0.13	15,15,15,15	0
3	CA	A	802	1/1	1.00	0.10	29,29,29,29	0
3	CA	A	801	1/1	1.00	0.13	15,15,15,15	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.