



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 19, 2020 – 07:53 pm BST

PDB ID : 4GLU  
Title : Crystal structure of the mirror image form of VEGF-A  
Authors : Mandal, K.; Uppalapati, M.; Ault-Riche, D.; Kenney, J.; Lowitz, J.; Sidhu, S.;  
Kent, S.B.H.  
Deposited on : 2012-08-14  
Resolution : 1.90 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

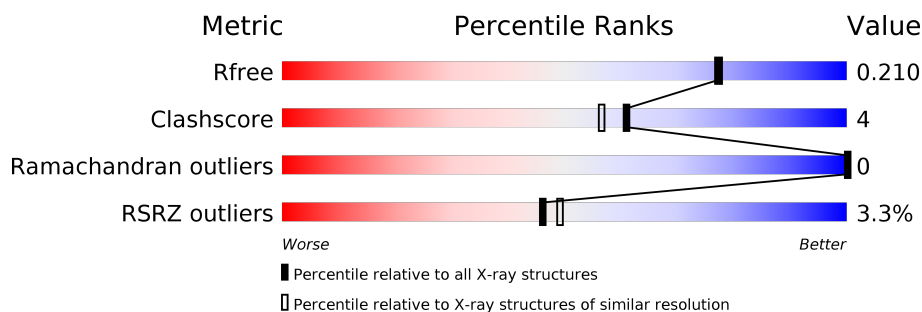
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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  $\geq 3$ , 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	102	
1	B	102	
1	C	102	
1	D	102	
1	E	102	
1	F	102	

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
2	ACT	B	202	-	-	X	-

## 2 Entry composition [i](#)

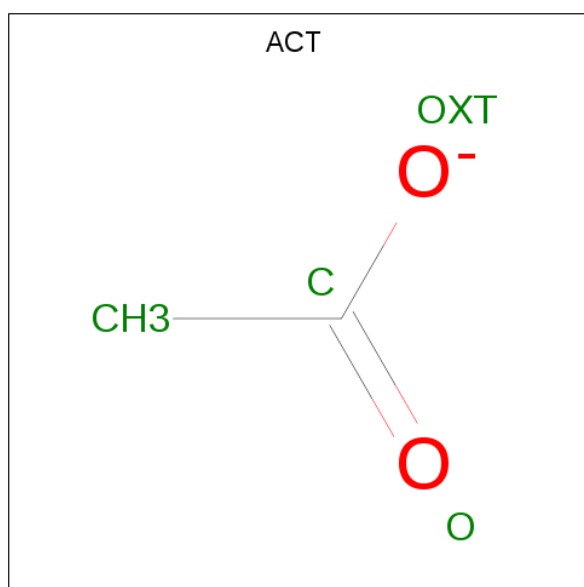
There are 5 unique types of molecules in this entry. The entry contains 5192 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (with D amino acids) called D- Vascular endothelial growth factor-A.

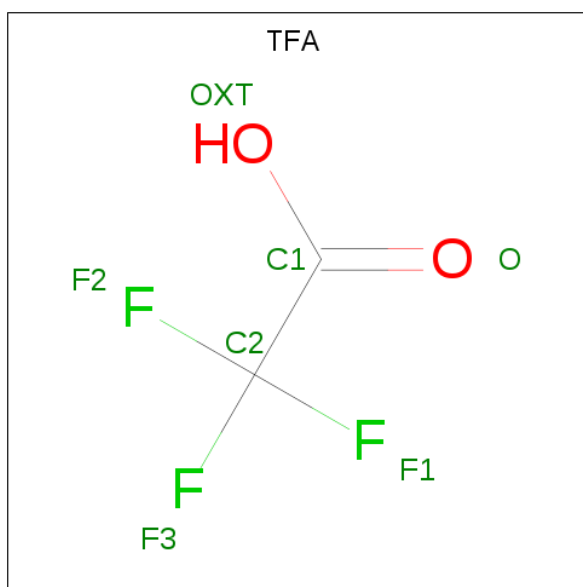
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	95	Total	C	N	O	S	0	1	0
			771	486	129	143	13			
1	D	95	Total	C	N	O	S	0	1	0
			773	485	129	146	13			
1	B	97	Total	C	N	O	S	0	2	0
			802	504	132	153	13			
1	C	96	Total	C	N	O	S	0	2	0
			793	497	136	147	13			
1	E	95	Total	C	N	O	S	0	0	0
			770	483	129	145	13			
1	F	97	Total	C	N	O	S	0	1	0
			791	495	132	151	13			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0

- Molecule 3 is trifluoroacetic acid (three-letter code: TFA) (formula:  $C_2HF_3O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C F O 7 2 3 2	0	0
3	D	1	Total C F O 7 2 3 2	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	F	O	0	0
			7	2	3	2		
3	D	1	Total	C	F	O	0	0
			7	2	3	2		
3	C	1	Total	C	F	O	0	0
			7	2	3	2		
3	F	1	Total	C	F	O	0	0
			7	2	3	2		
3	F	1	Total	C	F	O	0	0
			7	2	3	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	68	Total 68	O 68	0	0
5	D	53	Total 53	O 53	0	0
5	B	85	Total 85	O 85	0	0
5	C	53	Total 53	O 53	0	0
5	E	58	Total 58	O 58	0	0
5	F	62	Total 62	O 62	0	0



- Molecule 1: D- Vascular endothelial growth factor-A



- |     |     |     |     |     |     |    |    |    |    |  |  |     |  |     |  |     |     |  |     |     |  |     |     |     |  |     |     |     |     |  |  |     |     |     |     |  |      |     |     |
|-----|-----|-----|-----|-----|-----|----|----|----|----|--|--|-----|--|-----|--|-----|-----|--|-----|-----|--|-----|-----|-----|--|-----|-----|-----|-----|--|--|-----|-----|-----|-----|--|------|-----|-----|
| GLY | DGN | DGN | DGN | DHI | DHI | E6 | V7 | V8 | K9 |  |  | L28 |  | E35 |  | K41 | P42 |  | V45 | P46 |  | E60 | G61 | V62 |  | R75 | I76 | K77 | P78 |  |  | E96 | G97 | P98 | P99 |  | K100 | DLY | DAS |
|-----|-----|-----|-----|-----|-----|----|----|----|----|--|--|-----|--|-----|--|-----|-----|--|-----|-----|--|-----|-----|-----|--|-----|-----|-----|-----|--|--|-----|-----|-----|-----|--|------|-----|-----|

- GLY DGN DSG DHI DHI E6 V7 V8 R16 C54 N55 E86 E96 C97 R98 D102

- GLY DGN DSG DHI H5 R16 E23 Y38 K41 P42 S43 M71 R75 I76 K77 G81 K100 DLY DAS

- |     |     |     |     |     |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |     |     |
|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|
| GLY | DGN | DSG | DHI | DHI | E6 | F10 | M11 | D12 | R16 | S17 | L25 | F29 | Q30 | E31 | I36 | E37 | P46 | H79 | K94 | G95 | E96 | K100 | DLY | DAS |
|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|

- 





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	231.40 Å   43.99 Å   73.51 Å 90.00°   100.30°   90.00°	Depositor
Resolution (Å)	32.50 – 1.90 32.50 – 1.89	Depositor EDS
% Data completeness (in resolution range)	98.0 (32.50-1.90) 97.8 (32.50-1.89)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.12 (at 1.89 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1128)	Depositor
R, $R_{free}$	0.172   ,   0.209 0.174   ,   0.210	Depositor DCC
$R_{free}$ test set	2897 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.0	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 63.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5192	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: DIL, GOL, DTH, DPR, DLE, MED, DGN, DAS, DVA, DGL, DSN, DTY, DSG, DAR, ACT, DHI, DPN, DLY, DCY, TFA

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	0.31	0/17	0.78	0/16
1	B	0.36	0/17	0.62	0/16
1	C	0.25	0/17	0.61	0/16
1	D	0.30	0/17	0.79	0/16
1	E	0.44	0/17	0.90	0/16
1	F	0.39	0/17	0.68	0/16
All	All	0.35	0/102	0.74	0/96

There are no bond length outliers.

There are no bond angle outliers.

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	771	0	669	5	0
1	B	802	0	688	7	0
1	C	793	0	687	8	0
1	D	773	0	664	9	0
1	E	770	0	663	11	0
1	F	791	0	677	12	0
2	A	8	0	6	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	12	0	9	2	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
2	E	8	0	6	0	0
2	F	4	0	3	0	0
3	A	7	0	0	0	0
3	C	7	0	0	0	0
3	D	21	0	0	0	0
3	F	14	0	0	0	0
4	C	12	0	16	1	0
4	D	6	0	8	0	0
4	F	6	0	8	1	0
5	A	68	0	0	0	0
5	B	85	0	0	0	0
5	C	53	0	0	1	0
5	D	53	0	0	0	0
5	E	58	0	0	0	1
5	F	62	0	0	1	0
All	All	5192	0	4110	40	1

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 4.

The worst 5 of 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)
1:E:37:DGL:N	1:E:37:DGL:OE2	2.27	0.67
1:F:35:DGL:OE1	1:F:75:DAR:NH1	2.33	0.62
1:D:96:DGL:OE2	1:D:98:DAR:NH2	2.33	0.60
1:A:96:DGL:OE1	1:A:98:DAR:NE	2.34	0.59
1:B:96:DGL:OE2	1:B:98:DAR:NE	2.30	0.59

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:346:HOH:O	5:E:346:HOH:O[2_557]	2.13	0.07

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

552 non-standard protein/DNA/RNA residues are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

21 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
3	TFA	C	204	-	3,6,6	0.30	0	3,9,9	1.10	0
2	ACT	E	202	-	1,3,3	1.31	0	0,3,3	0.00	-
2	ACT	A	201	-	1,3,3	1.24	0	0,3,3	0.00	-
2	ACT	B	203	-	1,3,3	1.32	0	0,3,3	0.00	-
2	ACT	A	203	-	1,3,3	1.31	0	0,3,3	0.00	-
3	TFA	D	204	-	3,6,6	0.21	0	3,9,9	1.00	0
3	TFA	D	203	-	3,6,6	0.34	0	3,9,9	1.07	0
3	TFA	F	203	-	3,6,6	0.18	0	3,9,9	0.96	0
4	GOL	C	203	-	5,5,5	0.38	0	5,5,5	0.36	0
4	GOL	D	202	-	5,5,5	0.35	0	5,5,5	0.33	0
3	TFA	A	202	-	3,6,6	0.18	0	3,9,9	0.94	0
4	GOL	F	202	-	5,5,5	0.33	0	5,5,5	0.36	0
4	GOL	C	201	-	5,5,5	0.28	0	5,5,5	0.59	0
3	TFA	D	205	-	3,6,6	0.26	0	3,9,9	0.88	0
2	ACT	B	201	-	1,3,3	0.98	0	0,3,3	0.00	-
2	ACT	E	201	-	1,3,3	1.65	0	0,3,3	0.00	-
2	ACT	D	201	-	1,3,3	1.09	0	0,3,3	0.00	-
3	TFA	F	201	-	3,6,6	0.17	0	3,9,9	0.89	0
2	ACT	B	202	-	1,3,3	1.10	0	0,3,3	0.00	-
2	ACT	C	202	-	1,3,3	1.35	0	0,3,3	0.00	-
2	ACT	F	204	-	1,3,3	1.34	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
3	TFA	C	204	-	-	0/0/6/6	-
4	GOL	C	203	-	-	4/4/4/4	-
3	TFA	D	204	-	-	0/0/6/6	-
3	TFA	D	203	-	-	0/0/6/6	-
3	TFA	F	203	-	-	0/0/6/6	-
3	TFA	A	202	-	-	0/0/6/6	-
4	GOL	D	202	-	-	4/4/4/4	-
4	GOL	F	202	-	-	4/4/4/4	-
3	TFA	D	205	-	-	0/0/6/6	-
3	TFA	F	201	-	-	0/0/6/6	-
4	GOL	C	201	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	203	GOL	O1-C1-C2-C3
4	F	202	GOL	C1-C2-C3-O3
4	F	202	GOL	O2-C2-C3-O3
4	D	202	GOL	O1-C1-C2-C3
4	D	202	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	202	GOL	1	0
4	C	201	GOL	1	0
2	B	202	ACT	2	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	5/102 (4%)	-0.32	0	100 100	19, 22, 24, 34	0
1	B	5/102 (4%)	-0.31	0	100 100	16, 21, 23, 27	0
1	C	5/102 (4%)	0.61	1 (20%)	1 1	21, 23, 49, 68	0
1	D	5/102 (4%)	0.19	0	100 100	23, 23, 46, 50	0
1	E	5/102 (4%)	-0.07	0	100 100	22, 24, 38, 53	0
1	F	5/102 (4%)	-0.03	0	100 100	19, 21, 36, 53	0
All	All	30/612 (4%)	0.01	1 (3%)	46 49	16, 24, 53, 68	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	81	GLY	2.9

### 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
1	DGL	B	6	9/10	0.74	0.29	70,79,94,97	0
1	DGL	D	6	9/10	0.77	0.25	46,59,84,87	0
1	DHI	C	5	10/11	0.77	0.17	59,75,82,82	0
1	DTY	C	38	12/13	0.78	0.25	42,79,89,90	0
1	DLY	E	100	9/10	0.81	0.14	63,67,76,79	0
1	DGL	E	6	9/10	0.81	0.19	39,53,83,84	0
1	DGL	C	6	9/10	0.81	0.23	45,55,62,70	2
1	DHI	C	79	10/11	0.82	0.18	76,81,83,85	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	DGL	D	37	9/10	0.82	0.32	61,72,93,96	0
1	DGL	D	57	9/10	0.83	0.32	59,70,93,96	1
1	DGL	F	37	9/10	0.83	0.27	62,74,99,100	0
1	DGL	F	6	9/10	0.84	0.17	46,61,81,88	0
1	DGL	C	37	9/10	0.85	0.22	66,71,93,93	1
1	DAS	B	102	9/9	0.85	0.19	45,58,84,87	0
1	DAS	E	56	8/9	0.86	0.13	50,52,58,60	0
1	DGN	E	80	9/10	0.86	0.15	42,55,68,68	0
1	DTY	F	38	12/13	0.86	0.15	44,50,59,62	0
1	DGN	E	91	9/10	0.87	0.12	25,32,42,45	0
1	DGN	F	80	9/10	0.87	0.17	57,61,81,82	0
1	DGN	E	30	9/10	0.87	0.19	50,54,74,78	0
1	DGL	C	35	9/10	0.88	0.13	61,63,74,79	0
1	DGN	F	30	9/10	0.88	0.18	38,54,79,86	0
1	DLE	C	59	8/9	0.88	0.15	42,50,56,57	0
1	DGN	E	82	9/10	0.88	0.12	31,35,47,49	0
1	DLY	C	100	9/10	0.88	0.19	52,63,65,68	0
1	DHI	C	83	10/11	0.89	0.22	44,73,93,93	0
1	DTY	F	32	12/13	0.89	0.16	37,45,56,56	0
1	DAS	C	56	8/9	0.89	0.13	40,52,58,67	0
1	DTY	E	32	12/13	0.89	0.18	31,44,65,65	0
1	DGL	C	60	9/10	0.89	0.11	35,41,54,57	0
1	DGL	D	35	9/10	0.89	0.18	61,68,71,74	0
1	DHI	A	79	10/11	0.89	0.14	37,48,61,62	0
1	DAS	E	12	8/9	0.89	0.12	33,37,61,66	0
1	DPR	C	78	7/8	0.90	0.17	76,81,84,89	0
1	DAS	D	34	8/9	0.90	0.23	48,63,76,83	0
1	DPN	E	29	11/12	0.90	0.17	37,44,57,60	0
1	DGN	D	82	9/10	0.90	0.17	37,44,70,81	0
1	DGN	D	80	9/10	0.90	0.12	44,54,79,81	0
1	DAS	D	56	8/9	0.90	0.11	39,47,52,53	0
1	DAR	E	75	11/12	0.90	0.15	27,40,55,56	0
1	DHI	A	83	10/11	0.90	0.11	25,31,39,39	0
1	DTY	C	32	12/13	0.90	0.15	34,44,61,62	0
1	DGL	E	57	9/10	0.90	0.15	48,61,74,80	0
1	DTY	D	32	12/13	0.91	0.18	30,47,66,68	0
1	DAS	E	34	8/9	0.91	0.15	41,51,67,68	0
1	DIL	C	84	8/9	0.91	0.11	44,50,51,52	0
1	DGN	A	82	9/10	0.91	0.11	26,32,53,56	0
1	DGN	A	80	9/10	0.91	0.23	37,44,60,60	0
1	DAR	E	98	11/12	0.91	0.18	39,44,71,72	0
1	DGL	E	60	9/10	0.91	0.12	35,41,69,71	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	DSG	C	68[B]	8/9	0.91	0.15	35,41,50,58	5
1	DGL	D	66	9/10	0.91	0.12	31,34,43,54	0
1	DGL	C	57	9/10	0.91	0.15	53,59,81,85	0
1	DTY	E	38	12/13	0.91	0.10	34,39,44,46	0
1	DLE	E	59	8/9	0.91	0.14	40,44,46,48	0
1	DGL	F	35	9/10	0.91	0.14	60,64,75,84	0
1	DLY	F	77	9/10	0.91	0.22	43,49,83,83	0
1	DLY	B	101	9/10	0.91	0.16	45,60,71,72	0
1	DSG	C	68[A]	8/9	0.91	0.15	35,41,44,46	5
1	MED	E	11	8/9	0.91	0.13	35,39,54,78	0
1	DIL	D	36	8/9	0.91	0.20	63,69,70,71	0
1	DAR	C	98	11/12	0.91	0.16	46,53,72,78	0
1	MED	C	74	8/9	0.92	0.09	33,35,53,56	0
1	DGN	C	80	9/10	0.92	0.29	69,82,89,92	1
1	DGN	F	82	9/10	0.92	0.12	41,52,70,71	0
1	DTY	D	38	12/13	0.92	0.21	34,59,75,83	0
1	DGL	E	35	9/10	0.92	0.10	39,43,59,63	0
1	DGL	F	57	9/10	0.92	0.17	32,54,83,86	0
1	DIL	D	76	8/9	0.92	0.09	30,34,38,39	0
1	DPR	D	99	7/8	0.92	0.17	43,48,51,52	0
1	DAS	F	34	8/9	0.92	0.16	57,60,63,65	0
1	DLY	F	41	9/10	0.92	0.16	27,30,60,62	0
1	DLY	E	77	9/10	0.92	0.12	39,44,53,53	0
1	DAS	C	34	8/9	0.92	0.11	51,56,72,77	0
1	DVA	A	7	7/8	0.92	0.15	43,45,49,51	0
1	DSG	F	68	8/9	0.93	0.11	26,34,52,56	0
1	DTY	B	32[B]	12/13	0.93	0.13	22,24,33,33	9
1	DGL	E	37	9/10	0.93	0.18	40,44,76,82	0
1	DGL	D	60	9/10	0.93	0.12	30,41,53,56	0
1	DVA	B	7	7/8	0.93	0.16	38,43,49,49	0
1	DTY	B	32[A]	12/13	0.93	0.13	22,25,30,30	9
1	DPN	F	29	11/12	0.93	0.11	34,37,44,45	0
1	DIL	D	84	8/9	0.93	0.14	41,44,47,50	0
1	DSG	E	55	8/9	0.93	0.12	34,45,48,50	0
1	DAS	F	102	9/9	0.93	0.15	35,51,64,65	0
1	DLY	F	101	9/10	0.93	0.12	30,33,36,39	0
1	DGL	C	86	9/10	0.93	0.08	41,43,59,61	0
1	DGN	A	91	9/10	0.93	0.14	15,20,47,49	0
1	DIL	C	36	8/9	0.93	0.20	60,71,74,75	0
1	DAS	A	12	8/9	0.93	0.14	31,39,68,78	0
1	DGL	E	96	9/10	0.93	0.21	32,33,63,65	0
1	DGN	D	30	9/10	0.93	0.15	29,42,68,71	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	DIL	F	36	8/9	0.93	0.17	58,63,68,69	0
1	DLY	D	77	9/10	0.93	0.17	38,43,67,74	0
1	DAR	C	75	11/12	0.93	0.14	36,47,67,70	0
1	DGN	C	30	9/10	0.93	0.12	31,39,66,69	0
1	DSG	B	55	8/9	0.93	0.12	26,41,60,60	0
1	DPR	C	99	7/8	0.93	0.11	52,58,60,61	0
1	DLY	A	9	9/10	0.93	0.18	34,44,68,70	0
1	DGN	D	15	9/10	0.93	0.15	22,30,53,59	0
1	DCY	D	53	6/7	0.93	0.09	17,22,25,27	0
1	DLE	D	59	8/9	0.93	0.13	37,39,43,47	0
1	DLY	C	77	9/10	0.93	0.17	58,69,81,81	0
1	DGN	E	15	9/10	0.93	0.15	25,30,54,58	0
1	DGL	B	31	9/10	0.93	0.10	26,31,39,39	0
1	DLY	A	101	5/10	0.93	0.12	39,56,65,73	0
1	DSN	C	88	6/7	0.93	0.10	32,35,36,41	0
1	DAR	B	98	11/12	0.93	0.17	23,35,82,84	0
1	DPR	E	99	7/8	0.93	0.13	48,53,64,64	0
1	DGN	D	91	9/10	0.93	0.11	24,29,36,42	0
1	DHI	D	83	10/11	0.93	0.29	38,59,78,80	0
1	DIL	D	73	8/9	0.93	0.08	24,27,31,33	0
1	DSG	A	55	8/9	0.94	0.13	17,39,50,53	0
1	DGL	E	65	9/10	0.94	0.16	32,38,70,73	0
1	DPR	F	78	7/8	0.94	0.14	43,46,54,55	0
1	DAR	F	75	11/12	0.94	0.13	31,49,64,66	0
1	MED	C	87	8/9	0.94	0.09	34,37,40,50	0
1	DLY	D	100	9/10	0.94	0.15	45,56,59,64	0
1	DSN	E	67	6/7	0.94	0.11	29,37,39,40	0
1	DGN	B	15	9/10	0.94	0.16	27,30,59,66	0
1	DGL	F	86	9/10	0.94	0.09	30,32,42,49	0
1	DLY	C	41	9/10	0.94	0.13	28,31,53,63	0
1	DGN	C	91	9/10	0.94	0.11	28,32,42,47	0
1	DAS	B	12[B]	8/9	0.94	0.13	28,31,45,53	5
1	DLY	B	100	9/10	0.94	0.12	29,35,42,44	0
1	DHI	F	79	10/11	0.94	0.10	51,55,59,60	0
1	DIL	E	84	8/9	0.94	0.12	26,31,34,34	0
1	DAR	A	98	11/12	0.94	0.12	18,25,70,70	0
1	DGN	F	72	9/10	0.94	0.10	27,29,41,44	0
1	DLE	F	25	8/9	0.94	0.13	19,25,32,35	0
1	DHI	D	79	10/11	0.94	0.09	39,43,48,50	0
1	DSG	A	68	8/9	0.94	0.14	22,27,49,54	0
1	DGN	C	82	9/10	0.94	0.21	55,66,84,86	0
1	DAS	B	12[A]	8/9	0.94	0.13	28,31,41,44	5

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	DHI	E	83	10/11	0.94	0.11	31,36,48,52	0
1	MED	F	74	8/9	0.94	0.16	28,35,54,86	0
1	DAR	B	16	11/12	0.95	0.17	19,34,73,75	0
1	DPR	F	33	7/8	0.95	0.12	50,56,62,63	0
1	DAR	A	16	11/12	0.95	0.13	19,25,65,70	0
1	DAS	F	56	8/9	0.95	0.08	28,33,39,42	0
1	DIL	D	69	8/9	0.95	0.09	27,30,36,37	0
1	DVA	B	8	7/8	0.95	0.09	29,32,38,39	0
1	DGN	B	30	9/10	0.95	0.14	33,36,69,73	0
1	DLY	F	94	9/10	0.95	0.21	21,27,75,77	0
1	MED	A	11	8/9	0.95	0.10	40,49,58,90	0
1	DGL	D	96	9/10	0.95	0.11	29,31,64,68	0
1	DGL	C	96	9/10	0.95	0.13	29,31,67,75	0
1	DIL	E	76	8/9	0.95	0.10	31,32,40,45	0
1	DGL	A	96	9/10	0.95	0.11	15,19,51,51	0
1	DVA	D	13	7/8	0.95	0.09	17,21,24,27	0
1	DPR	C	42	7/8	0.95	0.07	25,26,30,31	0
1	DSG	E	93	8/9	0.95	0.12	26,35,42,43	0
1	DGL	F	65	9/10	0.95	0.13	25,33,58,63	0
1	DGN	F	91	9/10	0.95	0.08	21,25,34,37	0
1	DPN	C	40	11/12	0.95	0.10	30,32,40,40	0
1	DLY	E	9	9/10	0.95	0.19	31,37,64,66	0
1	DVA	F	26	7/8	0.95	0.12	22,25,28,28	0
1	DIL	D	39	8/9	0.95	0.09	28,32,36,41	0
1	DVA	B	62	7/8	0.95	0.08	18,19,23,31	0
1	DTH	C	70	7/8	0.95	0.09	33,34,41,45	0
1	DAR	D	75	11/12	0.95	0.14	31,34,71,73	0
1	DGL	A	86	9/10	0.95	0.09	20,23,41,45	0
1	DLE	D	25	8/9	0.95	0.10	16,21,29,32	0
1	DLY	D	94	9/10	0.95	0.14	27,31,59,60	0
1	DPR	E	33	7/8	0.95	0.14	39,43,52,53	0
1	DGL	E	31	9/10	0.95	0.08	37,40,47,49	0
1	DAS	B	56	8/9	0.95	0.09	23,34,37,39	0
1	DPN	D	40	11/12	0.95	0.12	24,28,42,42	0
1	DAR	E	16	11/12	0.95	0.14	25,33,79,82	0
1	DTY	A	14	12/13	0.95	0.11	22,35,51,55	0
1	DHI	E	79	10/11	0.95	0.08	42,47,51,52	0
1	DLY	E	94	9/10	0.95	0.24	30,33,65,67	0
1	DGN	A	15	9/10	0.95	0.18	24,29,64,66	0
1	DGL	D	65	9/10	0.95	0.07	29,32,48,52	0
1	DTY	B	14	12/13	0.95	0.13	26,36,54,54	0
1	DGN	A	30	9/10	0.95	0.12	22,27,56,58	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	DIL	A	84	8/9	0.95	0.09	23,28,31,43	0
1	MED	B	11	8/9	0.95	0.11	26,33,57,58	0
1	DPN	E	40	11/12	0.95	0.10	23,27,36,37	0
1	DGL	F	60	9/10	0.95	0.09	21,22,35,35	0
1	DPN	E	10	11/12	0.95	0.07	30,36,44,45	0
1	DLY	C	94	9/10	0.95	0.16	31,34,64,74	0
1	DGL	F	66	9/10	0.95	0.10	28,36,47,49	0
1	DAS	B	34	8/9	0.95	0.10	24,26,52,58	0
1	DGL	C	31	9/10	0.95	0.09	37,45,48,51	0
1	DGL	A	57	9/10	0.95	0.11	21,26,37,53	0
1	DGL	B	57	9/10	0.95	0.11	25,32,56,59	0
1	DIL	F	84	8/9	0.95	0.13	34,36,38,40	0
1	DSG	D	55	8/9	0.95	0.09	25,33,41,42	0
1	DHI	F	83	10/11	0.95	0.11	33,37,46,48	0
1	DSG	D	68	8/9	0.95	0.10	33,37,47,66	0
1	DGN	D	72	9/10	0.95	0.12	31,32,45,47	0
1	DGL	E	66	9/10	0.96	0.14	34,37,57,60	0
1	DGL	B	66	9/10	0.96	0.11	17,19,39,40	0
1	DIL	F	22	8/9	0.96	0.11	17,22,26,32	0
1	DIL	A	28	8/9	0.96	0.09	14,17,18,19	0
1	DTY	F	14	12/13	0.96	0.15	18,27,53,58	0
1	DLE	B	25	8/9	0.96	0.08	17,20,27,27	0
1	DPN	B	29	11/12	0.96	0.08	19,28,35,38	0
1	DGL	B	96	9/10	0.96	0.12	19,21,52,55	0
1	DPR	D	42	7/8	0.96	0.08	21,23,24,27	0
1	DGL	A	31	9/10	0.96	0.08	22,24,31,37	0
1	DGL	C	23	9/10	0.96	0.10	19,25,48,60	0
1	DGN	F	15	9/10	0.96	0.13	18,20,26,33	0
1	DCY	E	54	6/7	0.96	0.08	28,31,34,35	0
1	DSG	C	55	8/9	0.96	0.10	24,30,43,44	0
1	DIL	F	76	8/9	0.96	0.12	34,40,52,57	0
1	DAR	C	16[A]	11/12	0.96	0.14	15,22,24,28	8
1	DLY	D	41	9/10	0.96	0.09	25,28,55,61	0
1	DAR	F	16	11/12	0.96	0.15	16,21,65,67	0
1	DAS	A	56	8/9	0.96	0.14	19,24,34,34	0
1	DTH	A	70	7/8	0.96	0.08	18,20,23,26	0
1	MED	F	11	8/9	0.96	0.13	21,28,51,58	0
1	DGL	E	86	9/10	0.96	0.09	31,32,45,53	0
1	DLE	F	90	8/9	0.96	0.12	24,26,47,51	0
1	DGL	C	66	9/10	0.96	0.08	33,37,52,61	0
1	DVA	A	26	7/8	0.96	0.09	18,22,24,26	0
1	DLY	B	9	9/10	0.96	0.19	29,36,69,75	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	DLY	F	9	9/10	0.96	0.09	20,24,28,29	0
1	DPR	B	21	7/8	0.96	0.07	16,19,22,22	0
1	DTY	E	14	12/13	0.96	0.08	27,39,49,49	0
1	DIL	B	22	8/9	0.96	0.10	17,18,34,38	0
1	DAR	C	16[B]	11/12	0.96	0.14	14,22,30,34	8
1	MED	A	74	8/9	0.96	0.10	17,23,43,66	0
1	DPN	B	10	11/12	0.96	0.11	33,37,41,46	0
1	DGL	D	86	9/10	0.96	0.08	38,39,53,61	0
1	DVA	A	13	7/8	0.96	0.09	28,29,37,52	0
1	DPN	C	29	11/12	0.96	0.08	29,37,40,40	0
1	MED	D	11	8/9	0.96	0.12	24,26,53,67	0
1	DPN	A	89	11/12	0.96	0.09	13,15,19,22	0
1	DGL	B	65	9/10	0.96	0.11	17,21,37,39	0
1	DGL	F	23	9/10	0.96	0.09	18,22,38,38	0
1	DAR	D	98	11/12	0.96	0.14	39,41,50,50	0
1	DSN	D	67	6/7	0.96	0.10	30,31,39,39	0
1	DIL	C	76	8/9	0.96	0.14	42,44,54,54	0
1	DGN	B	91	9/10	0.96	0.08	14,17,27,33	0
1	DLY	A	100	9/10	0.96	0.11	23,25,29,34	0
1	DGL	B	35	9/10	0.96	0.08	19,21,37,48	0
1	DCY	A	44	6/7	0.96	0.10	17,19,21,23	0
1	DLE	C	90	8/9	0.96	0.09	26,31,41,41	0
1	DIL	E	39	8/9	0.96	0.11	30,33,53,54	0
1	DIL	C	39	8/9	0.96	0.12	39,39,52,53	0
1	DVA	F	7	7/8	0.96	0.09	30,32,42,44	0
1	DPR	A	78	7/8	0.96	0.10	30,38,44,45	0
1	DGL	C	65	9/10	0.96	0.12	32,44,75,76	0
1	DGL	F	96	9/10	0.96	0.10	21,26,56,61	0
1	DVA	B	13	7/8	0.96	0.11	26,26,36,37	0
1	DSG	F	93	8/9	0.96	0.10	21,31,45,52	0
1	DHI	F	20	10/11	0.96	0.11	16,18,23,25	0
1	DHI	B	20	10/11	0.96	0.08	16,19,26,30	0
1	DPR	E	21	7/8	0.96	0.09	22,23,26,27	0
1	DVA	A	8	7/8	0.96	0.09	34,36,39,43	0
1	DCY	E	97	6/7	0.96	0.09	32,35,43,44	0
1	DSN	D	17	6/7	0.96	0.07	20,21,30,31	0
1	DGL	F	31	9/10	0.96	0.07	36,42,51,54	0
1	DAR	F	98	11/12	0.96	0.15	25,29,72,74	0
1	DGN	B	82	9/10	0.96	0.08	16,22,31,34	0
1	DGN	B	80	9/10	0.96	0.09	24,34,47,54	0
1	DLE	C	47	8/9	0.97	0.07	21,23,26,27	0
1	DLE	A	47	8/9	0.97	0.09	16,17,20,23	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	DPR	F	99	7/8	0.97	0.06	30,32,33,36	0
1	DAR	B	49	11/12	0.97	0.07	15,17,23,24	0
1	DIL	E	36	8/9	0.97	0.18	44,60,68,74	0
1	MED	D	87	8/9	0.97	0.07	30,32,37,39	0
1	DPN	A	10	11/12	0.97	0.09	32,35,40,43	0
1	DIL	C	69	8/9	0.97	0.09	30,33,35,36	0
1	DIL	F	39	8/9	0.97	0.11	30,38,50,57	0
1	DGL	B	37	9/10	0.97	0.09	21,24,32,34	0
1	DSG	F	55	8/9	0.97	0.12	20,29,31,31	0
1	DVA	E	13	7/8	0.97	0.08	26,28,33,35	0
1	DVA	F	8	7/8	0.97	0.08	20,23,24,25	0
1	DIL	A	73	8/9	0.97	0.07	17,18,20,20	0
1	DSG	B	68	8/9	0.97	0.07	16,19,41,45	0
1	DLY	A	41	9/10	0.97	0.12	18,22,47,48	0
1	DGL	A	66	9/10	0.97	0.07	17,22,35,35	0
1	DTH	E	24	7/8	0.97	0.11	17,21,24,25	0
1	DTH	D	70	7/8	0.97	0.09	31,36,38,38	0
1	DPR	E	78	7/8	0.97	0.08	39,42,44,44	0
1	DGL	A	37	9/10	0.97	0.07	23,26,31,33	0
1	DLY	A	77	9/10	0.97	0.08	25,30,32,32	0
1	DTY	C	14	12/13	0.97	0.12	15,18,32,32	0
1	DAR	C	49	11/12	0.97	0.08	19,23,29,31	0
1	DPR	E	63	7/8	0.97	0.07	32,34,36,38	0
1	DPR	A	99	7/8	0.97	0.12	20,21,25,28	0
1	DTY	A	18	12/13	0.97	0.08	17,22,28,29	0
1	DAS	A	34	8/9	0.97	0.08	20,27,46,53	0
1	DAS	D	27	8/9	0.97	0.06	20,24,28,29	0
1	DIL	E	69	8/9	0.97	0.11	22,30,32,33	0
1	DCY	D	54	6/7	0.97	0.07	24,31,32,39	0
1	DTY	D	18	12/13	0.97	0.09	19,28,35,40	0
1	DSG	E	68	8/9	0.97	0.10	30,32,51,59	0
1	DGL	D	31	9/10	0.97	0.11	32,35,45,49	0
1	DAR	A	75	11/12	0.97	0.07	17,22,25,25	0
1	DIL	A	69	8/9	0.97	0.08	18,21,28,32	0
1	DHI	D	20	10/11	0.97	0.07	19,21,24,25	0
1	MED	E	48	8/9	0.97	0.09	19,22,27,31	0
1	DSN	E	88	6/7	0.97	0.06	26,30,33,57	0
1	DIL	C	22	8/9	0.97	0.09	21,25,44,51	0
1	DHI	A	20	10/11	0.97	0.07	15,21,23,28	0
1	DPN	A	29	11/12	0.97	0.08	18,24,29,30	0
1	DPR	B	33	7/8	0.97	0.09	26,30,35,36	0
1	DTH	C	64	7/8	0.97	0.15	34,36,44,46	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	DAS	F	27	8/9	0.97	0.07	25,27,33,34	0
1	DPN	C	89	11/12	0.97	0.07	27,30,32,35	0
1	DPN	D	29	11/12	0.97	0.06	24,29,36,39	0
1	DTH	A	64	7/8	0.97	0.07	17,20,25,26	0
1	DIL	A	22[B]	8/9	0.97	0.12	15,18,24,29	5
1	DLE	F	59	8/9	0.97	0.09	25,28,29,30	0
1	DGL	B	60	9/10	0.97	0.09	21,22,39,39	0
1	DHI	B	79	10/11	0.97	0.07	23,30,32,34	0
1	DAS	C	27	8/9	0.97	0.07	22,31,37,37	0
1	DHI	D	92	10/11	0.97	0.08	23,24,29,29	0
1	DVA	E	7	7/8	0.97	0.05	35,35,38,40	0
1	DCY	E	53	6/7	0.97	0.10	25,26,28,29	0
1	DAR	D	16	11/12	0.97	0.09	18,28,56,57	0
1	DCY	D	44	6/7	0.97	0.09	16,19,20,21	0
1	DSG	D	93	8/9	0.97	0.09	30,34,46,47	0
1	DTY	B	18	12/13	0.97	0.07	19,21,24,27	0
1	DPN	D	89	11/12	0.97	0.08	24,26,29,32	0
1	DTH	A	24	7/8	0.97	0.11	16,21,23,23	0
1	DTH	B	70	7/8	0.97	0.09	13,16,17,21	0
1	DAS	E	27	8/9	0.97	0.09	23,25,35,36	0
1	DTY	E	18	12/13	0.97	0.10	24,28,36,42	0
1	DTH	E	64	7/8	0.97	0.17	32,37,41,43	0
1	DLY	F	100	9/10	0.97	0.12	30,32,50,51	0
1	DTH	D	24	7/8	0.97	0.08	14,20,21,23	0
1	DTH	F	70	7/8	0.97	0.06	29,29,32,34	0
1	MED	E	74	8/9	0.97	0.11	22,25,29,29	0
1	DVA	A	62	7/8	0.97	0.09	14,17,24,26	0
1	DTY	B	38	12/13	0.97	0.11	17,20,26,29	0
1	DPR	D	78	7/8	0.97	0.09	43,45,55,60	0
1	DCY	A	53	6/7	0.97	0.08	16,19,23,28	0
1	DCY	F	44	6/7	0.97	0.11	22,24,26,27	0
1	DPN	B	89	11/12	0.97	0.08	13,15,17,18	0
1	DIL	C	73	8/9	0.97	0.10	28,31,37,39	0
1	DTH	E	70	7/8	0.97	0.07	25,29,33,35	0
1	DGL	A	65	9/10	0.97	0.11	16,20,37,37	0
1	DPR	E	46	7/8	0.97	0.12	18,20,23,24	0
1	DSN	A	43	6/7	0.97	0.07	20,23,24,24	0
1	DGN	C	72	9/10	0.97	0.11	30,33,40,41	0
1	DLE	E	25	8/9	0.97	0.17	21,23,28,36	0
1	DLE	B	47	8/9	0.97	0.07	13,15,20,21	0
1	DPN	F	89	11/12	0.97	0.08	22,24,27,27	0
1	DIL	F	73	8/9	0.97	0.10	24,26,29,31	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	DLE	B	59	8/9	0.97	0.14	22,24,26,26	0
1	DLY	D	9	9/10	0.97	0.12	23,26,64,71	0
1	DTH	F	24	7/8	0.97	0.09	20,21,24,28	0
1	DIL	F	28	8/9	0.97	0.11	23,26,32,32	0
1	DPR	A	33	7/8	0.97	0.07	25,28,32,34	0
1	DPN	E	89	11/12	0.97	0.08	21,25,28,30	0
1	DGN	E	72	9/10	0.97	0.07	20,23,27,27	0
1	DAS	D	12	8/9	0.97	0.08	24,28,39,44	0
1	DPR	E	42	7/8	0.97	0.15	18,19,21,23	0
1	DIL	B	76	8/9	0.97	0.10	14,19,23,24	0
1	DLY	B	77	9/10	0.97	0.08	16,19,34,36	0
1	DAR	F	49	11/12	0.97	0.10	17,19,28,29	0
1	DAR	E	49	11/12	0.97	0.07	19,22,32,32	0
1	DIL	A	22[A]	8/9	0.97	0.12	13,17,26,33	5
1	DPR	F	21	7/8	0.97	0.08	18,20,21,23	0
1	DGL	D	23	9/10	0.97	0.09	16,21,35,39	0
1	DSN	A	17	6/7	0.97	0.10	20,24,24,32	0
1	DPR	D	33	7/8	0.97	0.15	44,47,51,53	0
1	DLE	C	25	8/9	0.97	0.09	25,27,30,30	0
1	DLY	B	94	9/10	0.97	0.15	17,23,53,56	0
1	DPR	C	33	7/8	0.97	0.09	52,55,58,59	0
1	DPN	D	10	11/12	0.97	0.08	23,25,32,35	0
1	DAS	A	27	8/9	0.97	0.10	18,26,34,37	0
1	DGL	E	23	9/10	0.97	0.09	18,21,46,51	0
1	DPR	F	46	7/8	0.97	0.08	19,22,25,30	0
1	DPR	A	63	7/8	0.97	0.07	18,19,22,24	0
1	MED	D	74	8/9	0.97	0.07	28,35,43,47	0
1	DVA	B	45	7/8	0.97	0.08	12,14,17,17	0
1	DTY	C	18	12/13	0.97	0.11	16,21,34,36	0
1	DLY	A	94	9/10	0.97	0.13	17,22,54,58	0
1	DPR	A	46	7/8	0.97	0.08	16,19,21,25	0
1	DPR	C	21	7/8	0.97	0.07	19,25,27,27	0
1	DLE	A	59	8/9	0.97	0.12	18,19,22,25	0
1	DTH	C	24	7/8	0.97	0.07	18,22,25,33	0
1	DAS	C	12	8/9	0.97	0.10	14,16,26,28	0
1	DVA	F	13	7/8	0.98	0.12	18,19,23,29	0
1	DCY	D	61	6/7	0.98	0.10	21,26,27,28	0
1	DCY	B	44	6/7	0.98	0.12	15,17,18,20	0
1	DLE	E	47	8/9	0.98	0.09	18,21,23,24	0
1	DCY	B	53	6/7	0.98	0.06	19,20,24,30	0
1	DTH	D	64	7/8	0.98	0.10	29,32,33,35	0
1	DSG	B	93	8/9	0.98	0.07	16,21,27,31	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	DPR	A	21	7/8	0.98	0.06	16,18,20,21	0
1	DIL	D	28	8/9	0.98	0.07	22,22,24,28	0
1	DSN	C	17	6/7	0.98	0.11	14,15,18,20	0
1	DPR	D	63	7/8	0.98	0.07	27,29,32,36	0
1	DTH	B	64	7/8	0.98	0.07	19,20,28,29	0
1	DPR	B	63	7/8	0.98	0.07	17,19,23,28	0
1	DIL	B	84	8/9	0.98	0.11	13,15,18,23	0
1	DCY	D	95	6/7	0.98	0.08	23,30,34,36	0
1	DLE	D	47	8/9	0.98	0.09	18,19,26,26	0
1	DCY	C	95	6/7	0.98	0.08	25,30,32,37	0
1	DAS	B	27	8/9	0.98	0.10	19,23,28,32	0
1	DPR	B	78	7/8	0.98	0.05	18,24,31,32	0
1	DIL	C	28	8/9	0.98	0.08	25,27,29,33	0
1	DGN	B	72	9/10	0.98	0.10	12,13,21,23	0
1	MED	F	48	8/9	0.98	0.06	18,20,26,28	0
1	DSN	A	67	6/7	0.98	0.06	16,17,22,23	0
1	DLE	D	90	8/9	0.98	0.10	23,29,40,48	0
1	DHI	C	20	10/11	0.98	0.08	19,22,26,29	0
1	MED	E	71	8/9	0.98	0.10	22,24,26,27	0
1	DSN	C	43	6/7	0.98	0.07	24,26,26,27	0
1	DPR	D	46	7/8	0.98	0.11	18,21,26,30	0
1	MED	C	11	8/9	0.98	0.11	16,18,31,31	0
1	DLE	B	90	8/9	0.98	0.11	14,16,31,39	0
1	DIL	B	69	8/9	0.98	0.07	15,17,20,23	0
1	DPR	C	46	7/8	0.98	0.06	19,23,28,32	0
1	DTY	D	14	12/13	0.98	0.06	19,29,40,47	0
1	DPR	F	42	7/8	0.98	0.07	24,25,27,28	0
1	DGN	A	72	9/10	0.98	0.08	17,19,33,35	0
1	DIL	D	22	8/9	0.98	0.08	17,20,23,26	0
1	DPR	F	63	7/8	0.98	0.07	22,22,28,29	0
1	DVA	C	62	7/8	0.98	0.06	28,32,34,38	0
1	DAS	F	12	8/9	0.98	0.07	18,20,31,34	0
1	DPR	D	21	7/8	0.98	0.07	20,21,22,22	0
1	DSN	D	88[B]	6/7	0.98	0.11	31,33,37,37	3
1	DPN	C	10	11/12	0.98	0.15	16,17,21,23	0
1	DVA	C	7	7/8	0.98	0.09	19,20,21,24	0
1	DVA	A	45	7/8	0.98	0.09	14,15,17,18	0
1	DVA	E	8	7/8	0.98	0.07	30,31,33,35	0
1	DCY	E	50	6/7	0.98	0.05	22,25,28,31	0
1	DVA	D	26	7/8	0.98	0.06	18,19,22,24	0
1	DSN	F	88[B]	6/7	0.98	0.09	27,28,29,34	3
1	DSN	F	88[A]	6/7	0.98	0.09	27,28,34,35	3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	DCY	F	53	6/7	0.98	0.12	17,21,22,25	0
1	MED	D	48	8/9	0.98	0.07	19,21,26,29	0
1	DTH	B	24	7/8	0.98	0.08	15,18,21,26	0
1	DCY	C	44	6/7	0.98	0.07	22,23,25,29	0
1	DIL	E	28	8/9	0.98	0.08	19,23,27,31	0
1	DCY	E	61	6/7	0.98	0.06	27,32,34,34	0
1	DIL	E	73	8/9	0.98	0.10	20,21,23,23	0
1	DAR	D	49	11/12	0.98	0.07	18,20,25,29	0
1	DVA	D	45	7/8	0.98	0.10	18,18,23,25	0
1	DAR	B	75	11/12	0.98	0.13	13,17,21,27	0
1	DSG	C	93	8/9	0.98	0.12	30,35,54,56	0
1	DIL	E	22	8/9	0.98	0.08	18,19,28,29	0
1	DSN	D	88[A]	6/7	0.98	0.11	31,33,34,37	3
1	DCY	B	61	6/7	0.98	0.07	19,22,23,24	0
1	DTH	F	64	7/8	0.98	0.07	24,26,34,36	0
1	DIL	A	39	8/9	0.98	0.08	22,24,27,31	0
1	DCY	C	53	6/7	0.98	0.09	18,19,22,24	0
1	DSN	A	88	6/7	0.98	0.10	17,20,20,38	0
1	DPR	B	46	7/8	0.98	0.07	13,16,19,21	0
1	DCY	E	44	6/7	0.98	0.10	17,17,19,24	0
1	DSN	C	67	6/7	0.98	0.06	33,38,43,44	0
1	DLE	F	47	8/9	0.98	0.07	18,20,26,27	0
1	DCY	B	54	6/7	0.98	0.08	20,21,28,29	0
1	DPN	B	40	11/12	0.98	0.12	13,17,19,21	0
1	DVA	C	45	7/8	0.98	0.08	21,22,25,27	0
1	DSN	B	43	6/7	0.98	0.10	13,16,20,22	0
1	DLY	E	41	9/10	0.98	0.12	20,22,24,24	0
1	DCY	F	97	6/7	0.98	0.08	22,25,28,29	0
1	DPR	C	63	7/8	0.98	0.07	32,33,36,42	0
1	DLE	E	90	8/9	0.98	0.09	27,30,49,53	0
1	DCY	C	19	6/7	0.98	0.09	18,20,24,24	0
1	DSN	B	17	6/7	0.98	0.08	19,24,25,32	0
1	DGL	B	86	9/10	0.98	0.10	14,17,25,30	0
1	DHI	E	20	10/11	0.98	0.06	22,25,27,30	0
1	DVA	C	26	7/8	0.98	0.08	21,24,26,30	0
1	DGL	A	60	9/10	0.98	0.09	16,18,30,39	0
1	DGN	C	15	9/10	0.98	0.13	16,17,24,24	0
1	DVA	E	26	7/8	0.98	0.12	19,20,32,33	0
1	DVA	D	7	7/8	0.98	0.08	31,33,36,41	0
1	DIL	B	28	8/9	0.98	0.08	12,15,19,25	0
1	DCY	B	95	6/7	0.98	0.06	17,17,24,28	0
1	DPN	A	40	11/12	0.98	0.07	16,19,23,24	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	DGL	A	35	9/10	0.98	0.07	20,23,27,28	0
1	DIL	A	76	8/9	0.98	0.07	22,28,31,31	0
1	DVA	F	62	7/8	0.98	0.07	21,22,26,30	0
1	DSN	F	67	6/7	0.98	0.09	27,29,31,31	0
1	DGL	B	23	9/10	0.98	0.08	16,20,43,47	0
1	DHI	E	92	10/11	0.98	0.07	24,27,29,29	0
1	DIL	B	39	8/9	0.98	0.10	16,20,32,36	0
1	MED	E	87	8/9	0.98	0.09	25,29,34,40	0
1	DLE	A	90	8/9	0.98	0.09	17,18,36,42	0
1	DTY	A	38	12/13	0.98	0.07	19,21,25,25	0
1	DHI	B	92	10/11	0.98	0.06	15,16,19,20	0
1	DSG	A	93	8/9	0.98	0.09	14,22,29,31	0
1	DVA	B	26	7/8	0.98	0.08	15,21,28,29	0
1	DGL	A	23	9/10	0.98	0.08	15,17,30,32	0
1	DHI	C	92	10/11	0.98	0.07	24,28,31,33	0
1	DCY	D	97	6/7	0.98	0.07	26,29,38,39	0
1	DCY	E	95	6/7	0.98	0.07	29,30,36,39	0
1	DHI	F	92	10/11	0.98	0.07	19,23,24,24	0
1	DVA	E	45	7/8	0.98	0.12	15,16,18,20	0
1	DAR	A	49	11/12	0.98	0.09	14,20,26,28	0
1	DIL	A	36	8/9	0.98	0.11	24,29,38,48	0
1	DLY	C	9	9/10	0.98	0.09	15,16,30,32	0
1	DSN	D	43	6/7	0.98	0.14	19,22,24,25	0
1	DCY	C	54	6/7	0.98	0.10	21,26,30,39	0
1	DCY	F	95	6/7	0.98	0.08	20,21,30,30	0
1	DTY	A	32	12/13	0.98	0.06	18,23,40,41	0
1	DSN	B	88	6/7	0.98	0.09	14,15,24,34	0
1	DTY	F	18	12/13	0.98	0.13	16,20,28,31	0
1	DIL	B	36	8/9	0.98	0.09	26,29,39,41	0
1	DSN	F	17	6/7	0.98	0.14	16,17,18,27	0
1	DLE	A	25	8/9	0.98	0.09	19,22,28,30	0
1	DPN	F	40	11/12	0.98	0.12	26,31,37,38	0
1	DVA	D	62	7/8	0.98	0.07	26,29,34,40	0
1	MED	F	71	8/9	0.98	0.07	24,26,28,30	0
1	DSN	E	43	6/7	0.98	0.12	17,20,22,23	0
1	DSN	F	43	6/7	0.98	0.08	24,24,29,30	0
1	DCY	D	50	6/7	0.98	0.06	20,21,24,27	0
1	DCY	C	50	6/7	0.98	0.07	23,25,29,29	0
1	DCY	B	19	6/7	0.98	0.07	19,21,23,23	0
1	DCY	E	19	6/7	0.98	0.07	25,27,29,29	0
1	DCY	A	54	6/7	0.99	0.09	16,18,23,25	0
1	MED	D	71	8/9	0.99	0.06	23,30,34,37	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	DVA	D	8	7/8	0.99	0.07	20,23,27,29	0
1	DHI	B	83	10/11	0.99	0.08	14,20,24,26	0
1	DVA	F	45	7/8	0.99	0.10	20,21,24,25	0
1	DCY	A	19	6/7	0.99	0.08	16,16,18,19	0
1	MED	B	74	8/9	0.99	0.14	12,14,16,18	0
1	DCY	F	19	6/7	0.99	0.10	16,19,21,21	0
1	DCY	C	97	6/7	0.99	0.09	28,30,35,39	0
1	DPR	A	42	7/8	0.99	0.05	17,20,22,22	0
1	MED	B	87	8/9	0.99	0.10	14,16,20,20	0
1	MED	F	87	8/9	0.99	0.08	26,31,35,42	0
1	DCY	C	61	6/7	0.99	0.09	24,25,28,29	0
1	DVA	C	8	7/8	0.99	0.11	14,15,17,19	0
1	DIL	B	73	8/9	0.99	0.14	12,12,13,13	0
1	MED	A	48	8/9	0.99	0.06	14,18,24,24	0
1	DCY	F	61	6/7	0.99	0.08	19,20,21,25	0
1	DLY	B	41	9/10	0.99	0.15	13,14,18,19	0
1	DVA	C	13	7/8	0.99	0.11	13,14,15,16	0
1	MED	C	71	8/9	0.99	0.09	29,34,35,35	0
1	DCY	D	19	6/7	0.99	0.06	21,23,25,26	0
1	MED	B	71	8/9	0.99	0.10	12,15,21,21	0
1	DPR	B	42	7/8	0.99	0.12	13,14,15,16	0
1	DCY	B	97	6/7	0.99	0.10	20,21,24,27	0
1	DCY	A	95	6/7	0.99	0.08	15,19,20,25	0
1	DSN	E	17	6/7	0.99	0.10	23,24,27,32	0
1	DPR	B	99	7/8	0.99	0.15	26,28,29,34	0
1	DCY	A	61	6/7	0.99	0.11	15,17,20,22	0
1	DCY	F	54	6/7	0.99	0.09	17,20,24,28	0
1	DSN	B	67	6/7	0.99	0.06	16,17,21,23	0
1	DCY	A	97	6/7	0.99	0.13	17,19,25,28	0
1	MED	A	71	8/9	0.99	0.07	16,19,22,25	0
1	MED	A	87	8/9	0.99	0.06	16,18,20,22	0
1	DCY	F	50	6/7	0.99	0.06	17,19,23,23	0
1	DVA	E	62	7/8	0.99	0.09	29,32,37,37	0
1	DIL	F	69	8/9	0.99	0.08	23,27,31,33	0
1	DPN	F	10	11/12	0.99	0.13	19,21,25,26	0
1	MED	B	48	8/9	0.99	0.07	14,18,25,27	0
1	DHI	A	92	10/11	0.99	0.06	13,17,20,20	0
1	MED	C	48	8/9	0.99	0.07	23,25,29,30	0
1	DCY	B	50	6/7	0.99	0.05	17,19,21,22	0
1	DCY	A	50	6/7	0.99	0.08	13,15,20,23	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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
3	TFA	D	204	7/7	0.74	0.32	51,78,88,89	0
2	ACT	A	201	4/4	0.82	0.31	59,68,69,71	0
4	GOL	F	202	6/6	0.82	0.14	51,56,59,63	0
3	TFA	A	202	7/7	0.83	0.16	68,73,80,81	0
3	TFA	F	203	7/7	0.84	0.13	83,85,89,93	0
2	ACT	B	202	4/4	0.86	0.16	57,58,65,76	0
3	TFA	F	201	7/7	0.87	0.21	44,78,80,84	0
3	TFA	D	205	7/7	0.87	0.19	49,61,69,70	0
3	TFA	C	204	7/7	0.88	0.15	50,61,66,67	0
4	GOL	D	202	6/6	0.88	0.11	50,57,61,64	0
4	GOL	C	203	6/6	0.89	0.16	37,43,54,56	0
3	TFA	D	203	7/7	0.89	0.15	33,54,63,70	0
4	GOL	C	201	6/6	0.89	0.15	32,47,50,52	0
2	ACT	E	201	4/4	0.90	0.11	36,44,54,62	0
2	ACT	C	202	4/4	0.90	0.23	48,49,55,60	0
2	ACT	A	203	4/4	0.93	0.09	45,48,49,49	0
2	ACT	E	202	4/4	0.93	0.23	68,72,72,73	0
2	ACT	B	203	4/4	0.94	0.06	40,49,50,59	0
2	ACT	D	201	4/4	0.95	0.19	50,54,57,65	0
2	ACT	B	201	4/4	0.95	0.12	34,54,60,60	0
2	ACT	F	204	4/4	0.95	0.17	46,52,59,59	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.