



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2026 – 10:02 PM UTC

PDB ID : 9Z2H / pdb\_00009z2h  
Title : Crystal structure of A10 Fab in complex with the EGFR peptide  
Authors : Zhan, J.; Maslanka, C.; Xia, D.  
Deposited on : 2025-11-05  
Resolution : 2.45 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](mailto:validation@mail.wwpdb.org)

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

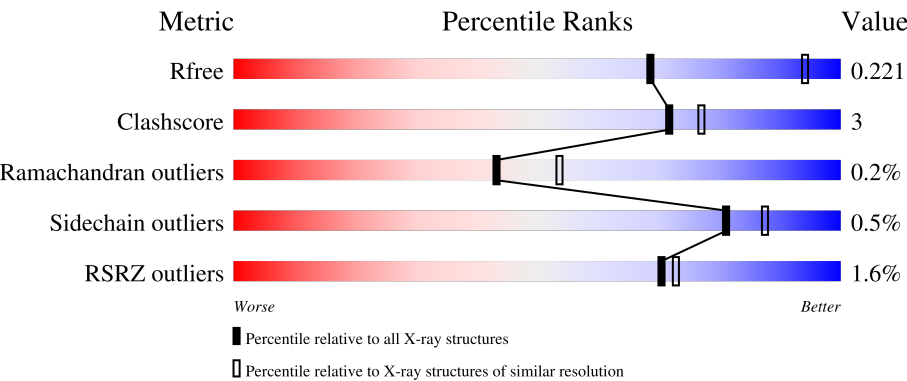
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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 <sub>free</sub>	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	24	<div><div>17%</div><div><div></div><div></div><div></div><div></div></div><div>58%</div><div>17%</div><div>25%</div></div>
1	E	24	<div><div>12%</div><div><div></div><div></div><div></div><div></div></div><div>71%</div><div>•</div><div>25%</div></div>
2	H	247	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>81%</div><div>8%</div><div>11%</div></div>
2	HH	247	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>84%</div><div>5%</div><div>11%</div></div>
3	L	214	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>91%</div><div>9%</div></div>

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Mol	Chain	Length	Quality of chain
3	LL	214	 91%8% .

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
4	ACT	H	301	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13673 atoms, of which 6693 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	18	Total	C	H	N	O	S	0	0	0
			258	79	123	23	30	3			
1	E	18	Total	C	H	N	O	S	0	0	0
			258	79	123	23	30	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	HIS	-	expression tag	UNP P00533
A	20	HIS	-	expression tag	UNP P00533
A	21	HIS	-	expression tag	UNP P00533
A	22	HIS	-	expression tag	UNP P00533
A	23	HIS	-	expression tag	UNP P00533
A	24	HIS	-	expression tag	UNP P00533
E	19	HIS	-	expression tag	UNP P00533
E	20	HIS	-	expression tag	UNP P00533
E	21	HIS	-	expression tag	UNP P00533
E	22	HIS	-	expression tag	UNP P00533
E	23	HIS	-	expression tag	UNP P00533
E	24	HIS	-	expression tag	UNP P00533

- Molecule 2 is a protein called Fab heavy chain of the A10 antibody.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	219	Total	C	H	N	O	S	0	0	0
			3261	1035	1632	269	316	9			
2	HH	219	Total	C	H	N	O	S	0	0	0
			3261	1035	1632	269	316	9			

- Molecule 3 is a protein called Fab light chain of the A10 antibody.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	L	213	Total	C	H	N	O	S	0	0	0
			3213	1023	1584	270	331	5			
3	LL	213	Total	C	H	N	O	S	0	0	0
			3213	1023	1584	270	331	5			

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	H	O	0	0
			7	2	3	2		
4	L	1	Total	C	H	O	0	0
			7	2	3	2		
4	LL	1	Total	C	H	O	0	0
			7	2	3	2		
4	LL	1	Total	C	H	O	0	0
			7	2	3	2		
4	LL	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	O	0	0
			2	2		
5	H	40	Total	O	0	0
			40	40		
5	L	27	Total	O	0	0
			27	27		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	4	Total 4	O 4	0	0
5	HH	59	Total 59	O 59	0	0
5	LL	42	Total 42	O 42	0	0



- Molecule 3: Fab light chain of the A10 antibody

Chain LL: 91% 8% .





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.62Å 129.62Å 144.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.25 – 2.45 33.25 – 2.45	Depositor EDS
% Data completeness (in resolution range)	61.2 (33.25-2.45) 71.9 (33.25-2.45)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.190 , 0.223 0.191 , 0.221	Depositor DCC
$R_{free}$ test set	1791 reflections (3.43%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.3	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 36.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.041 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13673	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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: 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	0.27	0/135	0.53	0/177
1	E	0.21	0/135	0.56	0/177
2	H	0.19	0/1669	0.45	0/2278
2	HH	0.18	0/1669	0.45	0/2278
3	L	0.18	0/1665	0.43	0/2264
3	LL	0.19	0/1665	0.44	0/2264
All	All	0.19	0/6938	0.45	0/9438

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	135	123	123	3	0
1	E	135	123	123	0	0
2	H	1629	1632	1632	16	0
2	HH	1629	1632	1632	6	0
3	L	1629	1584	1584	9	0
3	LL	1629	1584	1584	12	0
4	H	4	3	3	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	4	3	3	0	0
4	LL	12	9	9	2	0
5	A	2	0	0	0	0
5	E	4	0	0	0	0
5	H	40	0	0	0	0
5	HH	59	0	0	0	0
5	L	27	0	0	0	0
5	LL	42	0	0	0	0
All	All	6980	6693	6693	44	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 (44) 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:LL:63:SER:OG	3:LL:74:THR:HB	1.80	0.80
2:H:111:THR:CG2	4:H:301:ACT:H3	2.18	0.74
3:LL:78:LEU:HD11	3:LL:104:LEU:HD21	1.73	0.71
3:LL:63:SER:HG	3:LL:74:THR:HB	1.57	0.70
2:H:111:THR:HG21	4:H:301:ACT:H3	1.76	0.68
2:HH:139:THR:HG21	2:HH:187:THR:HB	1.76	0.68
3:L:4:MET:HE3	3:L:23:CYS:SG	2.38	0.64
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.78	0.64
2:H:63:PHE:HB3	2:H:67:LEU:HD13	1.86	0.57
2:H:8:GLY:O	4:H:301:ACT:H2	2.08	0.54
2:H:182:LEU:C	2:H:182:LEU:HD12	2.33	0.53
2:HH:182:LEU:HD12	2:HH:182:LEU:C	2.34	0.52
1:A:9:MET:HE2	1:A:11:GLU:HB2	1.94	0.50
2:H:155:THR:HG22	2:H:203:ASN:HB3	1.92	0.50
3:LL:4:MET:HG3	3:LL:23:CYS:SG	2.52	0.49
2:H:140:ALA:CB	2:H:193:LEU:HD11	2.42	0.49
1:A:13:GLY:HA2	2:H:102:MET:HA	1.94	0.49
3:LL:120:PRO:HD3	3:LL:132:VAL:HG22	1.95	0.48
2:H:111:THR:HG23	4:H:301:ACT:H3	1.93	0.48
3:LL:142:ARG:CZ	3:LL:163:VAL:HG21	2.44	0.48
3:LL:163:VAL:CG2	3:LL:175:LEU:HD12	2.44	0.47
2:H:149:TYR:CE1	2:H:154:VAL:HG13	2.49	0.47
2:HH:152:GLU:HG2	2:HH:153:PRO:HA	1.97	0.46
3:L:108:ARG:HG2	3:L:109:THR:N	2.31	0.46
3:LL:47:LEU:HD21	3:LL:62:PHE:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:76:SER:O	3:L:77:SER:C	2.58	0.44
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.99	0.44
2:H:123:PRO:HB2	2:H:146:VAL:HG13	1.98	0.44
3:L:50:GLY:O	3:L:51:ALA:HB3	2.17	0.44
2:H:154:VAL:HG23	2:H:182:LEU:HD21	1.99	0.44
3:LL:163:VAL:HG12	3:LL:164:THR:O	2.18	0.44
2:HH:66:ARG:HD2	2:HH:83:THR:O	2.18	0.44
2:H:7:SER:HA	4:H:301:ACT:H1	2.00	0.43
3:LL:59:PRO:HA	4:LL:303:ACT:H2	2.00	0.43
2:HH:12:VAL:HG11	2:HH:85:MET:HG3	2.00	0.43
2:H:218:LYS:O	2:H:219:SER:C	2.62	0.43
3:L:186:TYR:HA	3:L:192:TYR:OH	2.20	0.42
3:L:185:ASP:HA	3:L:188:LYS:HG2	2.03	0.41
2:HH:163:LEU:HD21	2:HH:186:VAL:HG21	2.03	0.41
2:H:205:LYS:N	2:H:206:PRO:CD	2.84	0.41
3:LL:125:LEU:HD12	3:LL:183:LYS:HG3	2.02	0.40
1:A:12:ASP:HA	2:H:98:LYS:HD2	2.04	0.40
3:LL:138:ASN:O	4:LL:302:ACT:H2	2.22	0.40
3:L:97:THR:HG22	3:L:98:PHE:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	16/24 (67%)	16 (100%)	0	0	100	100
1	E	16/24 (67%)	15 (94%)	1 (6%)	0	100	100
2	H	217/247 (88%)	214 (99%)	3 (1%)	0	100	100
2	HH	217/247 (88%)	209 (96%)	8 (4%)	0	100	100
3	L	211/214 (99%)	202 (96%)	8 (4%)	1 (0%)	24	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	LL	211/214 (99%)	204 (97%)	6 (3%)	1 (0%)	24	32
All	All	888/970 (92%)	860 (97%)	26 (3%)	2 (0%)	43	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	138	ASN
3	LL	138	ASN

### 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	14/20 (70%)	14 (100%)	0	100	100
1	E	14/20 (70%)	13 (93%)	1 (7%)	13	18
2	H	186/211 (88%)	186 (100%)	0	100	100
2	HH	186/211 (88%)	185 (100%)	1 (0%)	81	87
3	L	185/186 (100%)	185 (100%)	0	100	100
3	LL	185/186 (100%)	183 (99%)	2 (1%)	65	76
All	All	770/834 (92%)	766 (100%)	4 (0%)	81	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	2	CYS
2	HH	201	ASN
3	LL	4	MET
3	LL	123	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	39	GLN
3	L	38	GLN
2	HH	168	HIS
2	HH	175	GLN
2	HH	201	ASN
3	LL	137	ASN
3	LL	160	GLN
3	LL	199	GLN

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

5 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	$\# Z  > 2$
4	ACT	LL	302	-	3,3,3	1.45	1 (33%)	3,3,3	1.37	0
4	ACT	L	301	-	3,3,3	1.41	1 (33%)	3,3,3	0.97	0
4	ACT	LL	303	-	3,3,3	1.42	1 (33%)	3,3,3	1.03	0
4	ACT	LL	301	-	3,3,3	1.44	1 (33%)	3,3,3	0.89	0
4	ACT	H	301	-	3,3,3	1.42	1 (33%)	3,3,3	0.98	0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	LL	301	ACT	CH3-C	2.10	1.57	1.49
4	LL	303	ACT	CH3-C	2.05	1.57	1.49
4	L	301	ACT	CH3-C	2.05	1.57	1.49
4	LL	302	ACT	CH3-C	2.04	1.57	1.49
4	H	301	ACT	CH3-C	2.02	1.57	1.49

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	LL	302	ACT	1	0
4	LL	303	ACT	1	0
4	H	301	ACT	5	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	18/24 (75%)	0.99	4 (22%) 2 2	39, 67, 106, 133	0
1	E	18/24 (75%)	0.79	3 (16%) 4 3	36, 56, 111, 124	0
2	H	219/247 (88%)	-0.17	2 (0%) 81 82	29, 44, 69, 105	0
2	HH	219/247 (88%)	-0.23	3 (1%) 73 75	30, 43, 80, 111	0
3	L	213/214 (99%)	-0.13	1 (0%) 87 88	25, 43, 89, 120	0
3	LL	213/214 (99%)	-0.27	1 (0%) 87 88	28, 42, 66, 77	0
All	All	900/970 (92%)	-0.16	14 (1%) 70 73	25, 43, 83, 133	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	ALA	4.5
1	A	2	CYS	3.7
2	HH	139	THR	3.2
2	H	218	LYS	3.2
1	E	2	CYS	3.0
2	H	219	SER	2.6
3	L	213	GLU	2.6
2	HH	137	GLY	2.5
1	A	7	TYR	2.3
1	E	1	ALA	2.3
1	A	5	ASP	2.3
2	HH	190	SER	2.2
1	E	7	TYR	2.2
3	LL	212	GLY	2.0

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

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



### 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	ACT	L	301	4/4	0.75	0.26	45,54,61,71	0
4	ACT	H	301	4/4	0.83	0.15	53,61,64,64	0
4	ACT	LL	303	4/4	0.86	0.14	47,68,76,76	0
4	ACT	LL	301	4/4	0.89	0.34	44,53,60,74	0
4	ACT	LL	302	4/4	0.94	0.09	39,46,55,55	0

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

There are no such residues in this entry.