



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 06:22 PM GMT

PDB ID : 3BPS  
Title : PCSK9:EGF-A complex  
Authors : Kwon, H.J.  
Deposited on : 2007-12-19  
Resolution : 2.41 Å(reported)

This is a full wwPDB validation 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 <http://wwpdb.org/ValidationPDFNotes.html>

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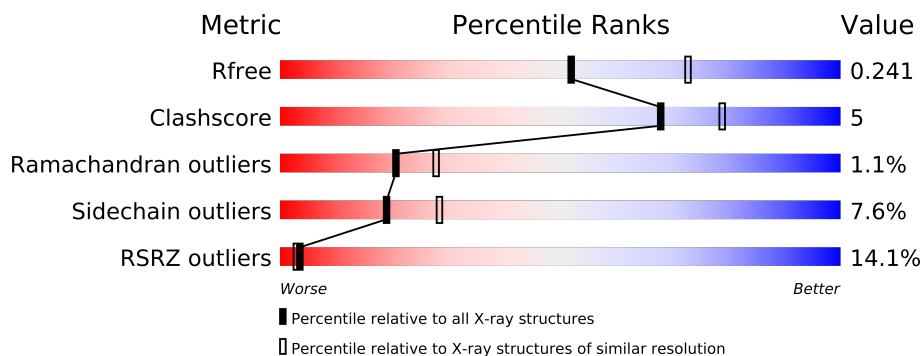
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 2.41 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))
$R_{free}$	66092	2496 (2.44-2.40)
Clashscore	79885	3124 (2.44-2.40)
Ramachandran outliers	78287	3067 (2.44-2.40)
Sidechain outliers	78261	3068 (2.44-2.40)
RSRZ outliers	66119	2499 (2.44-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	P	100	
2	A	540	
3	E	83	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4414 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	92	Total	C	N	O	S	0	0	0
			740	474	133	131	2			

- Molecule 2 is a protein called Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	435	Total	C	N	O	S	0	0	0
			3236	2006	589	616	25			

- Molecule 3 is a protein called Low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	41	Total	C	N	O	S	0	0	0
			308	183	56	62	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	290	GLY	-	EXPRESSION TAG	UNP P01130
E	291	ALA	-	EXPRESSION TAG	UNP P01130
E	292	MET	-	EXPRESSION TAG	UNP P01130

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

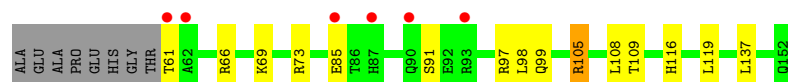
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	20	Total 20	O 20	0	0
5	A	105	Total 105	O 105	0	0
5	E	4	Total 4	O 4	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

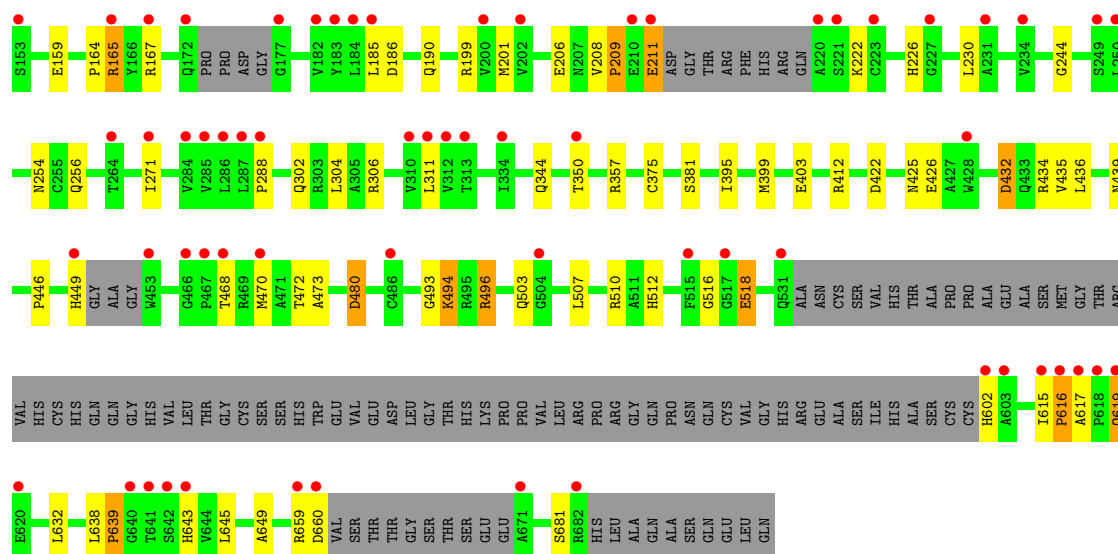
- Molecule 1: Proprotein convertase subtilisin/kexin type 9

Chain P: 



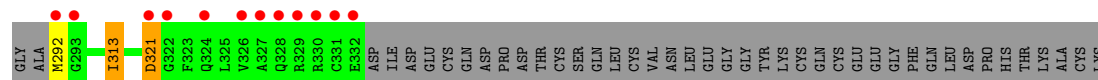
- Molecule 2: Proprotein convertase subtilisin/kexin type 9

Chain A: 



- Molecule 3: Low-density lipoprotein receptor

Chain E: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.95Å 116.95Å 134.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.41 41.33 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.00-2.41) 99.0 (41.33-2.41)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.03 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, $R_{free}$	0.203 , 0.240 0.204 , 0.241	Depositor DCC
$R_{free}$ test set	1831 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.7	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 66.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 36511 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4414	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

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

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

## 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: CA

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	P	0.65	0/757	0.64	0/1023
2	A	0.67	0/3292	0.75	2/4469 (0.0%)
3	E	0.53	0/311	0.62	0/417
All	All	0.66	0/4360	0.72	2/5909 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	412	ARG	NE-CZ-NH1	6.68	123.64	120.30
2	A	412	ARG	NE-CZ-NH2	-5.50	117.55	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	740	0	750	6	0
2	A	3236	0	3185	34	0
3	E	308	0	278	2	0
4	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	105	0	0	2	0
5	E	4	0	0	0	0
5	P	20	0	0	2	0
All	All	4414	0	4213	42	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (42) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:66:ARG:HH11	1:P:73:ARG:HD2	1.13	1.10
2:A:472:THR:HG21	2:A:510:ARG:HH21	1.21	1.03
1:P:66:ARG:NH1	1:P:73:ARG:HD2	1.84	0.92
2:A:472:THR:HG21	2:A:510:ARG:NH2	1.90	0.85
2:A:185:LEU:HD11	2:A:271:ILE:HD11	1.78	0.65
2:A:208:VAL:HG12	2:A:209:PRO:HD2	1.80	0.63
2:A:211:GLU:HB3	2:A:254:ASN:HB2	1.80	0.62
3:E:321:ASP:OD1	3:E:321:ASP:N	2.31	0.62
2:A:426:GLU:HB3	2:A:434:ARG:HG2	1.84	0.59
2:A:496:ARG:HH21	2:A:512:HIS:HB3	1.68	0.58
2:A:208:VAL:CG1	2:A:209:PRO:HD2	2.40	0.52
2:A:494:LYS:HG2	2:A:516:GLY:HA3	1.92	0.52
2:A:199:ARG:NH1	5:A:46:HOH:O	2.36	0.50
2:A:645:LEU:HD21	2:A:659:ARG:HE	1.77	0.49
2:A:186:ASP:OD2	2:A:288:PRO:HG2	2.13	0.49
2:A:493:GLY:O	2:A:643:HIS:NE2	2.30	0.49
2:A:615:ILE:HD13	2:A:619:GLN:HE22	1.78	0.48
2:A:209:PRO:HD3	5:A:67:HOH:O	2.14	0.47
2:A:472:THR:HG22	2:A:473:ALA:N	2.28	0.47
2:A:518:GLU:H	2:A:518:GLU:CD	2.19	0.46
2:A:226:HIS:CE1	2:A:230:LEU:HD11	2.51	0.46
2:A:165:ARG:NH1	2:A:446:PRO:HB2	2.32	0.45
1:P:97:ARG:NH2	5:P:167:HOH:O	2.50	0.45
2:A:357:ARG:HB3	2:A:436:LEU:HB3	1.99	0.44
2:A:199:ARG:CZ	2:A:244:GLY:HA2	2.47	0.44
2:A:395:ILE:HG22	2:A:399:MET:HE2	2.01	0.43
1:P:98:LEU:HB2	1:P:137:LEU:HD11	2.01	0.43
1:P:99:GLN:HG2	1:P:109:THR:OG1	2.19	0.42
2:A:302:GLN:O	2:A:306:ARG:HG2	2.20	0.42
2:A:480:ASP:N	2:A:480:ASP:OD1	2.45	0.42
2:A:632:LEU:HD23	2:A:649:ALA:HB1	2.00	0.42
2:A:422:ASP:HA	2:A:439:ASN:CG	2.40	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:E:313:ILE:O	3:E:313:ILE:HG22	2.20	0.41
2:A:344:GLN:OE1	2:A:425:ASN:HB3	2.21	0.41
2:A:403:GLU:HG2	2:A:449:HIS:HE1	1.85	0.41
1:P:105:ARG:NH2	5:P:163:HOH:O	2.53	0.41
2:A:660:ASP:N	2:A:660:ASP:OD1	2.54	0.41
2:A:638:LEU:HA	2:A:639:PRO:HD2	1.72	0.41
2:A:306:ARG:HA	2:A:306:ARG:HD3	1.91	0.41
2:A:304:LEU:HB3	2:A:311:LEU:HD11	2.02	0.41
2:A:472:THR:CG2	2:A:510:ARG:HG3	2.51	0.40
2:A:616:PRO:HB2	2:A:617:ALA:H	1.74	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	P	90/100 (90%)	88 (98%)	2 (2%)	0	100	100
2	A	423/540 (78%)	400 (95%)	17 (4%)	6 (1%)	16	21
3	E	39/83 (47%)	36 (92%)	3 (8%)	0	100	100
All	All	552/723 (76%)	524 (95%)	22 (4%)	6 (1%)	21	28

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	432	ASP
2	A	616	PRO
2	A	206	GLU
2	A	209	PRO
2	A	164	PRO
2	A	639	PRO

### 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	P	79/84 (94%)	71 (90%)	8 (10%)	11	15
2	A	346/431 (80%)	322 (93%)	24 (7%)	22	33
3	E	35/71 (49%)	32 (91%)	3 (9%)	15	22
All	All	460/586 (78%)	425 (92%)	35 (8%)	19	28

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	61	THR
1	P	69	LYS
1	P	85	GLU
1	P	91	SER
1	P	105	ARG
1	P	108	LEU
1	P	116	HIS
1	P	119	LEU
2	A	159	GLU
2	A	165	ARG
2	A	167	ARG
2	A	190	GLN
2	A	201	MET
2	A	211	GLU
2	A	222	LYS
2	A	256	GLN
2	A	350	THR
2	A	375	CYS
2	A	381	SER
2	A	432	ASP
2	A	435	VAL
2	A	468	THR
2	A	470	MET
2	A	480	ASP
2	A	494	LYS
2	A	496	ARG
2	A	503	GLN

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Mol	Chain	Res	Type
2	A	507	LEU
2	A	518	GLU
2	A	602	HIS
2	A	619	GLN
2	A	681	SER
3	E	292	MET
3	E	313	ILE
3	E	321	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	101	GLN
2	A	298	ASN
2	A	417	HIS
2	A	449	HIS
2	A	503	GLN
2	A	619	GLN
3	E	306	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

## 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 ⓘ

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	P	92/100 (92%)	0.31	6 (6%)	18 16	43, 52, 67, 73	0
2	A	435/540 (80%)	0.86	62 (14%)	3 3	42, 51, 70, 95	0
3	E	41/83 (49%)	1.39	12 (29%)	1 1	40, 53, 70, 73	0
All	All	568/723 (78%)	0.81	80 (14%)	3 3	40, 52, 70, 95	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	292	MET	7.9
2	A	660	ASP	6.4
2	A	220	ALA	5.4
2	A	617	ALA	5.2
2	A	153	SER	5.1
2	A	616	PRO	5.1
2	A	615	ILE	5.0
3	E	328	GLN	5.0
2	A	620	GLU	4.9
2	A	641	THR	4.6
3	E	327	ALA	4.3
2	A	618	PRO	4.3
3	E	330	ARG	4.3
3	E	326	VAL	4.2
3	E	293	GLY	4.1
2	A	449	HIS	4.1
2	A	642	SER	4.1
2	A	504	GLY	4.1
2	A	603	ALA	4.0
2	A	211	GLU	3.9
2	A	602	HIS	3.9
2	A	659	ARG	3.7
3	E	322	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
2	A	470	MET	3.5
2	A	453	TRP	3.5
1	P	85	GLU	3.3
2	A	167	ARG	3.2
2	A	165	ARG	3.0
2	A	221	SER	3.0
2	A	428	TRP	3.0
3	E	324	GLN	2.9
2	A	287	LEU	2.9
2	A	682	ARG	2.9
3	E	321	ASP	2.9
2	A	286	LEU	2.8
2	A	486	CYS	2.8
2	A	249	SER	2.8
2	A	271	ILE	2.8
3	E	332	GLU	2.7
2	A	183	TYR	2.6
2	A	671	ALA	2.6
2	A	288	PRO	2.6
2	A	185	LEU	2.6
2	A	619	GLN	2.6
2	A	177	GLY	2.5
2	A	310	VAL	2.5
2	A	466	GLY	2.5
3	E	329	ARG	2.5
2	A	285	VAL	2.5
2	A	312	VAL	2.5
2	A	531	GLN	2.5
2	A	184	LEU	2.5
2	A	467	PRO	2.5
2	A	231	ALA	2.4
1	P	61	THR	2.4
2	A	311	LEU	2.4
2	A	643	HIS	2.3
2	A	334	ILE	2.3
2	A	227	GLY	2.3
2	A	234	VAL	2.3
1	P	62	ALA	2.3
2	A	210	GLU	2.3
3	E	331	CYS	2.3
2	A	202	VAL	2.3
2	A	284	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	A	200	VAL	2.3
2	A	250	LEU	2.3
2	A	515	PHE	2.3
2	A	223	CYS	2.2
2	A	350	THR	2.2
2	A	468	THR	2.2
2	A	182	VAL	2.2
2	A	264	THR	2.2
2	A	517	GLY	2.2
2	A	313	THR	2.1
1	P	87	HIS	2.1
1	P	93	ARG	2.1
2	A	640	GLY	2.1
2	A	172	GLN	2.1
1	P	90	GLN	2.1

## 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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	CA	E	1	1/1	0.03	-1.51	47,47,47,47	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.