



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:40 AM 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 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)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

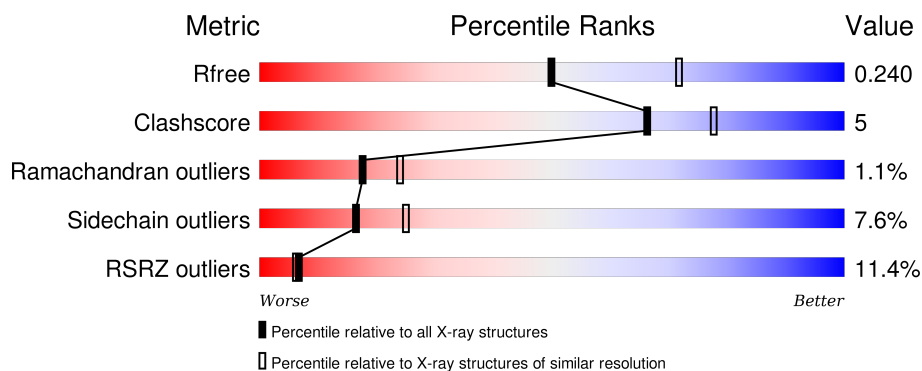
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (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. 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	P	100	 6% 77% 14% • 8%
2	A	540	 9% 67% 11% • 19%
3	E	83	 10% 46% • 51%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4414 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 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		

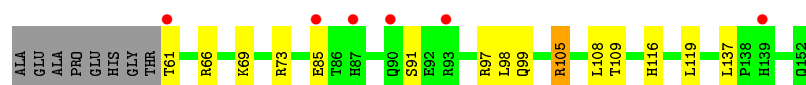
- Molecule 5 is water.

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

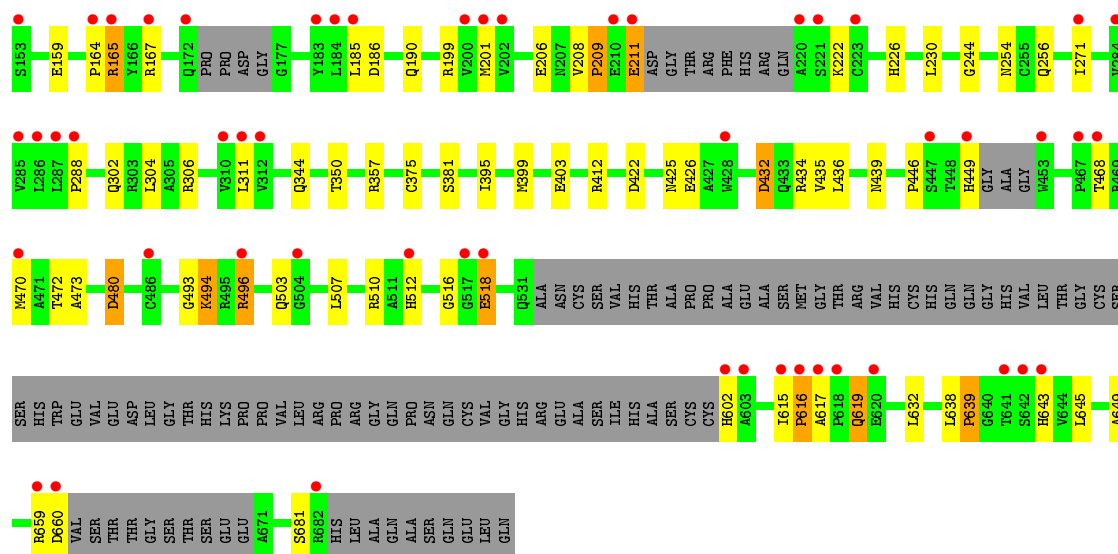
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

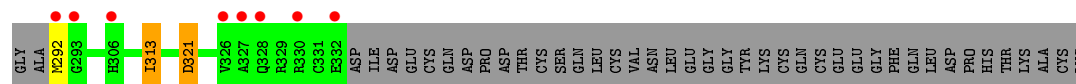
- Molecule 1: Proprotein convertase subtilisin/kexin type 9



- Molecule 2: Proprotein convertase subtilisin/kexin type 9



- Molecule 3: Low-density lipoprotein receptor



## 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 0.202 , 0.240	Depositor DCC
$R_{free}$ test set	1827 reflections (5.29%)	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> )	0.35 , 59.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 36511 reflections	Xtriage
$F_o, F_c$ correlation	0.94	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.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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 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	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
5	A	105	0	0	2	0
5	E	4	0	0	0	0

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

All (42) 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: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	Interatomic distance (Å)	Clash overlap (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 [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	P	90/100 (90%)	88 (98%)	2 (2%)	0	100	100
2	A	423/540 (78%)	400 (95%)	17 (4%)	6 (1%)	14	18
3	E	39/83 (47%)	36 (92%)	3 (8%)	0	100	100
All	All	552/723 (76%)	524 (95%)	22 (4%)	6 (1%)	17	24

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%)	9	13
2	A	346/431 (80%)	322 (93%)	24 (7%)	19	29
3	E	35/71 (49%)	32 (91%)	3 (9%)	13	19
All	All	460/586 (78%)	425 (92%)	35 (8%)	16	25

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

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Mol	Chain	Res	Type
2	A	503	GLN
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 [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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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%)	0.16	6 (6%)	22 22	43, 52, 67, 73	0
2	A	435/540 (80%)	0.69	51 (11%)	6 6	42, 51, 70, 95	0
3	E	41/83 (49%)	1.07	8 (19%)	1 1	40, 53, 70, 73	0
All	All	568/723 (78%)	0.63	65 (11%)	7 6	40, 52, 70, 95	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	292	MET	8.2
2	A	616	PRO	5.4
3	E	327	ALA	5.2
2	A	449	HIS	5.2
2	A	617	ALA	5.2
2	A	220	ALA	5.0
2	A	211	GLU	5.0
2	A	660	ASP	4.7
2	A	153	SER	4.6
2	A	642	SER	4.6
3	E	293	GLY	4.6
3	E	328	GLN	4.5
2	A	603	ALA	4.5
3	E	326	VAL	4.2
2	A	602	HIS	4.2
2	A	618	PRO	4.1
2	A	615	ILE	4.1
3	E	330	ARG	4.0
2	A	641	THR	3.9
2	A	620	GLU	3.9
2	A	470	MET	3.8
1	P	85	GLU	3.8
2	A	428	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
2	A	659	ARG	3.6
2	A	221	SER	3.6
2	A	504	GLY	3.6
2	A	165	ARG	3.4
2	A	172	GLN	3.4
2	A	453	TRP	3.3
2	A	167	ARG	3.2
2	A	210	GLU	3.1
2	A	447	SER	3.0
2	A	517	GLY	2.9
2	A	486	CYS	2.8
2	A	643	HIS	2.8
2	A	200	VAL	2.7
2	A	682	ARG	2.6
1	P	93	ARG	2.5
2	A	271	ILE	2.5
2	A	285	VAL	2.5
2	A	288	PRO	2.5
2	A	201	MET	2.5
3	E	332	GLU	2.5
1	P	61	THR	2.4
2	A	286	LEU	2.4
2	A	311	LEU	2.3
2	A	312	VAL	2.3
2	A	512	HIS	2.3
2	A	184	LEU	2.2
2	A	496	ARG	2.2
3	E	306	HIS	2.2
2	A	310	VAL	2.2
1	P	87	HIS	2.2
2	A	287	LEU	2.2
2	A	185	LEU	2.1
1	P	139	HIS	2.1
2	A	468	THR	2.1
2	A	202	VAL	2.1
1	P	90	GLN	2.1
2	A	467	PRO	2.1
2	A	223	CYS	2.1
2	A	284	VAL	2.0
2	A	164	PRO	2.0
2	A	518	GLU	2.0
2	A	183	TYR	2.0

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

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

## 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	E	1	1/1	0.98	0.07	-1.18	47,47,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.