



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 4, 2024 – 10:46 pm BST

PDB ID : 9EVG
Title : X-ray crystal structure of a de novo designed parallel coiled-coil heterohexamer with 3 heptad repeats, CCHex2-AB-g
Deposited on : 2024-03-29
Resolution : 1.90 Å(reported)

This wwPDB validation report is for manuscript review

This is a wwPDB X-ray Structure Validation Summary Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at 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 types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)

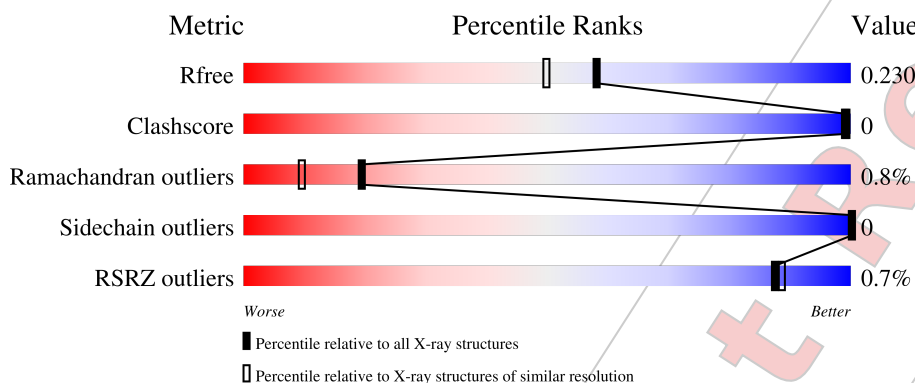
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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)
Sidechain outliers	138945	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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	25	<div> <div>4%</div> <div>96%</div> <div>.</div> </div>
1	E	25	<div> <div>92%</div> <div>8%</div> </div>
1	F	25	<div> <div>92%</div> <div>8%</div> </div>
1	G	25	<div> <div>92%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	25	 100%
1	K	25	 100%
2	B	25	 88% 8% •
2	C	25	 4% 92% • •
2	D	25	 92% 8%
2	I	25	 100%
2	J	25	 92% 8%
2	L	25	 88% • 8%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3629 atoms, of which 1718 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.

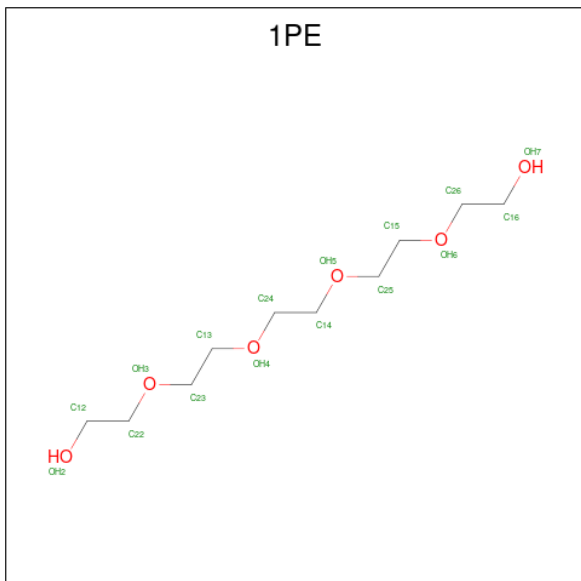
- Molecule 1 is a protein called CCHex2-B-g.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	23	Total	C	H	N	O	0	0	0
			292	98	143	23	28			
1	H	25	Total	C	H	N	O	0	0	1
			304	99	150	26	29			
1	K	25	Total	C	H	N	O	0	0	1
			304	101	149	25	29			
1	A	24	Total	C	H	N	O	0	0	0
			274	95	126	24	29			
1	F	25	Total	C	H	N	O	0	0	1
			288	98	137	25	28			
1	E	23	Total	C	H	N	O	0	0	0
			298	99	149	23	27			

- Molecule 2 is a protein called CCHex2-A-g.

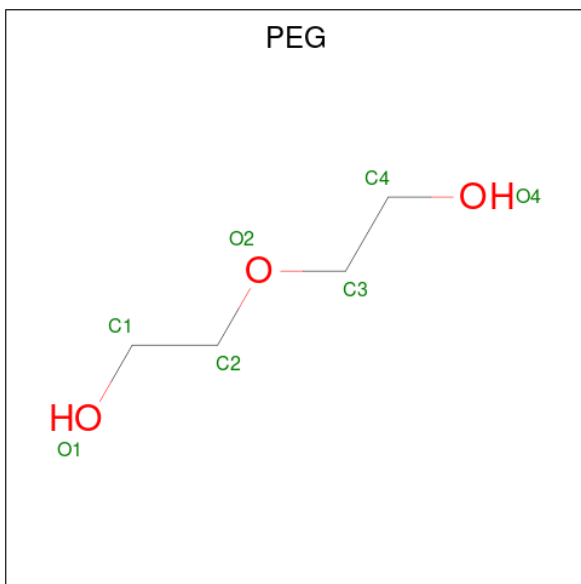
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	24	Total	C	H	N	O	0	0	0
			289	99	137	24	29			
2	J	23	Total	C	H	N	O	0	0	0
			263	88	125	22	28			
2	I	25	Total	C	H	N	O	0	0	1
			273	90	132	24	27			
2	L	23	Total	C	H	N	O	0	0	0
			271	91	128	22	30			
2	D	23	Total	C	H	N	O	0	0	0
			303	101	147	24	31			
2	C	24	Total	C	H	N	O	0	0	0
			298	102	141	24	31			

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			38	10	22	6		
3	L	1	Total	C	H	O	0	0
			38	10	22	6		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 5 is water.

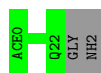
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	8	Total O 8 8	0	0
5	B	4	Total O 4 4	0	0
5	H	7	Total O 7 7	0	0
5	J	7	Total O 7 7	0	0
5	I	7	Total O 7 7	0	0
5	K	8	Total O 8 8	0	0
5	L	7	Total O 7 7	0	0
5	A	6	Total O 6 6	0	0
5	D	5	Total O 5 5	0	0
5	C	3	Total O 3 3	0	0
5	F	11	Total O 11 11	0	0
5	E	6	Total O 6 6	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: CCHex2-B-g

Chain G:  92% 8%



- Molecule 1: CCHex2-B-g

Chain H:  100%

There are no outlier residues recorded for this chain.

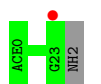
- Molecule 1: CCHex2-B-g

Chain K:  100%

There are no outlier residues recorded for this chain.

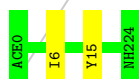
- Molecule 1: CCHex2-B-g

Chain A:  4% 96%



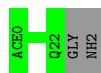
- Molecule 1: CCHex2-B-g

Chain F:  92% 8%

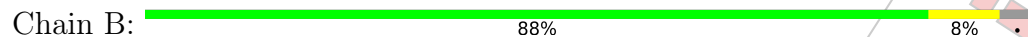


- Molecule 1: CCHex2-B-g

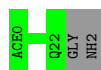
Chain E:  92% 8%



- Molecule 2: CCHex2-A-g



- Molecule 2: CCHex2-A-g

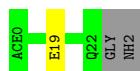
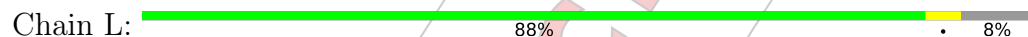


- Molecule 2: CCHex2-A-g

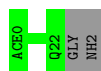


There are no outlier residues recorded for this chain.

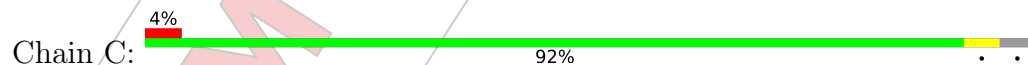
- Molecule 2: CCHex2-A-g



- Molecule 2: CCHex2-A-g



- Molecule 2: CCHex2-A-g



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	32.68Å 94.61Å 51.12Å 90.00° 91.75° 90.00°	Depositor
Resolution (Å)	47.31 – 1.90 47.31 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.31-1.90) 99.9 (47.31-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.200 , 0.227 0.199 , 0.230	Depositor DCC
R_{free} test set	1134 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 72.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3629	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ACE, NH2, PEG, 1PE

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	0.24	0/146	0.38	0/199
1	E	0.23	0/147	0.40	0/198
1	F	0.24	0/148	0.36	0/200
1	G	0.25	0/147	0.37	0/199
1	H	0.23	0/151	0.39	0/204
1	K	0.23	0/152	0.37	0/205
2	B	0.22	0/151	0.38	0/206
2	C	0.24	0/156	0.40	0/212
2	D	0.24	0/155	0.38	0/211
2	I	0.23	0/137	0.41	0/186
2	J	0.23	0/135	0.38	0/184
2	L	0.23	0/140	0.43	0/190
All	All	0.24	0/1765	0.39	0/2394

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	148	126	136	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	149	149	148	0	0
1	F	151	137	145	1	1
1	G	149	143	143	0	0
1	H	154	150	149	0	0
1	K	155	149	148	0	0
2	B	152	137	139	1	0
2	C	157	141	145	0	0
2	D	156	147	146	0	0
2	I	141	132	129	0	0
2	J	138	125	126	0	0
2	L	143	128	132	0	1
3	B	16	22	22	0	0
3	L	16	22	22	0	0
4	A	7	10	10	0	0
5	A	6	0	0	0	0
5	B	4	0	0	0	0
5	C	3	0	0	0	0
5	D	5	0	0	0	0
5	E	6	0	0	0	0
5	F	11	0	0	0	0
5	G	8	0	0	0	0
5	H	7	0	0	0	0
5	I	7	0	0	0	0
5	J	7	0	0	0	0
5	K	8	0	0	0	0
5	L	7	0	0	0	0
All	All	1911	1718	1740	1	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 0.

All (1) 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)
2:B:10:LEU:CD1	1:F:6:ILE:HG23	2.52	0.40

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)
2:L:19:GLU:OE2	1:F:15:TYR:OH[2_754]	2.12	0.08

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	22/25 (88%)	22 (100%)	0	0	100	100
1	E	21/25 (84%)	21 (100%)	0	0	100	100
1	F	23/25 (92%)	23 (100%)	0	0	100	100
1	G	21/25 (84%)	21 (100%)	0	0	100	100
1	H	23/25 (92%)	23 (100%)	0	0	100	100
1	K	23/25 (92%)	23 (100%)	0	0	100	100
2	B	22/25 (88%)	21 (96%)	0	1 (4%)	2	0
2	C	22/25 (88%)	21 (96%)	0	1 (4%)	2	0
2	D	21/25 (84%)	21 (100%)	0	0	100	100
2	I	23/25 (92%)	23 (100%)	0	0	100	100
2	J	21/25 (84%)	21 (100%)	0	0	100	100
2	L	21/25 (84%)	21 (100%)	0	0	100	100
All	All	263/300 (88%)	261 (99%)	0	2 (1%)	19	9

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1	GLY
2	C	1	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	11/18 (61%)	11 (100%)	0	100	100
1	E	11/18 (61%)	11 (100%)	0	100	100
1	F	11/18 (61%)	11 (100%)	0	100	100
1	G	11/18 (61%)	11 (100%)	0	100	100
1	H	12/18 (67%)	12 (100%)	0	100	100
1	K	11/18 (61%)	11 (100%)	0	100	100
2	B	11/18 (61%)	11 (100%)	0	100	100
2	C	12/18 (67%)	12 (100%)	0	100	100
2	D	13/18 (72%)	13 (100%)	0	100	100
2	I	9/18 (50%)	9 (100%)	0	100	100
2	J	10/18 (56%)	10 (100%)	0	100	100
2	L	11/18 (61%)	11 (100%)	0	100	100
All	All	133/216 (62%)	133 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	1PE	L	101	-	15,15,15	0.09	0	14,14,14	0.14	0
4	PEG	A	101	-	6,6,6	0.10	0	5,5,5	0.09	0
3	1PE	B	101	-	15,15,15	0.12	0	14,14,14	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1PE	L	101	-	-	4/13/13/13	-
4	PEG	A	101	-	-	2/4/4/4	-
3	1PE	B	101	-	-	7/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	101	1PE	OH4-C13-C23-OH3
3	B	101	1PE	OH6-C15-C25-OH5
3	L	101	1PE	OH5-C14-C24-OH4
3	L	101	1PE	OH6-C15-C25-OH5
4	A	101	PEG	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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.

For Manuscript Review

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, 95th 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 ²)	Q < 0.9
1	A	23/25 (92%)	0.20	1 (4%) 35 38	21, 25, 47, 89	0
1	E	22/25 (88%)	-0.19	0 100 100	25, 31, 42, 48	0
1	F	23/25 (92%)	-0.07	0 100 100	21, 28, 43, 79	0
1	G	22/25 (88%)	0.18	0 100 100	23, 28, 35, 57	0
1	H	23/25 (92%)	-0.08	0 100 100	26, 32, 43, 74	0
1	K	23/25 (92%)	-0.27	0 100 100	23, 28, 39, 55	0
2	B	23/25 (92%)	-0.04	0 100 100	24, 30, 43, 58	0
2	C	23/25 (92%)	0.06	1 (4%) 35 38	23, 29, 46, 82	0
2	D	22/25 (88%)	0.04	0 100 100	22, 29, 42, 57	0
2	I	23/25 (92%)	-0.14	0 100 100	26, 31, 43, 64	0
2	J	22/25 (88%)	-0.07	0 100 100	24, 30, 38, 61	0
2	L	22/25 (88%)	-0.03	0 100 100	22, 27, 45, 56	0
All	All	271/300 (90%)	-0.03	2 (0%) 87 88	21, 30, 51, 89	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	GLY	2.6
2	C	15	TRP	2.4

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 monosaccharides 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, 95th 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(\AA^2)	Q<0.9
4	PEG	A	101	7/7	0.83	0.15	40,53,57,64	0
3	1PE	B	101	16/16	0.86	0.13	36,51,65,66	0
3	1PE	L	101	16/16	0.90	0.14	38,48,60,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.