



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:39 AM GMT

PDB ID : 2I21  
Title : Bacteriorhodopsin/lipid complex, T46V mutant  
Authors : Lanyi, J.K.; Schobert, B.  
Deposited on : 2006-08-15  
Resolution : 1.84 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  
<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

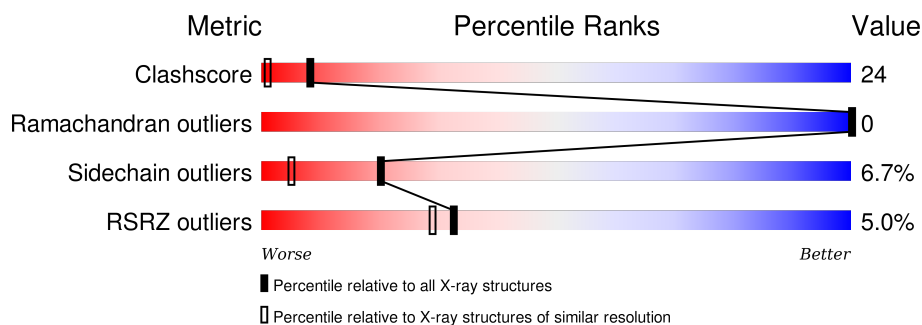
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.84 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))
Clashscore	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (1.86-1.82)
RSRZ outliers	91569	2639 (1.86-1.82)

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	A	249	

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
3	LI1	A	601	X	-	-	X
3	LI1	A	603	-	-	-	X
3	LI1	A	607	-	-	-	X
3	LI1	A	608	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LI1	A	609	-	-	-	X
3	LI1	A	610	-	-	-	X
3	LI1	A	611	X	-	-	X
3	LI1	A	612	-	-	-	X
3	LI1	A	613	X	-	-	X
4	SQU	A	701	X	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2074 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.

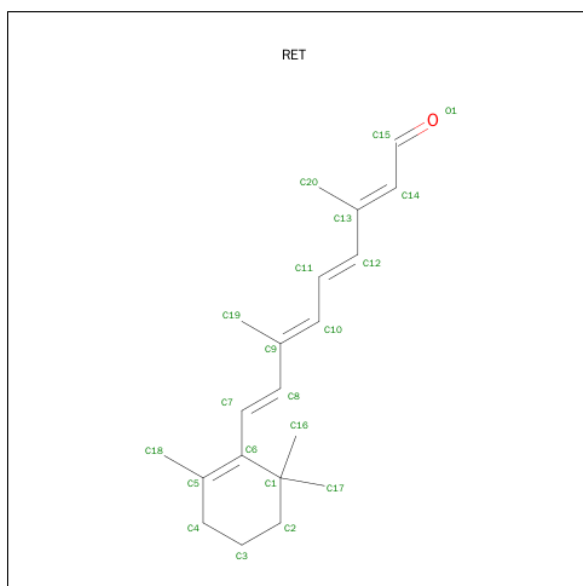
- Molecule 1 is a protein called Bacteriorhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1720	1160	262	289	9			

There is a discrepancy between the modelled and reference sequences:

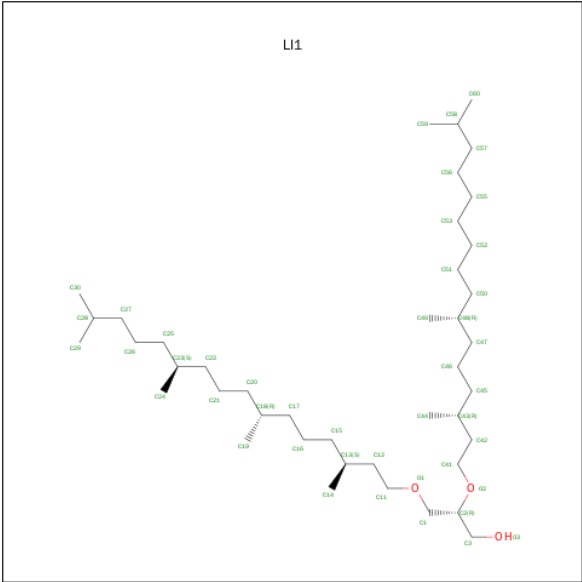
Chain	Residue	Modelled	Actual	Comment	Reference
A	46	VAL	THR	ENGINEERED	UNP P02945

- Molecule 2 is RETINAL (three-letter code: RET) (formula:  $C_{20}H_{28}O$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			20	20		

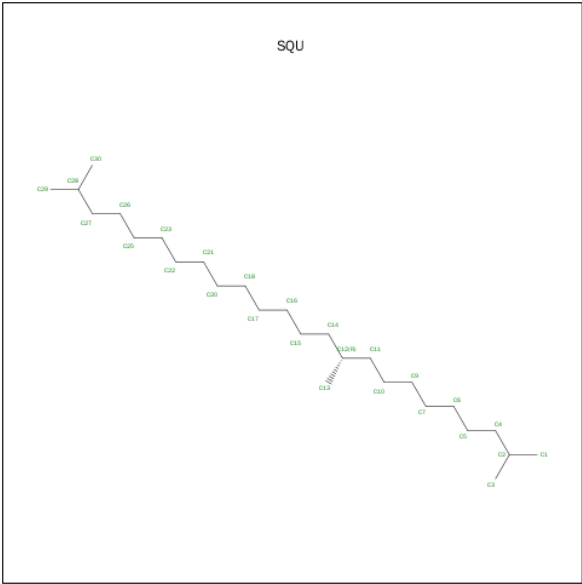
- Molecule 3 is 1-[2,6,10,14-TETRAMETHYL-HEXADECAN-16-YL]-2-[2,10,14-TRIMETHYLHEXADECAN-16-YL]GLYCEROL (three-letter code: LI1) (formula:  $C_{42}H_{86}O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 32 29 3	0	0
3	A	1	Total C O 41 38 3	0	0
3	A	1	Total C 18 18	0	0
3	A	1	Total C 16 16	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C O 38 35 3	0	0
3	A	1	Total C 18 18	0	0
3	A	1	Total C 16 16	0	0
3	A	1	Total C O 40 37 3	0	0
3	A	1	Total C 17 17	0	0
3	A	1	Total C 18 18	0	0
3	A	1	Total C 13 13	0	0

- Molecule 4 is 2,10,23-TRIMETHYL-TETRACOSANE (three-letter code: SQU) (formula:

C<sub>27</sub>H<sub>56</sub>).



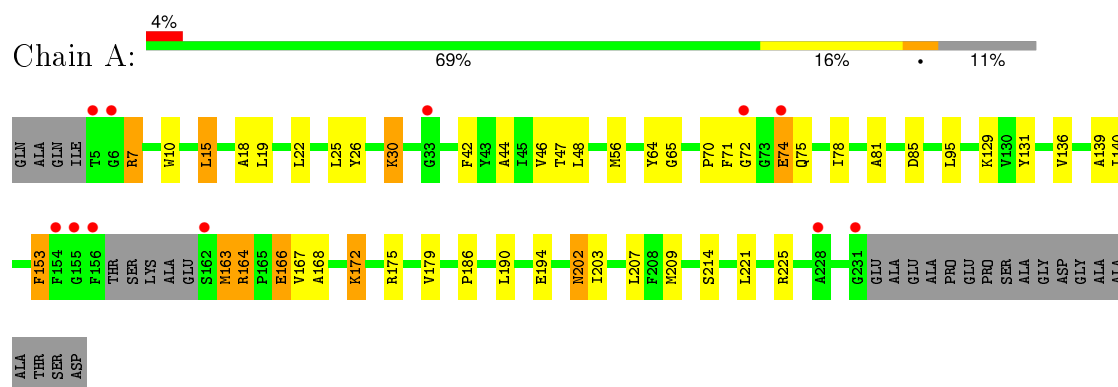
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			27	27		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	24	Total	O	0	0
			24	24		



- Molecule 1: Bacteriorhodopsin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.07Å 61.07Å 110.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 1.84 24.49 – 1.84	Depositor EDS
% Data completeness (in resolution range)	95.5 (25.00-1.84) 86.2 (24.49-1.84)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 1.84Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.195 , 0.260 0.180 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 99.6	EDS
Estimated twinning fraction	0.062 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 18360 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2074	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.56% 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: SQU, RET, LI1

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	0.32	0/1767	0.91	2/2413 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	7	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	7	ARG	NE-CZ-NH2	-5.21	117.70	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	A	1720	0	1778	64	0
2	A	20	0	27	3	0
3	A	283	0	452	72	0
4	A	27	0	53	4	0
5	A	24	0	0	1	0
All	All	2074	0	2310	106	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 24.

The worst 5 of 106 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:A:603:LI1:C25	3:A:603:LI1:C26	1.74	1.64
3:A:610:LI1:C25	3:A:610:LI1:C26	1.74	1.62
3:A:611:LI1:C25	3:A:611:LI1:C26	1.74	1.57
3:A:611:LI1:C25	3:A:611:LI1:C27	2.51	0.88
1:A:19:LEU:HD21	4:A:701:SQU:H32	1.55	0.88

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	218/249 (88%)	216 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	178/195 (91%)	166 (93%)	12 (7%)	20	5

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	LEU
1	A	153	PHE
1	A	166	GLU
1	A	75	GLN
1	A	164	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	ASN
1	A	202	ASN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

15 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	$\# Z  > 2$
2	RET	A	300	1	19,20,21	0.91	0	27,27,28	1.50	7 (25%)
3	LI1	A	601	-	31,31,44	1.09	2 (6%)	33,33,51	1.23	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	LI1	A	602	-	40,40,44	0.98	2 (5%)	41,45,51	3.09	7 (17%)
3	LI1	A	603	-	17,17,44	1.07	1 (5%)	18,18,51	1.14	1 (5%)
3	LI1	A	604	-	15,15,44	1.08	1 (6%)	14,14,51	1.09	1 (7%)
3	LI1	A	605	-	7,7,44	0.44	0	6,6,51	0.59	0
3	LI1	A	606	-	7,7,44	0.47	0	6,6,51	0.80	0
3	LI1	A	607	-	37,37,44	1.02	2 (5%)	36,38,51	1.03	3 (8%)
3	LI1	A	608	-	17,17,44	1.04	1 (5%)	18,18,51	1.24	3 (16%)
3	LI1	A	609	-	15,15,44	1.12	1 (6%)	14,14,51	1.17	2 (14%)
3	LI1	A	610	-	39,39,44	1.02	2 (5%)	41,41,51	1.08	2 (4%)
3	LI1	A	611	-	16,16,44	1.00	1 (6%)	17,18,51	2.05	3 (17%)
3	LI1	A	612	-	17,17,44	1.04	1 (5%)	18,18,51	1.14	1 (5%)
3	LI1	A	613	-	12,12,44	0.43	0	12,12,51	0.92	1 (8%)
4	SQU	A	701	-	26,26,26	1.35	5 (19%)	28,28,28	1.79	8 (28%)

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
2	RET	A	300	1	-	0/13/30/31	0/1/1/1
3	LI1	A	601	-	2/2/3/8	0/32/32/49	0/0/0/0
3	LI1	A	602	-	-	0/44/44/49	0/0/0/0
3	LI1	A	603	-	-	0/16/16/49	0/0/0/0
3	LI1	A	604	-	-	0/13/13/49	0/0/0/0
3	LI1	A	605	-	-	0/5/5/49	0/0/0/0
3	LI1	A	606	-	-	0/5/5/49	0/0/0/0
3	LI1	A	607	-	-	0/38/38/49	0/0/0/0
3	LI1	A	608	-	-	0/16/16/49	0/0/0/0
3	LI1	A	609	-	-	0/13/13/49	0/0/0/0
3	LI1	A	610	-	-	0/39/39/49	0/0/0/0
3	LI1	A	611	-	2/2/3/8	0/17/17/49	0/0/0/0
3	LI1	A	612	-	-	0/16/16/49	0/0/0/0
3	LI1	A	613	-	1/1/1/8	0/11/11/49	0/0/0/0
4	SQU	A	701	-	1/1/3/3	0/25/25/25	0/0/0/0

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	SQU	C14-C12	-3.28	1.35	1.52
4	A	701	SQU	C23-C22	-3.07	1.33	1.51
4	A	701	SQU	C9-C7	-2.82	1.35	1.51
4	A	701	SQU	C18-C17	-2.81	1.35	1.51
4	A	701	SQU	C4-C2	-2.23	1.34	1.51

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	LI1	C49-C48-C47	-9.66	73.94	111.08
3	A	602	LI1	C24-C23-C25	-9.33	75.20	111.08
3	A	610	LI1	C25-C26-C27	-3.55	101.06	113.66
3	A	612	LI1	C25-C26-C27	-3.54	101.10	113.66
3	A	603	LI1	C25-C26-C27	-3.53	101.13	113.66

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	611	LI1	C23
3	A	611	LI1	C13
4	A	701	SQU	C12
3	A	601	LI1	C2
3	A	601	LI1	C18

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	RET	3	0
3	A	601	LI1	8	0
3	A	602	LI1	17	0
3	A	603	LI1	10	0
3	A	606	LI1	1	0
3	A	607	LI1	4	0
3	A	608	LI1	2	0
3	A	610	LI1	19	0
3	A	611	LI1	10	0
3	A	612	LI1	3	0
3	A	613	LI1	1	0
4	A	701	SQU	4	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	222/249 (89%)	-0.15	11 (4%) 32 29	18, 26, 57, 128	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	GLY	4.1
1	A	162	SER	4.0
1	A	156	PHE	3.9
1	A	5	THR	3.6
1	A	6	GLY	3.4

### 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	LI1	A	611	17/45	0.69	0.38	10.26	104,114,144,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	LI1	A	603	18/45	0.71	0.22	7.34	44,54,78,80	0
3	LI1	A	613	13/45	0.86	0.16	6.59	39,52,71,73	0
3	LI1	A	610	40/45	0.52	0.35	6.55	63,108,131,135	0
3	LI1	A	612	18/45	0.84	0.22	6.48	27,44,55,77	0
4	SQU	A	701	27/27	0.69	0.26	6.44	55,62,96,105	0
3	LI1	A	607	38/45	0.76	0.15	4.57	34,55,84,102	0
3	LI1	A	609	16/45	0.65	0.33	4.11	53,69,84,85	0
3	LI1	A	601	32/45	0.76	0.21	3.94	37,64,89,97	0
3	LI1	A	608	18/45	0.78	0.20	3.33	35,65,82,84	0
3	LI1	A	602	41/45	0.73	0.22	1.84	30,73,91,92	0
2	RET	A	300	20/21	0.95	0.10	1.33	16,20,25,27	0
3	LI1	A	604	16/45	0.63	0.22	-	52,78,105,106	0
3	LI1	A	606	8/45	0.85	0.15	-	38,42,59,63	0
3	LI1	A	605	8/45	0.20	0.35	-	67,79,86,88	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.