



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2026 – 04:04 PM EDT

PDB ID : 12JR / pdb\_000012jr  
Title : Designed pentameric proton channel LQLL I6S/I13S  
Authors : Jacob, N.P.; Kratochvil, H.T.  
Deposited on : 2026-04-08  
Resolution : 2.25 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

<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>.

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

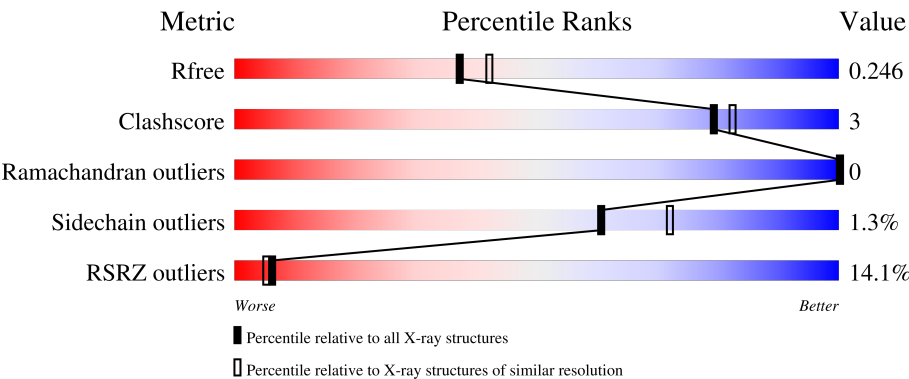
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.25 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))
$R_{free}$	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	26	<div><div>8%</div><div>92%</div><div></div></div>
1	B	26	<div><div>23%</div><div>92%</div><div></div></div>
1	C	26	<div><div>23%</div><div>88%</div><div>8%</div></div>
1	D	26	<div><div>12%</div><div>73%</div><div>23%</div></div>
1	E	26	<div><div>8%</div><div>96%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	26	<div><div></div><div>15%</div><div>81%</div><div>8%</div><div>•</div><div>8%</div></div>
1	G	26	<div><div></div><div>92%</div><div>8%</div></div>
1	H	26	<div><div></div><div>19%</div><div>88%</div><div>8%</div><div>•</div></div>
1	I	26	<div><div></div><div>15%</div><div>92%</div><div>8%</div></div>
1	J	26	<div><div></div><div>12%</div><div>88%</div><div>•</div><div>8%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4428 atoms, of which 2341 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 Proton channel LQLL I6S/I13S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	25	Total	C	H	N	O	3	0	0
			436	144	231	31	30			
1	B	25	Total	C	H	N	O	5	0	0
			421	141	222	28	30			
1	C	25	Total	C	H	N	O	3	2	0
			463	155	244	32	32			
1	D	25	Total	C	H	N	O	5	0	0
			422	141	222	30	29			
1	E	26	Total	C	H	N	O	5	0	0
			447	147	237	32	31			
1	F	24	Total	C	H	N	O	5	2	0
			436	148	229	30	29			
1	G	26	Total	C	H	N	O	3	0	0
			450	148	237	32	33			
1	H	25	Total	C	H	N	O	5	0	0
			421	141	222	28	30			
1	I	24	Total	C	H	N	O	3	2	0
			449	151	238	31	29			
1	J	24	Total	C	H	N	O	3	0	0
			428	142	228	30	28			

- Molecule 2 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	1	0
			23	6	13	4		

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total	C	H	O	2	0
			31	8	18	5		

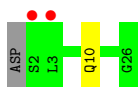
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	O	0	0
			1	1		

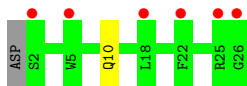
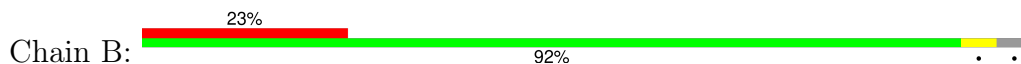
### 3 Residue-property plots

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.

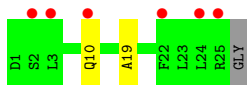
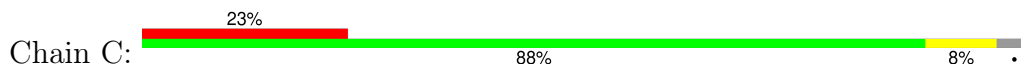
- Molecule 1: Proton channel LQLL I6S/I13S



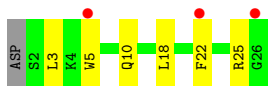
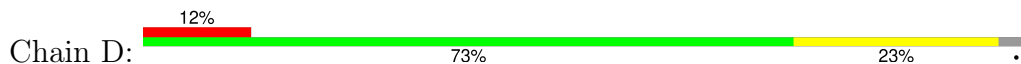
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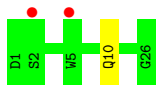
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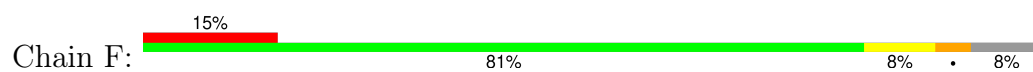
- Molecule 1: Proton channel LQLL I6S/I13S



- Molecule 1: Proton channel LQLL I6S/I13S



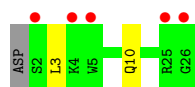
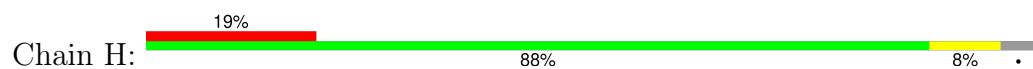
- Molecule 1: Proton channel LQLL I6S/I13S



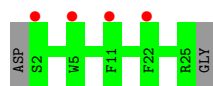
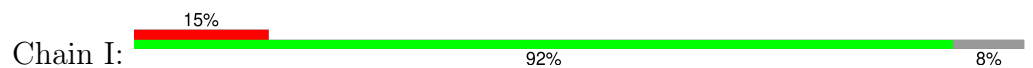
- Molecule 1: Proton channel LQLL I6S/I13S



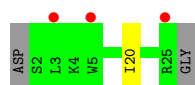
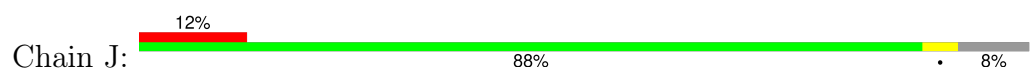
- Molecule 1: Proton channel LQLL I6S/I13S



- Molecule 1: Proton channel LQLL I6S/I13S



- Molecule 1: Proton channel LQLL I6S/I13S





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	40.86Å 45.09Å 47.52Å 117.73° 99.48° 106.02°	Depositor
Resolution (Å)	39.40 – 2.25 39.40 – 2.25	Depositor EDS
% Data completeness (in resolution range)	85.7 (39.40-2.25) 85.7 (39.40-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0431 (refmacat 0.4.126)	Depositor
R, $R_{free}$	0.207 , 0.247 0.206 , 0.246	Depositor DCC
$R_{free}$ test set	566 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.48 , 60.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.55$ , $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4428	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6790e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, PGE

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	0.50	0/209	0.91	0/281
1	B	0.59	0/203	0.85	0/274
1	C	0.49	0/232	0.91	0/314
1	D	0.55	0/204	1.18	1/277 (0.4%)
1	E	0.55	0/214	0.91	0/288
1	F	0.59	0/220	0.98	2/299 (0.7%)
1	G	0.51	0/217	0.98	0/292
1	H	0.56	0/203	0.85	0/274
1	I	0.52	0/224	0.88	0/303
1	J	0.54	0/204	0.91	0/276
All	All	0.54	0/2130	0.94	3/2878 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	22	PHE	CA-CB-CG	-12.41	101.39	113.80
1	F	22[A]	PHE	CA-CB-CG	5.63	119.43	113.80
1	F	22[B]	PHE	CA-CB-CG	5.63	119.43	113.80

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	205	231	230	1	0
1	B	199	222	219	1	0
1	C	219	244	232	4	0
1	D	200	222	219	2	0
1	E	210	237	235	1	0
1	F	207	229	214	4	0
1	G	213	237	237	4	0
1	H	199	222	219	4	0
1	I	211	238	225	0	0
1	J	200	228	227	1	0
2	A	10	13	14	0	0
3	G	13	18	18	2	0
4	H	1	0	0	0	0
All	All	2087	2341	2289	12	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 (12) 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:C:19:ALA:HA	1:F:8:PHE:CZ	2.31	0.65
1:G:3:LEU:HD21	1:H:3:LEU:CD1	2.32	0.60
1:G:10:GLN:NE2	1:H:10:GLN:HG3	2.19	0.57
1:D:5:TRP:HZ2	1:F:22[A]:PHE:CD1	2.29	0.51
1:G:3:LEU:HD21	1:H:3:LEU:HD12	1.93	0.51
1:C:19:ALA:CA	1:F:8:PHE:CZ	2.97	0.47
1:A:10:GLN:HE21	1:E:10:GLN:HE21	1.65	0.45
1:F:17:LEU:HD21	3:G:101:PG4:O1	2.17	0.44
1:B:10:GLN:NE2	1:C:10:GLN:HG3	2.33	0.44
1:C:10:GLN:OE1	1:D:10:GLN:HG2	2.18	0.44
1:G:3:LEU:HD21	1:H:3:LEU:HD11	1.98	0.44
3:G:101:PG4:H31	1:J:20:ILE:HG21	2.03	0.41

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	A	23/26 (88%)	23 (100%)	0	0	100	100
1	B	23/26 (88%)	23 (100%)	0	0	100	100
1	C	25/26 (96%)	25 (100%)	0	0	100	100
1	D	23/26 (88%)	22 (96%)	1 (4%)	0	100	100
1	E	24/26 (92%)	24 (100%)	0	0	100	100
1	F	24/26 (92%)	24 (100%)	0	0	100	100
1	G	24/26 (92%)	23 (96%)	1 (4%)	0	100	100
1	H	23/26 (88%)	22 (96%)	1 (4%)	0	100	100
1	I	24/26 (92%)	24 (100%)	0	0	100	100
1	J	22/26 (85%)	22 (100%)	0	0	100	100
All	All	235/260 (90%)	232 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	23/24 (96%)	23 (100%)	0	100	100
1	B	22/24 (92%)	22 (100%)	0	100	100
1	C	26/24 (108%)	26 (100%)	0	100	100
1	D	22/24 (92%)	19 (86%)	3 (14%)	3	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	23/24 (96%)	23 (100%)	0	100	100
1	F	24/24 (100%)	24 (100%)	0	100	100
1	G	24/24 (100%)	24 (100%)	0	100	100
1	H	22/24 (92%)	22 (100%)	0	100	100
1	I	25/24 (104%)	25 (100%)	0	100	100
1	J	23/24 (96%)	23 (100%)	0	100	100
All	All	234/240 (98%)	231 (99%)	3 (1%)	61	72

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3	LEU
1	D	18	LEU
1	D	25	ARG

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

Mol	Chain	Res	Type
1	A	10	GLN
1	B	10	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 ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

2 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	PGE	A	101	-	9,9,9	0.29	0	8,8,8	0.27	0
3	PG4	G	101	-	12,12,12	0.21	0	11,11,11	0.20	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
2	PGE	A	101	-	-	2/7/7/7	-
3	PG4	G	101	-	-	2/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	101	PG4	O2-C3-C4-O3
2	A	101	PGE	O3-C5-C6-O4
3	G	101	PG4	C4-C3-O2-C2
2	A	101	PGE	O2-C3-C4-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	101	PG4	2	0

## 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	A	25/26 (96%)	0.53	2 (8%) 18 16	22, 32, 61, 89	0
1	B	25/26 (96%)	1.02	6 (24%) 2 1	19, 31, 56, 86	0
1	C	25/26 (96%)	1.14	6 (24%) 2 1	16, 30, 51, 73	1 (4%)
1	D	25/26 (96%)	0.82	3 (12%) 9 8	20, 34, 69, 81	0
1	E	26/26 (100%)	0.71	2 (7%) 19 17	21, 32, 57, 72	0
1	F	24/26 (92%)	0.67	4 (16%) 4 3	17, 28, 50, 86	1 (4%)
1	G	26/26 (100%)	0.52	0 100 100	20, 30, 58, 81	0
1	H	25/26 (96%)	0.91	5 (20%) 3 2	22, 33, 61, 76	0
1	I	24/26 (92%)	0.84	4 (16%) 4 3	16, 32, 62, 64	1 (4%)
1	J	24/26 (92%)	0.50	3 (12%) 8 7	18, 31, 55, 68	0
All	All	249/260 (95%)	0.77	35 (14%) 6 5	16, 32, 68, 89	3 (1%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	22[A]	PHE	7.7
1	I	22[A]	PHE	6.0
1	D	26	GLY	5.1
1	B	25	ARG	4.5
1	I	2	SER	4.4
1	H	5	TRP	4.2
1	I	11	PHE	4.0
1	F	2	SER	3.4
1	D	5	TRP	3.3
1	H	2	SER	3.2
1	H	4	LYS	3.0
1	C	24	LEU	2.8
1	H	25	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	22	PHE	2.7
1	F	22[A]	PHE	2.6
1	F	5	TRP	2.6
1	B	26	GLY	2.6
1	H	26	GLY	2.5
1	C	25	ARG	2.5
1	D	22	PHE	2.4
1	I	5	TRP	2.4
1	C	3	LEU	2.3
1	C	2	SER	2.3
1	B	5	TRP	2.3
1	A	3	LEU	2.2
1	C	10	GLN	2.2
1	B	2	SER	2.2
1	E	5	TRP	2.1
1	F	23[A]	LEU	2.1
1	E	2	SER	2.1
1	B	18	LEU	2.1
1	J	5	TRP	2.1
1	J	3	LEU	2.1
1	J	25	ARG	2.1
1	A	2	SER	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 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(Å <sup>2</sup> )	Q<0.9
3	PG4	G	101	13/13	0.85	0.15	37,46,67,76	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PGE	A	101	10/10	0.89	0.11	28,35,52,67	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.