



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 01:21 AM UTC

PDB ID : 4I18 / pdb_00004i18
Title : Crystal structure of human prolactin receptor complexed with Fab fragment
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Deposited on : 2012-11-20
Resolution : 3.24 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

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:

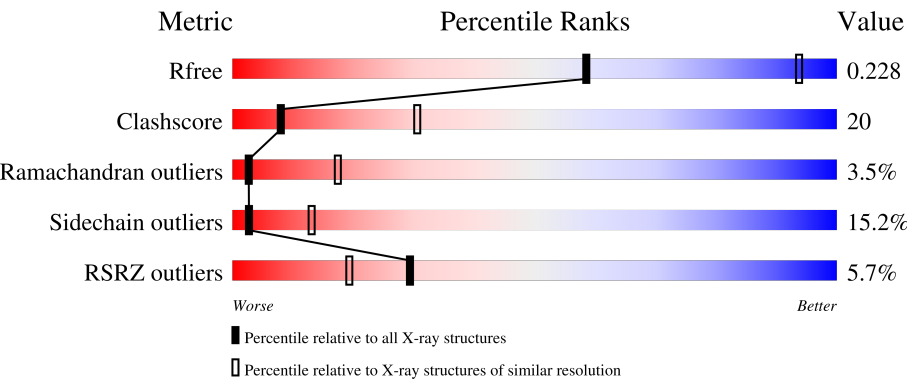
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 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	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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	B	217	11% 71% 24% • •
1	L	217	69% 26% •
2	A	236	% 67% 19% 7% • 7%
2	H	236	% 66% 22% 7% • •
3	C	211	10% 34% 30% 20% 5% 11%

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Mol	Chain	Length	Quality of chain
3	R	211	

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
6	ACT	R	301	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9903 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 antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	216	Total	C	N	O	S	0	0	0
			1673	1052	276	340	5			
1	B	215	Total	C	N	O	S	0	0	0
			1664	1047	275	337	5			

- Molecule 2 is a protein called antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	227	Total	C	N	O	S	0	0	0
			1686	1065	278	336	7			
2	A	220	Total	C	N	O	S	0	0	1
			1641	1039	270	325	7			

- Molecule 3 is a protein called Prolactin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	205	Total	C	N	O	S	0	0	0
			1677	1086	273	307	11			
3	C	188	Total	C	N	O	S	0	0	0
			1532	999	246	278	9			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

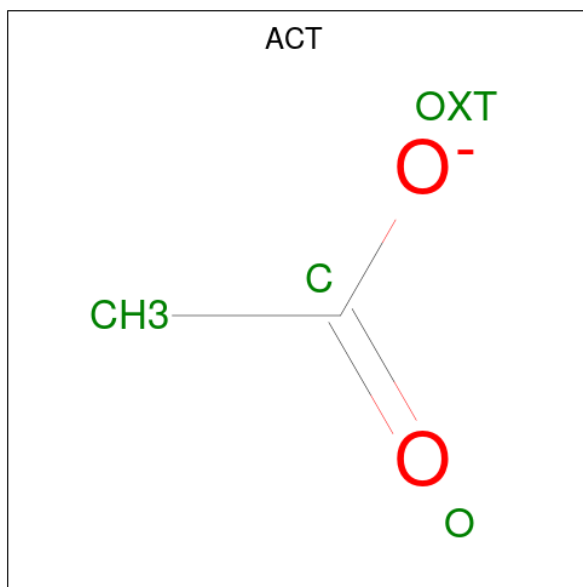


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

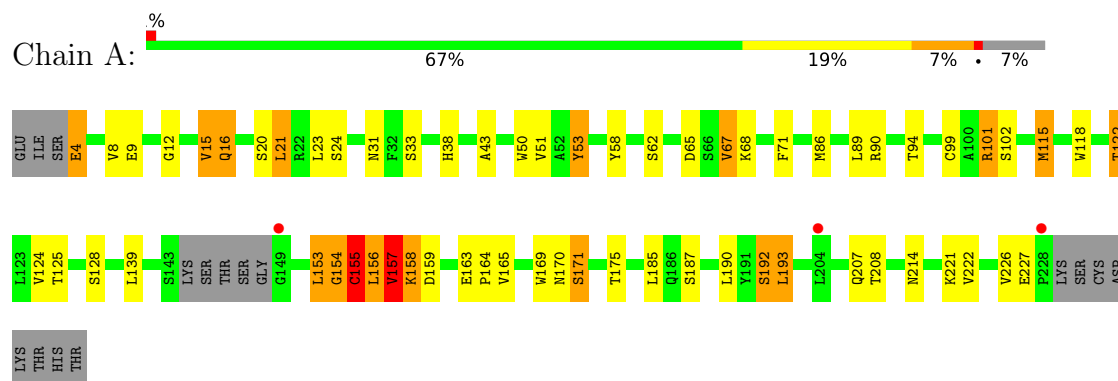
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).

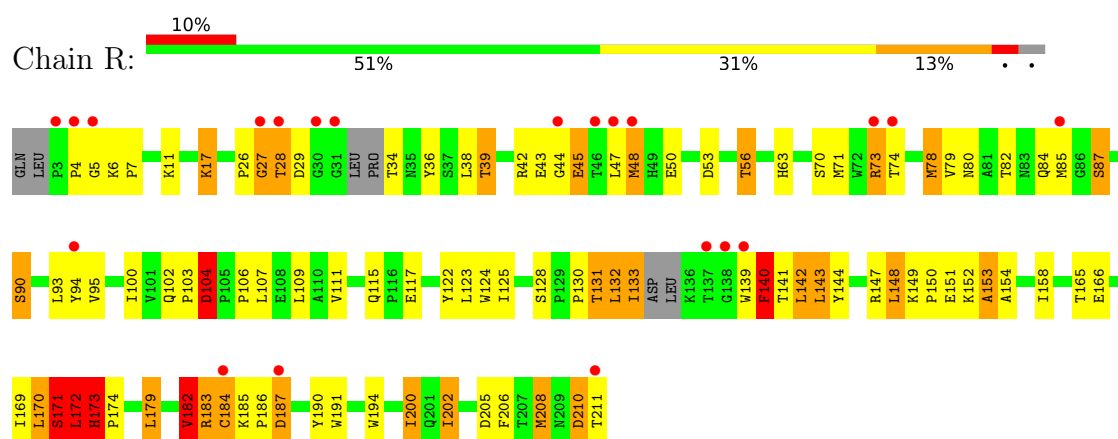


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	R	1	Total	C	O	0	0
			4	2	2		

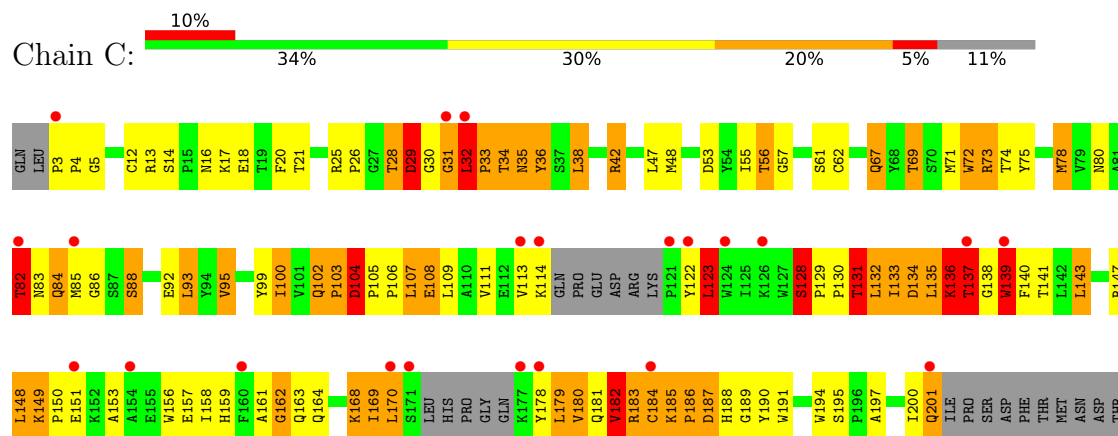
- Molecule 2: antibody heavy chain



- Molecule 3: Prolactin receptor



- Molecule 3: Prolactin receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	285.83Å 285.83Å 62.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.51 – 3.24 49.51 – 3.24	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.51-3.24) 99.3 (49.51-3.24)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.25Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.191 , 0.246 (Not available) , 0.228	Depositor DCC
R_{free} test set	2365 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9903	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, CA, GOL

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	B	0.90	0/1703	1.14	5/2313 (0.2%)
1	L	1.02	1/1712 (0.1%)	1.24	7/2325 (0.3%)
2	A	1.16	0/1685	1.36	11/2301 (0.5%)
2	H	1.19	0/1731	1.41	16/2363 (0.7%)
3	C	1.16	2/1588 (0.1%)	1.42	22/2168 (1.0%)
3	R	1.23	2/1737 (0.1%)	1.45	17/2368 (0.7%)
All	All	1.12	5/10156 (0.0%)	1.34	78/13838 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	2
2	H	0	1
3	C	0	3
3	R	0	1
All	All	0	7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	210	ASP	N-CA	6.22	1.54	1.46
3	C	178	TYR	N-CA	5.41	1.52	1.45
1	L	151	TRP	CA-C	-5.29	1.46	1.52
3	C	122	TYR	N-CA	5.22	1.52	1.46
3	R	6	LYS	CA-C	5.02	1.59	1.52

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	156	LEU	N-CA-C	-9.99	92.55	109.24
2	H	156	LEU	CA-C-N	9.89	139.51	121.70
2	H	156	LEU	C-N-CA	9.89	139.51	121.70
2	A	156	LEU	CA-C-N	9.84	139.41	121.70
2	A	156	LEU	C-N-CA	9.84	139.41	121.70

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	154	GLY	Peptide
2	A	155	CYS	Peptide
3	C	35	ASN	Peptide
2	H	154	GLY	Peptide
3	R	103	PRO	Peptide

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	B	1664	0	1610	43	0
1	L	1673	0	1616	46	0
2	A	1641	0	1567	56	0
2	H	1686	0	1605	65	0
3	C	1532	0	1446	112	0
3	R	1677	0	1586	88	0
4	A	6	0	8	0	0
4	C	6	0	8	0	0
4	H	6	0	8	3	0
4	L	6	0	8	0	0
5	B	1	0	0	0	0
5	H	1	0	0	0	0
6	R	4	0	3	2	0
All	All	9903	0	9465	380	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 20.

The worst 5 of 380 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:R:172:LEU:CA	3:R:173:HIS:HB2	1.69	1.20
3:C:30:GLY:HA2	3:C:31:GLY:O	1.43	1.17
1:L:119:PHE:CD1	2:H:145:SER:HA	1.81	1.16
3:R:170:LEU:O	3:R:171:SER:HB2	1.43	1.15
3:R:172:LEU:O	3:R:172:LEU:HD12	1.50	1.09

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	B	213/217 (98%)	201 (94%)	10 (5%)	2 (1%)	14	44
1	L	214/217 (99%)	201 (94%)	11 (5%)	2 (1%)	14	44
2	A	216/236 (92%)	199 (92%)	15 (7%)	2 (1%)	14	44
2	H	225/236 (95%)	207 (92%)	14 (6%)	4 (2%)	6	31
3	C	182/211 (86%)	148 (81%)	18 (10%)	16 (9%)	0	3
3	R	199/211 (94%)	159 (80%)	22 (11%)	18 (9%)	0	3
All	All	1249/1328 (94%)	1115 (89%)	90 (7%)	44 (4%)	3	17

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	145	SER
1	B	214	ARG
3	R	27	GLY
3	R	29	ASP
3	R	45	GLU

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	B	190/192 (99%)	173 (91%)	17 (9%)	9	32
1	L	191/192 (100%)	174 (91%)	17 (9%)	9	32
2	A	181/197 (92%)	152 (84%)	29 (16%)	2	11
2	H	185/197 (94%)	160 (86%)	25 (14%)	4	17
3	C	165/191 (86%)	121 (73%)	44 (27%)	0	2
3	R	183/191 (96%)	149 (81%)	34 (19%)	1	8
All	All	1095/1160 (94%)	929 (85%)	166 (15%)	3	13

5 of 166 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	R	179	LEU
3	C	131	THR
3	R	202	ILE
3	C	56	THR
3	C	141	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	67	GLN
3	C	83	ASN
1	B	201	HIS
1	B	192	HIS
3	C	159	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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	$\# Z > 2$
6	ACT	R	301	-	3,3,3	1.45	0	3,3,3	0.75	0
4	GOL	H	302	-	5,5,5	1.29	0	5,5,5	1.38	0
4	GOL	L	301	-	5,5,5	0.41	0	5,5,5	0.32	0
4	GOL	C	301	-	5,5,5	0.52	0	5,5,5	0.55	0
4	GOL	A	301	-	5,5,5	0.35	0	5,5,5	0.85	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
4	GOL	A	301	-	-	0/4/4/4	-
4	GOL	C	301	-	-	2/4/4/4	-
4	GOL	H	302	-	-	1/4/4/4	-
4	GOL	L	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	301	GOL	C1-C2-C3-O3
4	L	301	GOL	O2-C2-C3-O3
4	C	301	GOL	O1-C1-C2-C3
4	C	301	GOL	O1-C1-C2-O2
4	H	302	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	301	ACT	2	0
4	H	302	GOL	3	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 [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	B	215/217 (99%)	0.63	24 (11%) 10 7	34, 76, 121, 134	0
1	L	216/217 (99%)	-0.10	0 100 100	35, 51, 70, 89	0
2	A	220/236 (93%)	-0.21	3 (1%) 73 54	28, 42, 94, 116	0
2	H	227/236 (96%)	-0.17	3 (1%) 75 56	28, 42, 88, 105	0
3	C	188/211 (89%)	0.64	22 (11%) 9 7	37, 71, 119, 144	0
3	R	205/211 (97%)	0.47	21 (10%) 12 8	30, 53, 109, 159	0
All	All	1271/1328 (95%)	0.19	73 (5%) 29 19	28, 52, 108, 159	0

The worst 5 of 73 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	R	139	TRP	6.4
3	C	85	MET	6.3
3	C	121	PRO	5.9
3	R	3	PRO	5.9
1	B	215	GLY	5.9

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, 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(Å ²)	Q<0.9
4	GOL	H	302	6/6	0.89	0.18	37,53,61,62	0
6	ACT	R	301	4/4	0.92	0.25	43,47,50,51	0
4	GOL	L	301	6/6	0.94	0.11	46,55,66,75	0
5	CA	B	301	1/1	0.95	0.07	53,53,53,53	0
4	GOL	C	301	6/6	0.96	0.14	46,53,56,59	0
5	CA	H	301	1/1	0.97	0.06	52,52,52,52	0
4	GOL	A	301	6/6	0.98	0.06	32,34,37,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.