



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:44 AM GMT

PDB ID : 3N0P  
Title : A mutant human Prolactin receptor antagonist H30A in complex with the extracellular domain of the human prolactin receptor  
Authors : Kulkarni, M.V.; Tettamanzi, M.C.; Murphy, J.W.; Keeler, C.; Myszka, D.G.; Chayen, N.E.; Lolis, E.J.; Hodsdon, M.E.  
Deposited on : 2010-05-14  
Resolution : 2.10 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

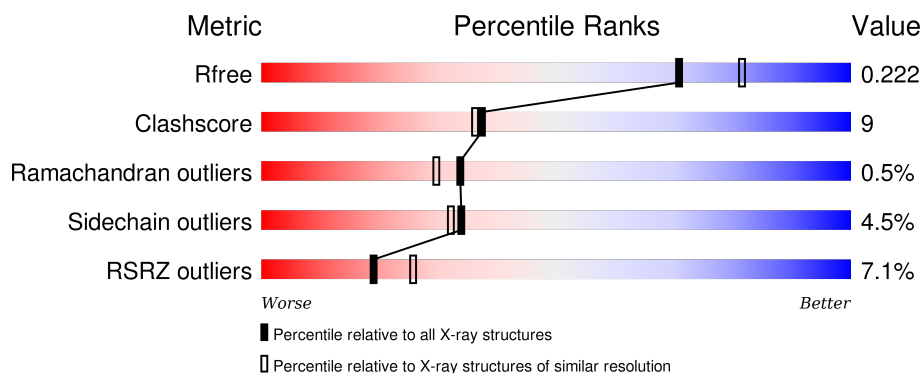
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	186	<div> <div>8%</div> <div>78%</div> <div>17%</div> <div>• •</div> </div>
2	B	210	<div> <div>6%</div> <div>79%</div> <div>19%</div> <div>•</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3581 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 Prolactin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	5	0
			1545	973	269	293	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	MET	-	INITIATING METHIONINE	UNP P01236
A	30	ALA	HIS	ENGINEERED MUTATION	UNP P01236
A	129	ARG	GLY	ENGINEERED MUTATION	UNP P01236

- Molecule 2 is a protein called Prolactin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	206	Total	C	N	O	S	0	3	0
			1701	1108	276	306	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	INITIATING METHIONINE	UNP P16471

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Na	0	0
			3	3		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		

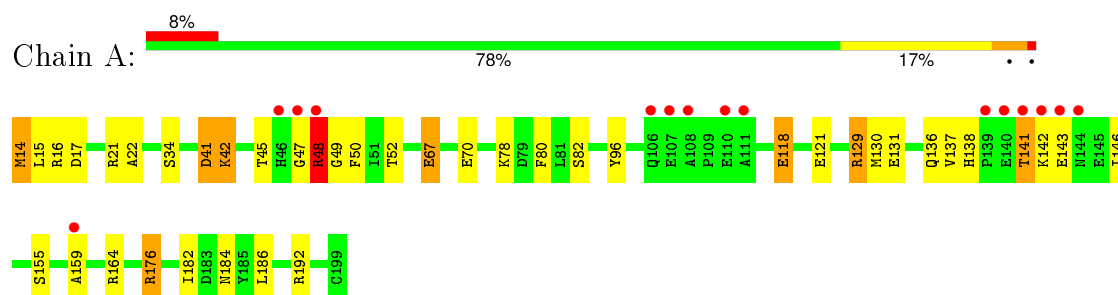
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	150	Total 150	O 150	0	0
5	B	181	Total 181	O 181	0	0

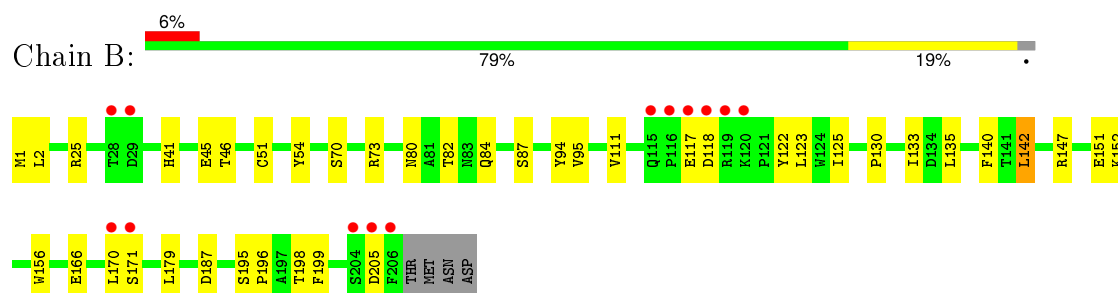
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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: Prolactin



#### • Molecule 2: Prolactin receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.54 Å 123.54 Å 73.33 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.67 – 2.10 29.67 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.67-2.10) 99.8 (29.67-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.36 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.180 , 0.224 0.180 , 0.222	Depositor DCC
$R_{free}$ test set	1902 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 53.5	EDS
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 37230 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3581	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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: NA, CL

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	1.13	6/1589 (0.4%)	1.04	9/2143 (0.4%)
2	B	1.18	0/1773	0.99	5/2420 (0.2%)
All	All	1.16	6/3362 (0.2%)	1.02	14/4563 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	GLU	CB-CG	10.01	1.71	1.52
1	A	121	GLU	CG-CD	5.80	1.60	1.51
1	A	70	GLU	CB-CG	5.27	1.62	1.52
1	A	131	GLU	CG-CD	5.27	1.59	1.51
1	A	96	TYR	CD2-CE2	5.25	1.47	1.39
1	A	131	GLU	CB-CG	5.04	1.61	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	ARG	NE-CZ-NH1	8.73	124.66	120.30
1	A	16	ARG	NE-CZ-NH2	-8.29	116.15	120.30
1	A	176	ARG	NE-CZ-NH1	7.35	123.98	120.30
2	B	187	ASP	CB-CG-OD1	7.20	124.78	118.30
1	A	192	ARG	NE-CZ-NH2	-7.17	116.72	120.30
2	B	142	LEU	CA-CB-CG	6.19	129.53	115.30
1	A	41	ASP	CB-CG-OD1	6.14	123.83	118.30
2	B	95	VAL	CB-CA-C	-5.73	100.51	111.40
2	B	25	ARG	NE-CZ-NH1	-5.71	117.44	120.30
2	B	187	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	A	129	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	176	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	129	ARG	NE-CZ-NH1	5.23	122.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	ARG	CB-CG-CD	-5.00	98.59	111.60

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	1545	0	1542	36	0
2	B	1701	0	1638	26	0
3	B	3	0	0	0	0
4	B	1	0	0	0	0
5	A	150	0	0	6	0
5	B	181	0	0	4	0
All	All	3581	0	3180	60	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 9.

All (60) 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:A:182:ILE:CD1	1:A:182:ILE:CG1	1.78	1.61
1:A:146:ILE:HG21	5:A:299:HOH:O	1.55	1.03
1:A:42:LYS:HB3	1:A:42:LYS:NZ	1.80	0.97
1:A:48:ARG:HG3	1:A:49:GLY:N	1.92	0.83
1:A:78:LYS:HD2	1:A:141:THR:CG2	2.09	0.82
1:A:42:LYS:CB	1:A:42:LYS:NZ	2.41	0.82
1:A:42:LYS:HB3	1:A:42:LYS:HZ3	1.43	0.80
2:B:84:GLN:HG2	5:B:230:HOH:O	1.82	0.79
1:A:182:ILE:CD1	1:A:182:ILE:CB	2.60	0.78
1:A:67:GLU:HG2	2:B:70:SER:HB2	1.68	0.74
1:A:48:ARG:HG3	1:A:49:GLY:H	1.50	0.73
2:B:45:GLU:HG3	2:B:73:ARG:NH2	2.04	0.72
2:B:41:HIS:ND1	5:B:261:HOH:O	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LYS:CB	1:A:42:LYS:HZ2	2.04	0.71
1:A:118[B]:GLU:OE2	5:A:307:HOH:O	2.10	0.69
2:B:46:THR:O	5:B:330:HOH:O	2.10	0.69
1:A:155:SER:HB2	5:A:334:HOH:O	1.92	0.68
1:A:42:LYS:HB3	1:A:42:LYS:HZ2	1.54	0.68
1:A:78:LYS:HD2	1:A:141:THR:HG23	1.77	0.67
1:A:17:ASP:O	5:A:259:HOH:O	2.14	0.65
2:B:111:VAL:CG1	2:B:123:LEU:HD11	2.27	0.65
2:B:179:LEU:HG	2:B:199:PHE:CE1	2.33	0.63
1:A:136[B]:GLN:HA	1:A:136[B]:GLN:NE2	2.16	0.60
2:B:45:GLU:HG3	2:B:73:ARG:HH21	1.68	0.56
1:A:34:SER:HA	1:A:176:ARG:HD3	1.88	0.54
2:B:130:PRO:HG2	2:B:133:ILE:HD12	1.91	0.53
1:A:130:MET:SD	1:A:186[A]:LEU:HD21	2.50	0.52
2:B:195:SER:HB2	2:B:196:PRO:HD2	1.92	0.52
1:A:137:VAL:HG12	1:A:138:HIS:CE1	2.46	0.51
1:A:48:ARG:HG2	1:A:50:PHE:CE2	2.46	0.50
2:B:133:ILE:HG22	2:B:135:LEU:HG	1.93	0.50
1:A:136[B]:GLN:HG2	5:A:322:HOH:O	2.11	0.50
2:B:151:GLU:HG2	2:B:152:LYS:HG3	1.93	0.50
2:B:80:ASN:C	2:B:80:ASN:OD1	2.49	0.49
1:A:48:ARG:CG	1:A:49:GLY:H	2.23	0.49
1:A:48:ARG:HG2	1:A:48:ARG:HH11	1.78	0.49
2:B:198:THR:HG22	5:B:266:HOH:O	2.11	0.49
2:B:80:ASN:O	2:B:80:ASN:OD1	2.31	0.48
1:A:48:ARG:CG	1:A:49:GLY:N	2.72	0.48
2:B:140:PHE:HE1	2:B:142:LEU:HD13	1.78	0.47
1:A:14:MET:HG3	1:A:17:ASP:HB2	1.96	0.47
1:A:159:ALA:O	1:A:164:ARG:NH2	2.47	0.47
1:A:146:ILE:O	1:A:146:ILE:HG23	2.14	0.46
1:A:47:GLY:O	1:A:48:ARG:HB2	2.15	0.46
2:B:147:ARG:HD2	2:B:156:TRP:CD2	2.51	0.46
2:B:111:VAL:HG13	2:B:123:LEU:HD11	1.97	0.46
2:B:122:TYR:HB3	2:B:170:LEU:HD13	1.97	0.46
2:B:45:GLU:CG	2:B:73:ARG:NH2	2.77	0.45
1:A:146:ILE:CG2	5:A:299:HOH:O	2.36	0.45
2:B:140:PHE:CE1	2:B:142:LEU:HD13	2.52	0.44
2:B:51:CYS:HB3	2:B:54:TYR:CZ	2.53	0.44
2:B:130:PRO:HD2	2:B:142:LEU:HD21	2.00	0.43
1:A:22:ALA:HB1	1:A:186[B]:LEU:HD21	2.00	0.43
1:A:21:ARG:HG2	1:A:129:ARG:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ASP:HA	1:A:45:THR:OG1	2.20	0.41
2:B:125:ILE:O	2:B:166:GLU:HA	2.20	0.41
1:A:52:THR:HG22	2:B:94:TYR:CZ	2.55	0.41
1:A:15:LEU:HA	1:A:15:LEU:HD23	1.72	0.40
2:B:82:THR:HG22	2:B:87:SER:CB	2.51	0.40
1:A:182:ILE:HB	1:A:182:ILE:CD1	2.48	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	A	189/186 (102%)	182 (96%)	6 (3%)	1 (0%)	34	30
2	B	207/210 (99%)	200 (97%)	6 (3%)	1 (0%)	34	30
All	All	396/396 (100%)	382 (96%)	12 (3%)	2 (0%)	34	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	118	ASP
1	A	48	ARG

### 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	177/172 (103%)	165 (93%)	12 (7%)	20	16
2	B	187/190 (98%)	182 (97%)	5 (3%)	52	56
All	All	364/362 (101%)	347 (95%)	17 (5%)	34	30

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	MET
1	A	42	LYS
1	A	48	ARG
1	A	67	GLU
1	A	80	PHE
1	A	82	SER
1	A	118[A]	GLU
1	A	118[B]	GLU
1	A	141	THR
1	A	142	LYS
1	A	143	GLU
1	A	184	ASN
2	B	1	MET
2	B	2	LEU
2	B	117	GLU
2	B	171	SER
2	B	205	ASP

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

Mol	Chain	Res	Type
1	A	138	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are 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 [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	186/186 (100%)	0.24	15 (8%)	15 20	17, 32, 65, 80	1 (0%)
2	B	206/210 (98%)	-0.12	13 (6%)	23 31	17, 29, 57, 77	0
All	All	392/396 (98%)	0.05	28 (7%)	19 26	17, 31, 63, 80	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	LYS	5.7
1	A	47	GLY	4.8
2	B	118	ASP	4.8
2	B	120	LYS	4.8
1	A	48	ARG	4.8
1	A	46	HIS	4.7
1	A	144	ASN	4.6
1	A	106	GLN	4.3
1	A	143	GLU	4.1
2	B	119	ARG	4.1
2	B	116	PRO	4.1
1	A	141	THR	4.0
1	A	159	ALA	3.7
1	A	107	GLU	3.5
1	A	140	GLU	3.1
2	B	117	GLU	3.0
2	B	205	ASP	2.9
2	B	171	SER	2.9
2	B	28	THR	2.9
1	A	139	PRO	2.8
2	B	29	ASP	2.5
1	A	111	ALA	2.4
2	B	115	GLN	2.4
2	B	170	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	110	GLU	2.3
1	A	108	ALA	2.2
2	B	206	PHE	2.2
2	B	204	SER	2.1

## 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(Å <sup>2</sup> )	Q<0.9
3	NA	B	211	1/1	0.99	0.14	0.70	17,17,17,17	0
3	NA	B	214	1/1	0.99	0.06	-1.27	35,35,35,35	0
3	NA	B	212	1/1	0.99	0.05	-2.28	26,26,26,26	0
4	CL	B	213	1/1	0.99	0.05	-	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.