



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:23 PM GMT

PDB ID : 4XNV
Title : The human P2Y1 receptor in complex with BPTU
Authors : Zhang, D.; Gao, Z.; Jacobson, K.; Han, G.W.; Stevens, R.; Zhao, Q.; Wu, B.
Deposited on : 2015-01-16
Resolution : 2.20 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

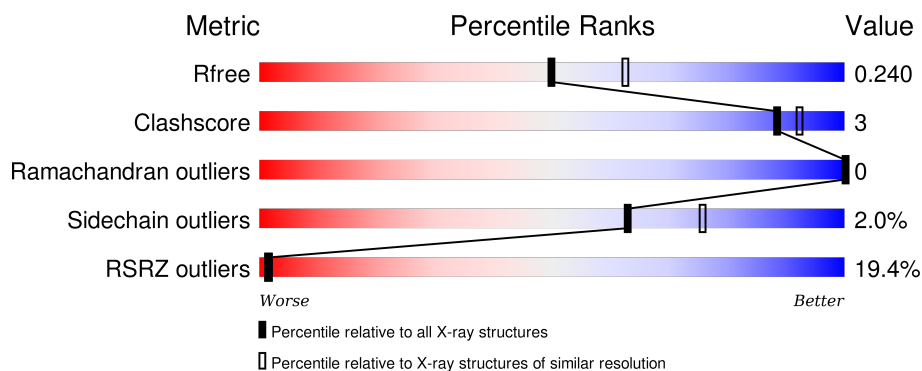
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	421	

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	CLR	A	1102	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	Y01	A	1105	-	-	-	X
5	OLC	A	1106	-	-	-	X
5	OLC	A	1107	-	-	-	X
5	OLC	A	1108	-	-	-	X
5	OLC	A	1109	-	-	-	X
5	OLC	A	1110	-	-	-	X
5	OLC	A	1111	-	-	-	X
5	OLC	A	1112	-	-	-	X
5	OLC	A	1113	-	-	-	X

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.

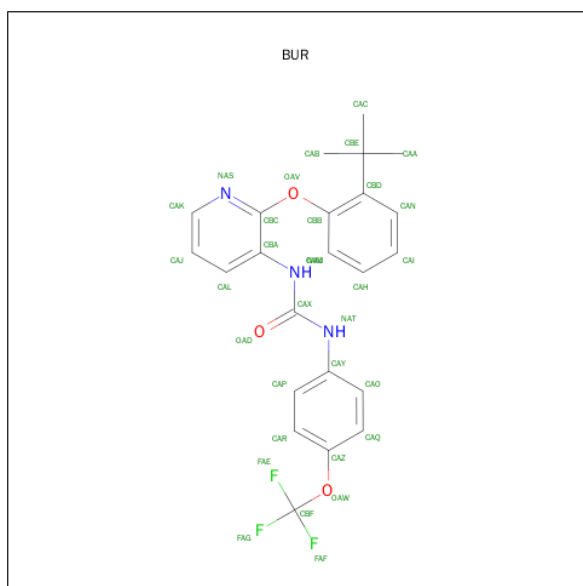
- Molecule 1 is a protein called P2Y purinoceptor 1, Rubredoxin, P2Y purinoceptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2713	1803	426	460	24			

There is a discrepancy between the modelled and reference sequences:

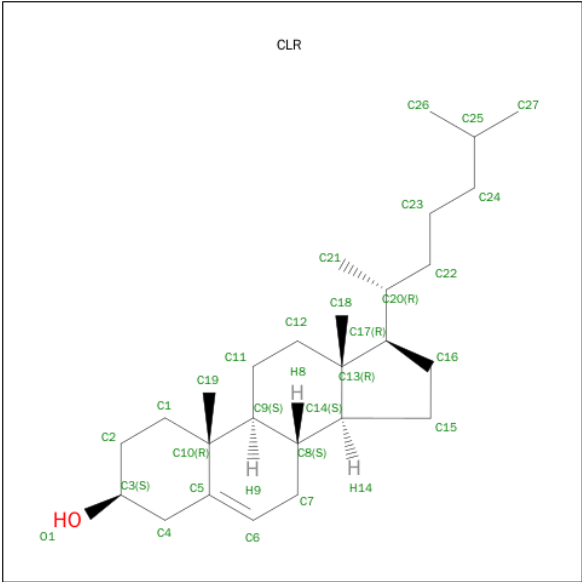
Chain	Residue	Modelled	Actual	Comment	Reference
A	320	ASN	ASP	engineered mutation	UNP P47900

- Molecule 2 is 1-[2-(2-tert-butylphenoxy)pyridin-3-yl]-3-[4-(trifluoromethoxy)phenyl]urea (three-letter code: BUR) (formula: C₂₃H₂₂F₃N₃O₃).



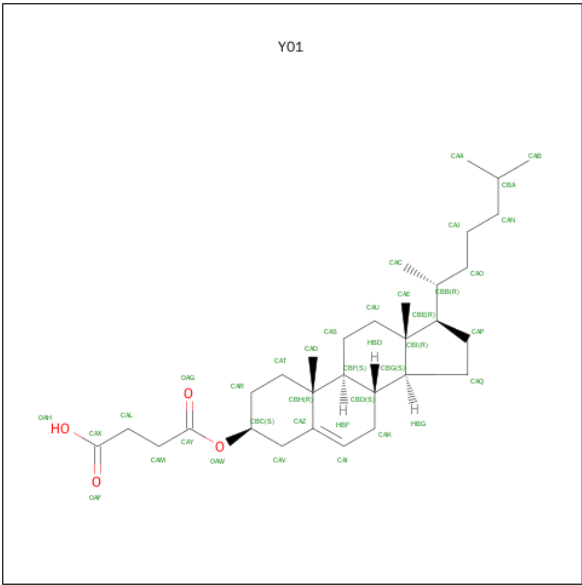
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			32	23	3	3	3		

- Molecule 3 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



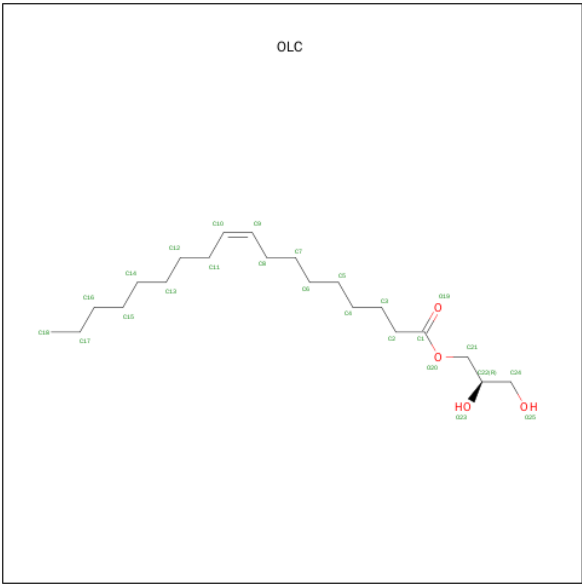
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			28	27	1		

- Molecule 4 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C₃₁H₅₀O₄).



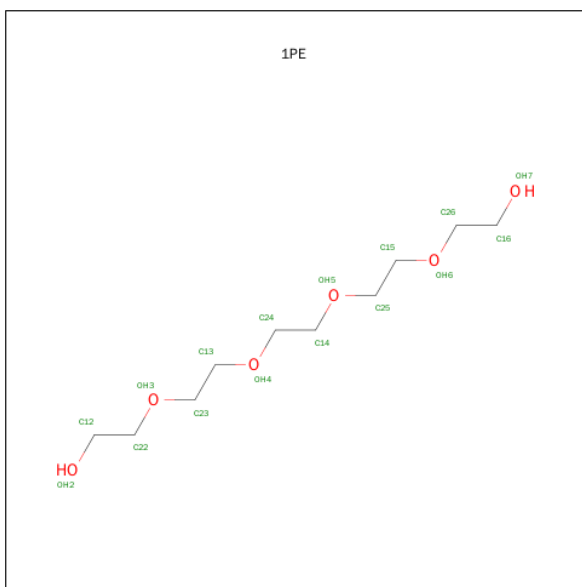
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			35	31	4		
4	A	1	Total	C	O	0	0
			35	31	4		
4	A	1	Total	C	O	0	0
			35	31	4		

- Molecule 5 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			21	17	4		
5	A	1	Total	C	O	0	0
			21	17	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			22	18	4		
5	A	1	Total	C	O	0	0
			25	21	4		

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	C O	0	0
			16	10 6		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	30	Total	O	0	0
			30	30		

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	66.27Å 66.27Å 239.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.40 – 2.20 41.40 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.40-2.20) 99.9 (41.40-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.207 , 0.230 0.211 , 0.240	Depositor DCC
R_{free} test set	1017 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.7	EDS
Estimated twinning fraction	0.055 for -h-k,k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 19881 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3114	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.26% 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, 0.375 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: ZN, OLC, BUR, 1PE, Y01, CLR

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	0.42	0/2787	0.59	0/3787

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	2713	0	2724	12	0
2	A	32	0	22	1	0
3	A	28	0	46	0	0
4	A	105	0	147	2	0
5	A	189	0	289	7	0
6	A	16	0	22	0	0
7	A	1	0	0	0	0
8	A	30	0	0	0	0
All	All	3114	0	3250	16	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.

The worst 5 of 16 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:282:MET:HG2	5:A:1112:OLC:H24A	1.84	0.59
1:A:125:LYS:HZ1	5:A:1110:OLC:H21A	1.69	0.58
1:A:312:LEU:HA	1:A:315:LEU:HD12	1.87	0.57
1:A:184:SER:HB2	5:A:1110:OLC:H11A	1.88	0.56
1:A:64:ILE:HG22	1:A:318:CYS:HB2	1.93	0.50

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	334/421 (79%)	323 (97%)	11 (3%)	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	295/367 (80%)	289 (98%)	6 (2%)	63	76

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	LEU
1	A	300	ASP
1	A	1041	LEU
1	A	49	PHE
1	A	268	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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	$\# Z > 2$
2	BUR	A	1101	-	29,34,34	1.58	5 (17%)	39,49,49	1.15	4 (10%)
3	CLR	A	1102	-	31,31,31	1.63	8 (25%)	48,48,48	1.10	4 (8%)
4	Y01	A	1103	-	35,38,38	1.78	6 (17%)	54,57,57	1.06	3 (5%)
4	Y01	A	1104	-	35,38,38	1.76	8 (22%)	54,57,57	1.12	3 (5%)
4	Y01	A	1105	-	35,38,38	1.79	8 (22%)	54,57,57	1.30	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	OLC	A	1106	-	20,20,24	1.03	1 (5%)	20,21,25	0.76	0
5	OLC	A	1107	-	20,20,24	1.06	1 (5%)	20,21,25	0.64	0
5	OLC	A	1108	-	24,24,24	1.02	1 (4%)	25,25,25	0.75	0
5	OLC	A	1109	-	24,24,24	1.02	1 (4%)	25,25,25	0.78	0
5	OLC	A	1110	-	24,24,24	1.00	1 (4%)	25,25,25	0.74	0
5	OLC	A	1111	-	24,24,24	0.99	1 (4%)	25,25,25	0.81	0
5	OLC	A	1112	-	21,21,24	1.06	1 (4%)	22,22,25	0.61	0
5	OLC	A	1113	-	24,24,24	1.05	1 (4%)	25,25,25	0.78	0
6	1PE	A	1114	-	15,15,15	0.55	0	14,14,14	0.50	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	BUR	A	1101	-	-	0/20/23/23	0/3/3/3
3	CLR	A	1102	-	-	0/10/68/68	0/4/4/4
4	Y01	A	1103	-	-	0/17/77/77	0/4/4/4
4	Y01	A	1104	-	-	0/17/77/77	0/4/4/4
4	Y01	A	1105	-	-	0/17/77/77	0/4/4/4
5	OLC	A	1106	-	-	0/20/20/24	0/0/0/0
5	OLC	A	1107	-	-	0/20/20/24	0/0/0/0
5	OLC	A	1108	-	-	0/24/24/24	0/0/0/0
5	OLC	A	1109	-	-	0/24/24/24	0/0/0/0
5	OLC	A	1110	-	-	0/24/24/24	0/0/0/0
5	OLC	A	1111	-	-	0/24/24/24	0/0/0/0
5	OLC	A	1112	-	-	0/21/21/24	0/0/0/0
5	OLC	A	1113	-	-	0/24/24/24	0/0/0/0
6	1PE	A	1114	-	-	0/13/13/13	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	BUR	CBE-CBD	-4.95	1.46	1.54
4	A	1105	Y01	CAK-CAI	-4.21	1.41	1.50
4	A	1105	Y01	CAV-CAZ	-4.16	1.41	1.51
4	A	1104	Y01	CAK-CAI	-4.13	1.41	1.50
4	A	1103	Y01	CAV-CAZ	-4.12	1.41	1.51

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	1105	Y01	CAV-CAZ-CAI	-3.51	114.61	120.57
4	A	1103	Y01	CAV-CAZ-CAI	-3.35	114.88	120.57
4	A	1104	Y01	CAV-CAZ-CAI	-3.31	114.96	120.57
4	A	1105	Y01	CAP-CAQ-CBG	-3.16	98.77	105.12
4	A	1105	Y01	CBG-CBI-CBE	-2.91	96.67	100.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	BUR	1	0
4	A	1104	Y01	1	0
4	A	1105	Y01	1	0
5	A	1107	OLC	2	0
5	A	1108	OLC	1	0
5	A	1110	OLC	4	0
5	A	1112	OLC	1	0
5	A	1113	OLC	1	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	A	340/421 (80%)	0.79	66 (19%) 1 1	28, 50, 149, 200	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1027	GLY	9.9
1	A	1010	GLY	6.8
1	A	159	SER	6.3
1	A	1008	VAL	6.1
1	A	1026	PRO	5.8

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, 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	LLDF	B-factors(Å ²)	Q<0.9
5	OLC	A	1107	21/25	0.71	0.28	7.26	57,62,82,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	OLC	A	1110	25/25	0.74	0.25	6.61	60,63,72,72	0
5	OLC	A	1108	25/25	0.67	0.25	6.17	78,85,88,88	0
5	OLC	A	1112	22/25	0.61	0.39	5.05	43,63,83,84	0
5	OLC	A	1113	25/25	0.45	0.35	4.30	63,70,81,82	0
3	CLR	A	1102	28/28	0.92	0.20	4.10	32,39,52,53	0
5	OLC	A	1106	21/25	0.72	0.33	3.46	50,54,74,75	0
5	OLC	A	1111	25/25	0.64	0.34	3.14	71,77,87,91	0
4	Y01	A	1105	35/35	0.74	0.23	2.81	65,70,88,89	0
5	OLC	A	1109	25/25	0.62	0.31	2.23	66,73,83,83	0
4	Y01	A	1103	35/35	0.91	0.18	0.82	35,41,59,62	0
2	BUR	A	1101	32/32	0.88	0.12	0.11	44,47,68,70	0
4	Y01	A	1104	35/35	0.88	0.15	-0.31	41,48,55,58	0
7	ZN	A	1115	1/1	0.96	0.04	-1.82	87,87,87,87	0
6	1PE	A	1114	16/16	0.76	0.28	-	84,88,91,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.