



# wwPDB X-ray Structure Validation Summary Report

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PDB ID : 3URO  
Title : Poliovirus receptor CD155 D1D2  
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Deposited on : 2011-11-22  
Resolution : 3.50 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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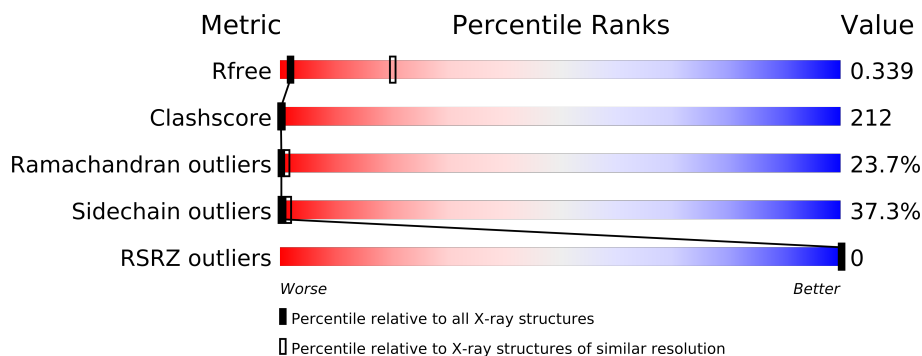
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance


The reported resolution of this entry is 3.50 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))
$R_{free}$	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	R	221	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1638 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Poliovirus receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	213	Total	C	N	O	S	0	0	0
			1638	1038	281	310	9			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	105	ASP	ASN	ENGINEERED MUTATION	UNP P15151
R	120	SER	ASN	ENGINEERED MUTATION	UNP P15151
R	188	GLN	ASN	ENGINEERED MUTATION	UNP P15151
R	218	GLN	ASN	ENGINEERED MUTATION	UNP P15151
R	237	SER	ASN	ENGINEERED MUTATION	UNP P15151
R	244	HIS	-	EXPRESSION TAG	UNP P15151
R	245	HIS	-	EXPRESSION TAG	UNP P15151
R	246	HIS	-	EXPRESSION TAG	UNP P15151
R	247	HIS	-	EXPRESSION TAG	UNP P15151
R	248	HIS	-	EXPRESSION TAG	UNP P15151
R	249	HIS	-	EXPRESSION TAG	UNP P15151



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.31Å 84.31Å 117.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.89 – 3.50 35.89 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (35.89-3.50) 99.3 (35.89-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.305 , 0.341 0.303 , 0.339	Depositor DCC
$R_{free}$ test set	276 reflections (4.86%)	DCC
Wilson B-factor (Å <sup>2</sup> )	126.4	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 327.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 5675 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	1638	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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	R	0.56	0/1678	1.16	13/2289 (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
1	R	0	2

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	92	LEU	CB-CA-C	15.51	139.68	110.20
1	R	93	GLU	N-CA-CB	12.02	132.24	110.60
1	R	92	LEU	N-CA-C	-8.53	87.96	111.00
1	R	91	ARG	CB-CA-C	7.60	125.60	110.40
1	R	146	GLN	N-CA-C	-6.72	92.87	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	R	140	ARG	Peptide
1	R	45	VAL	Peptide

### 5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	1638	0	1620	692	0
All	All	1638	0	1620	692	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 212.

The worst 5 of 692 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:122:THR:CB	1:R:136:ASP:HA	1.70	1.19
1:R:36:GLN:HA	1:R:139:LEU:CG	1.73	1.16
1:R:122:THR:HB	1:R:136:ASP:CA	1.74	1.15
1:R:144:LYS:HE2	1:R:145:PRO:O	1.45	1.15
1:R:59:THR:HG21	1:R:129:PRO:HG2	1.21	1.12

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	R	211/221 (96%)	111 (53%)	50 (24%)	50 (24%)	<b>0</b> <b>1</b>

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	45	VAL
1	R	55	ASN
1	R	72	SER
1	R	96	ALA
1	R	98	ARG

### 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	R	185/193 (96%)	116 (63%)	69 (37%)	<b>0</b> <b>1</b>

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	135	VAL
1	R	159	GLU
1	R	233	LEU
1	R	136	ASP
1	R	148	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	R	80	GLN
1	R	225	HIS
1	R	180	HIS
1	R	60	HIS
1	R	155	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

## 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	R	213/221 (96%)	-0.16	0 100 100	62, 98, 133, 166	0

There are no RSRZ outliers to report.

### 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 ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.