



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3URO / pdb_00003uro
Title : Poliovirus receptor CD155 D1D2
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Deposited on : 2011-11-22
Resolution : 3.50 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
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

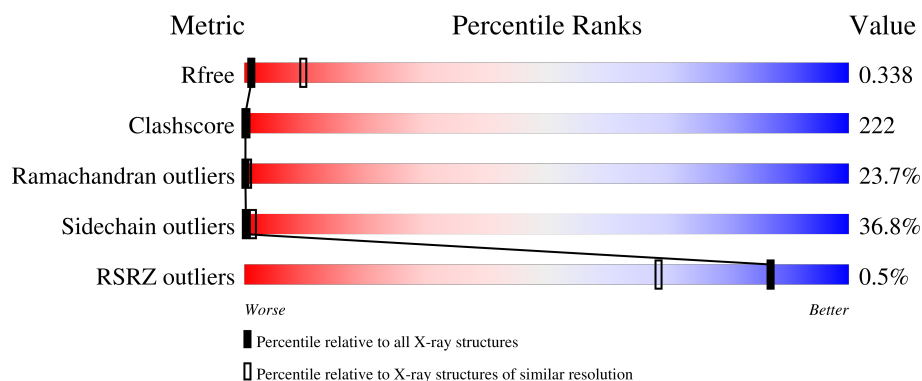
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	R	221	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1638 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 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

i

- Molecule 1: Poliovirus receptor

V209	A149	S89	VAL
P210	E150	K90	V30
S211	V151	R91	V31
S212	K152	L92	Q32
Q213	K153	E93	A33
V214	V154	F94	P34
D215	Q155	V95	T35
G216	L156	A96	Q36
K217	T157	A97	V37
Q218	G158	R98	P38
V219	E159	L99	G39
T220	P160	G100	F40
C221	V161	A101	L41
K222	P162	E102	G42
V223	M163	L103	D43
E224	A164	R104	S44
H225	R165	D105	V45
E226	C166	A106	T46
S227	V167	L107	L47
F228	S168	L108	P48
E229	T169	R109	C49
K230	G170	M110	Y50
P231	R171	F111	L51
Q232	R172	G112	Q52
L233	P173	L113	V53
L234	P174	R114	P54
T235	A175	V115	S55
V236	Q176	E116	S56
S237	T177	D117	E57
L238	T178	E118	V58
T239	W179	G119	T59
V240	H180	S120	H60
Y241	S181	T121	V61
Y242	D182	T122	S62
PRO	L183	C123	D63
HIS	G184	L124	L64
HIS	G185	F125	T65
HIS	M186	V126	H66
HIS	P187	T127	A67
HIS	Q188	F128	R68
HIS	T189	P129	H69
	G190	Q130	G70
	Q191	G131	E71
	V192	S132	S72
	P193	R133	G73
	G194	S134	S74
	F195	V135	M75
	L196	D136	A76
	S197	T137	V77
	G198	F138	F78
	T199	L139	H79
	T200	R140	Q80
	V201	V141	T81
	V202	T142	Q82
	T203	A143	G83
	S204	K144	P84
	L205	P145	S85
	W206	Q146	T86
	T207	S147	S87
	L208	T148	P88

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	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) 99.2 (35.89-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.305 , 0.341 0.304 , 0.338	Depositor DCC
R_{free} test set	277 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	126.4	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 310.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	1638	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.77	0/1678	1.59	42/2289 (1.8%)

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 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	R	92	LEU	CB-CA-C	14.70	139.68	110.42
1	R	93	GLU	N-CA-CB	12.87	132.24	110.49
1	R	37	VAL	N-CA-C	12.27	122.20	107.61
1	R	31	VAL	N-CA-C	10.95	123.72	108.93
1	R	92	LEU	N-CA-C	-10.72	87.96	110.80

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 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	R	1638	0	1620	722	0
All	All	1638	0	1620	722	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 222.

The worst 5 of 722 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: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 [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	R	211/221 (96%)	111 (53%)	50 (24%)	50 (24%)	0 0

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

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Mol	Chain	Res	Type
1	R	98	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	R	185/193 (96%)	117 (63%)	68 (37%)	0 1

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	208	LEU
1	R	215	ASP
1	R	238	LEU
1	R	115	VAL
1	R	114	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	R	218	GLN
1	R	225	HIS
1	R	232	GLN
1	R	80	GLN
1	R	146	GLN

5.3.3 RNA [i](#)

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](#)

There are no ligands in this entry.

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	R	213/221 (96%)	0.32	1 (0%)	87 68	62, 98, 133, 166	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	32	GLN	2.3

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.