



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 09:56 am GMT

PDB ID : 2P1Y
Title : 1.B2.D9, a bispecific alpha/beta TCR
Authors : McBeth, C.; Pizarro, J.C.; Strong, R.K.
Deposited on : 2007-03-06
Resolution : 2.42 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

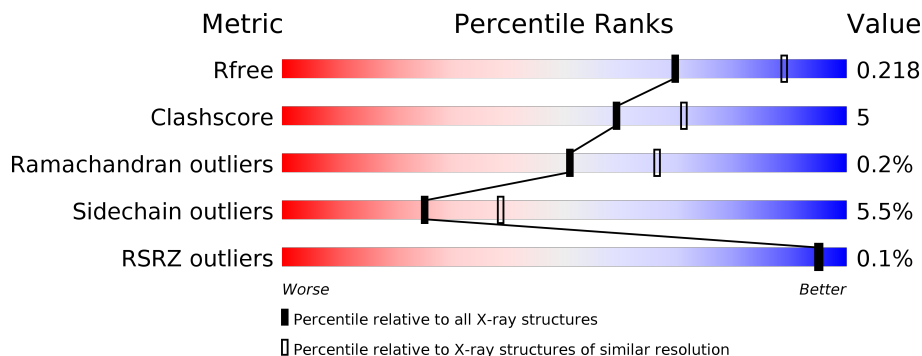
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.42 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}	100719	3709 (2.44-2.40)
Clashscore	112137	4241 (2.44-2.40)
Ramachandran outliers	110173	4178 (2.44-2.40)
Sidechain outliers	110143	4179 (2.44-2.40)
RSRZ outliers	101464	3740 (2.44-2.40)

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	238	
1	C	238	
1	E	238	
1	G	238	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7017 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 bispecific alpha/beta TCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1779	1124	304	346	5			
1	C	231	Total	C	N	O	S	0	0	0
			1771	1116	304	346	5			
1	E	217	Total	C	N	O	S	0	0	0
			1675	1064	283	323	5			
1	G	217	Total	C	N	O	S	0	0	0
			1690	1073	288	324	5			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	25	Total	O	0	0
			25	25		
2	C	15	Total	O	0	0
			15	15		
2	E	30	Total	O	0	0
			30	30		
2	G	32	Total	O	0	0
			32	32		

Y324	Y331	F332	P333	G342	L346	L350	D354	K355	K356	E357	R361	T364	R369	A386	A391	A392	I393	N396	A397	Y398	H407	L411	P412
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.68Å 105.48Å 81.53Å 90.00° 116.04° 90.00°	Depositor
Resolution (Å)	40.39 – 2.42 40.37 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.39-2.42) 99.2 (40.37-2.42)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.33 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.181 , 0.254 0.189 , 0.218	Depositor DCC
R_{free} test set	2073 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 3.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.488 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7017	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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

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	1.71	27/1821 (1.5%)	1.29	10/2465 (0.4%)
1	C	1.78	35/1814 (1.9%)	1.31	13/2459 (0.5%)
1	E	1.49	8/1717 (0.5%)	1.22	5/2329 (0.2%)
1	G	1.43	6/1733 (0.3%)	1.22	13/2350 (0.6%)
All	All	1.61	76/7085 (1.1%)	1.26	41/9603 (0.4%)

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	A	0	1
1	C	0	2
1	E	0	2
1	G	0	1
All	All	0	6

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	GLU	CG-CD	11.55	1.69	1.51
1	A	73	GLU	CG-CD	9.81	1.66	1.51
1	A	34	TRP	CB-CG	8.53	1.65	1.50
1	E	324	TYR	CE2-CZ	8.24	1.49	1.38
1	A	390	CYS	CB-SG	8.19	1.96	1.82

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	ASP	CB-CG-OD1	10.71	127.94	118.30
1	A	306	SER	N-CA-CB	-8.39	97.91	110.50
1	A	358	ASP	CB-CG-OD2	8.24	125.72	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	358	ASP	CB-CG-OD2	8.22	125.70	118.30
1	E	384	ASP	CB-CG-OD1	8.06	125.56	118.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	ARG	Peptide
1	C	116	LEU	Peptide
1	C	16	GLY	Peptide
1	E	305	GLN	Peptide
1	E	5	THR	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	A	1779	0	1697	24	0
1	C	1771	0	1671	16	0
1	E	1675	0	1590	21	0
1	G	1690	0	1608	13	0
2	A	25	0	0	0	0
2	C	15	0	0	1	0
2	E	30	0	0	0	0
2	G	32	0	0	1	0
All	All	7017	0	6566	73	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 5.

The worst 5 of 73 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:C:104:ARG:HG3	1:C:104:ARG:O	1.64	0.98
1:E:25:GLN:HE22	1:E:29:HIS:H	1.12	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:GLY:HA3	1:G:3:ALA:N	1.88	0.88
1:A:15:THR:HG22	1:A:116:LEU:O	1.79	0.82
1:G:109:HIS:CD2	1:G:342:GLY:H	2.02	0.77

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	225/238 (94%)	216 (96%)	9 (4%)	0	100	100
1	C	227/238 (95%)	216 (95%)	11 (5%)	0	100	100
1	E	211/238 (89%)	202 (96%)	8 (4%)	1 (0%)	32	45
1	G	211/238 (89%)	198 (94%)	12 (6%)	1 (0%)	32	45
All	All	874/952 (92%)	832 (95%)	40 (5%)	2 (0%)	51	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	84	PRO
1	E	84	PRO

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	190/199 (96%)	177 (93%)	13 (7%)	18	28
1	C	188/199 (94%)	173 (92%)	15 (8%)	14	21
1	E	180/199 (90%)	174 (97%)	6 (3%)	43	62
1	G	182/199 (92%)	175 (96%)	7 (4%)	38	56
All	All	740/796 (93%)	699 (94%)	41 (6%)	25	39

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	104	ARG
1	C	356	LYS
1	G	116	LEU
1	C	310	LEU
1	C	327	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	109	HIS
1	G	407	HIS
1	G	109	HIS
1	E	25	GLN
1	E	326	ASN

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 [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	A	231/238 (97%)	-0.61	1 (0%) 92 91	11, 23, 54, 67	0
1	C	231/238 (97%)	-0.65	0 100 100	11, 23, 55, 64	0
1	E	217/238 (91%)	-0.66	0 100 100	12, 28, 50, 59	0
1	G	217/238 (91%)	-0.65	0 100 100	12, 28, 51, 58	0
All	All	896/952 (94%)	-0.64	1 (0%) 95 95	11, 26, 53, 67	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	ALA	3.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.