



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 03:20 PM GMT

PDB ID : 2CDF  
Title : STRUCTURE AND BINDING KINETICS OF THREE DIFFERENT HUMAN CD1D-ALPHA-GALACTOSYLCERAMIDE-SPECIFIC CELL RECEPTORS (TCR 5E)  
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Deposited on : 2006-01-23  
Resolution : 2.25 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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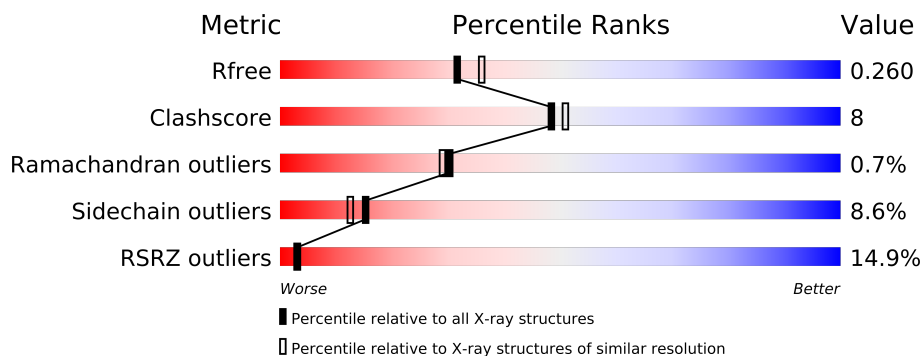
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.25 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	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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	A	191	
2	B	244	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3720 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 TCR 5E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1481	921	253	300	7			

- Molecule 2 is a protein called TCR 5E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1955	1229	335	383	8			

- Molecule 3 is water.

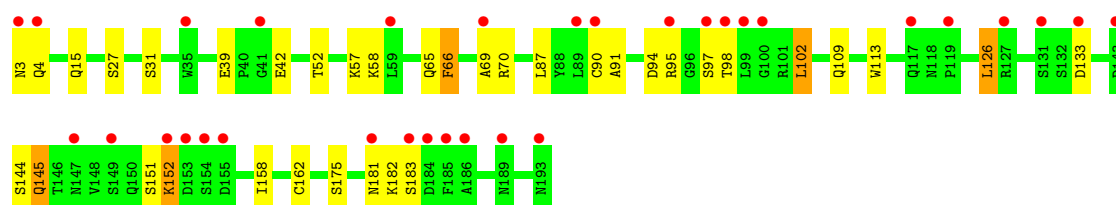
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	127	Total	O	0	0
			127	127		
3	B	157	Total	O	0	0
			157	157		

### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.

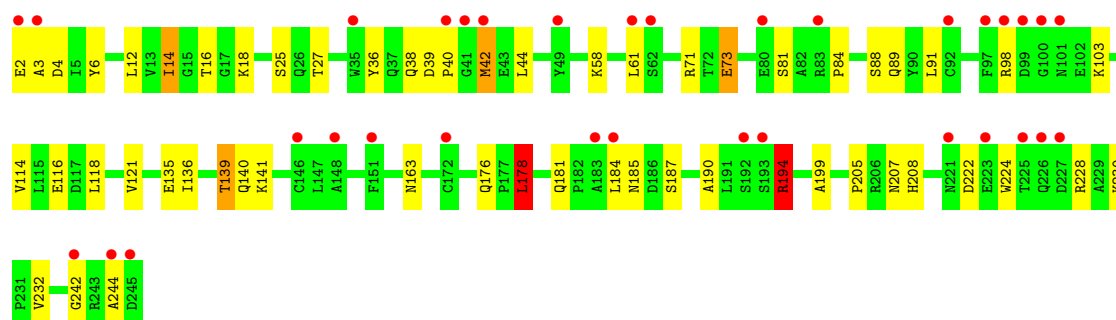
#### • Molecule 1: TCR 5E

Chain A: 



#### • Molecule 2: TCR 5E

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.45Å 64.45Å 184.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.25 28.56 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.7 (30.00-2.25) 98.7 (28.56-2.25)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.56 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.188 , 0.269 0.186 , 0.260	Depositor DCC
$R_{free}$ test set	1097 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.2	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 23.0	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 21654 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3720	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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	A	0.64	1/1510 (0.1%)	0.69	1/2045 (0.0%)
2	B	0.60	0/2008	0.72	2/2729 (0.1%)
All	All	0.62	1/3518 (0.0%)	0.70	3/4774 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	CYS	CB-SG	-6.65	1.71	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	178	LEU	CA-CB-CG	6.29	129.77	115.30
2	B	194	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	126	LEU	CA-CB-CG	5.45	127.83	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	A	1481	0	1413	20	0
2	B	1955	0	1844	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	127	0	0	4	0
3	B	157	0	0	9	0
All	All	3720	0	3257	52	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 8.

All (52) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:40:PRO:HA	3:B:2026:HOH:O	1.79	0.80
1:A:42:GLU:HG2	3:B:2025:HOH:O	1.82	0.78
2:B:14:ILE:HD11	2:B:114:VAL:HG22	1.70	0.74
2:B:44:LEU:HD21	2:B:91:LEU:HD12	1.69	0.74
1:A:109:GLN:OE1	3:A:2076:HOH:O	2.10	0.69
2:B:3:ALA:HB1	2:B:6:TYR:OH	1.92	0.69
1:A:39:GLU:OE2	3:A:2039:HOH:O	2.11	0.68
1:A:182:LYS:HB3	1:A:183:SER:CA	2.26	0.65
1:A:65:GLN:HG2	3:A:2059:HOH:O	1.97	0.65
2:B:163:ASN:HD21	2:B:207:ASN:HD22	1.45	0.64
2:B:36:TYR:HB3	2:B:44:LEU:HD22	1.80	0.62
1:A:182:LYS:HB3	1:A:183:SER:HA	1.83	0.61
2:B:84:PRO:HG3	2:B:116:GLU:HG3	1.83	0.59
2:B:121:VAL:O	2:B:228:ARG:NH2	2.38	0.57
2:B:230:LYS:HG2	2:B:232:VAL:HG13	1.87	0.56
1:A:145:GLN:HE21	1:A:145:GLN:H	1.54	0.55
2:B:136:ILE:HG23	2:B:199:ALA:HB1	1.87	0.55
2:B:208:HIS:HD2	3:B:2093:HOH:O	1.89	0.54
1:A:3:ASN:HB3	3:A:2003:HOH:O	2.07	0.54
2:B:228:ARG:NH1	3:B:2144:HOH:O	2.40	0.53
2:B:98:ARG:HB2	2:B:103:LYS:HD2	1.91	0.52
2:B:71:ARG:HA	3:B:2054:HOH:O	2.09	0.52
2:B:163:ASN:HD21	2:B:207:ASN:ND2	2.09	0.51
2:B:178:LEU:HD22	2:B:190:ALA:HB3	1.92	0.50
2:B:224:TRP:HB2	2:B:230:LYS:HD2	1.94	0.50
1:A:151:SER:HA	1:A:158:ILE:HD12	1.93	0.50
1:A:182:LYS:HB3	1:A:183:SER:CB	2.42	0.49
1:A:15:GLN:NE2	1:A:113:TRP:HB2	2.28	0.48
2:B:25:SER:HB2	2:B:73:GLU:OE1	2.14	0.48
1:A:31:SER:OG	1:A:95:ARG:HG3	2.15	0.47
2:B:139:THR:HG23	2:B:141:LYS:HB2	1.97	0.46
2:B:135:GLU:O	2:B:139:THR:HG22	2.14	0.46
2:B:84:PRO:CG	2:B:116:GLU:HG3	2.45	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:152:LYS:HB2	1:A:152:LYS:NZ	2.31	0.46
1:A:175:SER:OG	2:B:194:ARG:HD3	2.16	0.45
1:A:66:PHE:CE2	1:A:70:ARG:HG2	2.52	0.45
1:A:91:ALA:HB1	1:A:102:LEU:HG	2.00	0.44
2:B:181:GLN:HG2	3:B:2119:HOH:O	2.17	0.44
1:A:181:ASN:O	1:A:182:LYS:HG2	2.17	0.44
2:B:39:ASP:HB3	2:B:40:PRO:HD2	2.00	0.44
2:B:222:ASP:O	2:B:230:LYS:NZ	2.42	0.43
2:B:3:ALA:HB3	2:B:27:THR:OG1	2.18	0.43
2:B:208:HIS:CD2	3:B:2093:HOH:O	2.69	0.42
2:B:61:LEU:HG	3:B:2041:HOH:O	2.20	0.42
2:B:12:LEU:HG	2:B:14:ILE:HG23	2.01	0.42
2:B:205:PRO:HA	2:B:242:GLY:O	2.20	0.42
1:A:15:GLN:HE22	1:A:113:TRP:HB2	1.85	0.41
1:A:69:ALA:O	1:A:70:ARG:HB2	2.21	0.41
1:A:182:LYS:CB	1:A:183:SER:HA	2.48	0.41
2:B:42:MET:HE1	3:B:2032:HOH:O	2.21	0.41
2:B:181:GLN:O	2:B:187:SER:HB2	2.21	0.40
2:B:38:GLN:HG3	2:B:89:GLN:HB3	2.03	0.40

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	A	189/191 (99%)	182 (96%)	6 (3%)	1 (0%)	38	38
2	B	242/244 (99%)	233 (96%)	7 (3%)	2 (1%)	27	24
All	All	431/435 (99%)	415 (96%)	13 (3%)	3 (1%)	30	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	244	ALA

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Mol	Chain	Res	Type
1	A	97	SER
2	B	4	ASP

### 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	A	167/167 (100%)	151 (90%)	16 (10%)	12	8
2	B	216/216 (100%)	199 (92%)	17 (8%)	18	15
All	All	383/383 (100%)	350 (91%)	33 (9%)	15	12

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	27	SER
1	A	52	THR
1	A	57	LYS
1	A	58	LYS
1	A	66	PHE
1	A	87	LEU
1	A	94	ASP
1	A	98	THR
1	A	102	LEU
1	A	126	LEU
1	A	133	ASP
1	A	144	SER
1	A	145	GLN
1	A	152	LYS
1	A	162	CYS
2	B	2	GLU
2	B	14	ILE
2	B	16	THR
2	B	18	LYS
2	B	42	MET
2	B	58	LYS
2	B	73	GLU

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Mol	Chain	Res	Type
2	B	81	SER
2	B	88	SER
2	B	118	LEU
2	B	139	THR
2	B	140	GLN
2	B	176	GLN
2	B	178	LEU
2	B	184	LEU
2	B	185	ASN
2	B	194	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	4	GLN
1	A	15	GLN
1	A	109	GLN
1	A	145	GLN
1	A	189	ASN
2	B	138	HIS
2	B	140	GLN
2	B	168	HIS
2	B	207	ASN
2	B	208	HIS

### 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	A	191/191 (100%)	0.99	32 (16%) 2 2	10, 28, 51, 62	0
2	B	244/244 (100%)	0.82	33 (13%) 4 4	5, 27, 45, 68	0
All	All	435/435 (100%)	0.90	65 (14%) 3 3	5, 28, 48, 68	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	GLY	9.6
1	A	97	SER	6.7
2	B	245	ASP	5.4
2	B	183	ALA	5.4
1	A	184	ASP	5.3
1	A	133	ASP	4.8
2	B	227	ASP	4.2
2	B	3	ALA	3.9
2	B	184	LEU	3.9
2	B	99	ASP	3.8
2	B	101	ASN	3.7
1	A	152	LYS	3.7
2	B	225	THR	3.5
2	B	244	ALA	3.5
1	A	181	ASN	3.5
2	B	221	ASN	3.5
1	A	98	THR	3.4
1	A	3	ASN	3.3
1	A	99	LEU	3.3
1	A	185	PHE	3.2
1	A	183	SER	3.2
1	A	95	ARG	3.2
2	B	61	LEU	3.1
2	B	42	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	131	SER	3.0
2	B	40	PRO	3.0
1	A	35	TRP	3.0
1	A	186	ALA	2.9
2	B	62	SER	2.8
1	A	90	CYS	2.8
1	A	153	ASP	2.8
2	B	100	GLY	2.7
2	B	80	GLU	2.7
1	A	155	ASP	2.7
2	B	41	GLY	2.6
2	B	223	GLU	2.6
1	A	69	ALA	2.5
1	A	119	PRO	2.5
1	A	149	SER	2.5
1	A	89	LEU	2.5
2	B	2	GLU	2.4
2	B	49	TYR	2.4
1	A	189	ASN	2.4
1	A	147	ASN	2.3
2	B	192	SER	2.3
2	B	172	CYS	2.3
2	B	226	GLN	2.3
1	A	154	SER	2.3
2	B	98	ARG	2.2
2	B	83	ARG	2.2
1	A	41	GLY	2.2
2	B	146	CYS	2.2
1	A	193	ASN	2.2
2	B	151	PHE	2.1
2	B	97	PHE	2.1
1	A	117	GLN	2.1
2	B	92	CYS	2.1
2	B	35	TRP	2.1
1	A	4	GLN	2.0
1	A	127	ARG	2.0
2	B	148	ALA	2.0
2	B	242	GLY	2.0
1	A	59	LEU	2.0
2	B	193	SER	2.0
1	A	143	ASP	2.0

## 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.