



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:22 PM UTC

PDB ID : 2CDG / pdb_00002cdg
Title : Structure and binding kinetics of three different human CD1d-alpha- Galactosylceramide-specific T cell receptors (TCR 5B)
Authors : Gadola, S.D.; Koch, M.; Marles-Wright, J.; Lissin, N.M.; Sheperd, D.; Matulis, G.; Harlos, K.; Villiger, P.M.; Stuart, D.I.; Jakobsen, B.K.; Cerundolo, V.; Jones, E.Y.
Deposited on : 2006-01-23
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
Xtrriage (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

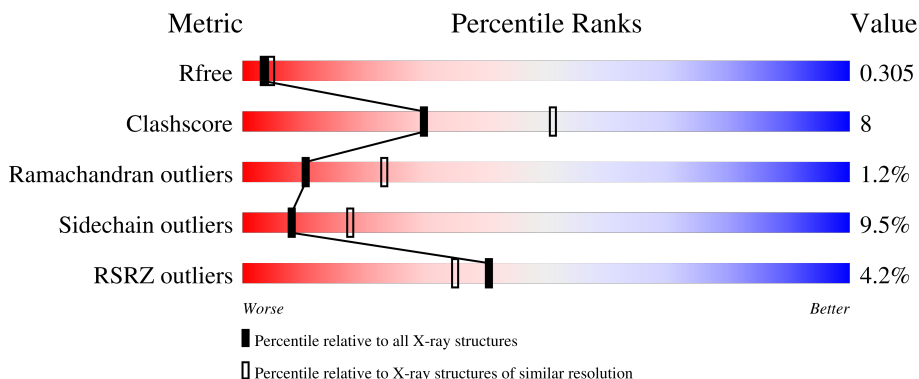
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	A	184	 3% 73% 18% 8%
2	B	244	 5% 78% 20% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3453 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 TCR 5E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	184	1444	888	259	289	8	0	0	0

- Molecule 2 is a protein called TCR 5E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	244	1948	1223	336	381	8	0	0	0

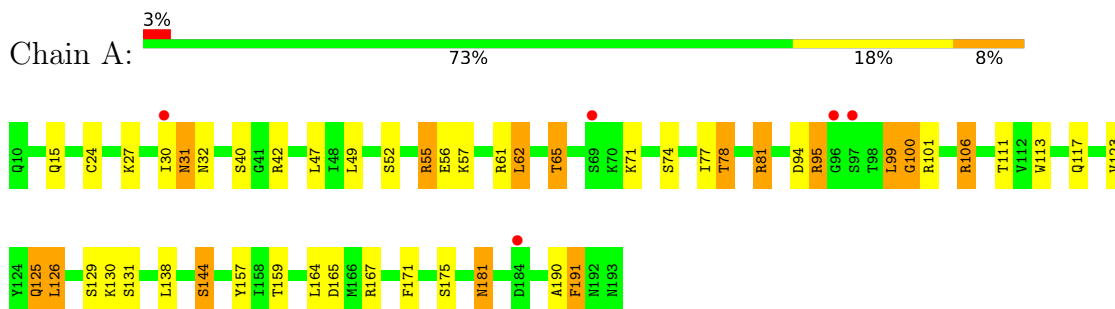
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	45	Total	O	0	0
			45	45		

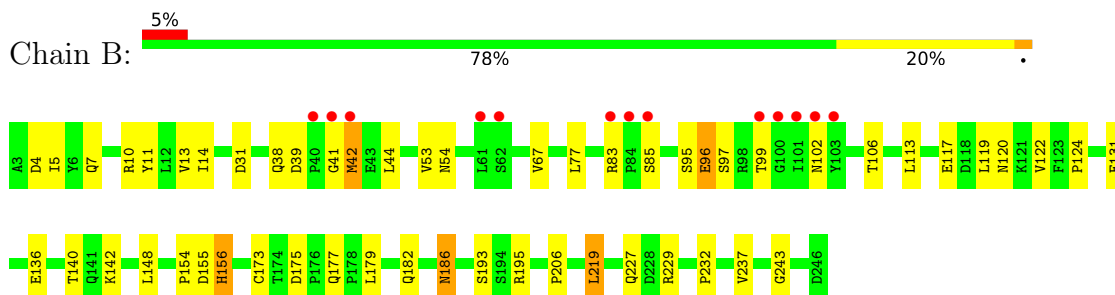
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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



- Molecule 2: TCR 5E



4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	64.06Å 64.06Å 185.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.66 – 2.60 61.66 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.0 (61.66-2.60) 96.0 (61.66-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.59Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.217 , 0.318 0.211 , 0.305	Depositor DCC
R_{free} test set	656 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtrriage
Anisotropy	0.112	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.055 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3453	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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	A	0.56	0/1469	0.82	0/1983
2	B	0.58	0/2001	0.88	3/2723 (0.1%)
All	All	0.57	0/3470	0.85	3/4706 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	95	SER	N-CA-C	5.19	116.17	108.60
2	B	177	GLN	N-CA-C	5.10	116.50	108.23
2	B	156	HIS	N-CA-C	5.05	117.48	107.98

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	1444	0	1390	35	0
2	B	1948	0	1842	25	0
3	A	16	0	0	1	0
3	B	45	0	0	1	0
All	All	3453	0	3232	56	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 8.

All (56) 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:81:ARG:HH11	1:A:81:ARG:HG3	1.16	1.09
1:A:106:ARG:HH11	1:A:106:ARG:HG3	1.30	0.92
1:A:81:ARG:HG3	1:A:81:ARG:NH1	1.89	0.84
1:A:181:ASN:HD22	1:A:181:ASN:N	1.76	0.84
1:A:181:ASN:HD22	1:A:181:ASN:H	1.27	0.81
1:A:106:ARG:HH11	1:A:106:ARG:CG	1.98	0.76
1:A:65:THR:HG23	1:A:74:SER:HB3	1.70	0.72
1:A:181:ASN:H	1:A:181:ASN:ND2	1.88	0.72
1:A:190:ALA:O	1:A:191:PHE:HB2	1.88	0.71
1:A:106:ARG:HG3	1:A:106:ARG:NH1	2.02	0.67
1:A:81:ARG:HH11	1:A:81:ARG:CG	2.01	0.66
2:B:140:THR:HG23	2:B:142:LYS:H	1.61	0.65
2:B:96:GLU:CD	2:B:97:SER:H	2.06	0.62
2:B:136:GLU:O	2:B:140:THR:HG22	2.01	0.61
1:A:30:ILE:HG22	1:A:94:ASP:HB3	1.82	0.60
1:A:15:GLN:HE22	1:A:144:SER:HB3	1.66	0.60
2:B:99:THR:HG23	2:B:102:ASN:HB2	1.87	0.56
1:A:111:THR:HG21	1:A:113:TRP:CZ2	2.42	0.54
1:A:190:ALA:O	1:A:191:PHE:CB	2.56	0.54
2:B:83:ARG:HB3	3:B:2013:HOH:O	2.07	0.54
1:A:42:ARG:HD3	2:B:10:ARG:HH12	1.74	0.53
1:A:181:ASN:N	1:A:181:ASN:ND2	2.43	0.52
1:A:95:ARG:HB3	1:A:99:LEU:HD22	1.91	0.52
2:B:122:VAL:O	2:B:229:ARG:NH2	2.41	0.51
1:A:123:VAL:HA	1:A:138:LEU:O	2.13	0.49
2:B:175:ASP:OD1	2:B:195:ARG:NH2	2.41	0.48
2:B:206:PRO:HA	2:B:243:GLY:O	2.14	0.47
2:B:186:ASN:OD1	2:B:186:ASN:N	2.37	0.47
1:A:31:ASN:HA	1:A:52:SER:HB3	1.97	0.47
1:A:125:GLN:HE21	1:A:125:GLN:HB2	1.58	0.46
1:A:61:ARG:HD2	1:A:78:THR:O	2.17	0.45
2:B:41:GLY:O	2:B:42:MET:HG2	2.15	0.45
2:B:53:VAL:O	2:B:54:ASN:HB2	2.17	0.45
1:A:164:LEU:HB3	2:B:173:CYS:HB2	1.99	0.44
2:B:67:VAL:HG13	2:B:77:LEU:HD23	1.99	0.44
1:A:126:LEU:HB3	2:B:131:GLU:O	2.17	0.44
2:B:5:ILE:HG21	2:B:106:THR:HG22	1.98	0.44
2:B:39:ASP:C	2:B:41:GLY:H	2.24	0.44
1:A:27:LYS:O	1:A:71:LYS:HD3	2.17	0.44
1:A:40:SER:O	1:A:42:ARG:NH1	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ASP:OD1	1:A:167:ARG:NH1	2.51	0.43
1:A:117:GLN:NE2	1:A:171:PHE:HA	2.33	0.43
1:A:32:ASN:HD21	1:A:49:LEU:HD11	1.83	0.43
1:A:95:ARG:HB3	1:A:100:GLY:HA2	1.99	0.43
1:A:65:THR:CG2	1:A:74:SER:HB3	2.45	0.42
2:B:11:TYR:CD1	2:B:156:HIS:HB3	2.55	0.42
2:B:120:ASN:OD1	2:B:227:GLN:HG3	2.19	0.42
2:B:154:PRO:HB2	2:B:155:ASP:H	1.54	0.42
2:B:41:GLY:O	2:B:42:MET:CB	2.67	0.42
1:A:159:THR:HG21	2:B:193:SER:OG	2.20	0.42
1:A:47:LEU:HD22	1:A:62:LEU:HD21	2.02	0.41
2:B:38:GLN:HE21	2:B:38:GLN:HB3	1.71	0.41
2:B:219:LEU:HD12	2:B:219:LEU:HA	1.84	0.41
2:B:124:PRO:HD3	2:B:232:PRO:HB3	2.02	0.41
1:A:55:ARG:HE	1:A:56:GLU:H	1.69	0.40
1:A:157:TYR:HA	3:A:2012:HOH:O	2.21	0.40

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	182/184 (99%)	158 (87%)	21 (12%)	3 (2%)	7	16
2	B	242/244 (99%)	228 (94%)	12 (5%)	2 (1%)	16	34
All	All	424/428 (99%)	386 (91%)	33 (8%)	5 (1%)	10	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	SER
1	A	191	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	42	MET
2	B	85	SER
1	A	100	GLY

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	163/163 (100%)	143 (88%)	20 (12%)	4 9
2	B	215/215 (100%)	199 (93%)	16 (7%)	13 29
All	All	378/378 (100%)	342 (90%)	36 (10%)	8 18

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	CYS
1	A	31	ASN
1	A	55	ARG
1	A	57	LYS
1	A	62	LEU
1	A	65	THR
1	A	77	ILE
1	A	78	THR
1	A	81	ARG
1	A	95	ARG
1	A	99	LEU
1	A	101	ARG
1	A	106	ARG
1	A	125	GLN
1	A	126	LEU
1	A	129	SER
1	A	130	LYS
1	A	144	SER
1	A	175	SER
1	A	181	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	4	ASP
2	B	7	GLN
2	B	13	VAL
2	B	14	ILE
2	B	31	ASP
2	B	44	LEU
2	B	96	GLU
2	B	113	LEU
2	B	117	GLU
2	B	119	LEU
2	B	148	LEU
2	B	179	LEU
2	B	182	GLN
2	B	186	ASN
2	B	219	LEU
2	B	237	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	23	ASN
1	A	32	ASN
1	A	34	GLN
1	A	38	GLN
1	A	125	GLN
1	A	147	ASN
1	A	174	ASN
1	A	181	ASN
2	B	38	GLN
2	B	48	HIS
2	B	89	GLN
2	B	139	HIS
2	B	141	GLN
2	B	156	HIS
2	B	169	HIS
2	B	208	ASN
2	B	227	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	A	184/184 (100%)	0.14	5 (2%) 56 50	11, 23, 35, 43	0
2	B	244/244 (100%)	0.18	13 (5%) 32 26	5, 21, 40, 58	0
All	All	428/428 (100%)	0.16	18 (4%) 40 35	5, 22, 38, 58	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	100	GLY	4.1
1	A	97	SER	3.8
2	B	99	THR	3.5
1	A	96	GLY	3.4
2	B	61	LEU	3.3
2	B	103	TYR	3.1
2	B	85	SER	3.1
1	A	69	SER	3.0
2	B	40	PRO	2.9
2	B	102	ASN	2.8
2	B	41	GLY	2.8
2	B	84	PRO	2.7
1	A	30	ILE	2.7
2	B	83	ARG	2.6
1	A	184	ASP	2.6
2	B	42	MET	2.4
2	B	62	SER	2.4
2	B	101	ILE	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.