WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 3, 2023 – 03:24 pm GMT

PDB ID : 2CDE

Title : Structure and binding kinetics of three different human CD1d-alpha- Galacto-sylceramide specific T cell receptors - iNKT-TCR

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 : 3.50 Å(reported)

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

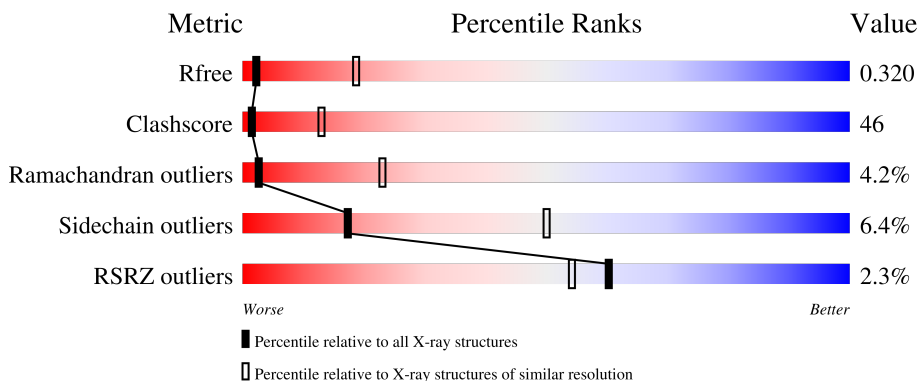|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Rfree		0.320
Clashscore		46
Ramachandran outliers		4.2%
Sidechain outliers		6.4%
RSRZ outliers		2.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 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 <=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	192	4% · 40% 53% 6% ·
1	C	192	3% · 36% 57% 6% ·
1	E	192	% · 38% 56% 6% ·
2	B	244	2% · 42% 51% 7%
2	D	244	2% · 42% 49% 8% ·

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Mol	Chain	Length	Quality of chain
2	F	244	2% 41% 51% 8%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 10330 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 INKT-TCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1495	923	256	308	8			
1	C	192	Total	C	N	O	S	0	0	0
			1495	923	256	308	8			
1	E	192	Total	C	N	O	S	0	0	0
			1483	915	255	305	8			

- Molecule 2 is a protein called INKT-TCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1952	1227	334	384	7			
2	D	244	Total	C	N	O	S	0	0	0
			1952	1227	334	384	7			
2	F	244	Total	C	N	O	S	0	0	0
			1953	1227	334	385	7			

3 Residue-property plots ⓘ

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: INKT-TCR

Chain A:

- Molecule 1: INKT-TCR

Chain C:

- Molecule 1: INKT-TCR

Chain E:

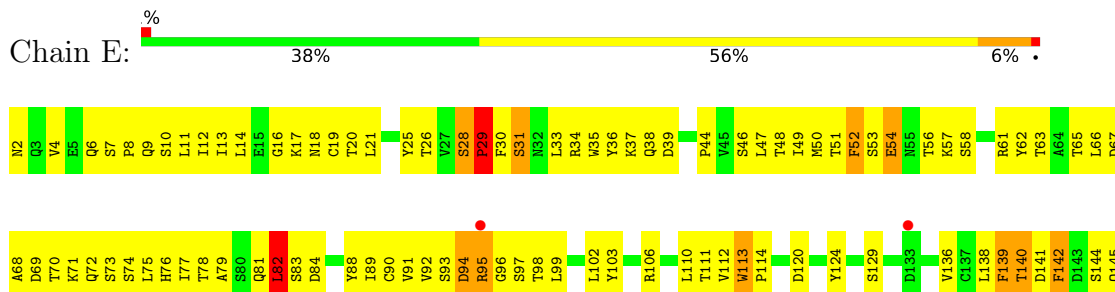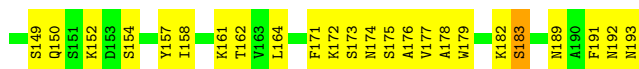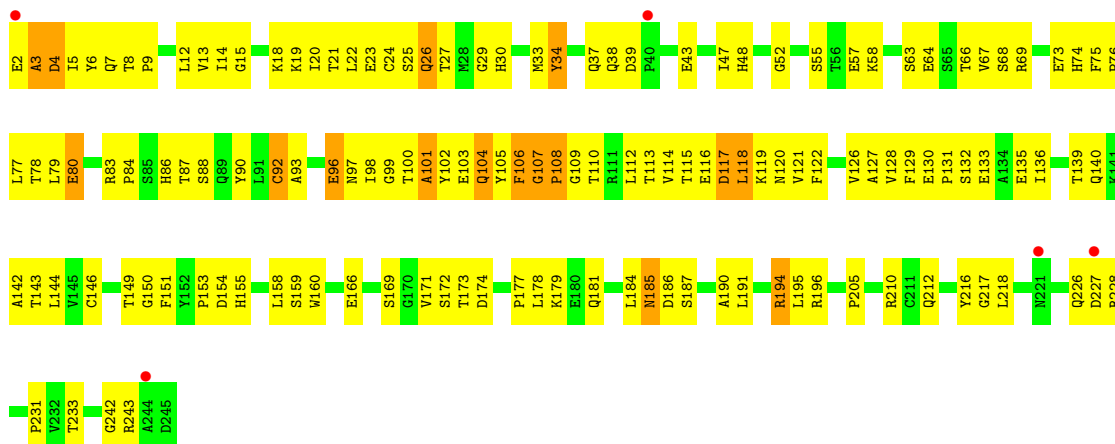S149 Q150 S151 K152 D153 S154 Y157 I158 K161 T162 V163 L164 F171 K172 S173 N174 S175 A176 V177 A178 W179 K182 S183 N189 A190 F191 N192 N193

• Molecule 2: INKT-TCR

Chain B:

| 2% | 42% | 51% | 7% |

E2 A3 D4 I5 Y6 Q7 T8 P9 L12 V13 I14 G15 K18 K19 I20 T21 L22 E23 C24 S25 Q26 T27 M28 G29 H30 M33 Y34 Q37 Q38 D39 P40 E43 I47 H48 G52 S55 T56 E57 K58 S63 E64 S65 T66 V67 S68 R69 E73 H74 F75 P76

L77 T78 L79 E80 R83 P84 S85 H86 T87 S88 Q89 Y90 L91 C92 A93 E96 N97 I98 G99 T100 A101 Y102 E103 Q104 Y105 F106 G107 P108 G109 T110 R111 L112 T113 V114 T115 E116 D117 L118 K119 N120 V121 F122 V126 A127 V128 F129 E130 P131 S132 E133 A134 E135 I136 T139 Q140 K141

A142 T143 L144 V145 C146 T149 G150 F151 Y152 P153 D154 H155 L158 S159 W160 E166 S169 G170 V171 S172 T173 D174 P177 L178 K179 E180 Q181 L184 N185 D186 S187 A190 L191 R194 L195 R196 P205 R210 C211 Q212 Y216 G217 L218 N221 Q226 D227 R228

P231 V232 T233 G242 R243 A244 D245

• Molecule 2: INKT-TCR

Chain D:

| 2% | 42% | 49% | 8% | • |

E2 A3 D4 I5 Y6 Q7 T8 P9 R10 Y11 L12 V13 I14 G15 T16 I20 T21 L22 E23 C24 S25 Q26 T27 M28 G29 H30 Y34 W35 Y36 Q37 Q38 D39 P40 E43 L44 H45 L46 I47 H48 Y49 G59 D60 L61 S62 S63 E64 S65 T66 V67 S68 R69 E73 H74 F75 P76

L77 T78 L79 R83 P84 S85 H86 T87 S88 Q89 Y90 L91 C92 A93 E96 N97 I98 G99 T100 A101 Y102 E103 Q104 Y105 F106 G107 P108 G109 T110 R111 L112 T113 V114 T115 E116 D117 L118 K119 N120 V121 F122 P123 P124 V128 P131 S132 E133 I136 T139 Q140 K141 A142 T143 L144

V145 C146 L147 A148 T149 G150 F151 Y152 P153 D154 H155 L158 S159 W160 E166 V171 S172 T173 D174 P177 L178 K179 E180 Q181 L184 N185 D186 S187 A190 L191 R194 L195 R196 A199 Q203 D204 P205 H208 F209 R210 C211 Q212 Y216 G217 L218 S219 E220 Q226

D227 P231 V232 T233 E239 A240 W241 G242 R243 A244 D245

• Molecule 2: INKT-TCR

Chain F:

| 2% | 41% | 51% | 8% |

E2 A3 D4 I5 Y6 Q7 T8 P9 R10 Y11 L12 V13 I14 G17 I20 T21 L22 E23 C24 S25 Q26 T27 M28 G29 H30 D31 K32 M33 Y34 W35 Y36 Q37 Q38 D39 P40 E43 L44 I47 H48 G52 E57 K58 S63 E64 S65 T66 V67 S68 R69 E73 H74 F75

P76 L77 T78 L79 E80 S81 A82 R83 H86 T87 S88 Q89 Y90 L91 C92 A93 E96 N97 I98 G99 T100 A101 Y102 E103 Q104 Y105 F106 G107 P108 G109 T110 R111 L112 T113 V114 D117 L118 K119 N120 V121 F122 P123 P124 V126 A127 E130 P131 S132 E133 A134 E135 I136 T139 Q140

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	289.36Å 84.95Å 78.86Å 90.00° 103.30° 90.00°	Depositor
Resolution (Å)	30.00 – 3.50 19.99 – 3.48	Depositor EDS
% Data completeness (in resolution range)	98.9 (30.00-3.50) 97.9 (19.99-3.48)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.96 (at 3.44Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.283 , 0.350 0.268 , 0.320	Depositor DCC
R_{free} test set	1203 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	79.8	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 56.1	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.035 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	10330	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.34	0/1522	0.59	0/2064
1	C	0.35	0/1522	0.58	0/2064
1	E	0.39	0/1509	0.62	1/2046 (0.0%)
2	B	0.34	0/2006	0.59	0/2733
2	D	0.35	0/2006	0.61	1/2733 (0.0%)
2	F	0.36	0/2007	0.61	0/2733
All	All	0.36	0/10572	0.60	2/14373 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	114	PRO	N-CA-CB	5.53	109.94	103.30
2	D	152	TYR	C-N-CD	5.03	138.96	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	1495	0	1434	160	0
1	C	1495	0	1434	160	0
1	E	1483	0	1411	165	0
2	B	1952	0	1840	180	0
2	D	1952	0	1840	168	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1953	0	1840	169	0
All	All	10330	0	9799	930	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 46.

The worst 5 of 930 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)
2:D:8:THR:HB	2:D:9:PRO:HD2	1.16	1.12
1:C:136:VAL:HG12	1:C:179:TRP:HB3	1.35	1.07
1:E:82:LEU:H	1:E:82:LEU:HD23	1.21	1.06
2:F:34:TYR:HB2	2:F:93:ALA:HB3	1.37	1.03
1:E:13:ILE:HG12	1:E:17:LYS:HD2	1.40	1.03

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	190/192 (99%)	157 (83%)	25 (13%)	8 (4%)	3	23
1	C	190/192 (99%)	153 (80%)	28 (15%)	9 (5%)	2	20
1	E	190/192 (99%)	155 (82%)	27 (14%)	8 (4%)	3	23
2	B	242/244 (99%)	206 (85%)	27 (11%)	9 (4%)	3	26
2	D	242/244 (99%)	200 (83%)	30 (12%)	12 (5%)	2	19
2	F	242/244 (99%)	203 (84%)	30 (12%)	9 (4%)	3	26
All	All	1296/1308 (99%)	1074 (83%)	167 (13%)	55 (4%)	3	23

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	GLU
1	A	95	ARG
1	A	154	SER
1	C	54	GLU
1	C	55	ASN

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	174/174 (100%)	162 (93%)	12 (7%)	15	47
1	C	174/174 (100%)	163 (94%)	11 (6%)	18	51
1	E	170/174 (98%)	157 (92%)	13 (8%)	13	43
2	B	215/215 (100%)	204 (95%)	11 (5%)	24	57
2	D	215/215 (100%)	199 (93%)	16 (7%)	13	44
2	F	215/215 (100%)	204 (95%)	11 (5%)	24	57
All	All	1163/1167 (100%)	1089 (94%)	74 (6%)	17	50

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	94	ASP
2	F	176	GLN
1	E	113	TRP
2	F	26	GLN
1	C	28	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	76	HIS
2	F	176	GLN
1	E	145	GLN
2	F	89	GLN

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Mol	Chain	Res	Type
2	F	207	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 monosaccharides 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, 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(Å²)	Q<0.9
1	A	192/192 (100%)	0.07	7 (3%)	42	38	19, 64, 91, 98	0
1	C	192/192 (100%)	0.01	5 (2%)	56	49	9, 51, 85, 104	0
1	E	192/192 (100%)	-0.23	2 (1%)	82	77	7, 38, 82, 102	0
2	B	244/244 (100%)	-0.05	5 (2%)	65	60	16, 57, 85, 93	0
2	D	244/244 (100%)	-0.16	6 (2%)	57	51	9, 52, 82, 95	0
2	F	244/244 (100%)	-0.28	5 (2%)	65	60	7, 37, 74, 106	0
All	All	1308/1308 (100%)	-0.11	30 (2%)	60	54	7, 51, 85, 106	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	133	ASP	5.2
1	A	133	ASP	4.3
1	C	133	ASP	4.0
2	F	2	GLU	3.9
2	D	185	ASN	3.5

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 monosaccharides 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.