WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Aug 26, 2024 – 02:21 PM JST

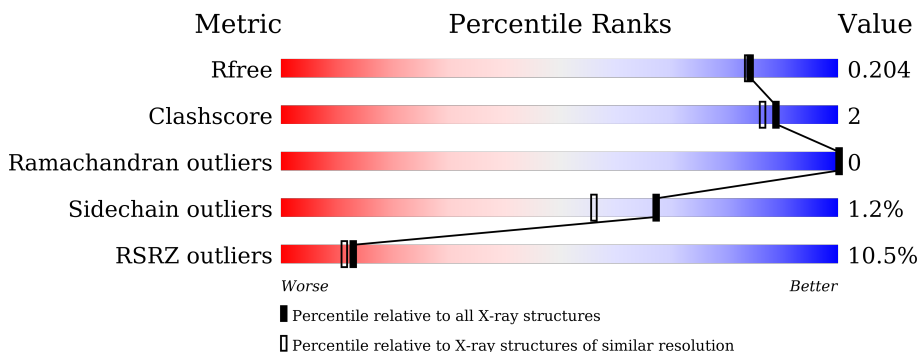|		
PDB ID	:	8W90
Title	:	crystal structure of CD4-D1D2 with Nb457
Authors	:	Wang, X.Y.; Wang, Y.X.
Deposited on	:	2023-09-04
Resolution	:	1.81 Å(reported)

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 1.81 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		0.204
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		1.2%
RSRZ outliers		10.5%

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$_{free}$	164625	9242 (1.84-1.80)
Clashscore	180529	1080 (1.82-1.82)
Ramachandran outliers	177936	1073 (1.82-1.82)
Sidechain outliers	177891	1073 (1.82-1.82)
RSRZ outliers	164620	9241 (1.84-1.80)

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	134	3% / 89% · 10%
1	C	134	3% / 91% · 7%
1	E	134	5% / 87% 6% 7%
2	B	178	3% / 94% 6%
2	D	178	9% / 88% 6% · 5%
2	F	178	31% / 83% 7% 10%

2   Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 6936 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 NB457.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	0	0	0
			913	569	158	182	4			
1	C	125	Total	C	N	O	S	0	0	0
			937	581	165	186	5			
1	E	124	Total	C	N	O	S	0	0	0
			935	581	164	186	4			

- Molecule 2 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	178	Total	C	N	O	S	0	0	0
			1383	865	242	272	4			
2	D	169	Total	C	N	O	S	0	0	0
			1308	821	226	257	4			
2	F	161	Total	C	N	O	S	0	0	0
			1250	781	219	246	4			

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total	O	0	0
			42	42		
3	B	59	Total	O	0	0
			59	59		
3	C	38	Total	O	0	0
			38	38		
3	D	37	Total	O	0	0
			37	37		
3	E	28	Total	O	0	0
			28	28		
3	F	6	Total	O	0	0
			6	6		

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.

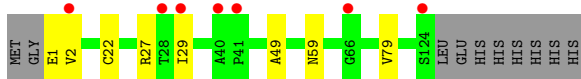- Molecule 1: NB457
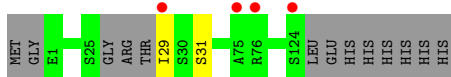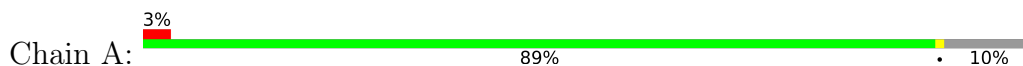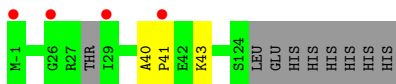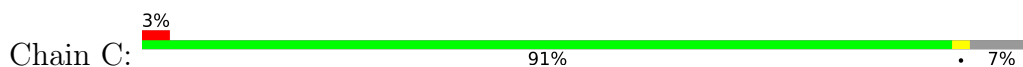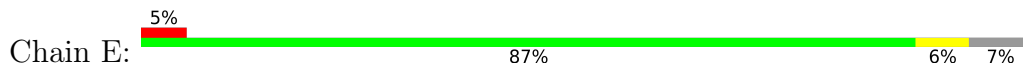
Chain A:

- Molecule 1: NB457

Chain C:

- Molecule 1: NB457

Chain E:

- Molecule 2: T-cell surface glycoprotein CD4

Chain B:

- Molecule 2: T-cell surface glycoprotein CD4

Chain D:

- Molecule 2: T-cell surface glycoprotein CD4

Chain F:

31%

83%

7% 10%

K1 K2 G6 T17 A18 SER GLN LYS LYS SER I24 Q25 F26 H27 W28 K29 Q33 I34 K35 I36 L37 G38 N39 GLN GLY SER PHE LEU THR LYS GLY PRO S49 K50 L51 N52 D53 S60 L61 W62 N66 F67 P68 L69 I70 I71 K72 N73 I83 V86 V93

S104 L109 Q110 G111 L118 S125 C130 R131 S132 P133 R134 G135 K136 N137 I138 Q139 G140 G141 K142 V146 S147 Q148 L149 GLU LEU Q152 D153 S154 T158 C159 T160 V161 L162 I172 L177 ALA
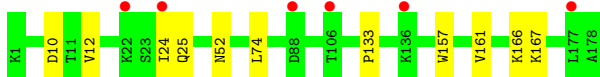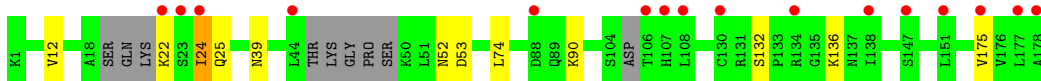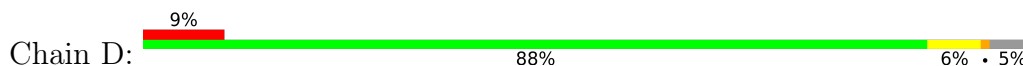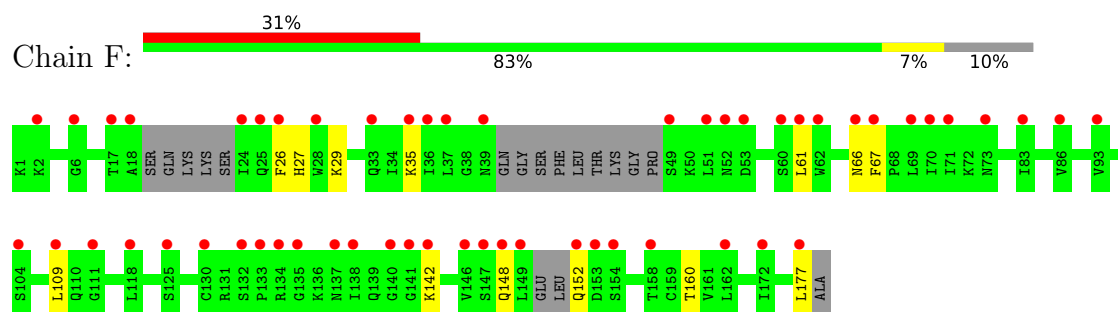
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	47.08Å 141.98Å 81.66Å 90.00° 97.93° 90.00°	Depositor
Resolution (Å)	24.25 – 1.81 24.25 – 1.81	Depositor EDS
% Data completeness (in resolution range)	99.3 (24.25-1.81) 99.3 (24.25-1.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 1.80Å)	Xtriage
Refinement program	PHENIX dev_3942	Depositor
R, R_{free}	0.186 , 0.206 0.185 , 0.204	Depositor DCC
R_{free} test set	4782 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 48.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6936	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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	0.39	0/928	0.56	0/1256
1	C	0.39	0/952	0.58	0/1286
1	E	0.37	0/951	0.58	0/1288
2	B	0.38	0/1402	0.54	0/1891
2	D	0.33	0/1323	0.51	0/1783
2	F	0.27	0/1264	0.46	0/1703
All	All	0.35	0/6820	0.53	0/9207

There are no bond length outliers.

There are no bond angle outliers.

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	913	0	884	1	0
1	C	937	0	903	2	0
1	E	935	0	908	4	0
2	B	1383	0	1414	6	0
2	D	1308	0	1324	7	0
2	F	1250	0	1264	5	0
3	A	42	0	0	0	0
3	B	59	0	0	1	0
3	C	38	0	0	0	0
3	D	37	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	28	0	0	0	0
3	F	6	0	0	0	0
All	All	6936	0	6697	24	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 2.

The worst 5 of 24 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:B:52:ASN:HB2	3:B:203:HOH:O	1.98	0.63
1:A:29:ILE:HG23	1:A:31:SER:H	1.70	0.56
2:F:61:LEU:HB3	2:F:66:ASN:HB2	1.89	0.55
1:C:41:PRO:O	1:C:43:LYS:HD2	2.06	0.55
1:C:40:ALA:HB3	1:C:43:LYS:HD3	1.94	0.49

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	117/134 (87%)	116 (99%)	1 (1%)	0	100	100
1	C	121/134 (90%)	118 (98%)	3 (2%)	0	100	100
1	E	122/134 (91%)	120 (98%)	2 (2%)	0	100	100
2	B	176/178 (99%)	171 (97%)	5 (3%)	0	100	100
2	D	161/178 (90%)	157 (98%)	4 (2%)	0	100	100
2	F	153/178 (86%)	147 (96%)	6 (4%)	0	100	100
All	All	850/936 (91%)	829 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	95/106 (90%)	95 (100%)	0	100	100
1	C	96/106 (91%)	96 (100%)	0	100	100
1	E	97/106 (92%)	96 (99%)	1 (1%)	73	62
2	B	161/161 (100%)	160 (99%)	1 (1%)	84	78
2	D	151/161 (94%)	148 (98%)	3 (2%)	50	35
2	F	145/161 (90%)	141 (97%)	4 (3%)	38	21
All	All	745/801 (93%)	736 (99%)	9 (1%)	67	56

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	152	GLN
2	F	160	THR
2	D	175	VAL
1	E	27	ARG
2	F	142	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides 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 (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(Å²)	Q<0.9
1	A	121/134 (90%)	0.22	4 (3%)	49	49	22, 31, 51, 65	0
1	C	125/134 (93%)	0.21	4 (3%)	50	50	22, 30, 57, 73	0
1	E	124/134 (92%)	0.34	7 (5%)	31	30	23, 33, 59, 73	0
2	B	178/178 (100%)	0.16	6 (3%)	48	48	20, 31, 59, 87	0
2	D	169/178 (94%)	0.56	16 (9%)	15	14	22, 37, 71, 84	0
2	F	161/178 (90%)	1.65	55 (34%)	1	1	39, 61, 90, 110	0
All	All	878/936 (93%)	0.55	92 (10%)	13	11	20, 35, 77, 110	0

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	29	ILE	7.0
1	C	29	ILE	5.4
2	F	24	ILE	5.3
2	D	44	LEU	4.7
1	C	41	PRO	4.1

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 monosaccharides 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.