WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 13, 2024 – 08:47 AM EDT

PDB ID	:	1OAY
Title	:	Antibody multispecificity mediated by conformational diversity
Authors	:	James, L.C.; Roversi, P.; Tawfik, D.
Deposited on	:	2003-01-21
Resolution	:	2.66 Å(reported)

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

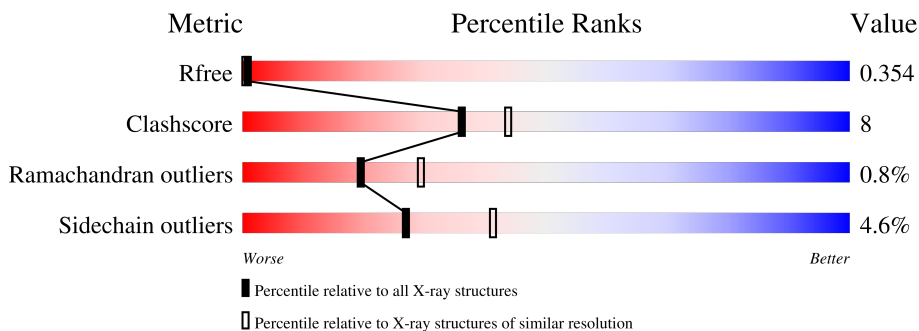|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.66 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		0.354
Clashscore		8
Ramachandran outliers		0.8%
Sidechain outliers		4.6%

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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)

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%

Mol	Chain	Length	Quality of chain
1	H	122	90% 9% •
1	J	122	89% 10% •
2	L	110	91% • • • •
2	M	110	63% 13% • 23%
2	N	110	90% • • • •
2	O	110	68% 14% • 16%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 5134 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 IMMUNOGLOBULIN E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	121	Total	C	N	O	S	0	0	0
			952	611	157	179	5			
1	J	121	Total	C	N	O	S	0	0	0
			952	611	157	179	5			

- Molecule 2 is a protein called IMMUNOGLOBULIN E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	108	Total	C	N	O	S	0	0	0
			796	500	138	156	2			
2	M	85	Total	C	N	O	S	0	0	0
			625	390	109	124	2			
2	N	107	Total	C	N	O	S	0	0	0
			788	496	136	154	2			
2	O	92	Total	C	N	O	S	0	0	0
			671	419	117	133	2			

- Molecule 3 is Furazolidone (three-letter code: FUR) (formula: $C_8H_5N_3O_5$).

FUR
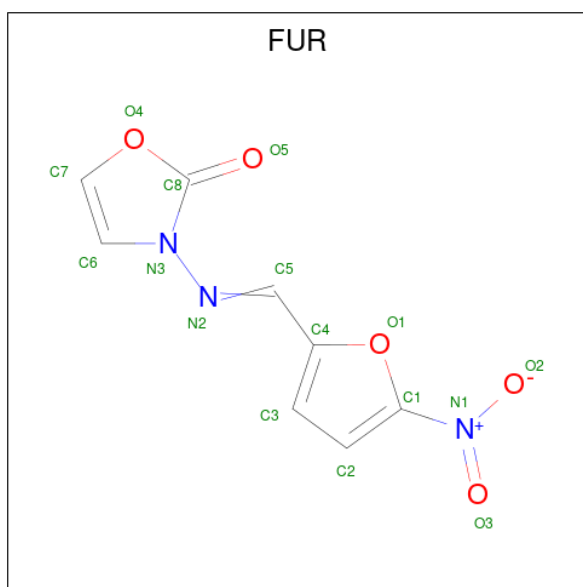
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total 16	C 8	N 3	O 5	0	0
3	J	1	Total 16	C 8	N 3	O 5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	80	Total 80	O 80	0	0
4	J	58	Total 58	O 58	0	0
4	L	65	Total 65	O 65	0	0
4	M	22	Total 22	O 22	0	0
4	N	74	Total 74	O 74	0	0
4	O	19	Total 19	O 19	0	0

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. 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. 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: IMMUNOGLOBULIN E

Chain H:

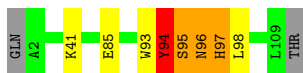- Molecule 1: IMMUNOGLOBULIN E

Chain J:
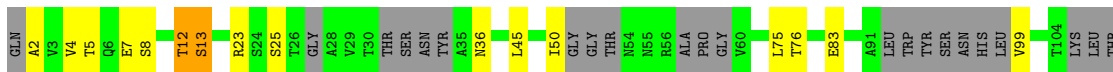
- Molecule 2: IMMUNOGLOBULIN E

Chain L:

- Molecule 2: IMMUNOGLOBULIN E

Chain M:

- Molecule 2: IMMUNOGLOBULIN E

Chain N:

- Molecule 2: IMMUNOGLOBULIN E

Chain O:

GLN A2 V3 V4 T5 Q6 E7 S8 S13 R23 T26 GLY A28 V29 T30 THR SER ASN TYR ALA N36 W37 V38 Q39 L45 I50 A57 PRO GLY VAL P61 L75 A86 I87 Y88 A91 LEU TRP TYR SER ASN HIS LEU V99 T104 K105 V108 L109 THR

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.17Å 79.14Å 168.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.66 37.26 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.00-2.66) 99.4 (37.26-2.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.258 , 0.280 0.340 , 0.354	Depositor DCC
R_{free} test set	2421 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 8.9	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.459 for k,h,-l	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	5134	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FUR

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	H	0.26	0/980	0.56	2/1329 (0.2%)
1	J	0.27	0/980	0.56	2/1329 (0.2%)
2	L	1.69	3/810 (0.4%)	0.95	6/1106 (0.5%)
2	M	0.32	0/628	0.59	0/845
2	N	1.89	5/801 (0.6%)	0.96	6/1093 (0.5%)
2	O	0.72	1/673 (0.1%)	0.66	2/906 (0.2%)
All	All	1.08	9/4872 (0.2%)	0.73	18/6608 (0.3%)

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
2	L	0	1
2	N	0	1
All	All	0	2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	94	TYR	CB-CG	38.60	2.09	1.51
2	L	94	TYR	CB-CG	38.56	2.09	1.51
2	N	97	HIS	CB-CG	26.01	1.96	1.50
2	L	97	HIS	CB-CG	26.01	1.96	1.50
2	N	95	SER	CA-CB	20.16	1.83	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	94	TYR	CB-CG-CD1	-13.67	112.80	121.00
2	L	94	TYR	CB-CG-CD1	-13.63	112.82	121.00
2	N	94	TYR	CA-CB-CG	-12.52	89.62	113.40
2	L	94	TYR	CA-CB-CG	-12.51	89.63	113.40
2	L	94	TYR	CB-CG-CD2	12.31	128.39	121.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	94	TYR	Sidechain
2	N	94	TYR	Sidechain

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	H	952	0	913	5	0
1	J	952	0	913	6	0
2	L	796	0	777	17	0
2	M	625	0	611	21	0
2	N	788	0	771	18	0
2	O	671	0	662	18	0
3	H	16	0	2	0	0
3	J	16	0	2	0	0
4	H	80	0	0	0	0
4	J	58	0	0	0	0
4	L	65	0	0	0	0
4	M	22	0	0	1	0
4	N	74	0	0	0	0
4	O	19	0	0	1	0
All	All	5134	0	4651	76	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.

The worst 5 of 76 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:N:95:SER:CA	2:N:95:SER:CB	1.83	1.54
2:N:97:HIS:CB	2:N:97:HIS:CG	1.96	1.48
2:L:97:HIS:CB	2:L:97:HIS:CG	1.96	1.48
2:O:7:GLU:C	2:O:8:SER:N	1.72	1.41
2:N:94:TYR:CB	2:N:94:TYR:CG	2.09	1.36

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	H	119/122 (98%)	112 (94%)	7 (6%)	0	100	100
1	J	119/122 (98%)	114 (96%)	5 (4%)	0	100	100
2	L	106/110 (96%)	94 (89%)	10 (9%)	2 (2%)	8	11
2	M	69/110 (63%)	57 (83%)	12 (17%)	0	100	100
2	N	103/110 (94%)	93 (90%)	8 (8%)	2 (2%)	8	11
2	O	78/110 (71%)	62 (80%)	15 (19%)	1 (1%)	12	18
All	All	594/684 (87%)	532 (90%)	57 (10%)	5 (1%)	19	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	95	SER
2	L	85	GLU
2	N	85	GLU
2	N	95	SER
2	O	86	ALA

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	H	99/101 (98%)	93 (94%)	6 (6%)	18	29
1	J	99/101 (98%)	93 (94%)	6 (6%)	18	29
2	L	84/87 (97%)	83 (99%)	1 (1%)	71	84
2	M	67/87 (77%)	62 (92%)	5 (8%)	13	21
2	N	83/87 (95%)	81 (98%)	2 (2%)	49	67
2	O	71/87 (82%)	68 (96%)	3 (4%)	30	45
All	All	503/550 (92%)	480 (95%)	23 (5%)	27	41

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	13	SER
2	M	83	GLU
2	M	45	LEU
2	N	41	LYS
1	J	11	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	5	GLN
1	H	112	GLN
1	J	5	GLN
1	J	112	GLN

5.3.3 RNA (i)

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 ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	FUR	H	500	-	7,17,17	3.54	4 (57%)	4,23,23	27.88	3 (75%)
3	FUR	J	500	-	7,17,17	3.54	4 (57%)	4,23,23	27.58	3 (75%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUR	H	500	-	-	1/1/9/9	0/2/2/2
3	FUR	J	500	-	-	1/1/9/9	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	500	FUR	C1-N1	-6.51	1.33	1.45
3	H	500	FUR	C1-N1	-6.49	1.33	1.45
3	H	500	FUR	C3-C2	-5.30	1.12	1.39
3	J	500	FUR	C3-C2	-5.29	1.12	1.39
3	J	500	FUR	C6-N3	3.11	1.46	1.38

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	500	FUR	C4-C5-N2	53.17	172.28	121.06
3	J	500	FUR	C4-C5-N2	52.56	171.70	121.06
3	H	500	FUR	C2-C3-C4	16.43	120.46	106.30
3	J	500	FUR	C2-C3-C4	16.35	120.39	106.30
3	H	500	FUR	C7-C6-N3	-3.12	101.37	109.93

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	500	FUR	C4-C5-N2-N3
3	J	500	FUR	C4-C5-N2-N3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	O	3
2	M	2
2	N	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	22:CYS	C	23:ARG	N	3.21
1	O	22:CYS	C	23:ARG	N	3.18
1	O	104:THR	C	105:LYS	N	2.86
1	M	7:GLU	C	8:SER	N	2.66
1	O	7:GLU	C	8:SER	N	1.72

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.