wwPDB X-ray Structure Validation Summary Report (i)

Nov 10, 2024 – 01:56 am GMT

PDB ID	:	1OAX
Title	:	Fv Structure of the IgE SPE-7 in complex with acenaphthenequinone
Authors	:	James, L.C.; Roversi, P.; Tawfik, D.
Deposited on	:	2003-01-21
Resolution	:	2.67 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

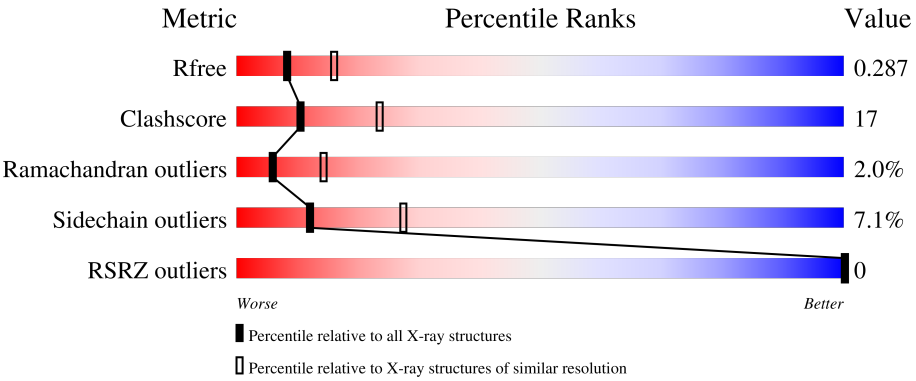
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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}	164625	4708 (2.70-2.66)
Clashscore	180529	5138 (2.70-2.66)
Ramachandran outliers	177936	5071 (2.70-2.66)
Sidechain outliers	177891	5071 (2.70-2.66)
RSRZ outliers	164620	4708 (2.70-2.66)

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	H	122	87% 11% •
1	J	122	89% 9% •
2	L	110	87% 9% • •
2	M	110	45% 45% 7% • •
2	N	110	85% 11% • •

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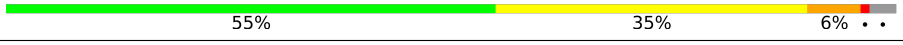
Mol	Chain	Length	Quality of chain
2	O	110	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5206 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.

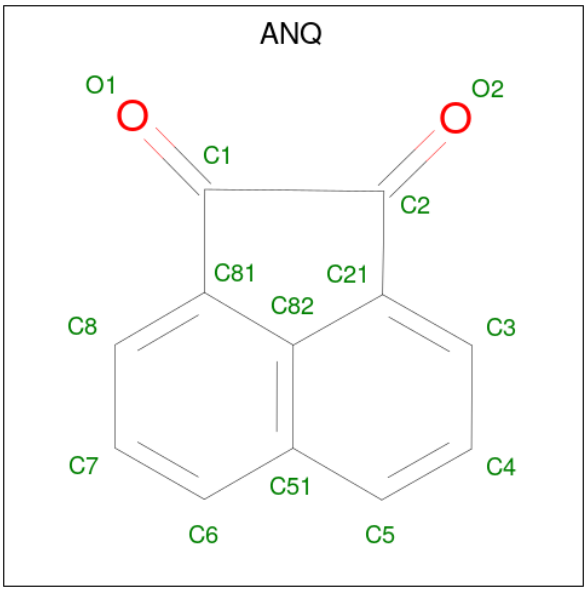
- Molecule 1 is a protein called IMMUNOGLOBULIN E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	122	Total	C	N	O	S	0	0	0
			961	616	158	182	5			
1	J	122	Total	C	N	O	S	0	0	0
			961	616	158	182	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
			798	502	138	156	2			
2	M	108	Total	C	N	O	S	0	0	0
			798	502	138	156	2			
2	N	108	Total	C	N	O	S	0	0	0
			798	502	138	156	2			
2	O	107	Total	C	N	O	S	0	0	0
			792	498	137	155	2			

- Molecule 3 is ACENAPHTHENEQUINONE (three-letter code: ANQ) (formula: $C_{12}H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total C O 14 12 2	0	0
3	J	1	Total C O 14 12 2	0	0

- Molecule 4 is water.

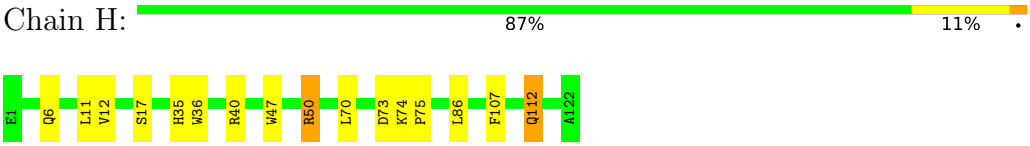
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	13	Total O 13 13	0	0
4	J	13	Total O 13 13	0	0
4	L	17	Total O 17 17	0	0
4	M	5	Total O 5 5	0	0
4	N	18	Total O 18 18	0	0
4	O	4	Total O 4 4	0	0

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.

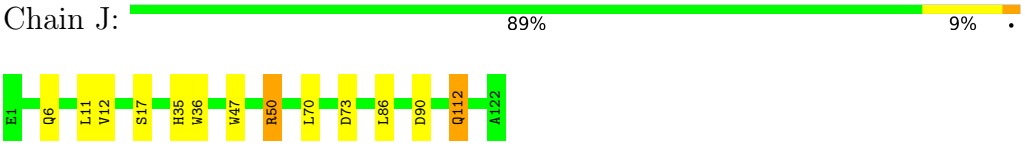
• Molecule 1: IMMUNOGLOBULIN E

Chain H:



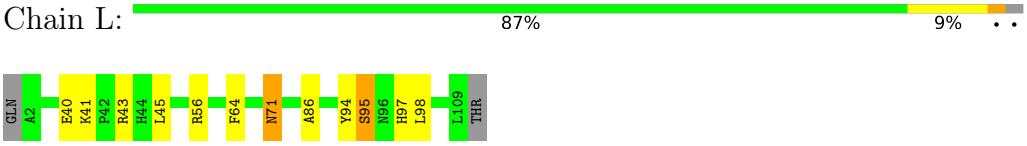
• Molecule 1: IMMUNOGLOBULIN E

Chain J:



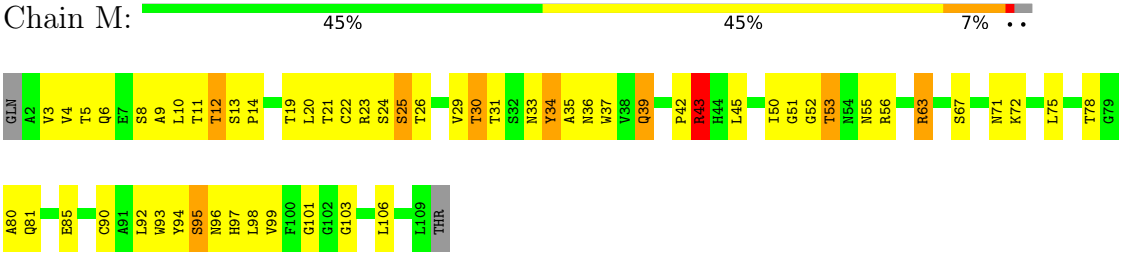
• Molecule 2: IMMUNOGLOBULIN E

Chain L:



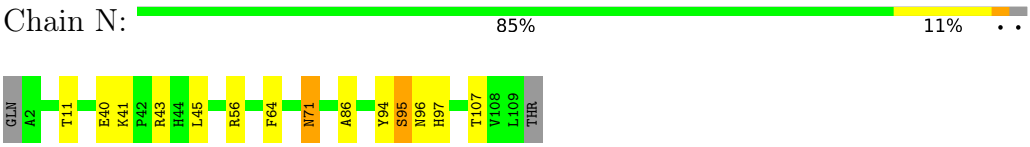
• Molecule 2: IMMUNOGLOBULIN E

Chain M:



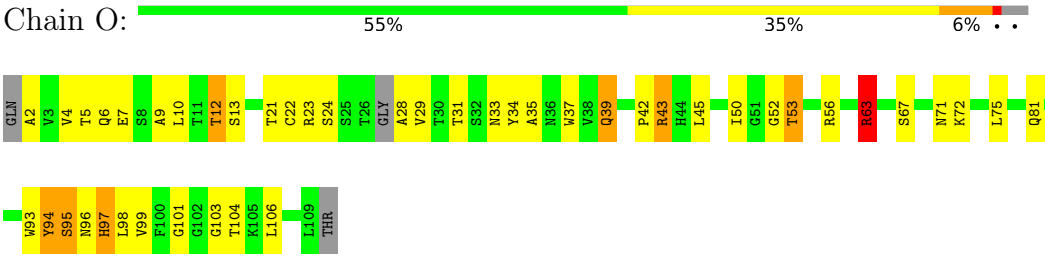
• Molecule 2: IMMUNOGLOBULIN E

Chain N:



• Molecule 2: IMMUNOGLOBULIN E

Chain O:


55%
35%
6%
GLN A2 V3 V4 T5 Q6 E7 S8 A9 L10 T11 T12 S13 T21 C22 R23 S24 S25 T26 GLY A28 V29 T30 T31 S32 N33 Y34 A35 N36 W37 V38 Q39 P42 R43 H44 L45 I50 G51 G52 T53 R56 R63 S67 N71 K72 L75 Q81 E85 C90
W93 Y94 S95 N96 H97 L98 V99 F100 G101 G102 G103 T104 K105 L106 L109 THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.73Å 78.64Å 167.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.53 – 2.67 39.53 – 2.67	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.53-2.67) 99.5 (39.53-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.238 , 0.282 0.284 , 0.287	Depositor DCC
R_{free} test set	1527 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	41.8	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 26.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.477 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5206	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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

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	0.35	0/989	0.68	1/1341 (0.1%)
1	J	0.34	0/989	0.67	2/1341 (0.1%)
2	L	0.40	1/814 (0.1%)	0.70	1/1112 (0.1%)
2	M	0.88	1/814 (0.1%)	1.03	2/1112 (0.2%)
2	N	0.42	1/814 (0.1%)	0.71	1/1112 (0.1%)
2	O	0.55	0/803	0.87	3/1096 (0.3%)
All	All	0.51	3/5223 (0.1%)	0.78	10/7114 (0.1%)

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	O	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	98	LEU	CB-CG	-14.54	1.10	1.52
2	N	97	HIS	CB-CG	5.73	1.60	1.50
2	L	97	HIS	CB-CG	5.18	1.59	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	98	LEU	CB-CG-CD1	-8.80	96.04	111.00
2	O	97	HIS	CA-CB-CG	6.46	124.58	113.60
2	O	63	ARG	NE-CZ-NH1	6.25	123.42	120.30
2	L	97	HIS	CA-CB-CG	6.06	123.91	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	94	TYR	CB-CG-CD1	5.93	124.56	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	O	28	ALA	Peptide

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	H	961	0	922	18	0
1	J	961	0	922	8	0
2	L	798	0	786	6	0
2	M	798	0	786	80	0
2	N	798	0	786	8	0
2	O	792	0	774	48	0
3	H	14	0	5	3	0
3	J	14	0	5	1	0
4	H	13	0	0	1	0
4	J	13	0	0	0	0
4	L	17	0	0	0	0
4	M	5	0	0	0	0
4	N	18	0	0	2	0
4	O	4	0	0	0	0
All	All	5206	0	4986	167	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 17.

The worst 5 of 167 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:M:5:THR:CG2	2:M:23:ARG:HD2	1.71	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:93:TRP:CE3	2:O:97:HIS:O	1.98	1.17
2:M:5:THR:CB	2:M:23:ARG:HD2	1.84	1.06
1:H:35:HIS:CD2	1:H:50:ARG:HB3	1.91	1.05
2:M:4:VAL:HG23	2:M:99:VAL:HG12	1.39	1.02

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	H	120/122 (98%)	119 (99%)	1 (1%)	0	100 100
1	J	120/122 (98%)	119 (99%)	1 (1%)	0	100 100
2	L	106/110 (96%)	98 (92%)	7 (7%)	1 (1%)	14 32
2	M	106/110 (96%)	88 (83%)	12 (11%)	6 (6%)	1 2
2	N	106/110 (96%)	98 (92%)	7 (7%)	1 (1%)	14 32
2	O	103/110 (94%)	87 (84%)	11 (11%)	5 (5%)	2 3
All	All	661/684 (97%)	609 (92%)	39 (6%)	13 (2%)	6 14

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	53	THR
2	O	53	THR
2	M	34	TYR
2	M	103	GLY
2	O	34	TYR

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	100/101 (99%)	96 (96%)	4 (4%)	27 51
1	J	100/101 (99%)	96 (96%)	4 (4%)	27 51
2	L	85/87 (98%)	81 (95%)	4 (5%)	22 45
2	M	85/87 (98%)	73 (86%)	12 (14%)	3 6
2	N	85/87 (98%)	81 (95%)	4 (5%)	22 45
2	O	83/87 (95%)	73 (88%)	10 (12%)	4 9
All	All	538/550 (98%)	500 (93%)	38 (7%)	12 27

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	12	THR
2	O	67	SER
2	O	24	SER
2	O	43	ARG
2	O	90	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	54	ASN
2	O	36	ASN
2	O	44	HIS
1	J	112	GLN
1	H	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 (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)

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	ANQ	H	500	-	16,16,16	3.28	11 (68%)	24,24,24	5.07	10 (41%)
3	ANQ	J	500	-	16,16,16	3.28	11 (68%)	24,24,24	5.04	9 (37%)

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	ANQ	H	500	-	-	-	0/3/3/3
3	ANQ	J	500	-	-	-	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	500	ANQ	C4-C3	-7.13	1.23	1.38
3	J	500	ANQ	C4-C3	-7.11	1.24	1.38
3	J	500	ANQ	C2-C1	-4.83	1.50	1.58
3	H	500	ANQ	C2-C1	-4.65	1.51	1.58
3	J	500	ANQ	C5-C51	4.00	1.51	1.41

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	500	ANQ	C4-C3-C21	15.47	147.34	119.56
3	J	500	ANQ	C4-C3-C21	15.41	147.24	119.56
3	J	500	ANQ	C3-C21-C82	-10.70	106.14	118.87
3	H	500	ANQ	C3-C21-C82	-10.70	106.15	118.87
3	H	500	ANQ	C3-C21-C2	8.05	143.06	133.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	500	ANQ	3	0
3	J	500	ANQ	1	0

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

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^{th} 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	H	122/122 (100%)	-1.39	0	100	100	27, 36, 51, 60	0
1	J	122/122 (100%)	-1.42	0	100	100	27, 36, 51, 60	0
2	L	108/110 (98%)	-1.46	0	100	100	25, 33, 42, 63	0
2	M	108/110 (98%)	-0.92	0	100	100	28, 60, 74, 81	0
2	N	108/110 (98%)	-1.52	0	100	100	25, 33, 42, 63	0
2	O	107/110 (97%)	-0.78	0	100	100	28, 60, 75, 80	0
All	All	675/684 (98%)	-1.26	0	100	100	25, 38, 72, 81	0

There are no RSRZ outliers to report.

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ANQ	H	500	14/14	0.98	0.08	54,54,55,56	0
3	ANQ	J	500	14/14	0.99	0.06	54,54,56,56	0

6.5 Other polymers (i)

There are no such residues in this entry.