wwPDB X-ray Structure Validation Summary Report (i)

Mar 5, 2026 – 01:57 AM UTC

PDB ID	:	3QMW / pdb_00003qmw
Title	:	RedJ with PEG molecule bound in the active site
Authors	:	Whicher, J.R.; Smith, J.L.
Deposited on	:	2011-02-05
Resolution	:	2.50 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:

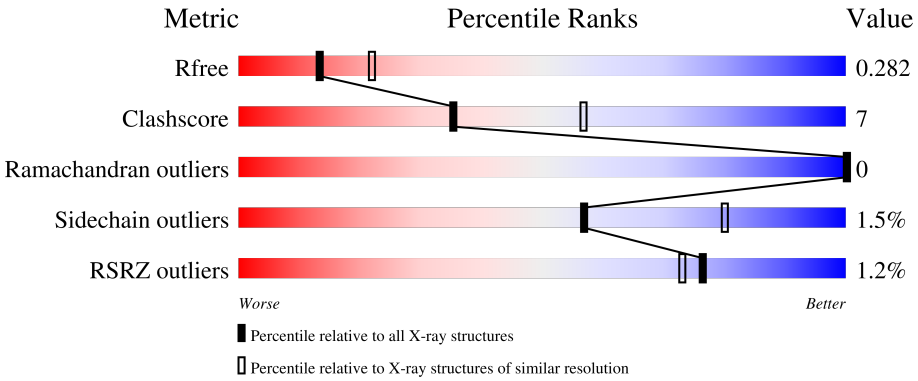
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	259	81% 12% • 5%
1	B	259	86% 9% 5%
1	C	259	3% 71% 21% • 7%
1	D	259	2% 77% 19% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7867 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.

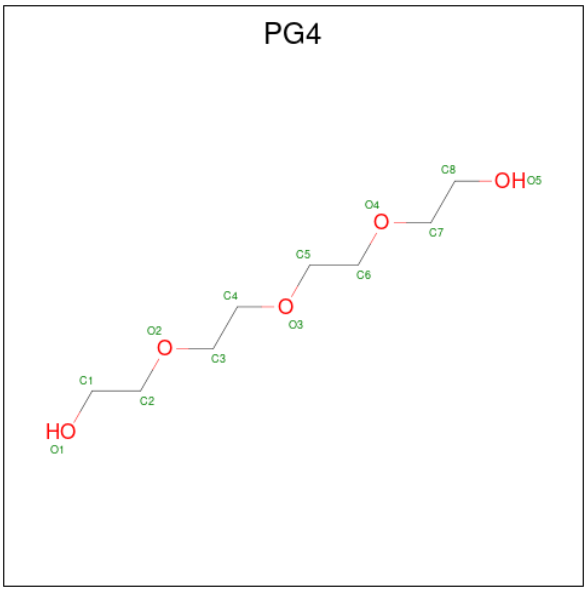
- Molecule 1 is a protein called Thioesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1926	1219	361	339	7			
1	B	246	Total	C	N	O	S	0	0	0
			1932	1221	361	343	7			
1	C	241	Total	C	N	O	S	0	0	0
			1888	1194	357	330	7			
1	D	249	Total	C	N	O	S	0	1	0
			1957	1237	368	345	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	SER	-	expression tag	UNP O54157
A	4	ASN	-	expression tag	UNP O54157
A	5	ALA	-	expression tag	UNP O54157
B	3	SER	-	expression tag	UNP O54157
B	4	ASN	-	expression tag	UNP O54157
B	5	ALA	-	expression tag	UNP O54157
C	3	SER	-	expression tag	UNP O54157
C	4	ASN	-	expression tag	UNP O54157
C	5	ALA	-	expression tag	UNP O54157
D	3	SER	-	expression tag	UNP O54157
D	4	ASN	-	expression tag	UNP O54157
D	5	ALA	-	expression tag	UNP O54157

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 13 8 5	0	0

- Molecule 3 is water.

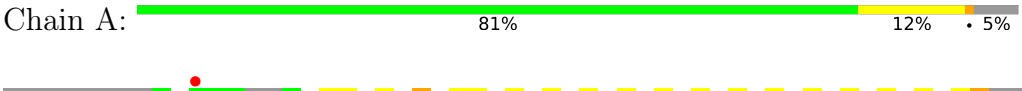
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	37	Total O 37 37	0	0
3	B	76	Total O 76 76	0	0
3	C	18	Total O 18 18	0	0
3	D	20	Total O 20 20	0	0

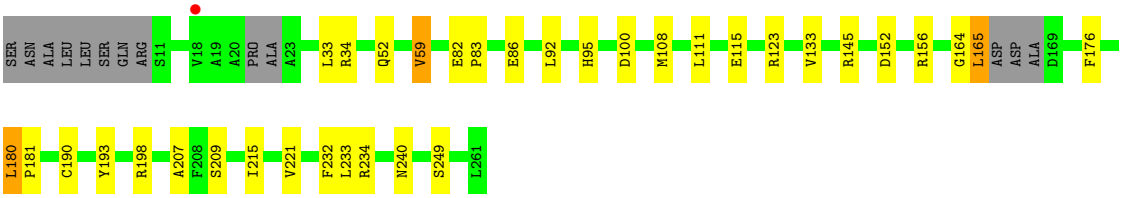
3 Residue-property plots (i)

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: Thioesterase

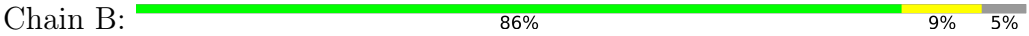
Chain A:

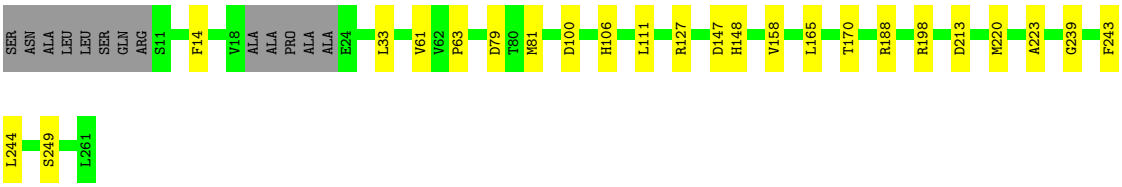




• Molecule 1: Thioesterase

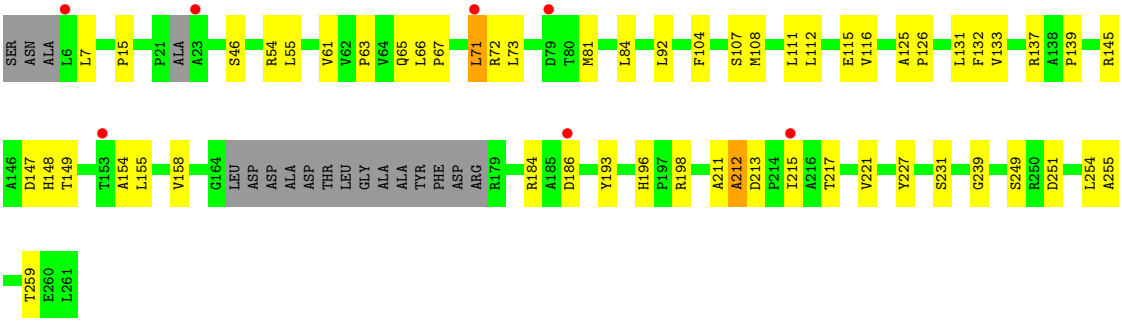
Chain B:





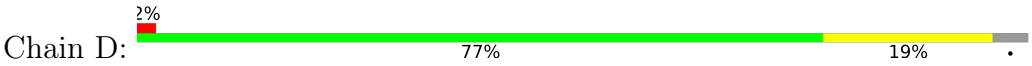
• Molecule 1: Thioesterase

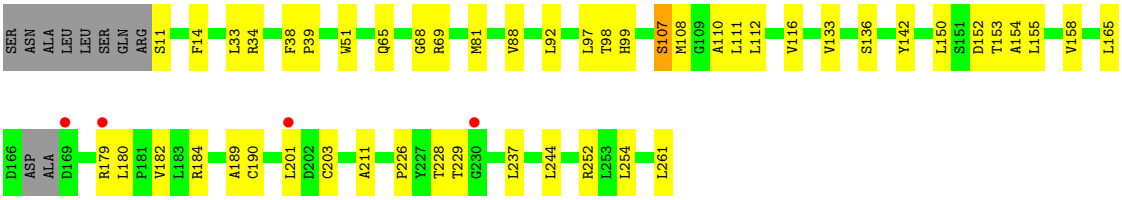
Chain C:



• Molecule 1: Thioesterase

Chain D:




SER ASN ALA LEU LEU SER GLN ARG S11 F14 L33 R34 F38 P39 W51 Q65 G68 R69 M81 V88 L92 L97 T98 H99 S107 M108 G109 A110 L111 L112 V116 V133 S136 Y142 L150 S151 D152 T153 A154 L155 V158 L165
D166 ASP ALA D169 R179 L180 P181 V182 L183 R184 A189 C190 L201 D202 C203 A211 P226 Y227 T228 T229 G230 L237 L244 R252 L253 L254 L261

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	155.54Å 45.01Å 156.40Å 90.00° 109.49° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.50) 92.3 (50.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.214 , 0.284 0.213 , 0.282	Depositor DCC
R_{free} test set	1630 reflections (4.52%)	wwPDB-VP
Wilson B-factor (Å^2)	39.9	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 34.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7867	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 5.51% 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: PG4

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	0.82	0/1983	0.86	0/2704
1	B	0.83	1/1990 (0.1%)	0.90	0/2715
1	C	0.72	3/1944 (0.2%)	0.81	1/2651 (0.0%)
1	D	0.66	2/2016 (0.1%)	0.80	0/2751
All	All	0.76	6/7933 (0.1%)	0.84	1/10821 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	212	ALA	CA-CB	-6.09	1.44	1.53
1	D	107	SER	C-O	-5.59	1.19	1.24
1	C	15	PRO	C-O	-5.53	1.17	1.23
1	D	211	ALA	CA-CB	-5.42	1.44	1.53
1	B	239	GLY	C-O	-5.18	1.18	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	71	LEU	N-CA-C	-5.16	107.15	112.93

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	1926	0	1877	24	0
1	B	1932	0	1876	14	0
1	C	1888	0	1851	39	0
1	D	1957	0	1906	41	0
2	B	13	0	18	2	0
3	A	37	0	0	2	0
3	B	76	0	0	2	0
3	C	18	0	0	0	0
3	D	20	0	0	2	0
All	All	7867	0	7528	112	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 7.

The worst 5 of 112 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:C:71:LEU:HD11	1:D:226:PRO:O	1.53	1.07
1:B:158:VAL:HG11	2:B:1:PG4:H52	1.63	0.78
1:C:213:ASP:C	1:C:213:ASP:OD1	2.29	0.73
1:A:115:GLU:CD	1:A:198:ARG:HH12	1.99	0.71
1:C:71:LEU:HG	1:D:226:PRO:HB2	1.72	0.70

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	240/259 (93%)	233 (97%)	7 (3%)	0	100	100
1	B	242/259 (93%)	237 (98%)	5 (2%)	0	100	100
1	C	235/259 (91%)	224 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	246/259 (95%)	236 (96%)	10 (4%)	0	100	100
All	All	963/1036 (93%)	930 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	194/204 (95%)	190 (98%)	4 (2%)	47	74
1	B	196/204 (96%)	194 (99%)	2 (1%)	68	86
1	C	192/204 (94%)	188 (98%)	4 (2%)	47	74
1	D	197/204 (97%)	195 (99%)	2 (1%)	68	86
All	All	779/816 (96%)	767 (98%)	12 (2%)	57	80

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	73	LEU
1	C	231	SER
1	D	158	VAL
1	C	249	SER
1	A	249	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	256	HIS
1	B	99	HIS

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

1 ligand is 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	$\#\|Z\| > 2$
2	PG4	B	1	-	12,12,12	0.59	0	11,11,11	0.33	0

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
2	PG4	B	1	-	-	4/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	PG4	O4-C7-C8-O5
2	B	1	PG4	C5-C6-O4-C7
2	B	1	PG4	O3-C5-C6-O4
2	B	1	PG4	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	PG4	2	0

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, 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	A	246/259 (94%)	-0.05	1 (0%) 88 86	17, 34, 55, 63	0
1	B	246/259 (94%)	-0.24	0 100 100	18, 29, 49, 68	0
1	C	241/259 (93%)	0.40	7 (2%) 53 49	25, 54, 67, 72	0
1	D	249/259 (96%)	0.53	4 (1%) 70 67	23, 56, 67, 70	1 (0%)
All	All	982/1036 (94%)	0.16	12 (1%) 76 73	17, 42, 65, 72	1 (0%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	71	LEU	2.7
1	C	23	ALA	2.6
1	A	18	VAL	2.5
1	C	79	ASP	2.4
1	C	6	LEU	2.3

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 oligosaccharides 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
2	PG4	B	1	13/13	0.89	0.11	38,39,43,44	0

6.5 Other polymers (i)

There are no such residues in this entry.