



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:16 PM GMT

PDB ID : 1O5W
Title : The structure basis of specific recognitions for substrates and inhibitors of rat monoamine oxidase A
Authors : Ma, J.; Yoshimura, M.; Yamashita, E.; Nakagawa, A.; Ito, A.; Tsukihara, T.
Deposited on : 2003-10-06
Resolution : 3.20 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

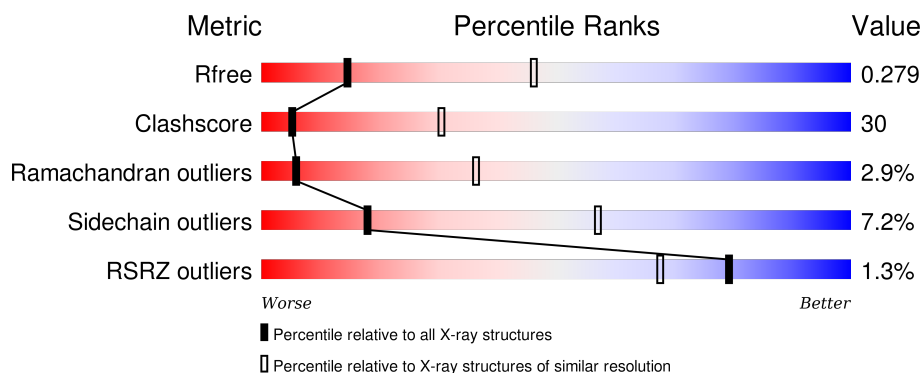
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. 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	534	<div> <div>2%</div> <div>51%40%5% .</div> </div>
1	B	534	<div> <div>47%41%5% • 6%</div> </div>
1	C	534	<div> <div>%50%40%5% • •</div> </div>
1	D	534	<div> <div>%50%39%5% 5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MLG	B	1709	-	-	-	X
2	MLG	C	2709	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16456 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 Amine oxidase [flavin-containing] A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	511	Total	C	N	O	S	0	0	0
			4071	2620	691	738	22			
1	B	503	Total	C	N	O	S	0	0	0
			4002	2570	682	729	21			
1	C	512	Total	C	N	O	S	0	0	0
			4079	2626	692	739	22			
1	D	506	Total	C	N	O	S	0	0	0
			4024	2585	685	732	22			

There are 44 discrepancies between the modelled and reference sequences:

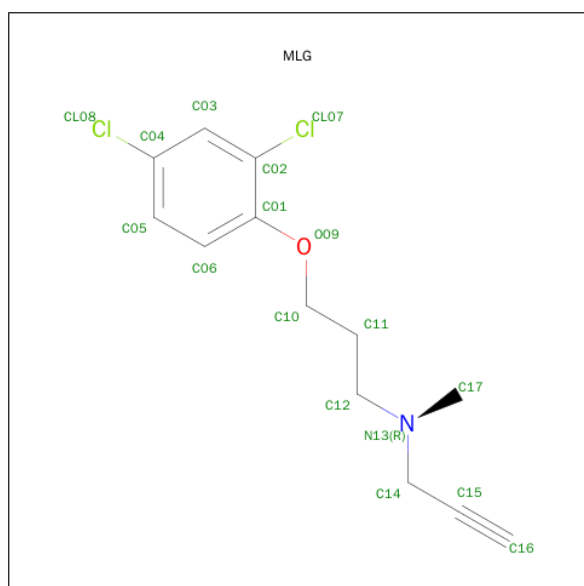
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	EXPRESSION TAG	UNP P21396
A	-6	GLY	-	EXPRESSION TAG	UNP P21396
A	-5	HIS	-	EXPRESSION TAG	UNP P21396
A	-4	HIS	-	EXPRESSION TAG	UNP P21396
A	-3	HIS	-	EXPRESSION TAG	UNP P21396
A	-2	HIS	-	EXPRESSION TAG	UNP P21396
A	-1	HIS	-	EXPRESSION TAG	UNP P21396
A	0	HIS	-	EXPRESSION TAG	UNP P21396
A	17	VAL	GLY	SEE REMARK 999	UNP P21396
A	18	VAL	LEU	SEE REMARK 999	UNP P21396
A	361	LEU	GLN	SEE REMARK 999	UNP P21396
B	993	MET	-	EXPRESSION TAG	UNP P21396
B	994	GLY	-	EXPRESSION TAG	UNP P21396
B	995	HIS	-	EXPRESSION TAG	UNP P21396
B	996	HIS	-	EXPRESSION TAG	UNP P21396
B	997	HIS	-	EXPRESSION TAG	UNP P21396
B	998	HIS	-	EXPRESSION TAG	UNP P21396
B	999	HIS	-	EXPRESSION TAG	UNP P21396
B	1000	HIS	-	EXPRESSION TAG	UNP P21396
B	1017	VAL	GLY	SEE REMARK 999	UNP P21396
B	1018	VAL	LEU	SEE REMARK 999	UNP P21396

Continued on next page...

Continued from previous page...


Chain	Residue	Modelled	Actual	Comment	Reference
B	1361	LEU	GLN	SEE REMARK 999	UNP P21396
C	1993	MET	-	EXPRESSION TAG	UNP P21396
C	1994	GLY	-	EXPRESSION TAG	UNP P21396
C	1995	HIS	-	EXPRESSION TAG	UNP P21396
C	1996	HIS	-	EXPRESSION TAG	UNP P21396
C	1997	HIS	-	EXPRESSION TAG	UNP P21396
C	1998	HIS	-	EXPRESSION TAG	UNP P21396
C	1999	HIS	-	EXPRESSION TAG	UNP P21396
C	2000	HIS	-	EXPRESSION TAG	UNP P21396
C	2017	VAL	GLY	SEE REMARK 999	UNP P21396
C	2018	VAL	LEU	SEE REMARK 999	UNP P21396
C	2361	LEU	GLN	SEE REMARK 999	UNP P21396
D	2993	MET	-	EXPRESSION TAG	UNP P21396
D	2994	GLY	-	EXPRESSION TAG	UNP P21396
D	2995	HIS	-	EXPRESSION TAG	UNP P21396
D	2996	HIS	-	EXPRESSION TAG	UNP P21396
D	2997	HIS	-	EXPRESSION TAG	UNP P21396
D	2998	HIS	-	EXPRESSION TAG	UNP P21396
D	2999	HIS	-	EXPRESSION TAG	UNP P21396
D	3000	HIS	-	EXPRESSION TAG	UNP P21396
D	3017	VAL	GLY	SEE REMARK 999	UNP P21396
D	3018	VAL	LEU	SEE REMARK 999	UNP P21396
D	3361	LEU	GLN	SEE REMARK 999	UNP P21396

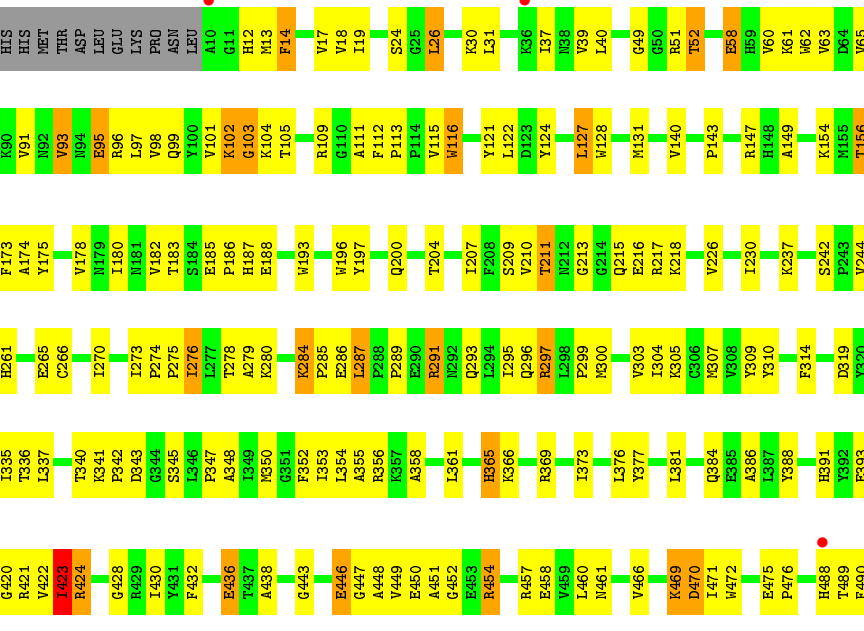
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: MLG, FAD) (formula: $C_{13}H_{15}Cl_2NO$, $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	2	Total	C	Cl	N	O	P	0	0
			70	40	2	10	16	2		
2	B	2	Total	C	Cl	N	O	P	0	0
			70	40	2	10	16	2		
2	C	2	Total	C	Cl	N	O	P	0	0
			70	40	2	10	16	2		
2	D	2	Total	C	Cl	N	O	P	0	0
			70	40	2	10	16	2		

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

- Chain A: 



- [illegible]





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	157.56Å 157.56Å 257.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.19 – 3.20 16.18 – 3.08	Depositor EDS
% Data completeness (in resolution range)	99.2 (16.19-3.20) 98.9 (16.18-3.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.07Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.282 0.221 , 0.279	Depositor DCC
R_{free} test set	2684 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	106.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 74.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 59281 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16456	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MLG, FAD

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	0.41	0/4171	0.65	1/5657 (0.0%)
1	B	0.39	1/4100 (0.0%)	0.64	2/5561 (0.0%)
1	C	0.39	1/4179 (0.0%)	0.65	2/5668 (0.0%)
1	D	0.39	1/4122 (0.0%)	0.65	1/5591 (0.0%)
All	All	0.40	3/16572 (0.0%)	0.65	6/22477 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	3210	VAL	CB-CG1	-5.23	1.41	1.52
1	C	2210	VAL	CB-CG2	-5.17	1.42	1.52
1	B	1210	VAL	CB-CG1	-5.06	1.42	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	406	CYS	N-CA-C	6.98	129.84	111.00
1	C	2406	CYS	N-CA-C	6.91	129.66	111.00
1	B	1406	CYS	N-CA-C	6.83	129.46	111.00
1	D	3406	CYS	N-CA-C	6.79	129.35	111.00
1	B	1406	CYS	CA-CB-SG	-5.38	104.31	114.00

There are no chirality outliers.

There are no planarity outliers.

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	A	4071	0	4085	256	0
1	B	4002	0	4007	270	0
1	C	4079	0	4096	260	0
1	D	4024	0	4034	257	0
2	A	70	0	44	4	0
2	B	70	0	44	3	0
2	C	70	0	44	2	0
2	D	70	0	44	2	0
All	All	16456	0	16398	997	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 30.

The worst 5 of 997 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:B:1464:GLY:HA3	1:D:3145:GLN:HG2	1.18	1.15
1:A:458:GLU:HA	1:A:471:ILE:HD11	1.33	1.10
1:C:2458:GLU:HA	1:C:2471:ILE:HD11	1.33	1.10
1:D:3458:GLU:HA	1:D:3471:ILE:HD11	1.34	1.06
1:B:1458:GLU:HA	1:B:1471:ILE:HD11	1.34	1.03

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	509/534 (95%)	428 (84%)	67 (13%)	14 (3%)	6	37
1	B	501/534 (94%)	416 (83%)	70 (14%)	15 (3%)	5	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	510/534 (96%)	422 (83%)	73 (14%)	15 (3%)	6	36
1	D	504/534 (94%)	418 (83%)	71 (14%)	15 (3%)	5	35
All	All	2024/2136 (95%)	1684 (83%)	281 (14%)	59 (3%)	6	36

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	LYS
1	A	408	THR
1	A	423	ILE
1	B	1102	LYS
1	B	1127	LEU

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	433/455 (95%)	402 (93%)	31 (7%)	18	57
1	B	425/455 (93%)	395 (93%)	30 (7%)	18	57
1	C	434/455 (95%)	401 (92%)	33 (8%)	16	55
1	D	428/455 (94%)	398 (93%)	30 (7%)	19	58
All	All	1720/1820 (94%)	1596 (93%)	124 (7%)	18	57

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1446	GLU
1	C	2095	GLU
1	D	3291	ARG
1	B	1454	ARG
1	C	2014	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1418	GLN
1	C	2260	ASN
1	D	3418	GLN
1	B	1494	ASN
1	C	2293	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
2	FAD	A	652	1,2	48,58,58	2.52	13 (27%)	54,89,89	2.47	9 (16%)
2	MLG	A	709	2	16,17,17	3.82	10 (62%)	20,21,21	9.61	5 (25%)
2	FAD	B	1652	1,2	48,58,58	2.59	13 (27%)	54,89,89	2.49	9 (16%)
2	MLG	B	1709	2	16,17,17	3.79	9 (56%)	20,21,21	9.77	5 (25%)
2	FAD	C	2652	1,2	48,58,58	2.57	12 (25%)	54,89,89	2.48	10 (18%)
2	MLG	C	2709	2	16,17,17	3.81	10 (62%)	20,21,21	9.63	5 (25%)
2	FAD	D	3652	1,2	48,58,58	2.56	13 (27%)	54,89,89	2.43	10 (18%)
2	MLG	D	3709	2	16,17,17	3.81	10 (62%)	20,21,21	9.70	5 (25%)

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	FAD	A	652	1,2	-	0/30/50/50	0/6/6/6
2	MLG	A	709	2	-	0/9/10/10	0/1/1/1
2	FAD	B	1652	1,2	-	0/30/50/50	0/6/6/6
2	MLG	B	1709	2	-	0/9/10/10	0/1/1/1
2	FAD	C	2652	1,2	-	0/30/50/50	0/6/6/6
2	MLG	C	2709	2	-	0/9/10/10	0/1/1/1
2	FAD	D	3652	1,2	-	0/30/50/50	0/6/6/6
2	MLG	D	3709	2	-	0/9/10/10	0/1/1/1

The worst 5 of 90 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1709	MLG	C14-C15	-7.34	1.37	1.47
2	D	3709	MLG	C14-C15	-7.19	1.37	1.47
2	C	2709	MLG	C14-C15	-6.74	1.38	1.47
2	A	709	MLG	C14-C15	-6.57	1.38	1.47
2	C	2652	FAD	C1'-N10	-5.48	1.42	1.48

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1709	MLG	C14-C15-C16	-43.23	121.67	177.76
2	D	3709	MLG	C14-C15-C16	-42.96	122.02	177.76
2	C	2709	MLG	C14-C15-C16	-42.66	122.40	177.76
2	A	709	MLG	C14-C15-C16	-42.52	122.58	177.76
2	C	2652	FAD	N3A-C2A-N1A	-7.97	122.79	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	709	MLG	4	0
2	B	1709	MLG	3	0
2	C	2709	MLG	2	0
2	D	3709	MLG	2	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, 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(Å ²)	Q<0.9
1	A	511/534 (95%)	-0.49	11 (2%) 65 50	41, 78, 146, 201	0
1	B	503/534 (94%)	-0.44	2 (0%) 93 90	43, 93, 152, 188	0
1	C	512/534 (95%)	-0.49	7 (1%) 78 65	41, 87, 151, 201	0
1	D	506/534 (94%)	-0.47	6 (1%) 81 69	48, 89, 150, 201	0
All	All	2032/2136 (95%)	-0.47	26 (1%) 79 67	41, 86, 150, 201	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3515	CYS	6.9
1	C	2519	TYR	6.8
1	C	2518	LEU	5.8
1	A	10	ALA	5.1
1	A	519	TYR	4.7

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
2	MLG	C	2709	17/17	0.73	0.35	3.47	62,91,140,149	0
2	MLG	B	1709	17/17	0.76	0.34	2.31	46,121,168,184	0
2	MLG	A	709	17/17	0.79	0.28	1.70	48,67,114,126	0
2	MLG	D	3709	17/17	0.74	0.31	1.70	61,111,159,175	0
2	FAD	A	652	53/53	0.97	0.16	0.09	32,62,102,113	0
2	FAD	C	2652	53/53	0.96	0.15	-0.07	33,67,98,126	0
2	FAD	B	1652	53/53	0.95	0.17	-0.21	34,72,138,153	0
2	FAD	D	3652	53/53	0.96	0.16	-0.25	35,75,119,148	0

6.5 Other polymers [i](#)

There are no such residues in this entry.