



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 20, 2016 – 12:36 PM EDT

PDB ID : 4Z14
Title : Recombinantly expressed latent aurone synthase (polyphenol oxidase)
Authors : Molitor, C.; Mauracher, S.G.; Rompel, A.
Deposited on : 2015-03-26
Resolution : 2.53 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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
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) : rb-20027790

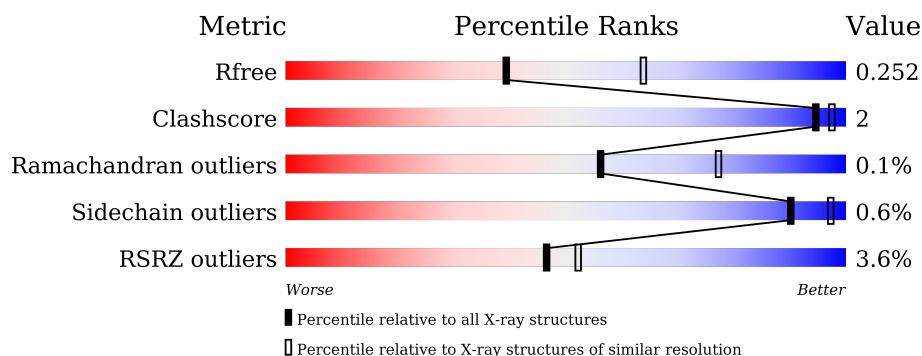
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	4241 (2.54-2.50)
Clashscore	102246	4968 (2.54-2.50)
Ramachandran outliers	100387	4873 (2.54-2.50)
Sidechain outliers	100360	4875 (2.54-2.50)
RSRZ outliers	91569	4253 (2.54-2.50)

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 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	520	<div> <div>5%</div> <div> <div></div> <div>92%</div> <div></div> </div> <div></div> </div>
1	B	520	<div> <div>4%</div> <div> <div></div> <div>93%</div> <div></div> </div> <div></div> </div>
1	C	520	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div></div> </div> <div></div> </div>
1	D	520	<div> <div>7%</div> <div> <div></div> <div>92%</div> <div></div> </div> <div></div> </div>
1	E	520	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>5%</div> </div> <div></div> </div>
1	F	520	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>5%</div> </div> <div></div> </div>

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Mol	Chain	Length	Quality of chain
1	G	520	<div> <div></div> <div>3%</div> <div>93%</div> <div></div> <div></div> </div>
1	H	520	<div> <div></div> <div>4%</div> <div>93%</div> <div></div> <div></div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 61726 atoms, of which 29358 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 Aurone synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	D	501	Total	C	H	N	O	S	0	0	0
			7456	2479	3570	677	715	15			
1	B	504	Total	C	H	N	O	S	0	0	0
			7739	2545	3741	691	747	15			
1	H	498	Total	C	H	N	O	S	0	0	0
			7623	2507	3698	682	721	15			
1	F	498	Total	C	H	N	O	S	0	0	0
			7520	2486	3618	675	726	15			
1	C	499	Total	C	H	N	O	S	0	0	0
			7683	2519	3731	682	736	15			
1	E	497	Total	C	H	N	O	S	0	0	0
			7555	2495	3649	680	716	15			
1	G	509	Total	C	H	N	O	S	0	0	0
			7725	2547	3731	694	738	15			
1	A	501	Total	C	H	N	O	S	0	0	0
			7543	2493	3620	685	730	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	MET	-	initiating methionine	UNP A0A075DN54
D	-1	ALA	-	expression tag	UNP A0A075DN54
D	0	LEU	-	expression tag	UNP A0A075DN54
B	-2	MET	-	initiating methionine	UNP A0A075DN54
B	-1	ALA	-	expression tag	UNP A0A075DN54
B	0	LEU	-	expression tag	UNP A0A075DN54
H	-2	MET	-	initiating methionine	UNP A0A075DN54
H	-1	ALA	-	expression tag	UNP A0A075DN54
H	0	LEU	-	expression tag	UNP A0A075DN54
F	-2	MET	-	initiating methionine	UNP A0A075DN54
F	-1	ALA	-	expression tag	UNP A0A075DN54
F	0	LEU	-	expression tag	UNP A0A075DN54
C	-2	MET	-	initiating methionine	UNP A0A075DN54

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	ALA	-	expression tag	UNP A0A075DN54
C	0	LEU	-	expression tag	UNP A0A075DN54
E	-2	MET	-	initiating methionine	UNP A0A075DN54
E	-1	ALA	-	expression tag	UNP A0A075DN54
E	0	LEU	-	expression tag	UNP A0A075DN54
G	-2	MET	-	initiating methionine	UNP A0A075DN54
G	-1	ALA	-	expression tag	UNP A0A075DN54
G	0	LEU	-	expression tag	UNP A0A075DN54
A	-2	MET	-	initiating methionine	UNP A0A075DN54
A	-1	ALA	-	expression tag	UNP A0A075DN54
A	0	LEU	-	expression tag	UNP A0A075DN54

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Cu 2 2	0	0
2	D	2	Total Cu 2 2	0	0
2	E	2	Total Cu 2 2	0	0
2	H	2	Total Cu 2 2	0	0
2	B	2	Total Cu 2 2	0	0
2	C	2	Total Cu 2 2	0	0
2	A	2	Total Cu 2 2	0	0
2	F	2	Total Cu 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	61	Total O 61 61	0	0
3	B	130	Total O 130 130	0	0
3	H	95	Total O 95 95	0	0
3	F	90	Total O 90 90	0	0

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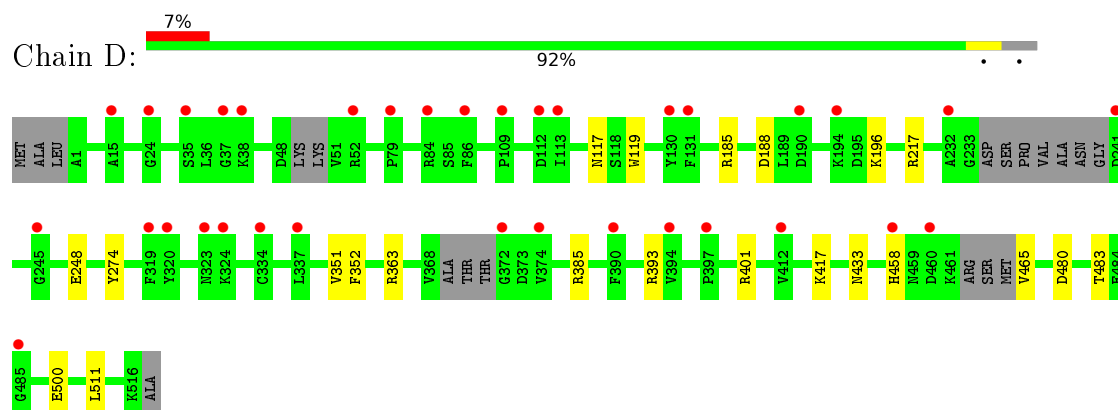
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	136	Total 136	O 136	0	0
3	E	133	Total 133	O 133	0	0
3	G	103	Total 103	O 103	0	0
3	A	118	Total 118	O 118	0	0

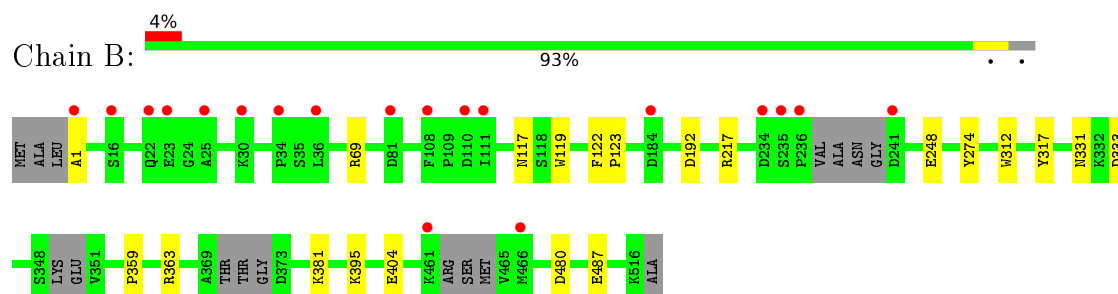
3 Residue-property plots [i](#)

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.

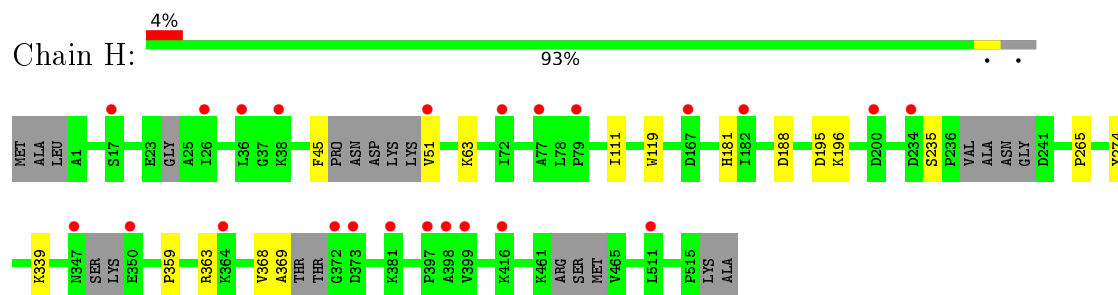
- Molecule 1: Aurone synthase



- Molecule 1: Aurone synthase

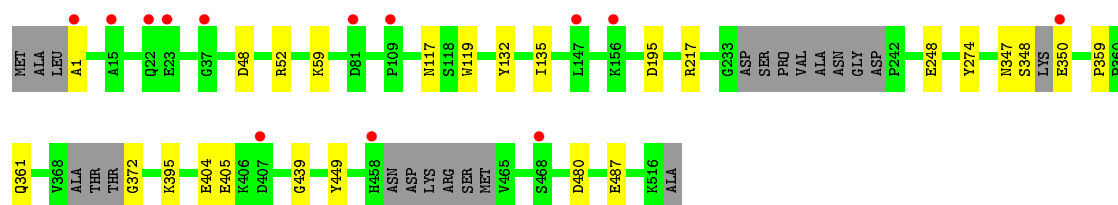


- Molecule 1: Aurone synthase

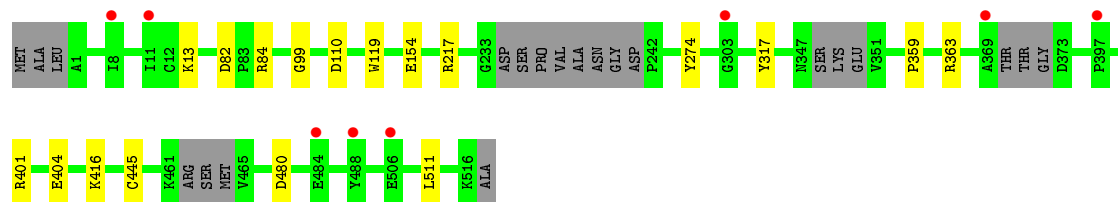
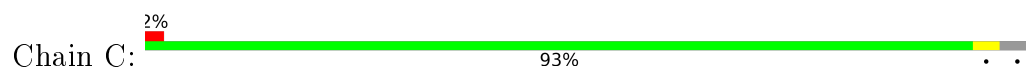


- Molecule 1: Aurone synthase

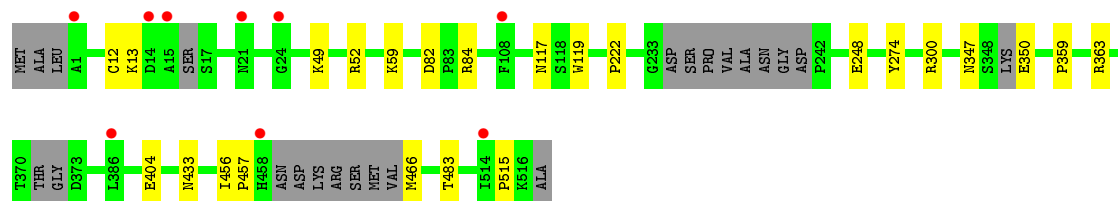




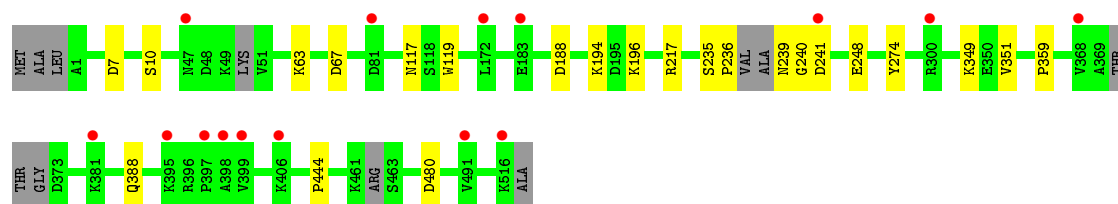
• Molecule 1: Aurone synthase



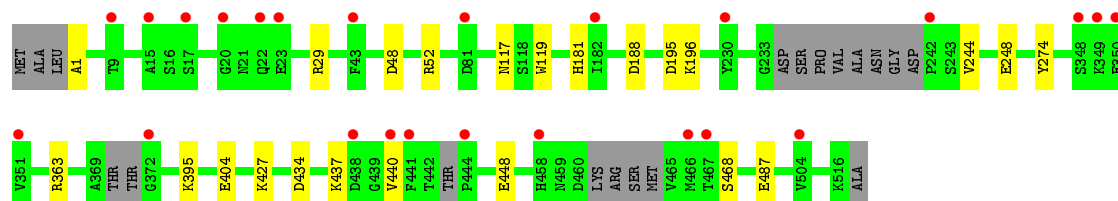
• Molecule 1: Aurone synthase



• Molecule 1: Aurone synthase



• Molecule 1: Aurone synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.85Å 103.79Å 175.56Å 100.69° 91.90° 105.18°	Depositor
Resolution (Å)	47.54 – 2.53 47.91 – 2.53	Depositor EDS
% Data completeness (in resolution range)	97.9 (47.54-2.53) 91.3 (47.91-2.53)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.208 , 0.253 0.208 , 0.252	Depositor DCC
R_{free} test set	6844 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	61726	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.48 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.7184e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: CU

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	0.22	0/4029	0.37	0/5481
1	B	0.21	0/4106	0.36	0/5585
1	C	0.21	0/4059	0.35	0/5522
1	D	0.21	0/3993	0.36	0/5442
1	E	0.21	0/4012	0.35	0/5458
1	F	0.21	0/4009	0.36	0/5459
1	G	0.21	0/4102	0.36	0/5582
1	H	0.21	0/4030	0.36	0/5479
All	All	0.21	0/32340	0.36	0/44008

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
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	437	LYS	Peptide

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	3923	3620	3671	13	0
1	B	3998	3741	3780	14	0
1	C	3952	3731	3744	10	0
1	D	3886	3570	3608	14	0
1	E	3906	3649	3678	18	0
1	F	3902	3618	3640	16	0
1	G	3994	3731	3775	12	0
1	H	3925	3698	3725	12	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	118	0	0	5	0
3	B	130	0	0	6	0
3	C	136	0	0	3	0
3	D	61	0	0	4	0
3	E	133	0	0	5	0
3	F	90	0	0	7	0
3	G	103	0	0	2	0
3	H	95	0	0	2	0
All	All	32368	29358	29621	101	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 101 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:A:468:SER:O	3:A:801:HOH:O	2.01	0.78
1:F:135:ILE:N	3:F:801:HOH:O	2.19	0.76
1:G:359:PRO:O	1:A:363:ARG:NH2	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:132:TYR:O	3:F:801:HOH:O	2.07	0.72
1:C:110:ASP:OD2	3:C:801:HOH:O	2.08	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	491/520 (94%)	474 (96%)	16 (3%)	1 (0%)	52	74
1	B	494/520 (95%)	480 (97%)	14 (3%)	0	100	100
1	C	489/520 (94%)	469 (96%)	20 (4%)	0	100	100
1	D	491/520 (94%)	474 (96%)	17 (4%)	0	100	100
1	E	485/520 (93%)	462 (95%)	23 (5%)	0	100	100
1	F	488/520 (94%)	472 (97%)	15 (3%)	1 (0%)	52	74
1	G	499/520 (96%)	481 (96%)	15 (3%)	3 (1%)	30	49
1	H	484/520 (93%)	470 (97%)	14 (3%)	0	100	100
All	All	3921/4160 (94%)	3782 (96%)	134 (3%)	5 (0%)	56	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	349	LYS
1	G	351	VAL
1	A	440	VAL
1	F	439	GLY
1	G	444	PRO

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	406/456 (89%)	404 (100%)	2 (0%)	92	98
1	B	422/456 (92%)	419 (99%)	3 (1%)	88	97
1	C	418/456 (92%)	414 (99%)	4 (1%)	82	94
1	D	395/456 (87%)	392 (99%)	3 (1%)	86	96
1	E	403/456 (88%)	400 (99%)	3 (1%)	88	97
1	F	403/456 (88%)	401 (100%)	2 (0%)	92	98
1	G	417/456 (91%)	415 (100%)	2 (0%)	92	98
1	H	411/456 (90%)	409 (100%)	2 (0%)	92	98
All	All	3275/3648 (90%)	3254 (99%)	21 (1%)	90	97

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	274	TYR
1	C	274	TYR
1	G	119	TRP
1	F	119	TRP
1	G	274	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	264	GLN
1	E	264	GLN
1	G	323	ASN
1	F	347	ASN
1	G	264	GLN

5.3.3 RNA ⓘ

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](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	501/520 (96%)	0.46	24 (4%) 34 39	30, 55, 93, 141	0
1	B	504/520 (96%)	0.39	19 (3%) 44 50	27, 51, 90, 144	0
1	C	499/520 (95%)	0.40	8 (1%) 74 78	34, 56, 82, 145	0
1	D	501/520 (96%)	0.65	34 (6%) 20 23	39, 70, 102, 148	0
1	E	497/520 (95%)	0.25	9 (1%) 71 75	27, 53, 90, 130	0
1	F	498/520 (95%)	0.36	13 (2%) 59 64	31, 58, 94, 120	0
1	G	509/520 (97%)	0.44	15 (2%) 55 60	36, 58, 92, 117	0
1	H	498/520 (95%)	0.44	23 (4%) 36 42	40, 61, 97, 120	0
All	All	4007/4160 (96%)	0.42	145 (3%) 46 52	27, 58, 94, 148	0

The worst 5 of 145 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	369	ALA	4.8
1	D	319	PHE	4.7
1	F	458	HIS	4.3
1	F	37	GLY	4.3
1	F	350	GLU	4.2

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 [i](#)

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(Å ²)	Q<0.9
2	CU	D	701	1/1	0.97	0.14	-1.36	74,74,74,74	0
2	CU	C	700	1/1	0.98	0.12	-1.64	52,52,52,52	0
2	CU	H	701	1/1	0.99	0.11	-1.80	58,58,58,58	0
2	CU	A	701	1/1	0.99	0.12	-1.91	49,49,49,49	0
2	CU	G	701	1/1	0.98	0.13	-2.03	59,59,59,59	0
2	CU	C	701	1/1	0.99	0.13	-2.15	61,61,61,61	0
2	CU	F	700	1/1	0.97	0.09	-2.32	66,66,66,66	0
2	CU	F	701	1/1	0.98	0.09	-2.44	64,64,64,64	0
2	CU	D	700	1/1	0.99	0.10	-2.76	67,67,67,67	0
2	CU	B	701	1/1	0.99	0.08	-2.79	48,48,48,48	0
2	CU	E	700	1/1	0.98	0.07	-2.86	78,78,78,78	0
2	CU	E	701	1/1	0.97	0.09	-3.03	51,51,51,51	0
2	CU	B	700	1/1	0.95	0.07	-3.23	69,69,69,69	0
2	CU	A	700	1/1	0.96	0.09	-3.34	61,61,61,61	0
2	CU	G	700	1/1	0.98	0.10	-4.33	58,58,58,58	0
2	CU	H	700	1/1	0.94	0.08	-4.59	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.