



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:03 PM GMT

PDB ID : 3SQC
Title : SQUALENE-HOPENE CYCLASE
Authors : Wendt, K.U.; Schulz, G.E.
Deposited on : 1998-09-04
Resolution : 2.80 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

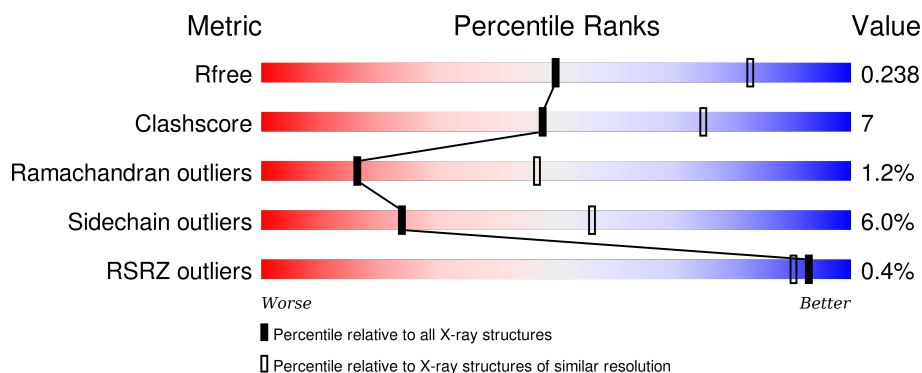
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	631	<div> <div></div> <div>78%</div> <div>17%</div> <div>••</div> </div>
1	B	631	<div> <div></div> <div>80%</div> <div>16%</div> <div>••</div> </div>
1	C	631	<div> <div></div> <div>79%</div> <div>17%</div> <div>••</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14997 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 SQUALENE-HOPENE CYCLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	619	Total	C	N	O	S	0	0	0
			4961	3187	858	895	21			
1	B	619	Total	C	N	O	S	0	0	0
			4961	3187	858	895	21			
1	C	619	Total	C	N	O	S	0	0	0
			4961	3187	858	895	21			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	376	CYS	ASP	ENGINEERED	UNP P33247
B	376	CYS	ASP	ENGINEERED	UNP P33247
C	376	CYS	ASP	ENGINEERED	UNP P33247

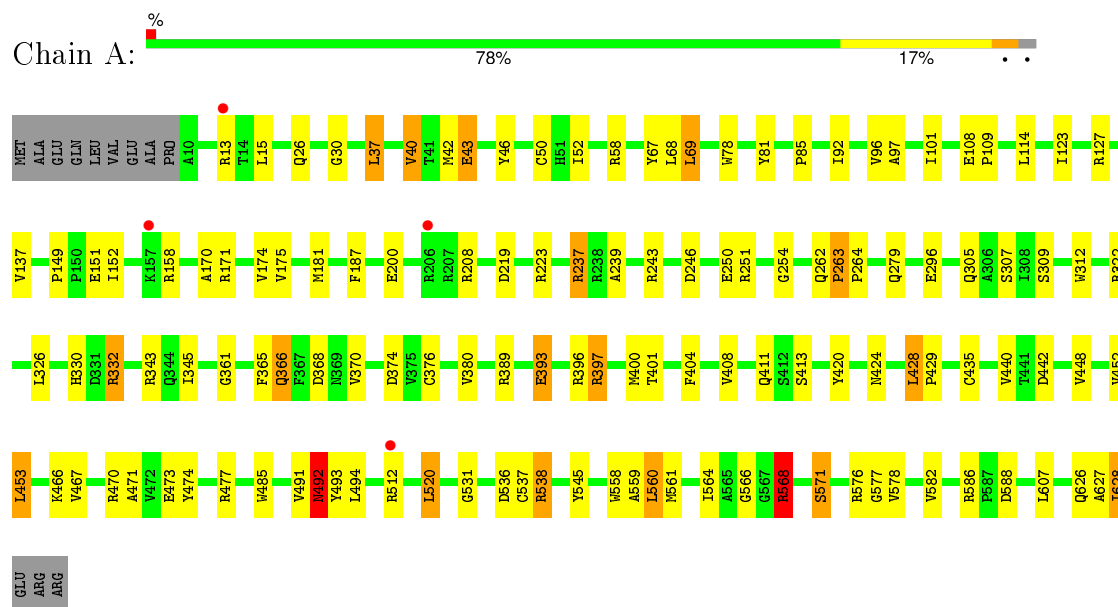
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	38	Total	O	0	0
			38	38		
2	B	38	Total	O	0	0
			38	38		
2	C	38	Total	O	0	0
			38	38		

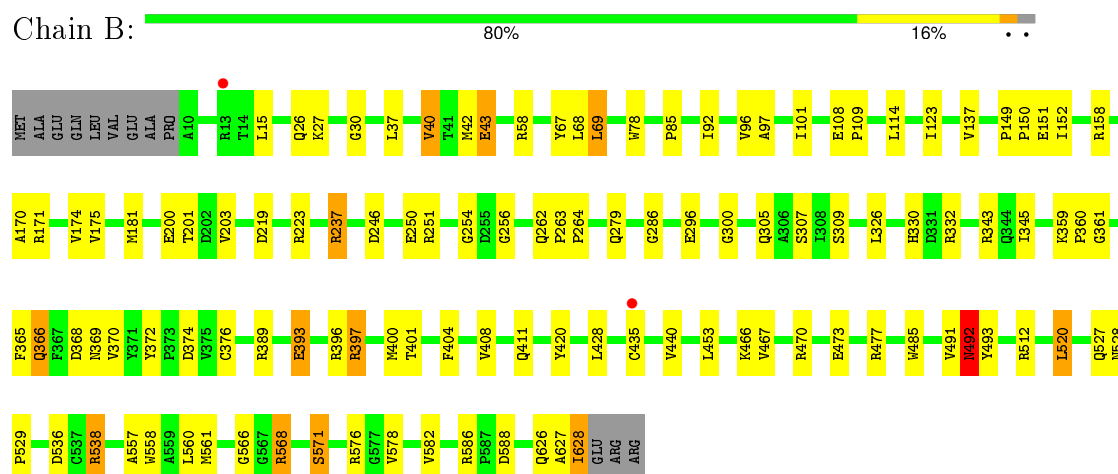
3 Residue-property plots

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.

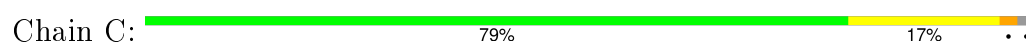
• Molecule 1: SQUALENE-HOPENE CYCLASE



• Molecule 1: SQUALENE-HOPENE CYCLASE



• Molecule 1: SQUALENE-HOPENE CYCLASE



Y493	F365	P149	MET
I509	F366	P150	ALA
D510	F367	E151	GLU
T511	D368	I152	GLN
R512	N369	R158	LEU
L520	V370	A170	VAL
N528	F372	R171	GLU
P529	D373	V174	ALA
D536	P374	V175	PRO
C537	V375	A176	Y11
R538	C376	L177	T14
A544	Y380	M181	L15
K548	R389	E200	L22
L560	E393	D219	Q26
I564	R396	R223	G30
A565	R397	R237	L37
G566	N400	D246	V40
G587	T401	E250	T41
R588	F404	R251	M42
A569	Y408	G254	E43
E570	Q411	Q262	Y46
S571	S412	P263	C50
R576	S413	P264	R58
G577	Y420	Q279	Y67
V578	L428	E296	L68
V582	P429	Q305	L69
Q626	C435	S307	W78
A627	V440	S308	Y81
I628	L453	S309	P85
GLU	K466	W312	I92
ARG	V467	L326	Y96
ARG	R470	H330	A97
	A471	D331	I101
	V472	R332	E108
	Y473	R343	P109
	Y474	Q344	L114
	R477	I345	R115
	W485	G361	I123
	V491		I137
	R492		

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.96Å 140.96Å 243.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80 40.14 – 2.80	Depositor EDS
% Data completeness (in resolution range)	82.4 (20.00-2.80) 82.4 (40.14-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.81Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.209 , 0.236 0.211 , 0.238	Depositor DCC
R_{free} test set	2890 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 38.7	EDS
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	2 of 57421 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14997	wwPDB-VP
Average B, all atoms (Å ²)	49.0	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 25.62 % 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 3.0674e-03. 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.47	0/5114	0.64	1/6962 (0.0%)
1	B	0.43	0/5114	0.63	1/6962 (0.0%)
1	C	0.44	0/5114	0.63	1/6962 (0.0%)
All	All	0.45	0/15342	0.63	3/20886 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	492	ASN	N-CA-C	6.68	129.05	111.00
1	A	492	ASN	N-CA-C	6.58	128.75	111.00
1	B	492	ASN	N-CA-C	6.51	128.58	111.00

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	4961	0	4788	78	0
1	B	4961	0	4788	68	0
1	C	4961	0	4788	72	0
2	A	38	0	0	0	0
2	B	38	0	0	0	0
2	C	38	0	0	0	0
All	All	14997	0	14364	215	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 215 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:42:MET:SD	1:B:262:GLN:HG2	2.25	0.77
1:B:568:ARG:HH11	1:B:568:ARG:HG2	1.49	0.77
1:A:568:ARG:HG2	1:A:568:ARG:HH11	1.51	0.76
1:C:568:ARG:HH11	1:C:568:ARG:HG2	1.52	0.75
1:B:40:VAL:HG13	1:B:68:LEU:HD22	1.67	0.75

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	617/631 (98%)	579 (94%)	30 (5%)	8 (1%)	15	44
1	B	617/631 (98%)	580 (94%)	30 (5%)	7 (1%)	17	50
1	C	617/631 (98%)	581 (94%)	29 (5%)	7 (1%)	17	50
All	All	1851/1893 (98%)	1740 (94%)	89 (5%)	22 (1%)	16	47

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	VAL
1	B	40	VAL
1	C	40	VAL
1	A	200	GLU
1	A	492	ASN

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	503/513 (98%)	473 (94%)	30 (6%)	24	56
1	B	503/513 (98%)	473 (94%)	30 (6%)	24	56
1	C	503/513 (98%)	473 (94%)	30 (6%)	24	56
All	All	1509/1539 (98%)	1419 (94%)	90 (6%)	24	56

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	237	ARG
1	B	401	THR
1	C	485	TRP
1	B	251	ARG
1	B	343	ARG

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

Mol	Chain	Res	Type
1	B	279	GLN
1	C	517	GLN
1	B	517	GLN
1	A	517	GLN
1	C	279	GLN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	619/631 (98%)	-0.58	4 (0%)	90 86	15, 46, 85, 100	0
1	B	619/631 (98%)	-0.62	2 (0%)	94 92	15, 46, 85, 100	0
1	C	619/631 (98%)	-0.63	1 (0%)	95 94	15, 46, 85, 100	0
All	All	1857/1893 (98%)	-0.61	7 (0%)	93 90	15, 46, 85, 100	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	512	ARG	2.3
1	A	157	LYS	2.3
1	B	13	ARG	2.2
1	C	570	GLU	2.2
1	A	13	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.